



## wwPDB EM Validation Summary Report ⓘ

Dec 19, 2022 – 09:03 am GMT

PDB ID : 7NH3  
EMDB ID : EMD-12319  
Title : Nematocida Huwel in open conformation  
Authors : Petrova, O.; Grishkovskaya, I.; Grabarczyk, D.B.; Kessler, D.; Haselbach, D.; Clausen, T.  
Deposited on : 2021-02-09  
Resolution : 6.37 Å(reported)  
Based on initial model : 7BII

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.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

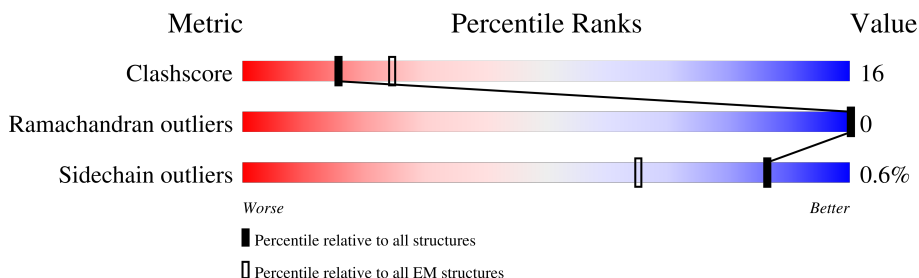
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.37 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	2490	

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 17417 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.

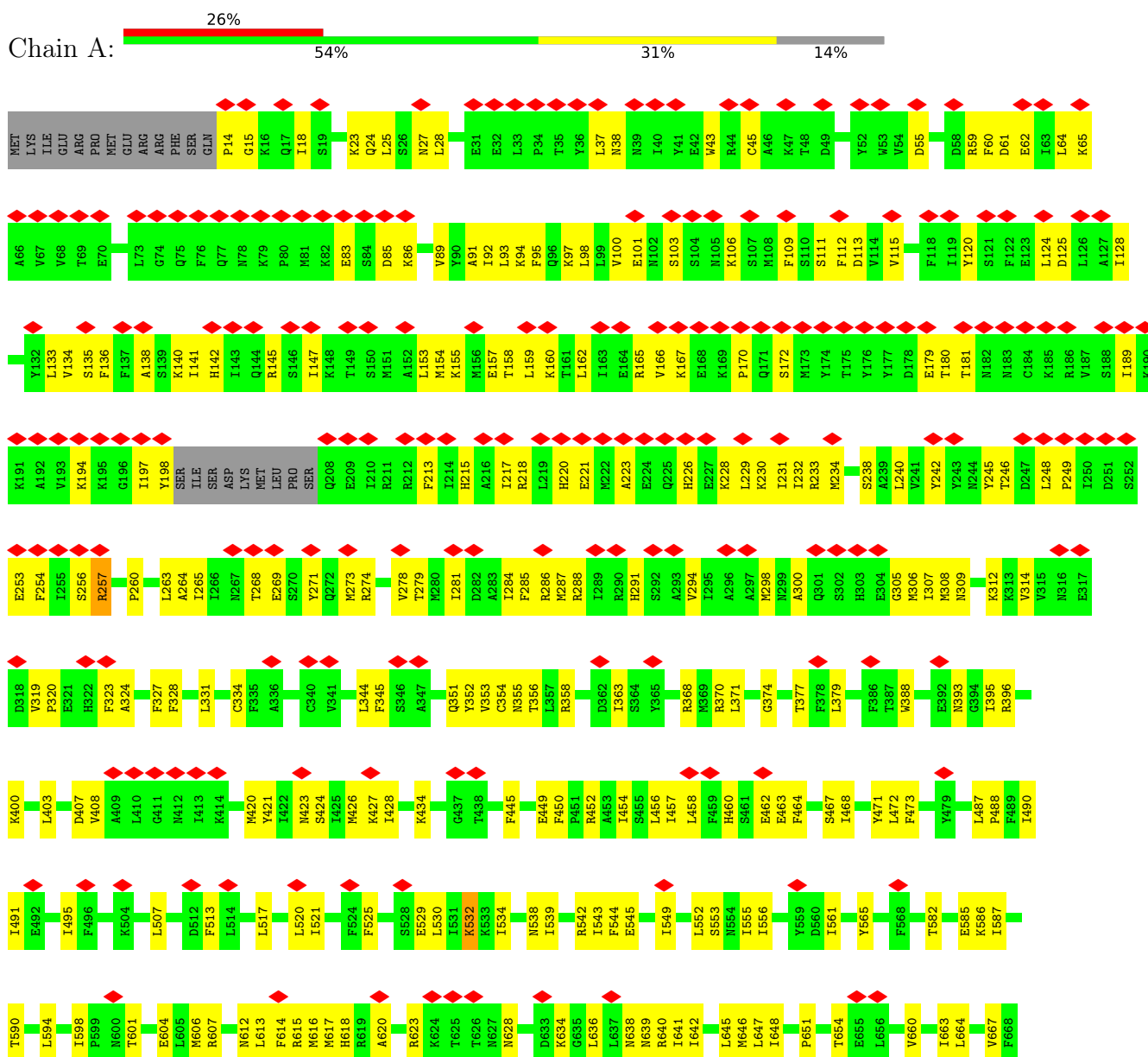
- Molecule 1 is a protein called E3 ubiquitin-protein ligase HUWE1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2138	17417	11256	2856	3208	97	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: E3 ubiquitin-protein ligase HUWE1





H2442	N2381	F2249	E2173	T2112	E2035	T1951	V1878	V1808	GLU
K2443	T2382	L2254	E2174	L2113	S2036	D1952	F1879	R1809	HIS
A2444	I2383	S2255	G2175	D2114	L2037	R1953	S1880	I1810	GLU
S2445	N2318	I2256	V2176	F2115	L2038	R1956	N1882	F1811	ALA
G2446	R2319	P2257	D2177	K2118	A2039	P1957	T1883	E1814	ARG
G2447	R2386	A2178	A2178	R2119	S2040	Y1962	E1884		TYR
S2448	Y2387	G2179	G2179	L2120	S2041	L1963	I1885	V1817	MET
S2449	T2388	D2259	G2180	T2120	L2042	M1964	I1886	N1818	GLU
R2450	S2389	L2260	G2181	Y2121	L2043	G1965	N1887	I1820	THR
L2451	D2390	T2261	L2181	F2122	P2044	K1969	K1888	I1821	PHE
P2452	S2391	V2263	T2182	Y2123	K2047	S1970	I1889	Q1822	ALA
T2453	Q2392	E2264	R2183	K2124		L1971	A1823	Y1822	GLY
A2454	V2393	A2265	E2184	R2125			V1824	Q1823	GLU
H2455	R2395	Y2186	Y2185	T2126	V2050	T1897	G1827	I1827	ILE
T2456	R2396	S2187	E2188	R2127	V2051	I1898			VAL
C2457	F2270	E2269	S2189	E2128	V2052	S1899			PRO
F2458	H2271	F2270	L2189	D2129	T2054	E1900	ALA		ARG
N2459	R2272	R2272	A2196	Q2130	I2055	S1901	SER		GLU
Q2460	S2273	L2274	N2197	Q2131	Q2056	S1902	SER		GLU
L2461	R2274	V2275	Y2198	L2132	M2057	K1903	SER		GLU
D2462	L2274	W2276	A2199	R2133	Y2058	L1904	ALA		LYS
L2463	V2276	L2277	L2200	T2135	I2059	L1905	GLY		LYS
P2464	W2277	I2277	F2201	S2137	E2063	S1906	ALA		LYS
E2465	L2278	E2279	I2204	L2138	N2064		ALA		PRO
Y2466	L2278	E2279	G2205	W2139	I2065		GLY		GLN
S2468	E2344	N2280	S2206	V2140	E2070		SER		GLU
Y2469	E2348	D2281	Q2209	Q2141	I2071		THR		MET
E2470	I2349	I2282	P2210	R2142	P2072		VAL		PRO
Q2471	L2350	E2283	Q2209	G2143	D2075		ASN		PHE
L2472	D2351	N2284	I2213	A2144	S2076		ALA		
V2473	V2352	V2285	S2214	W2145	S2077		SER		
K2474	D2353	L2286	H2215	F2146	I2078		GLY		
A2475	K2356	D2287	I2216	E2147	Y2079		SER		
L2476	N2359	N2288	Y2223	D2148	Y2080		GLY		
L2477	E2360	F2289	F2224	T2149	V2083		ASN		
F2478	K2361	S2291	I2227	H2151	L2089		GLU		
S2479	L2363	L2292	G2228	Q2152	I2090		V1851		
L2480	E2364	E2293	R2229	L2153	N2091		I1852		
E2481	L2365	L2293	I2230	W2154			A1853		
E2482	L2366	R2296	G2232	L2155	Q2095		P1854		
CYS	I2367	F2297	K2233	N2157	A2096		E1855		
THR	L2370	G2298	A2234	W2156	D2097		V1856		
SER	F2371	L2299	V2235	N2157	Q2097		I1857		
GLY	L2372	T2300	Y2236	E2159	L2100		T1858		
GLY	T2373	I2302	D2237	Q2160	H2103		T1859		
PHE	D2374	L2305	E2238	V2161	A2104		R1860		
PHE	V2375	K2306	W2239	R2162	F2105		G1861		
ALA	D2376	E2307	T2240	N2163	Q2109		F1862		
	Q2433	N2308	D2242	A2164	K2110		L1865		
	N2434	G2309	T2246	F2166	K2111		T1866		
	G2435	R2310	R2247	N2167			L1867		
	N2436	N2311	A2248	I2168			L1868		
	Q2437	I2312		K2169			F1875		
	F2438	A2313		F2170					
	Q2440	V2314		G2172					
	I2441								

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57866	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 ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.035	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00778	Depositor
Map size (Å)	344.0, 344.0, 344.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	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	0.25	0/17754	0.49	0/23950

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	17417	0	17695	569	0
All	All	17417	0	17695	569	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 16.

The worst 5 of 569 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:294:VAL:O	1:A:298:MET:HB2	1.67	0.94
1:A:1540:LEU:HD12	1:A:1544:LYS:HD2	1.63	0.80
1:A:556:ILE:HA	1:A:561:ILE:HD13	1.62	0.80
1:A:1008:PHE:HA	1:A:1011:LEU:HD13	1.65	0.79
1:A:814:LEU:HA	1:A:817:TYR:HD2	1.50	0.77



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	2123/2490 (85%)	2033 (96%)	90 (4%)	0	100	100

There are no Ramachandran outliers to report.

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

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	1951/2267 (86%)	1939 (99%)	12 (1%)	86	92

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1306	LYS
1	A	1387	LYS
1	A	2337	ARG
1	A	2142	ARG
1	A	886	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	855	ASN

*Continued on next page...*

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Mol	Chain	Res	Type
1	A	1116	ASN
1	A	1822	GLN
1	A	1563	GLN
1	A	809	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 monosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	246:THR	C	247:ASP	N	8.66
1	A	208:GLN	C	209:GLU	N	3.54

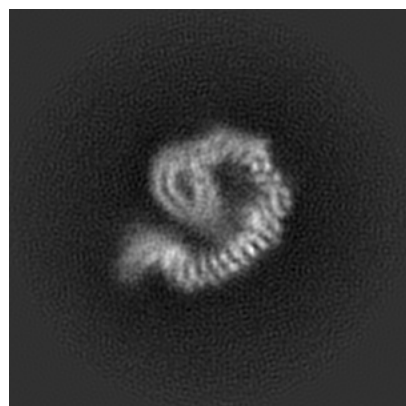
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12319. These allow visual inspection of the internal detail of the map and identification of artifacts.

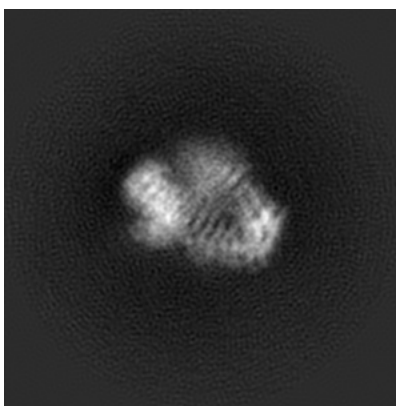
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

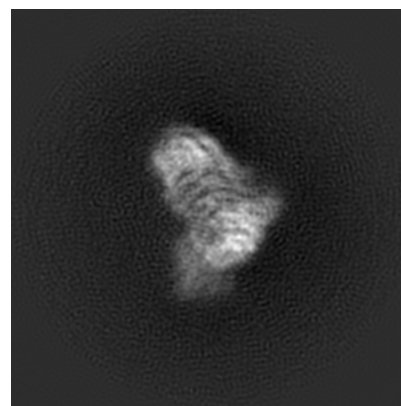
#### 6.1.1 Primary map



X

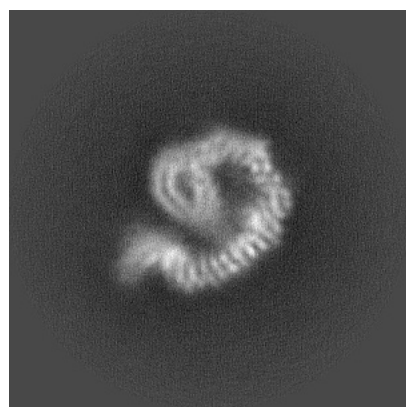


Y

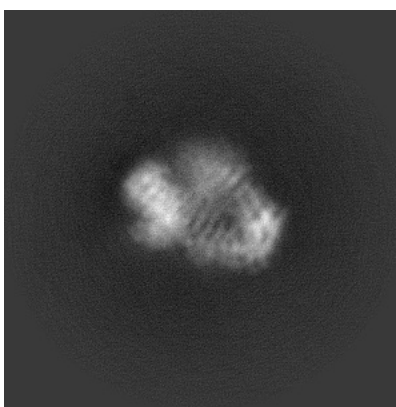


Z

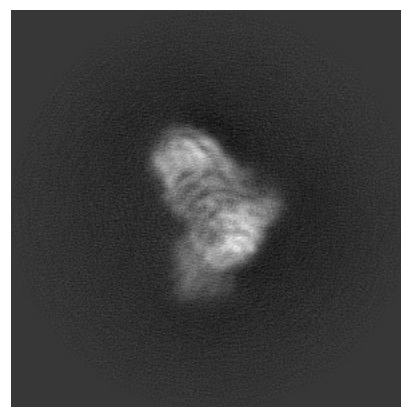
#### 6.1.2 Raw map



X



Y

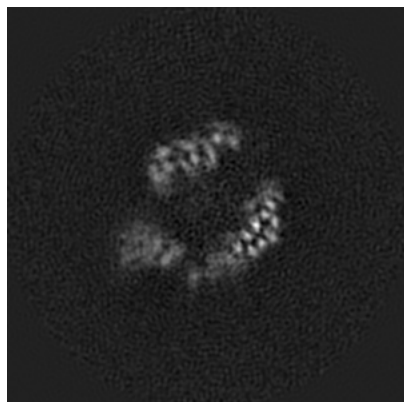


Z

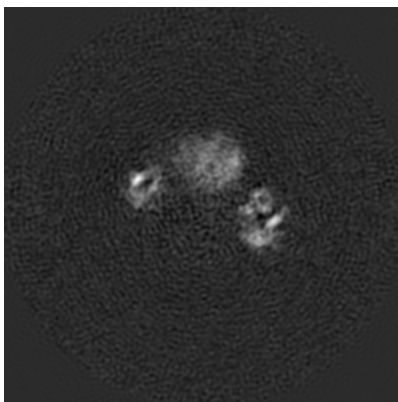
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

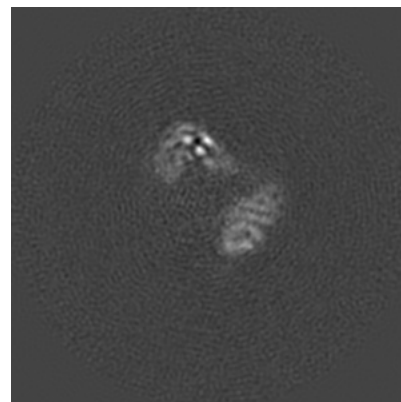
### 6.2.1 Primary map



X Index: 200

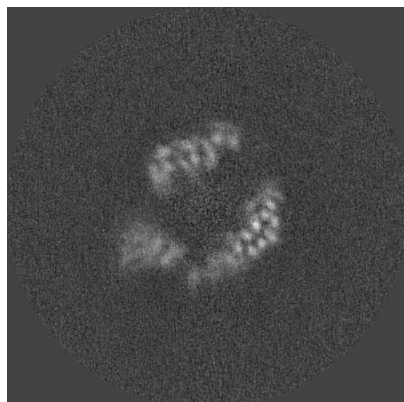


Y Index: 200

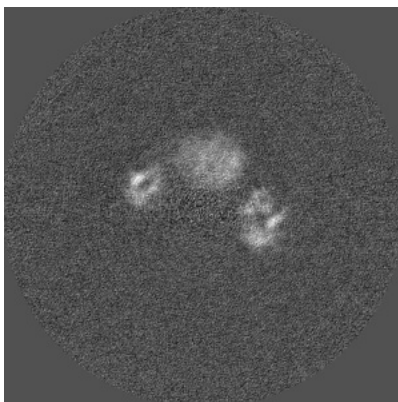


Z Index: 200

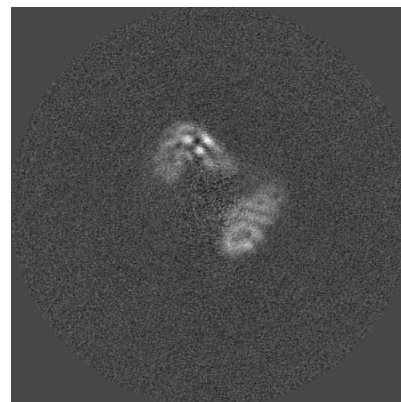
### 6.2.2 Raw map



X Index: 200



Y Index: 200

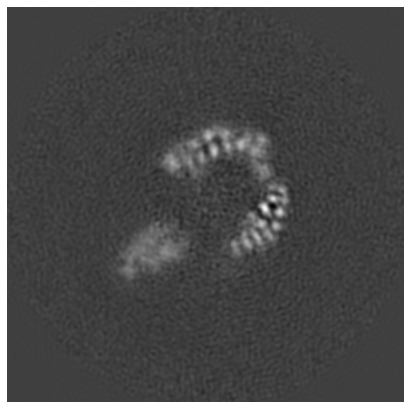


Z Index: 200

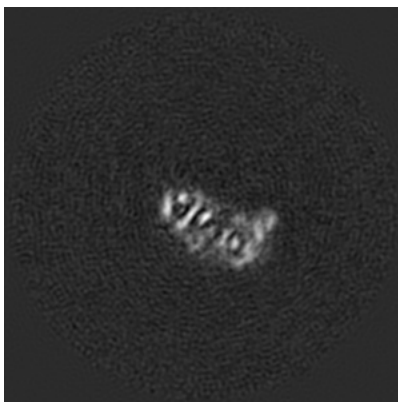
The images above show central slices of the map in three orthogonal directions.

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

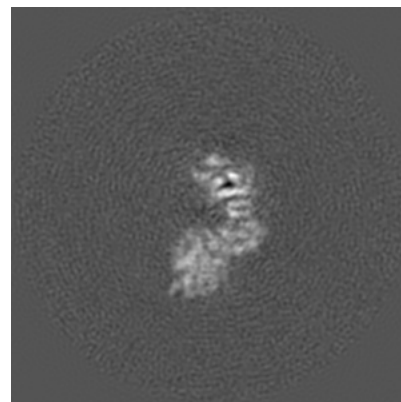
### 6.3.1 Primary map



X Index: 187

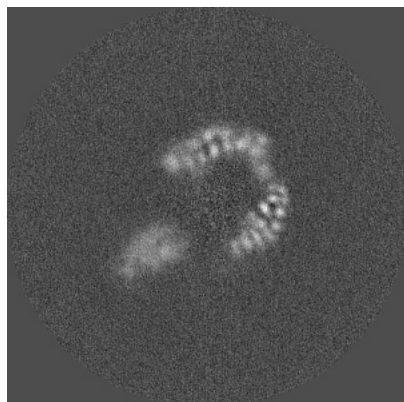


Y Index: 255

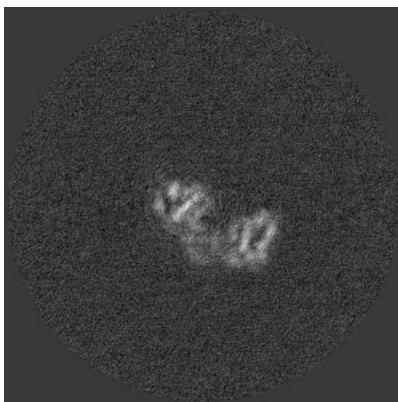


Z Index: 152

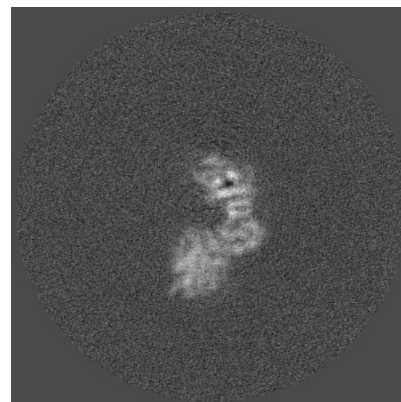
### 6.3.2 Raw map



X Index: 187



Y Index: 247

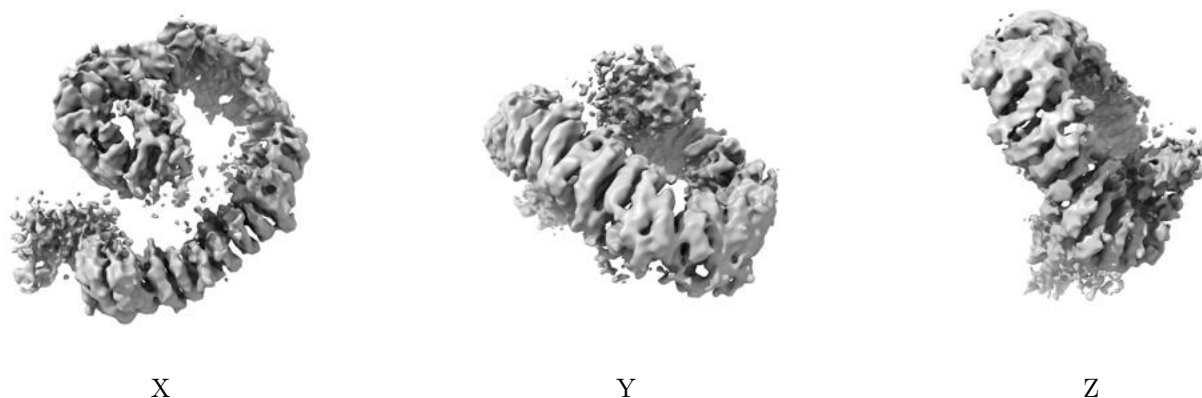


Z Index: 151

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

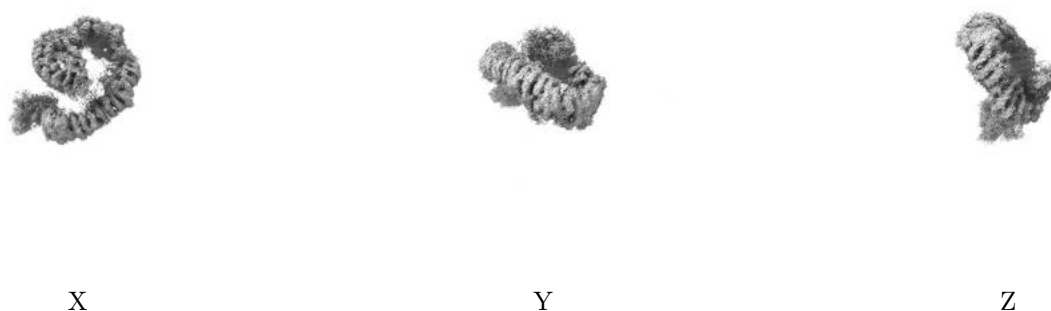
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00778. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.



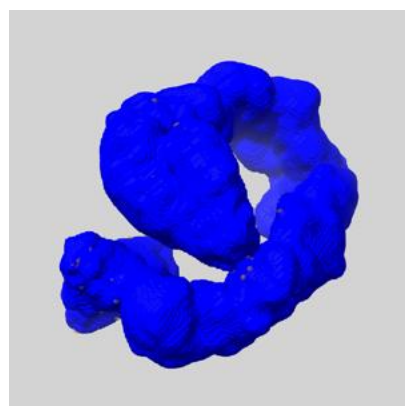
## 6.5 Mask visualisation [i](#)

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

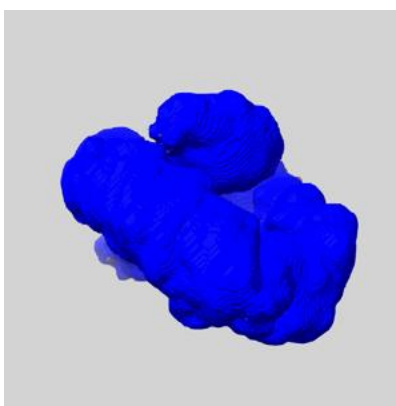
A mask typically either:

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

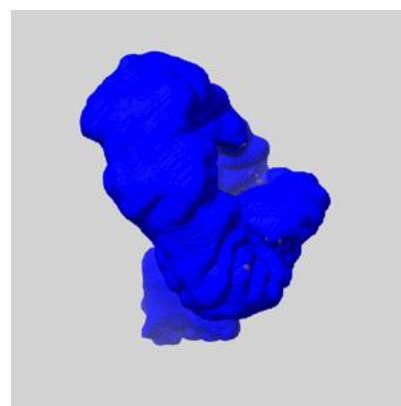
### 6.5.1 emd\_12319\_msk\_1.map [i](#)



X



Y

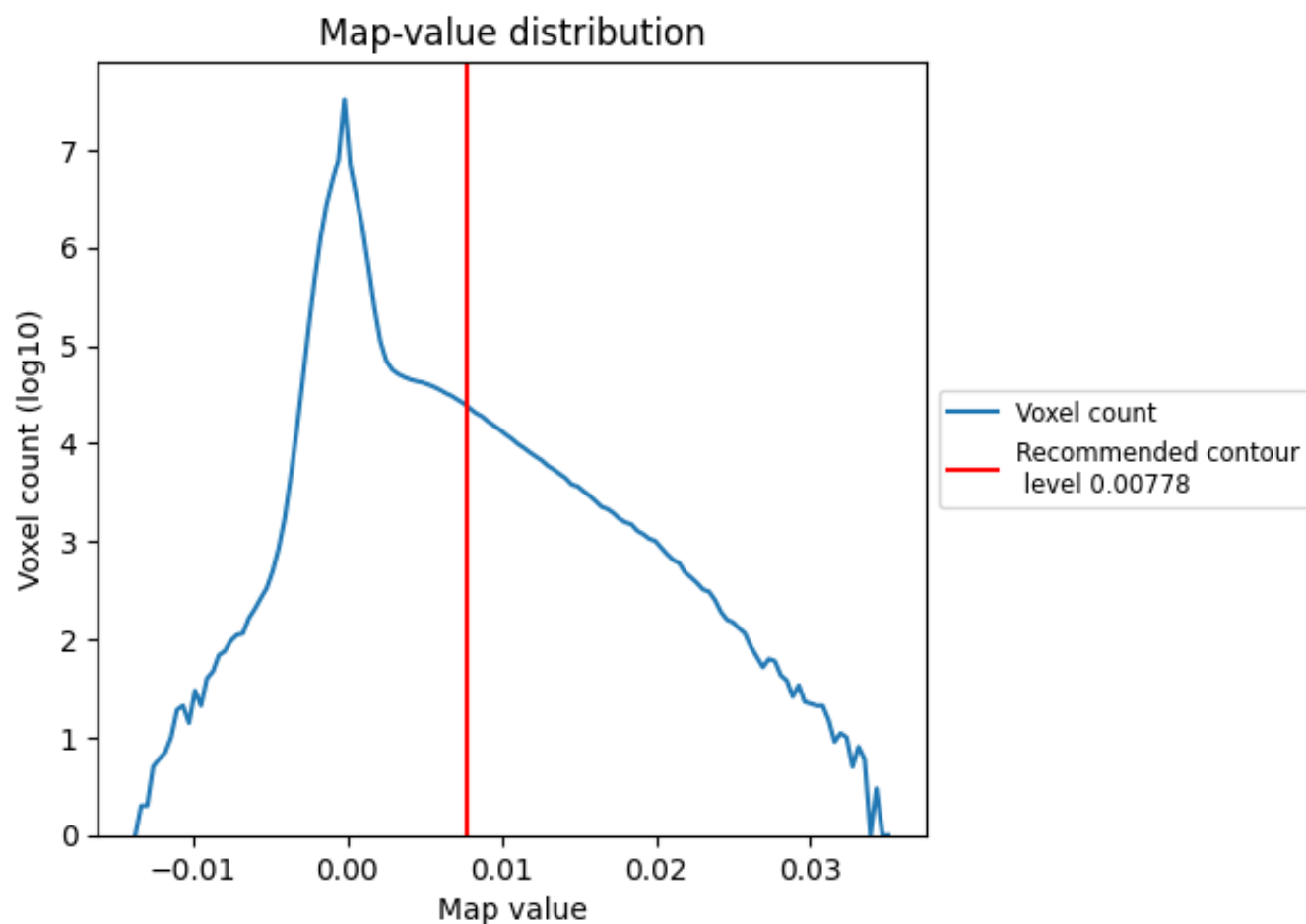


Z

## 7 Map analysis [i](#)

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

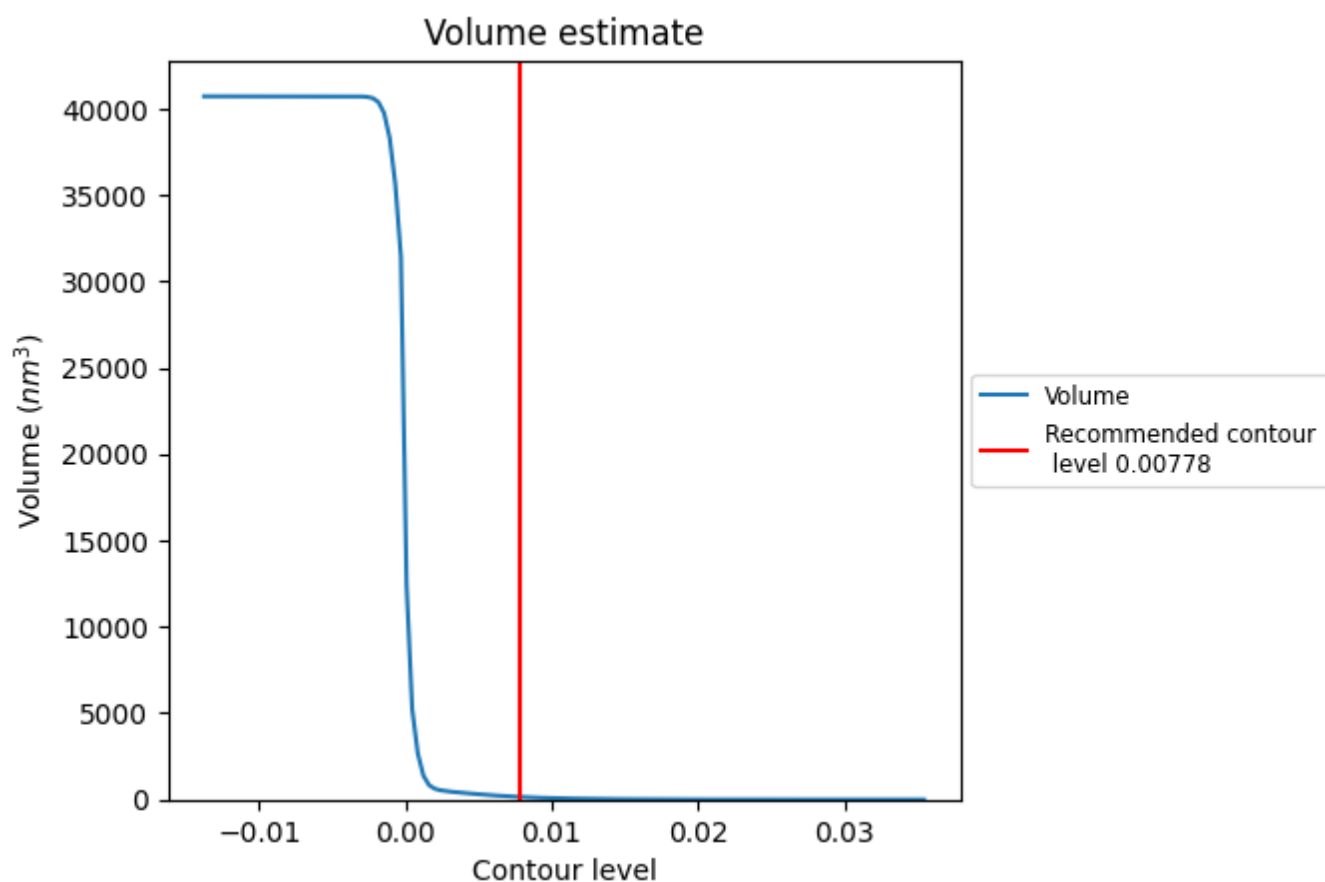
### 7.1 Map-value distribution [i](#)



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.



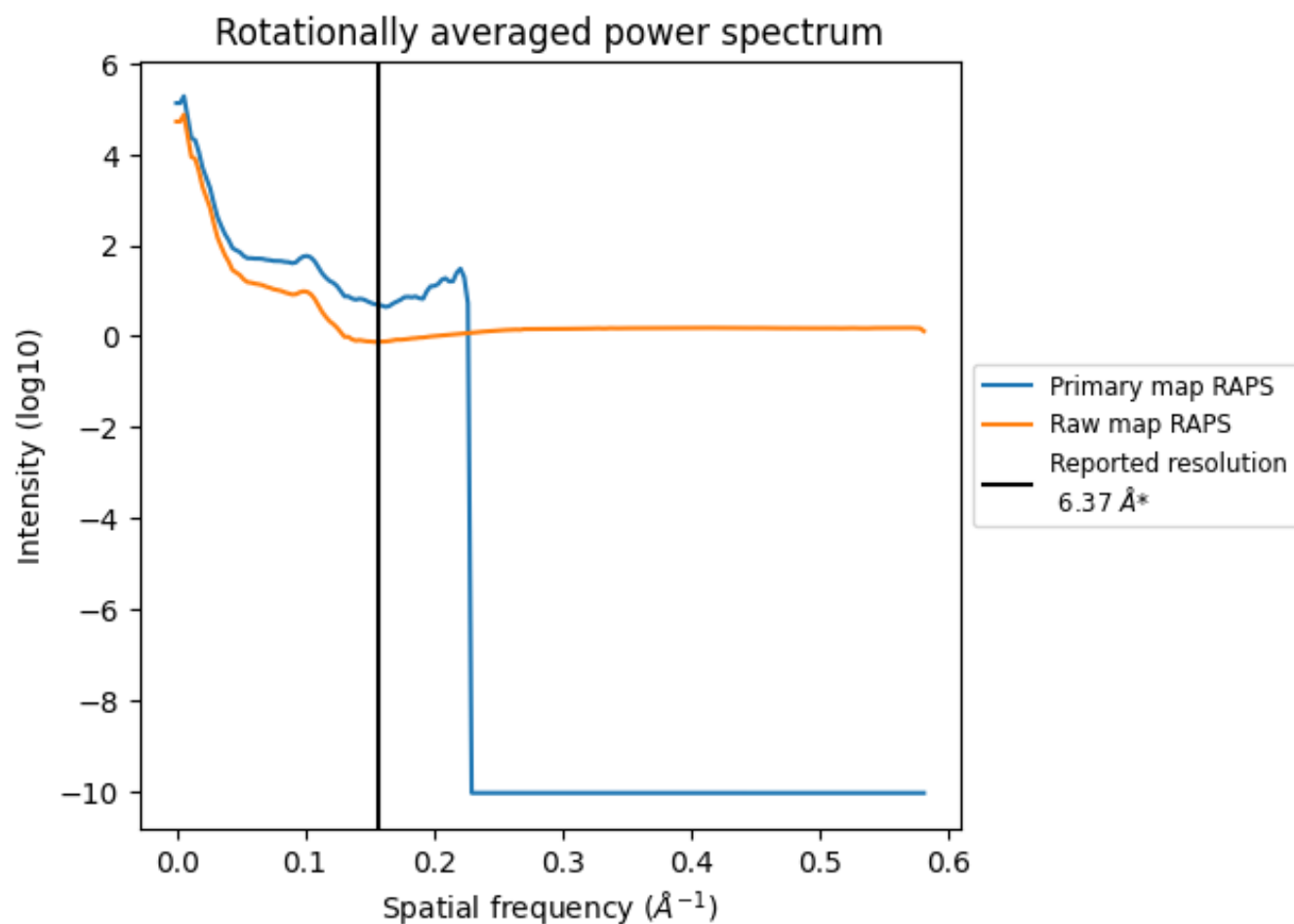
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 154 nm<sup>3</sup>; this corresponds to an approximate mass of 139 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 ⓘ

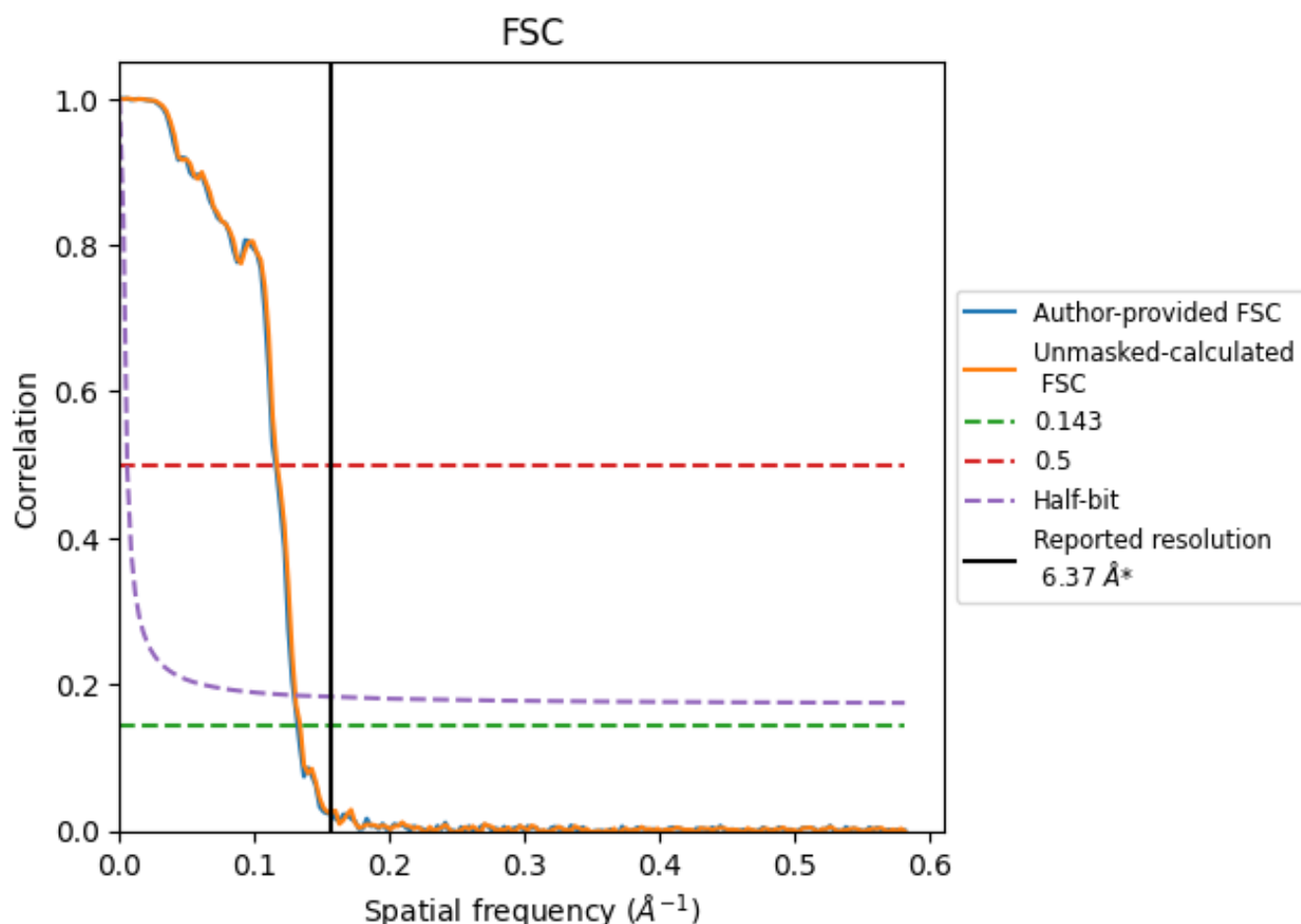


\*Reported resolution corresponds to spatial frequency of 0.157 Å<sup>-1</sup>

## 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 0.157 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	6.37	-	-
Author-provided FSC curve	7.58	8.66	7.74
Unmasked-calculated*	7.47	8.57	7.67

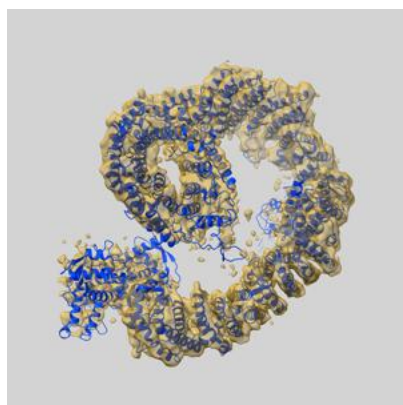
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 7.58 differs from the reported value 6.37 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.47 differs from the reported value 6.37 by more than 10 %

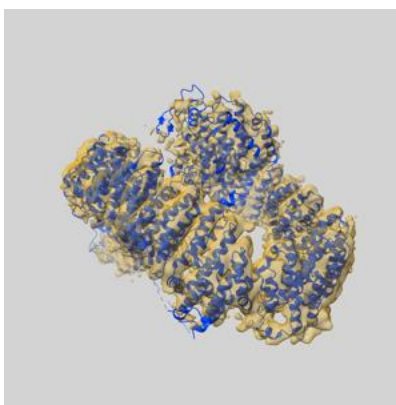
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12319 and PDB model 7NH3. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

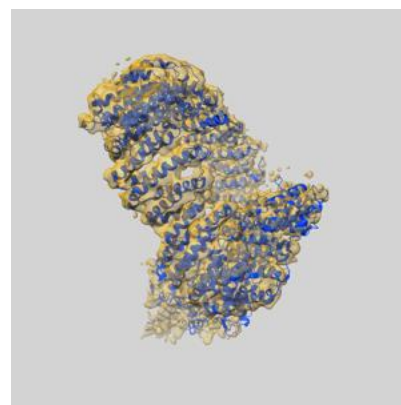
### 9.1 Map-model overlay [i](#)



X



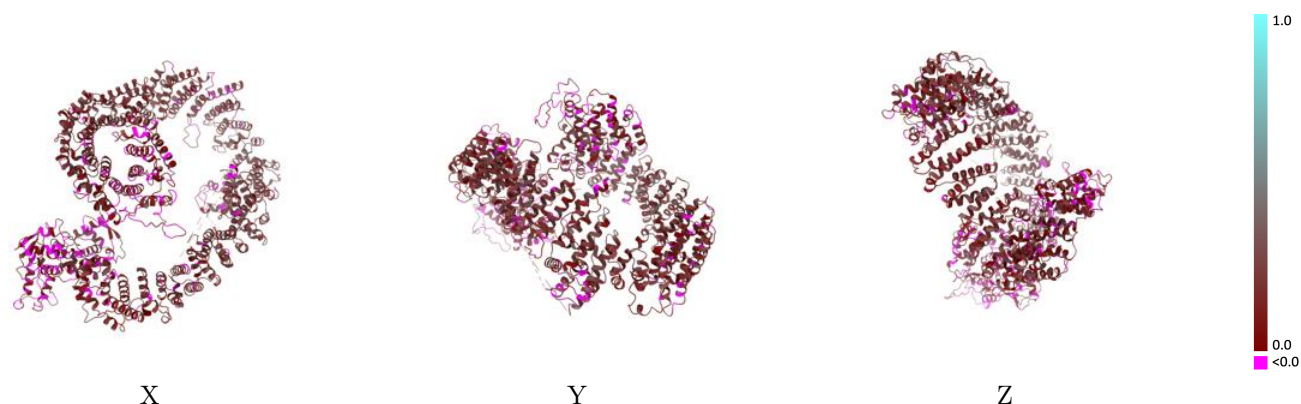
Y



Z

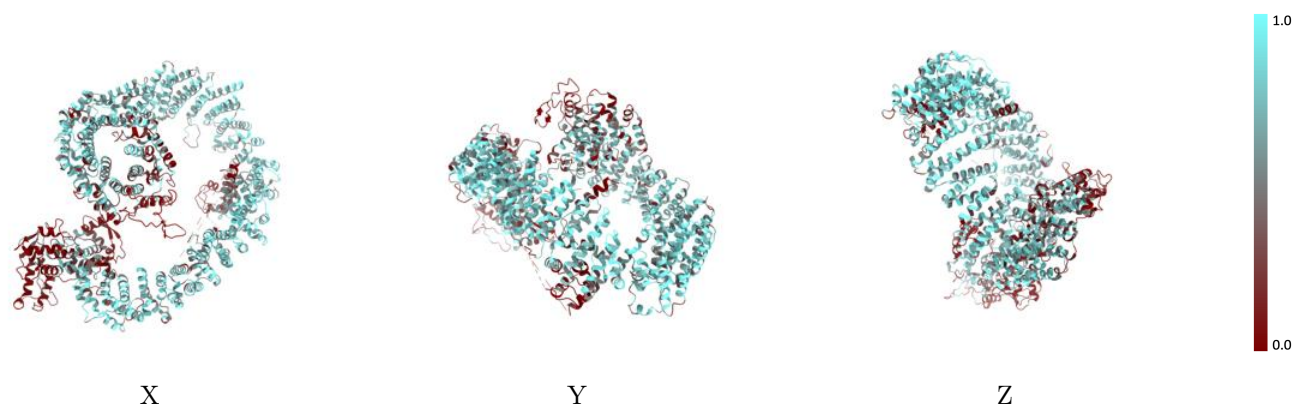
The images above show the 3D surface view of the map at the recommended contour level 0.00778 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



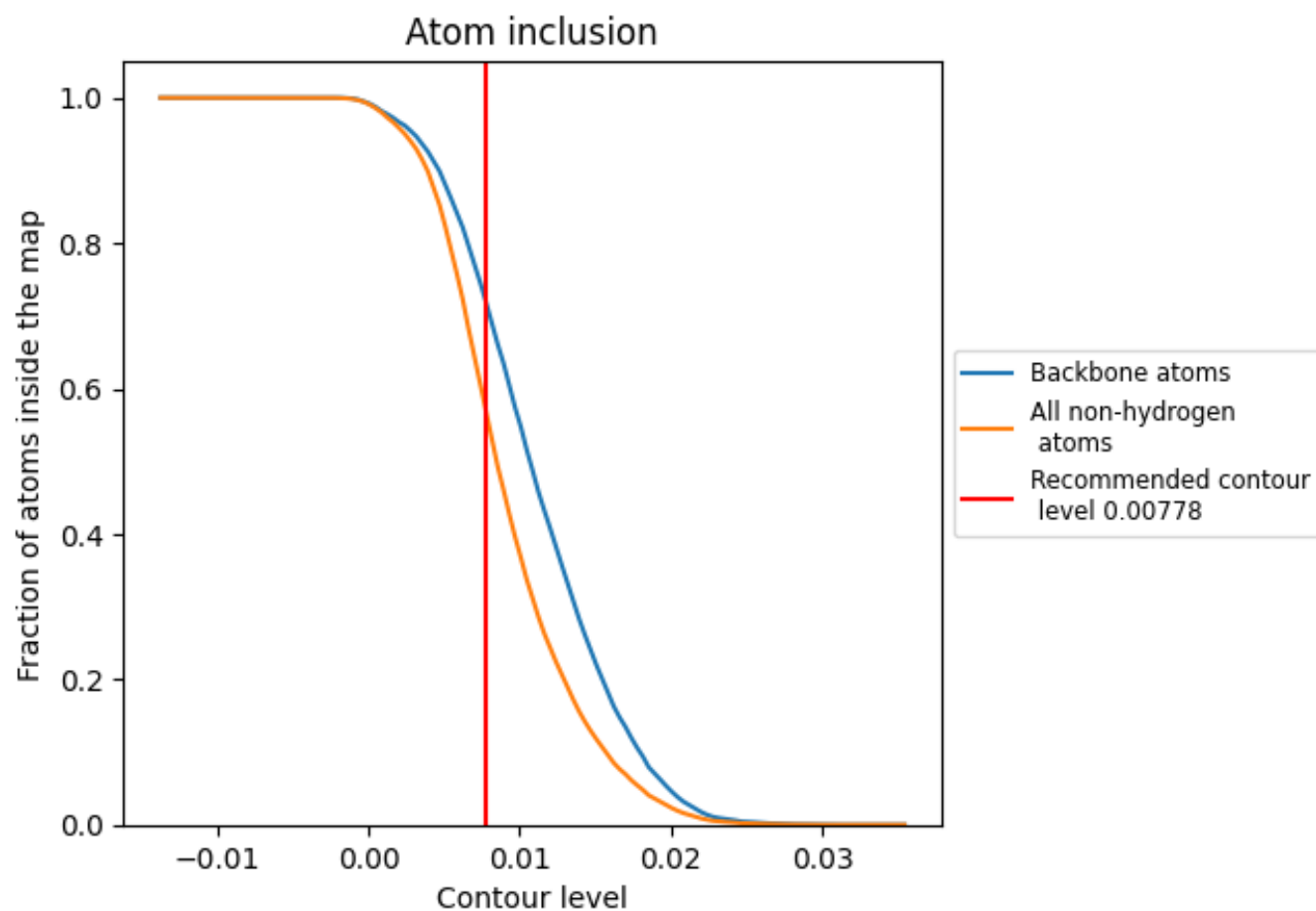
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00778).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 57% 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 (0.00778) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5669	<div></div> 0.1590
A	<div></div> 0.5669	<div></div> 0.1590

