



## wwPDB EM Validation Summary Report ⓘ

Sep 21, 2024 – 12:36 pm BST

PDB ID : 8QU8  
EMDB ID : EMD-18657  
Title : PROTAC-mediated complex of KRAS with VHL/Elongin-B/Elongin-C/Cullin-2/Rbx1  
Authors : Fischer, G.; Peter, D.; Arce-Solano, S.  
Deposited on : 2023-10-14  
Resolution : 3.50 Å(reported)  
Based on initial model : 5n4w

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.dev112  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : **FAILED**  
buster-report : 1.1.7 (2018)  
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) : 2.38.2

## 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10846 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 von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	139	Total	C	N	O	S	0	0
			1136	723	205	206	2		

- Molecule 2 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	103	Total	C	N	O	S	0	0
			814	515	137	158	4		

- Molecule 3 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	96	Total	C	N	O	S	0	0
			760	487	122	145	6		

- Molecule 4 is a protein called Cullin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	729	Total	C	N	O	S	0	0
			5974	3792	1014	1125	43		

- Molecule 5 is a protein called E3 ubiquitin-protein ligase RBX1, N-terminally processed.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	88	Total	C	N	O	S	0	0
			696	435	129	123	9		

- Molecule 6 is a protein called GTPase KRas.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	170	Total	C	N	O	S	1	0
			1364	854	234	270	6		

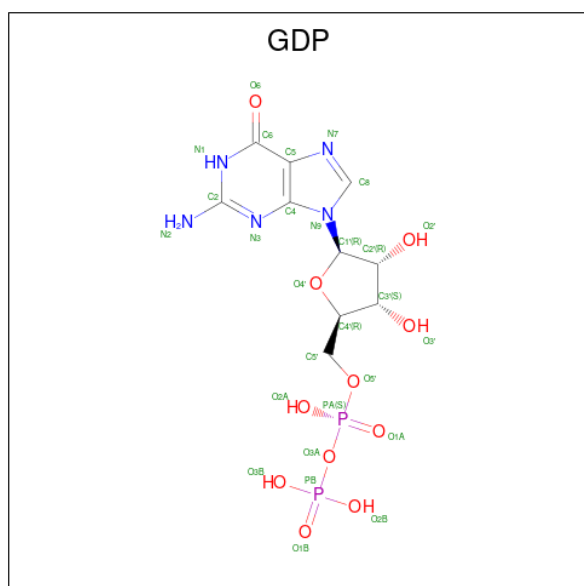
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	0	GLY	-	expression tag	UNP P01116
F	12	VAL	GLY	engineered mutation	UNP P01116
F	118	SER	CYS	engineered mutation	UNP P01116
F	151	GLY	ARG	variant	UNP P01116
F	153	ASP	GLU	variant	UNP P01116
F	165	LYS	-	expression tag	UNP P01116
F	166	HIS	-	expression tag	UNP P01116
F	167	LYS	-	expression tag	UNP P01116
F	168	GLU	-	expression tag	UNP P01116
F	169	LYS	-	expression tag	UNP P01116

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	E	2	Total	Zn	0
			2	2	

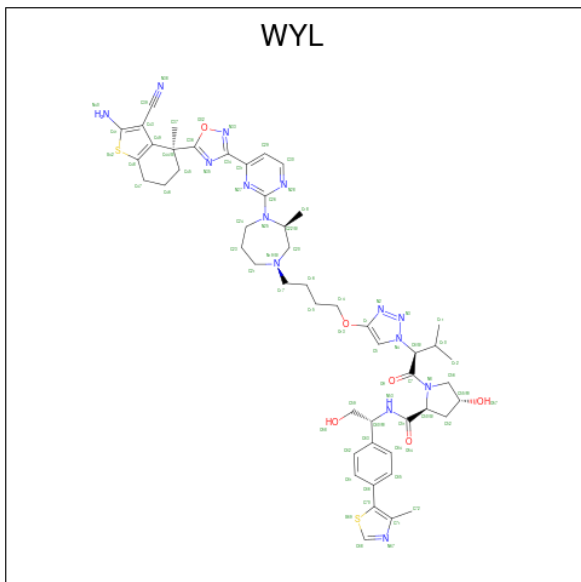
- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					AltConf
8	F	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 9 is (2S,4R)-1-[(2S)-2-[4-[4-[(3S)-4-[4-[5-[(4S)-2-azanyl-3-cyano-4-methyl-6,7-dihydro-5H-1-benzothiophen-4-yl]-1,2,4-oxadiazol-3-yl]pyrimidin-2-yl]-3-methyl-1,4-diazepan-1

-yl]butoxy]-1,2,3-triazol-1-yl]-3-methyl-butanoyl]-N-[(1R)-1-[4-(4-methyl-1,3-thiazol-5-yl)phenyl]-2-oxidanyl-ethyl]-4-oxidanyl-pyrrolidine-2-carboxamide (three-letter code: WYL) (formula: C<sub>50</sub>H<sub>62</sub>N<sub>14</sub>O<sub>6</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
9	F	1	72	50	14	6	2	0

MolProbity failed to run properly - this section is therefore empty.

### 3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	217000	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.355	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.5	Depositor
Map size ( $\text{\AA}$ )	381.44, 381.44, 381.44	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.99333334, 0.99333334, 0.99333334	Depositor

## 4 Model quality [i](#)

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

MolProbity failed to run properly - this section is therefore empty.

### 4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

### 4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 4.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
8	GDP	F	201	-	24,30,30	0.94	1 (4%)	30,47,47	1.30	4 (13%)
9	WYL	F	202	-	67,80,80	0.67	1 (1%)	62,116,116	1.23	6 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GDP	F	201	-	-	6/12/32/32	0/3/3/3
9	WYL	F	202	-	-	7/42/97/97	0/9/9/9

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	201	GDP	C6-N1	-2.31	1.34	1.37
9	F	202	WYL	C34-N35	2.03	1.38	1.35

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	202	WYL	C5-N4-C6	5.54	131.74	125.62
9	F	202	WYL	C37-C44-C49	4.25	117.89	107.66
8	F	201	GDP	PA-O3A-PB	-3.41	121.13	132.83
9	F	202	WYL	C14-O13-C1	-3.27	112.44	117.59
8	F	201	GDP	C3'-C2'-C1'	3.07	105.60	100.98

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

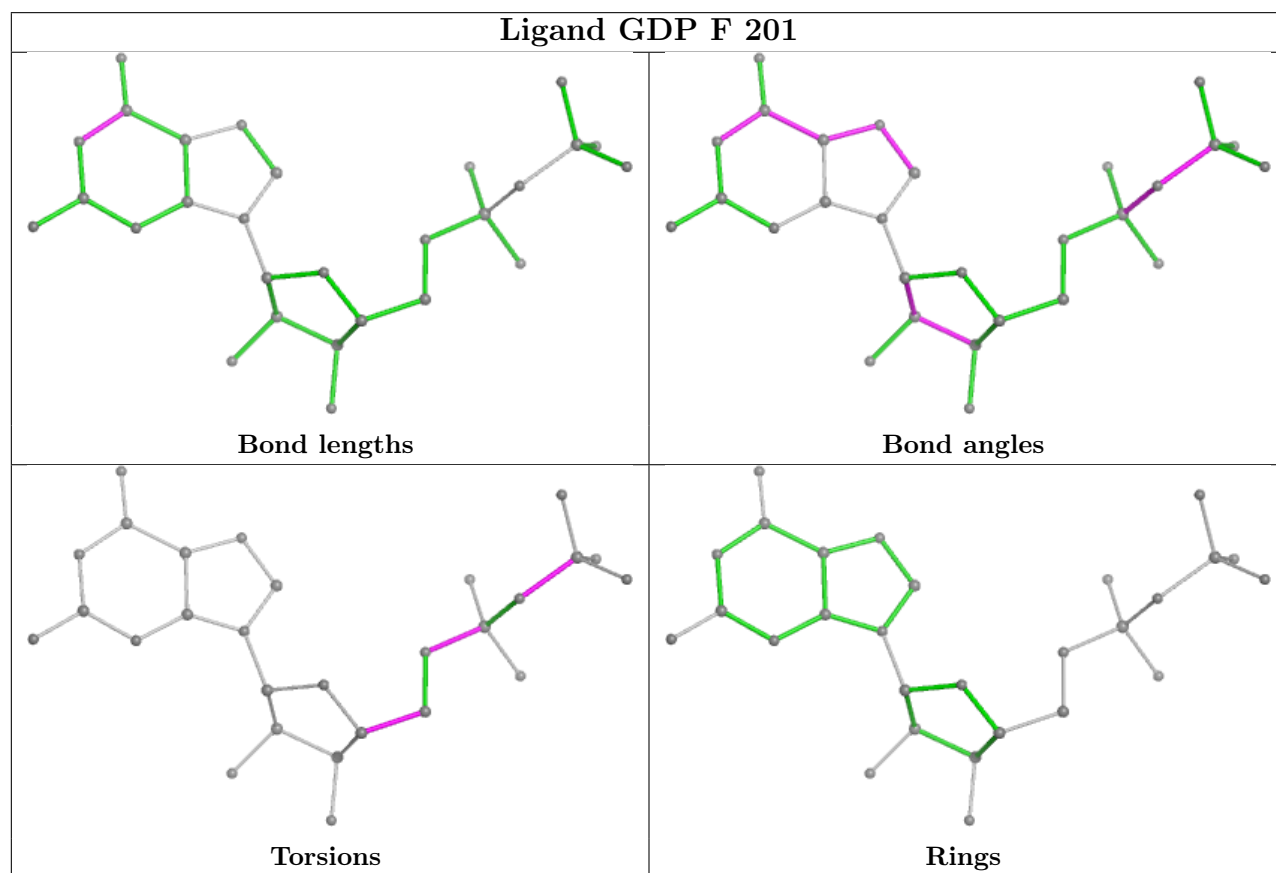
Mol	Chain	Res	Type	Atoms
8	F	201	GDP	PA-O3A-PB-O3B
9	F	202	WYL	C11-C10-C6-N4
9	F	202	WYL	C12-C10-C6-N4
9	F	202	WYL	C15-C16-C17-N19
8	F	201	GDP	O4'-C4'-C5'-O5'

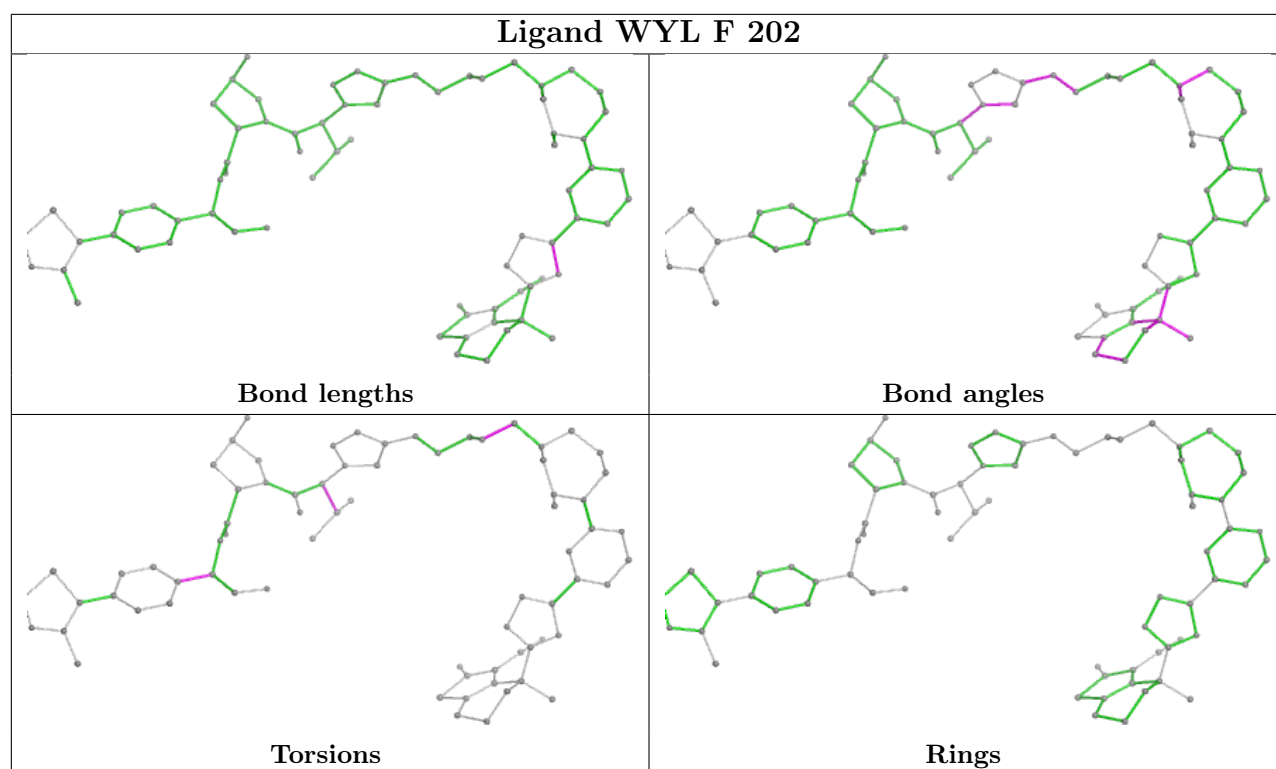


There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

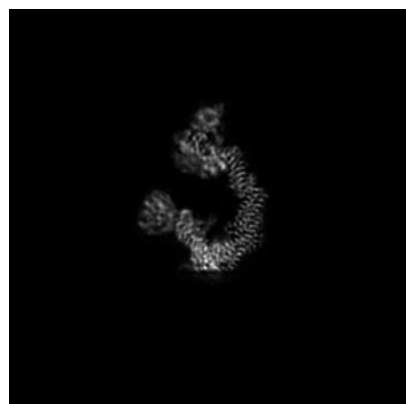
## 5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18657. These allow visual inspection of the internal detail of the map and identification of artifacts.

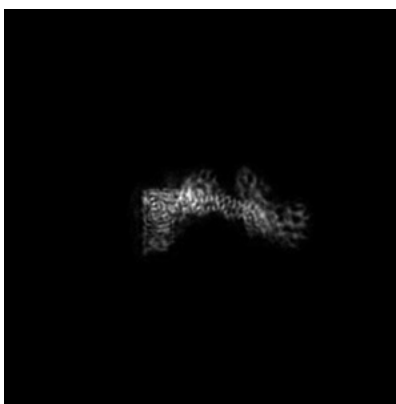
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

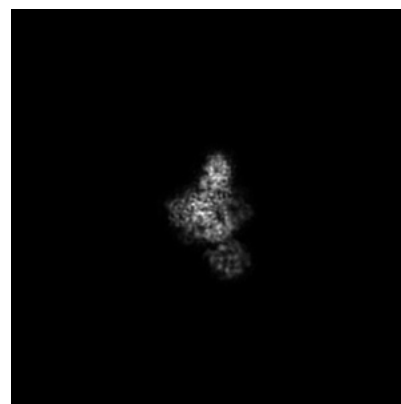
#### 5.1.1 Primary map



X

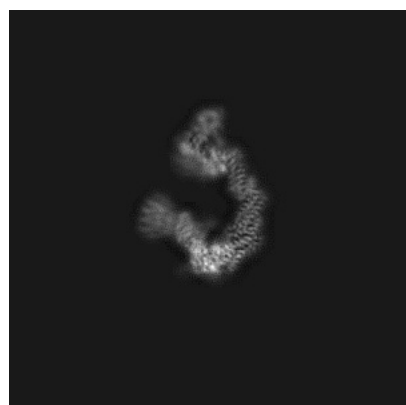


Y

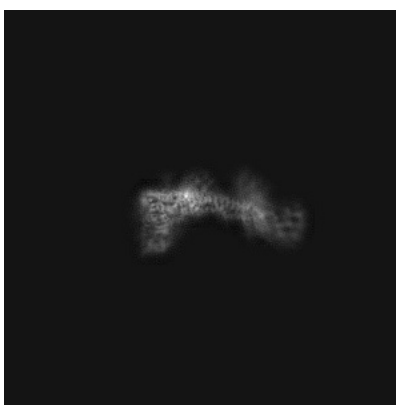


Z

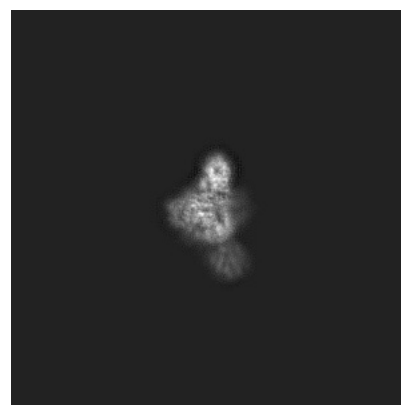
#### 5.1.2 Raw map



X



Y

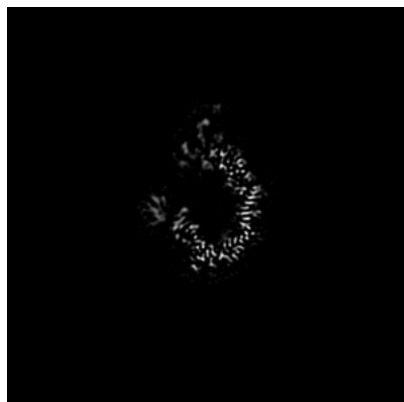


Z

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

## 5.2 Central slices [i](#)

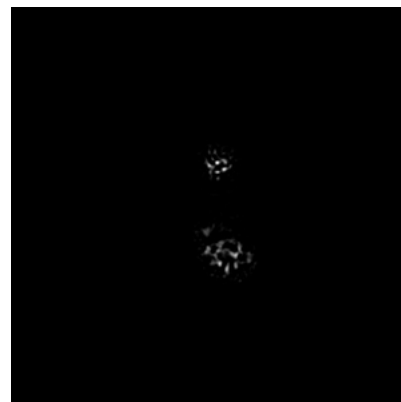
### 5.2.1 Primary map



X Index: 192

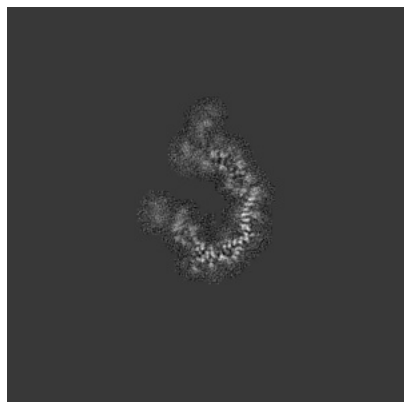


Y Index: 192

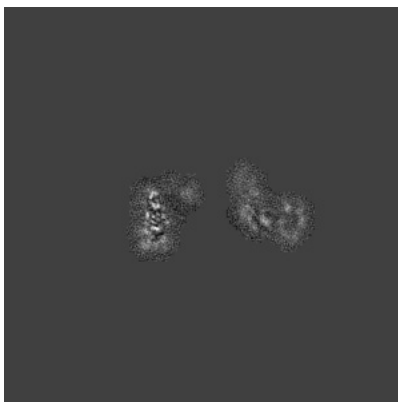


Z Index: 192

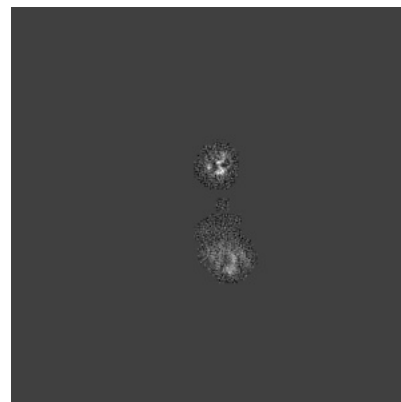
### 5.2.2 Raw map



X Index: 192



Y Index: 192

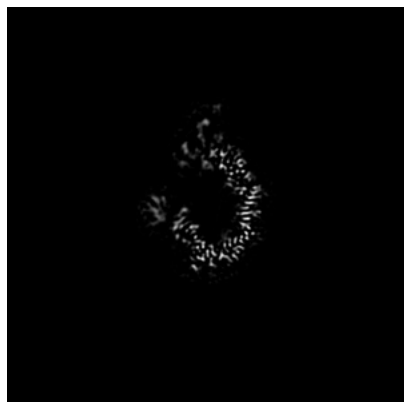


Z Index: 192

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

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

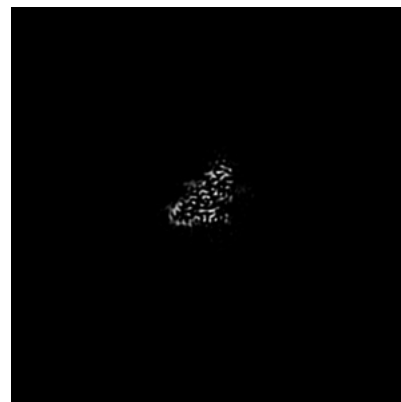
### 5.3.1 Primary map



X Index: 192

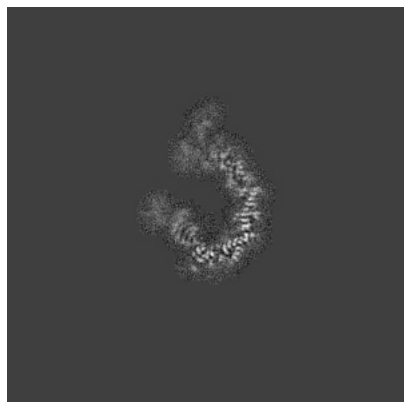


Y Index: 188

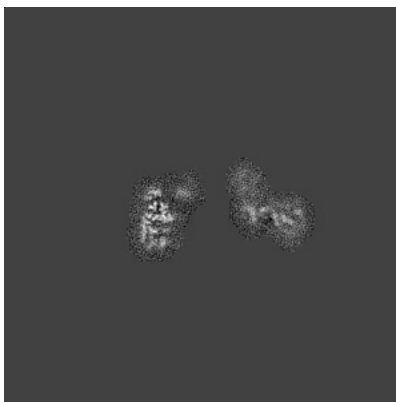


Z Index: 153

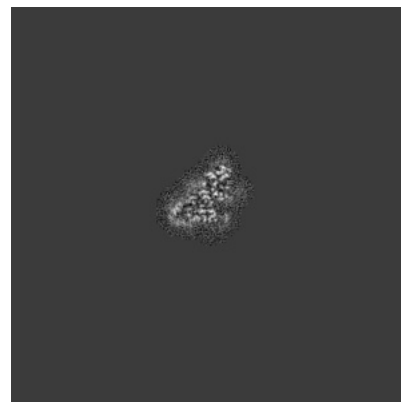
### 5.3.2 Raw map



X Index: 193



Y Index: 188

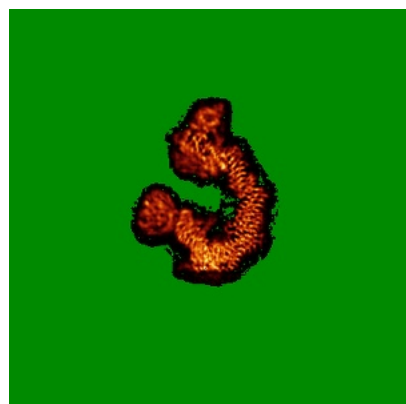


Z Index: 152

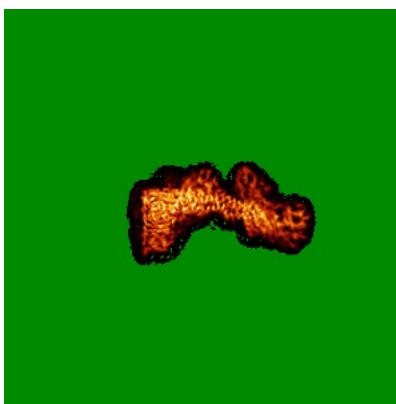
The images above show the largest variance slices of the map in three orthogonal directions.

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

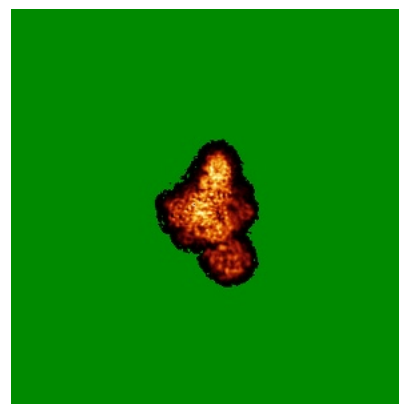
### 5.4.1 Primary map



X

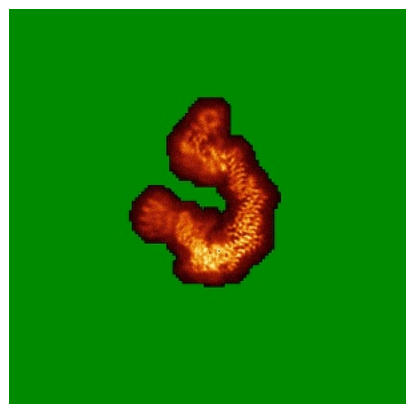


Y

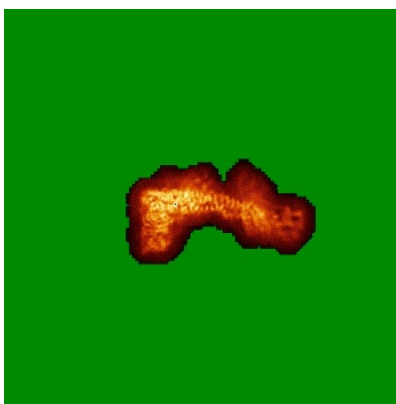


Z

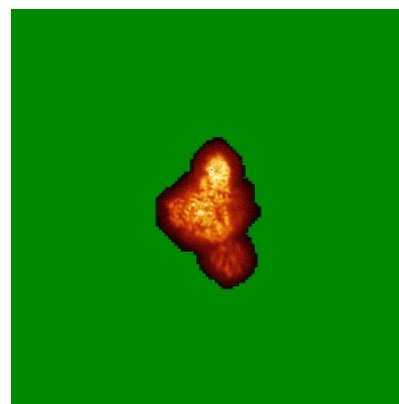
### 5.4.2 Raw map



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.

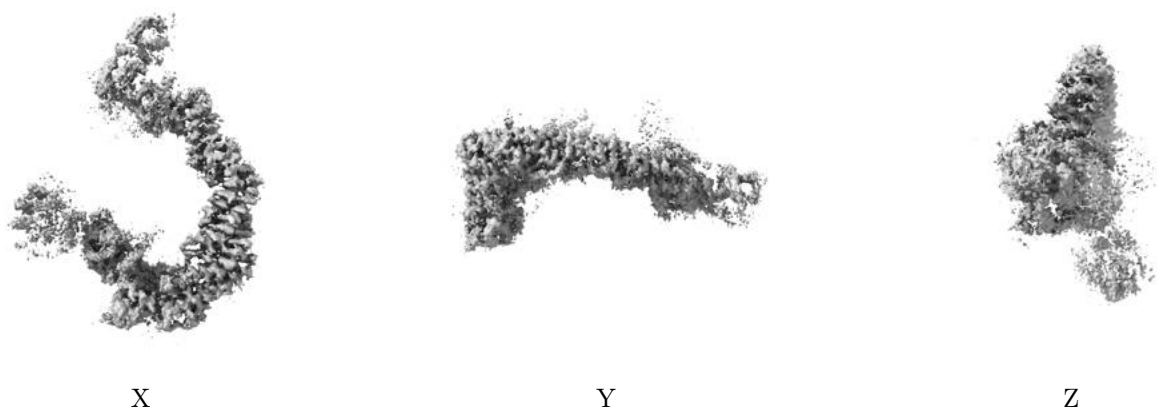
## 5.5 Orthogonal surface views [i](#)

### 5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 5.5.2 Raw map



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

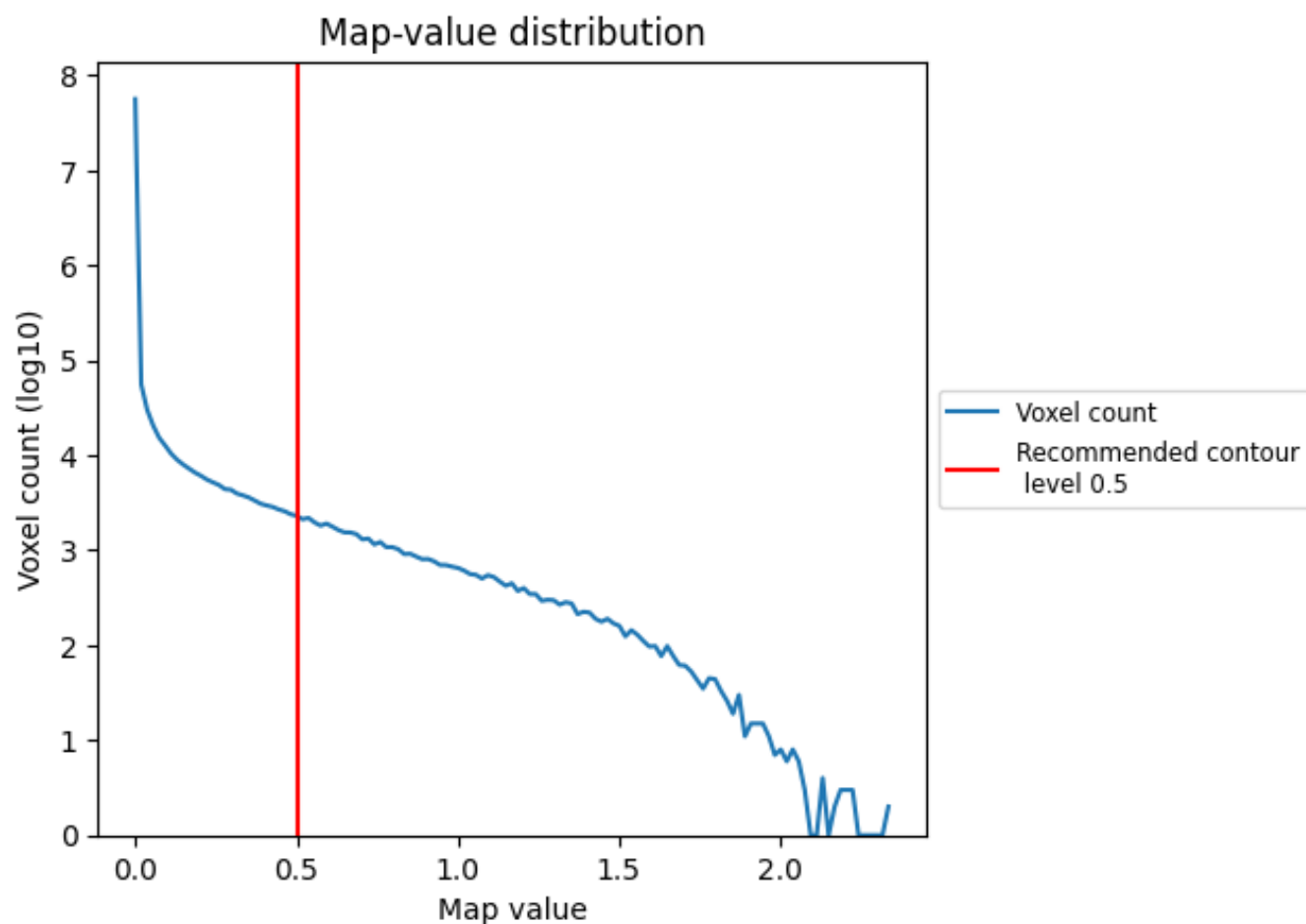
## 5.6 Mask visualisation [i](#)

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

## 6 Map analysis [i](#)

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

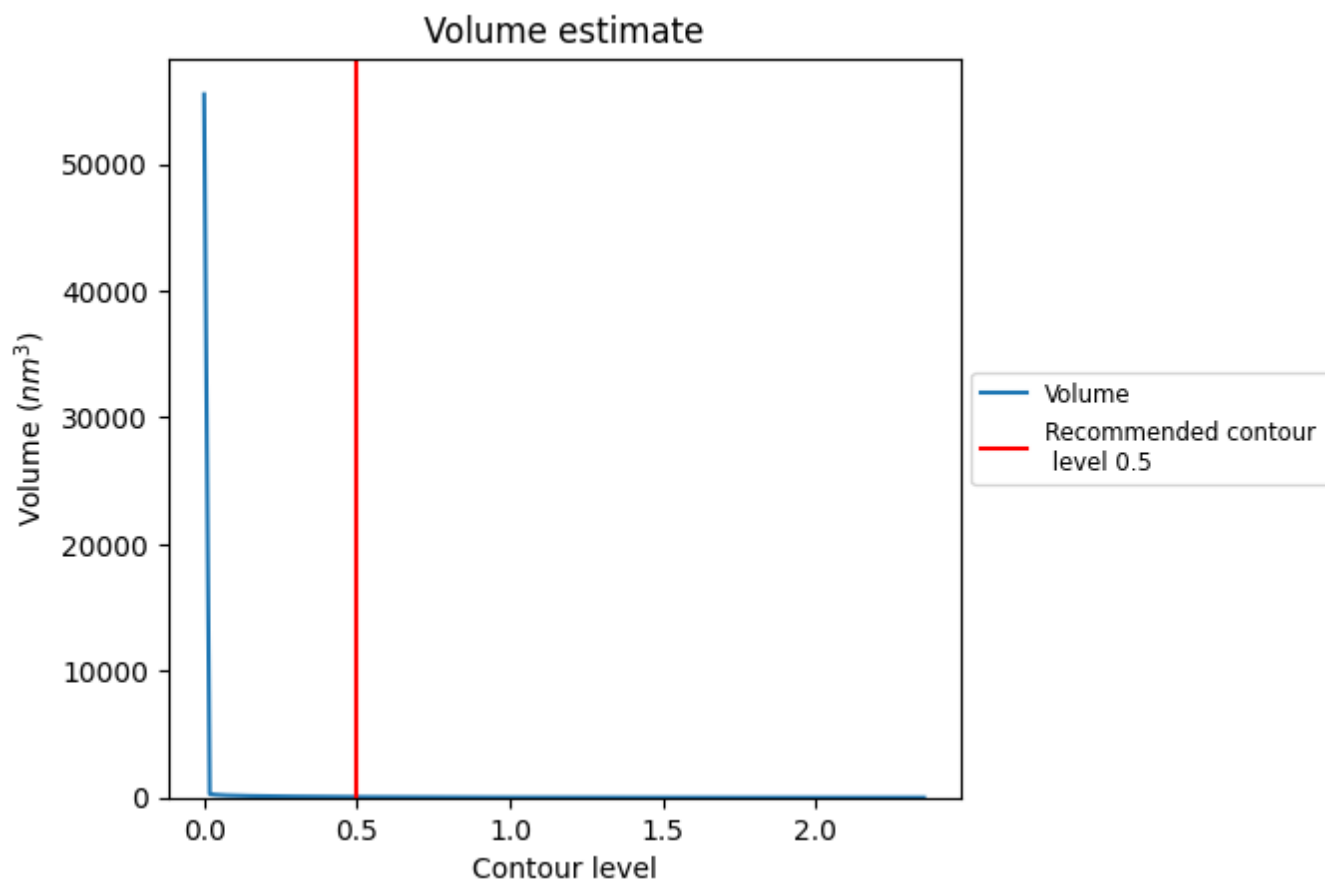
### 6.1 Map-value distribution [i](#)



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.



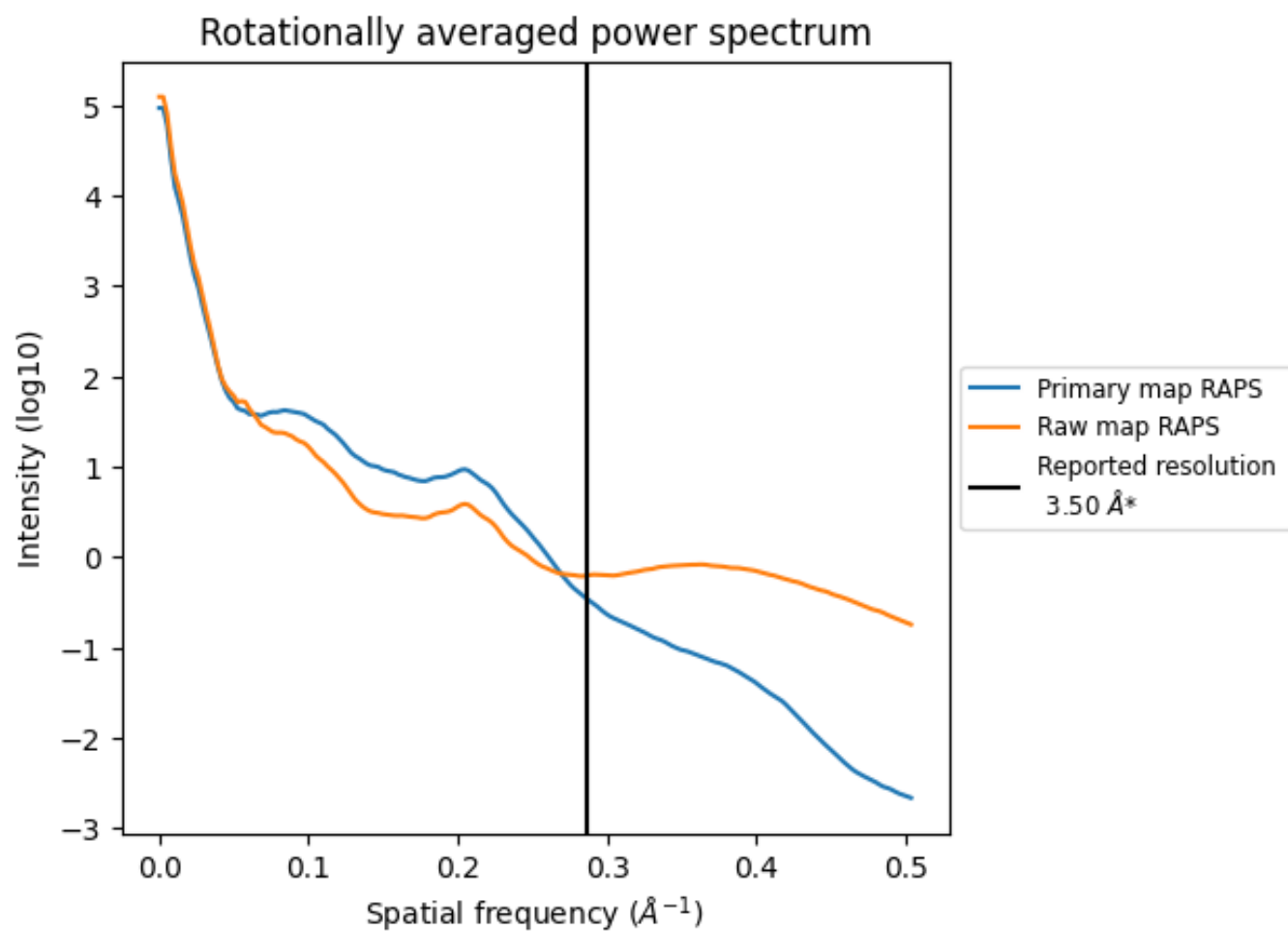
## 6.2 Volume estimate [i](#)



The volume at the recommended contour level is 46  $\text{nm}^3$ ; this corresponds to an approximate mass of 42 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.

### 6.3 Rotationally averaged power spectrum ⓘ

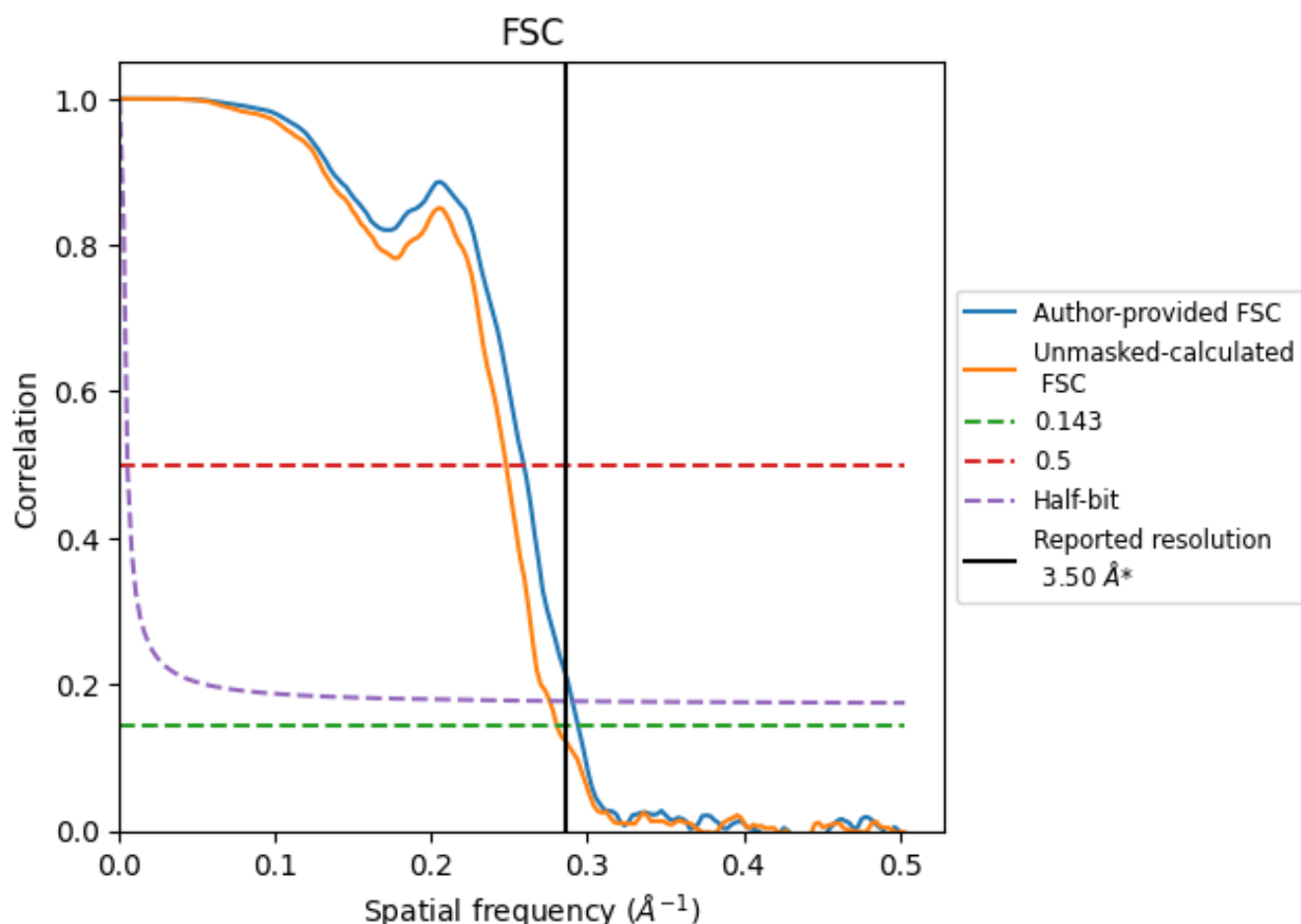


\*Reported resolution corresponds to spatial frequency of 0.286 Å<sup>-1</sup>

## 7 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.

### 7.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.286 Å<sup>-1</sup>

## 7.2 Resolution estimates [i](#)

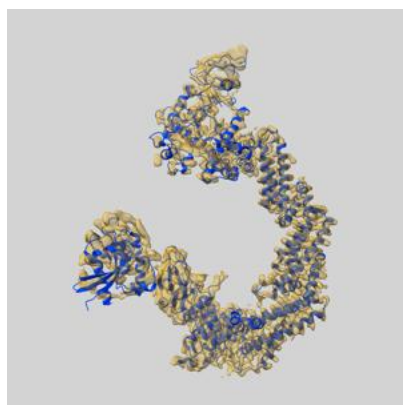
Resolution estimate (Å)	Estimation criterion (FSC cut-off)			
	0.143	0.5	Half-bit	Other
Reported by author	-	-	-	3.50
Author-provided FSC curve	3.40	3.86	3.44	-
Unmasked-calculated*	3.57	4.04	3.63	-

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

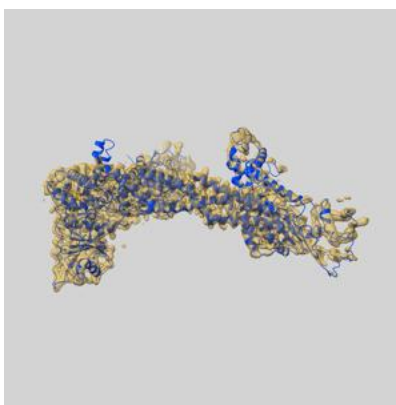
## 8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18657 and PDB model 8QU8. Per-residue inclusion information can be found in section ?? on page ??.

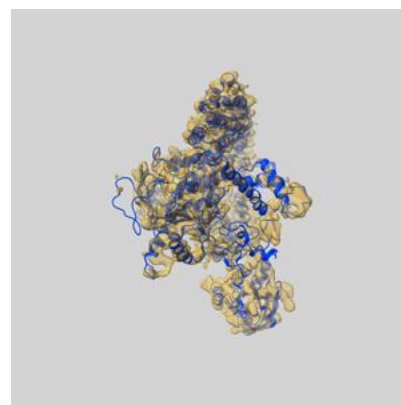
### 8.1 Map-model overlay [i](#)



X



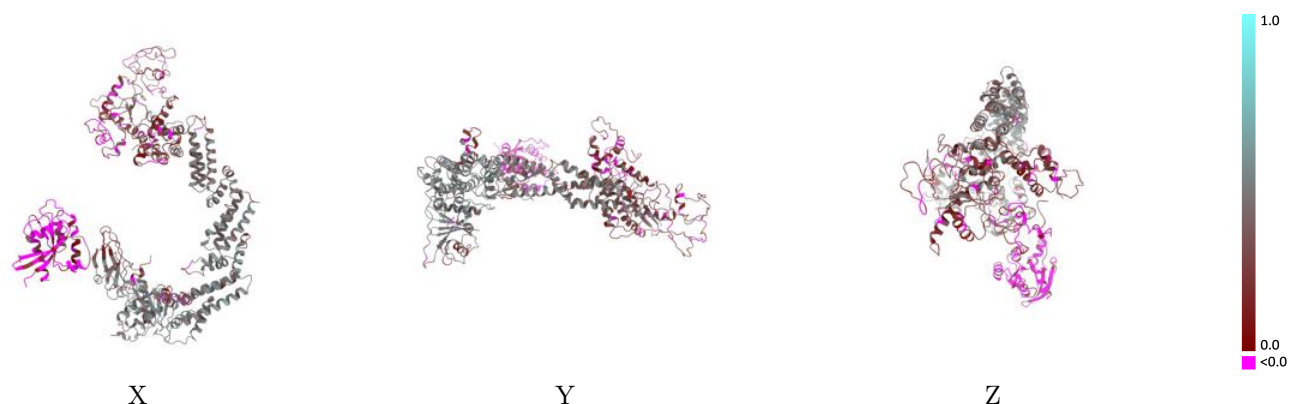
Y



Z

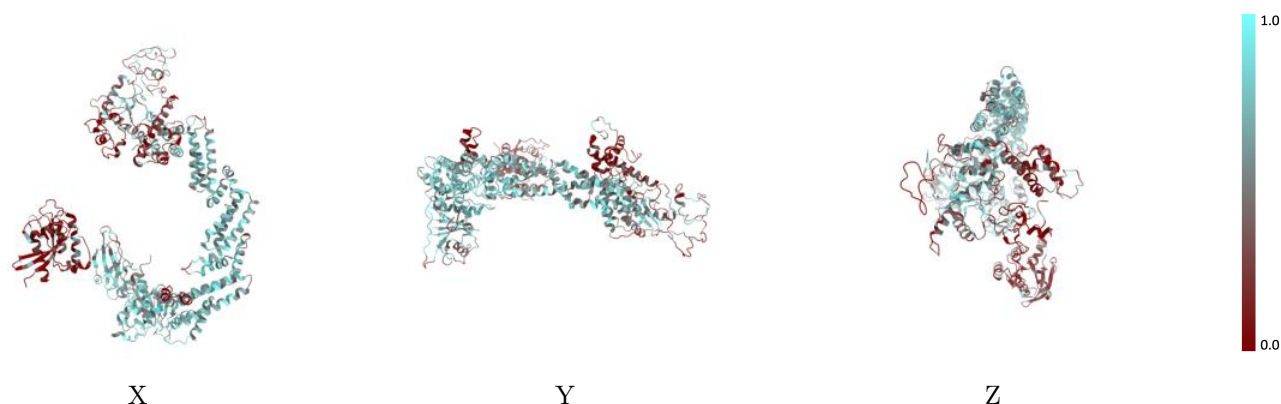
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



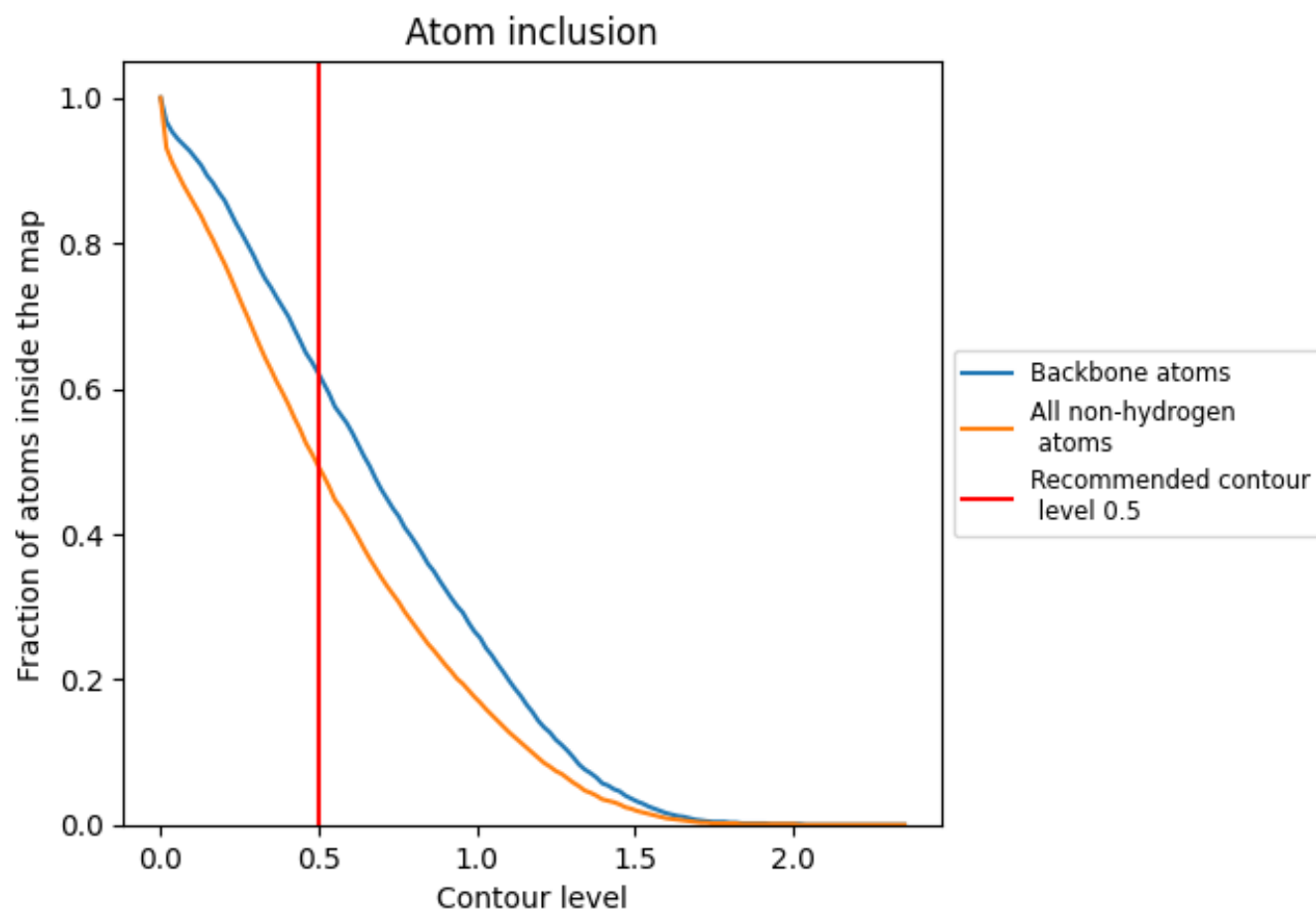
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 8.3 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 (0.5).

## 8.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 49% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4920	<div></div> 0.3060
A	<div></div> 0.6360	<div></div> 0.3920
B	<div></div> 0.6010	<div></div> 0.3970
C	<div></div> 0.6760	<div></div> 0.4610
D	<div></div> 0.5260	<div></div> 0.3480
E	<div></div> 0.2340	<div></div> 0.1550
F	<div></div> 0.2090	<div></div> 0.0040

