



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 06:27 PM UTC

PDB ID : 7NH1 / pdb_00007nh1
EMDB ID : EMD-12318
Title : Nematocida Huwe1 in closed conformation
Authors : Petrova, O.; Grishkovskaya, I.; Grabarczyk, D.B.; Kessler, D.; Haselbach, D.; Clausen, T.
Deposited on : 2021-02-09
Resolution : 5.29 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

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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

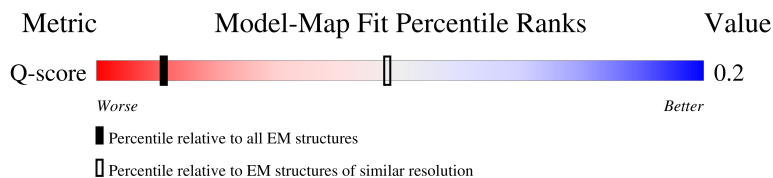
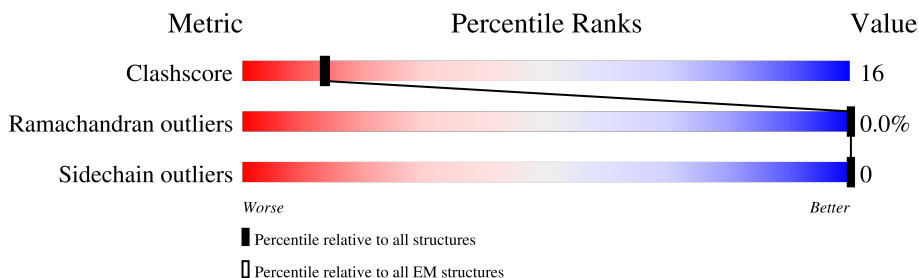
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.29 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	587 (4.79 - 5.75)

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 ≥ 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

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.

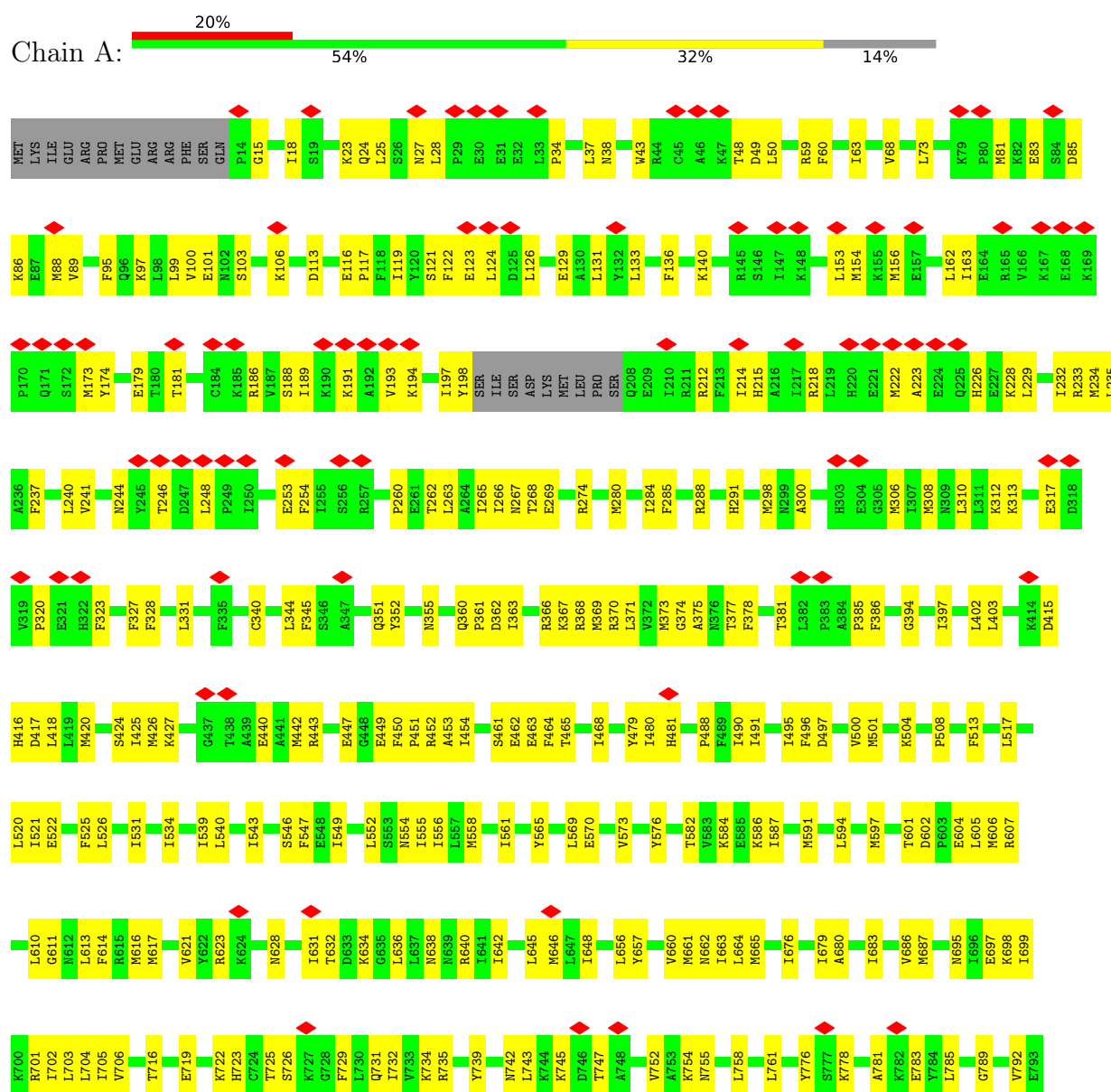
- Molecule 1 is a protein called E3 ubiquitin-protein ligase HUWE1.

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





PHE	F2427	S2367	K2306	T2246	W2185	K2124	S2036	L1932	I1852
GLY	A2428	S2368	E2307	R2247	Y2186	K2125	A2039	E1933	A1853
PHE	G2429	G2369	N2308	A2248	S2187	I2126	S2040	M1936	V1856
ALA	L2430	L2370	G2309	F2249	E2188	R2127	S2041	T1937	I1857
		P2371	R2310	Y2250	L2189	E2128	L2042	D1938	T1858
		E2372	N2311	K2251	K2191	D2129	L2043	T1939	K1859
		L2373	I2312	R2252	E2192	V2130	P2044	T1940	R1860
		D2374	A2313	L2254	M2193	Q2131	L2045	F1941	G1861
		V2375	V2314	S2255	F2194	L2132	F2046	K1942	F1862
		D2376	T2315	S2256	A2196	R2133	K2047	H1943	
		D2377	N2316	T2257	N2197	P2134		T1866	
		W2378	E2317	P2257	Y2198	T2135		Y1867	
		R2379	N2318	V2258	A2199	I2136		L1868	
		N2380	K2319	D2259	Y2199	T2054		G1869	
		W2381	R2320	L2260	L2200	I2055		R1963	
		T2382	E2321	T2261	F2201	M2139		F1875	
		L2383	Y2322	D2262	T2202	V2140		V1878	
		Y2384	V2323	V2263	P2203	G1965		F1879	
		F2385	E2324	E2264	I2204	G1966		S1880	
		G2386	L2325	A2265	G2205	S1987		Y1881	
		Y2387	V2326	L2266	S2206	I2058		N1882	
		T2388	C2327	D2267	S2207	I2059		T1883	
		S2389	R2328	P2268	Q2208	G2060		T1884	
		D2390	F2329	E2269	P2210	M2062		L1885	
		S2391	K2330	F2270	H2211	N2064		S1970	
		Q2392	L2331	H2271	H2212	I2065		I1887	
		V2393	V2332	R2272	I2213	E2067		K1888	
		L2394	R2333	S2273	S2214	S2069		T1897	
		R2395	V2334	L2274	H2215	K1978		I1898	
		W2396	I2335	V2275	I2216	D2148		S1889	
		Y2397	E2336	W2276	N2217	T2149		E1900	
		W2398	R2337	L2277	P2218	F2150		N1982	
		R2399	Q2338	L2278	E2219	H2151		F1981	
		A2400	L2339	E2279	H2220	Q2152		S1983	
		V2401	S2340	W2280	L2221	L2153		H1987	
		R2402	A2341	D2281	V2222	R2155		I1990	
		N2403	F2342	T2282	Y2223	L2156		L1905	
		F2404	A2343	E2283	F2224	N2157		S1906	
		S2405	E2344	W2284	K2225	G2158		T1907	
		M2406	G2345	V2285	F2226	E2159		V1908	
		E2407	F2346	L2286	I2227	Q2160		D1910	
		E2408	F2347	D2287	Q2228	V2161		C1911	
		R2409	E2348	W2288	R2229	K2162		F1912	
		A2410	I2349	N2289	I2230	F2166		M1913	
		K2411	L2350	F2290	I2231	M2167		V1917	
		L2412	D2351	S2291	G2232	T2170		A1918	
		L2413	V2352	T2292	K2233	A2171		E1919	
		Q2414	M2354	E2293	A2234	G2172		P1920	
		F2415	L2355	Q2294	V2235	K2173		E1924	
		A2416	K2356	D2295	Y2236	E2174		V1925	
		T2417	N2359	R2296	D2237	I2120		R1926	
		G2418	E2360	F2297	E2238	Y2121		I1929	
		T2419	K2361	G2298	M2239	F2122			
		S2420	E2362	T2299	T2240	D2177			
		K2421	L2363	T2300	V2241	A2178			
		L2422	E2364	D2242	D2242	G2179			
		P2423	L2365	T2302	F2245	G2180			
		L2424	L2366	T2303		L2181			
		E2481		D2304		T2182			
		E2482				K2183			
CYS						E2184			
THR									
SER									
GLY									

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	56284	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	0.038	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	0.13	0/17756	0.36	0/23956

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	17697	559	0
All	All	17417	0	17697	559	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 559 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:556:ILE:HA	1:A:561:ILE:HD13	1.62	0.79
1:A:591:MET:HE1	1:A:613:LEU:HD11	1.65	0.79
1:A:2286:LEU:HD23	1:A:2288:MET:H	1.45	0.79
1:A:369:MET:HG2	1:A:373:MET:HE1	1.66	0.77
1:A:241:VAL:HG22	1:A:248:LEU:HD21	1.67	0.76

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	2126/2490 (85%)	2035 (96%)	90 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2297	PHE

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%)	1951 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1247	ASN
1	A	2131	GLN
1	A	1887	ASN
1	A	2359	ASN
1	A	589	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

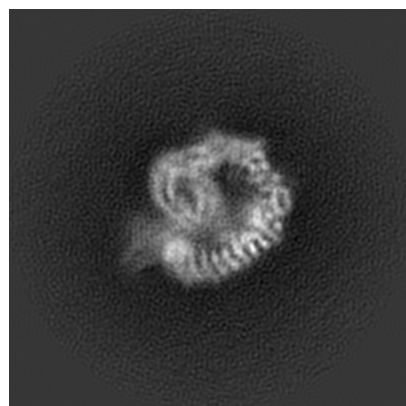
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12318. These allow visual inspection of the internal detail of the map and identification of artifacts.

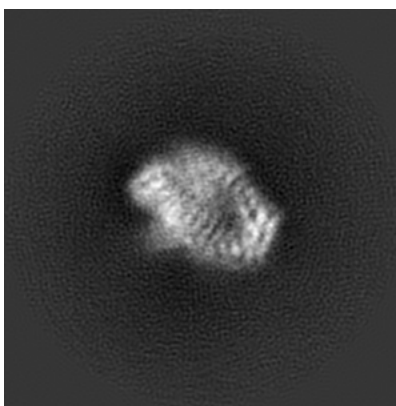
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

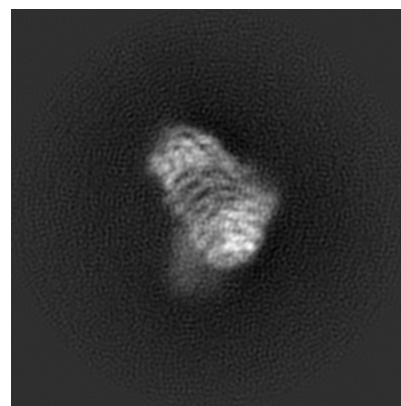
6.1.1 Primary map



X

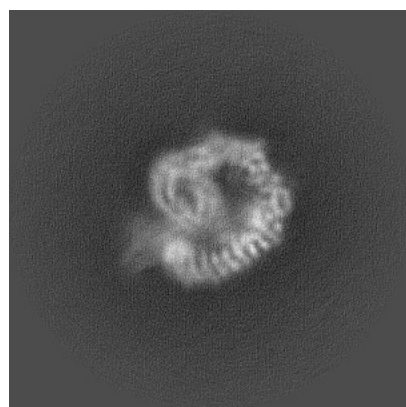


Y

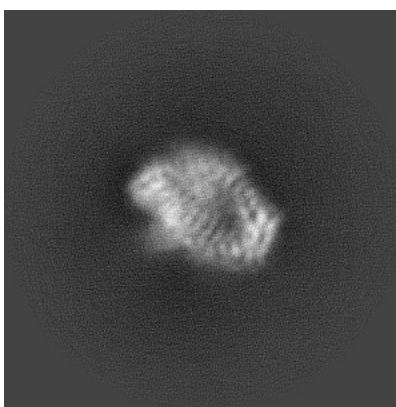


Z

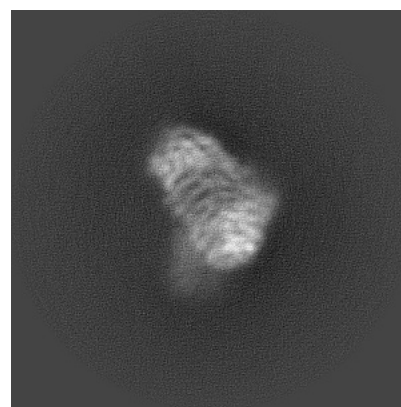
6.1.2 Raw map



X



Y



Z

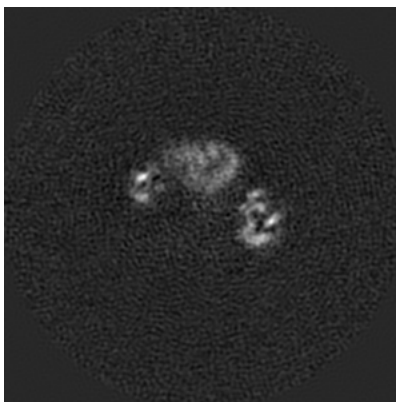
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

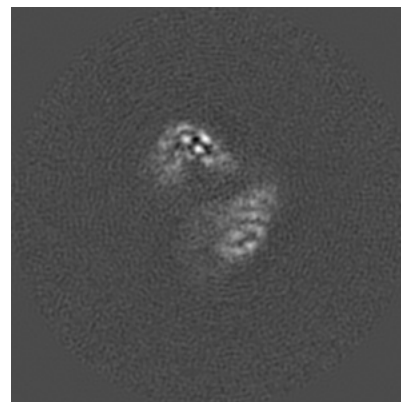
6.2.1 Primary map



X Index: 200

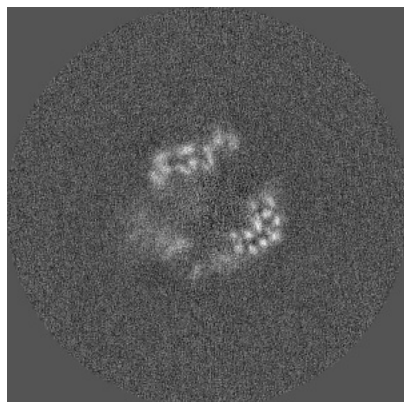


Y Index: 200

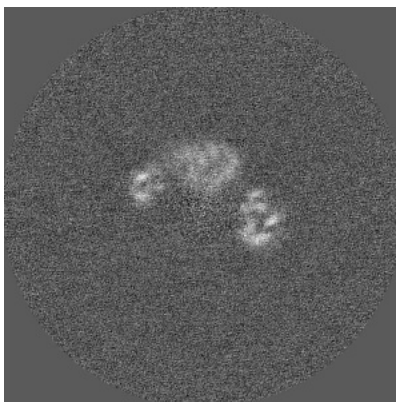


Z Index: 200

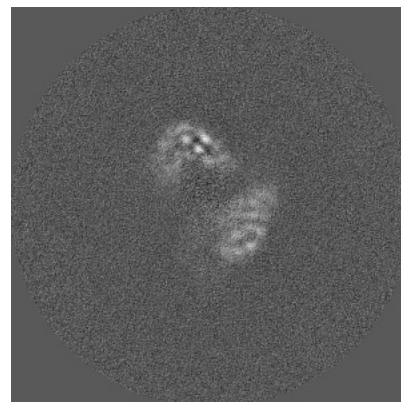
6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

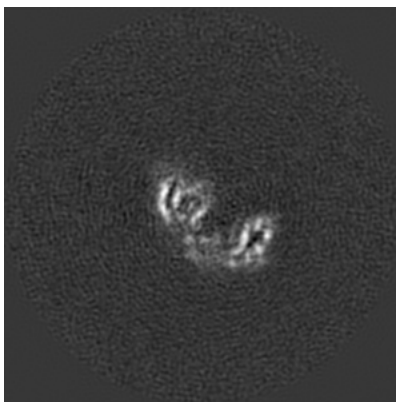
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 216

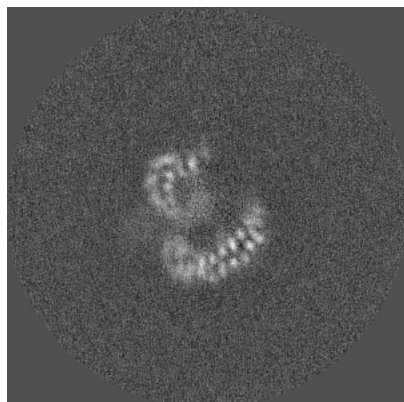


Y Index: 244

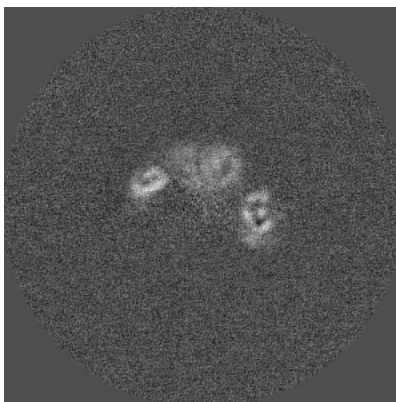


Z Index: 244

6.3.2 Raw map



X Index: 216



Y Index: 194

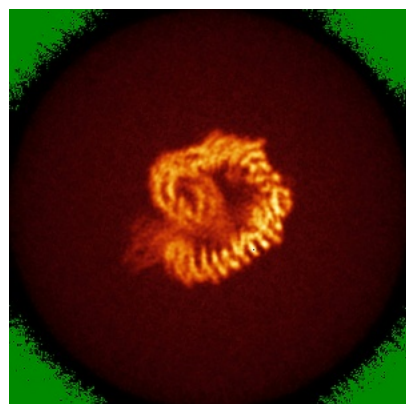


Z Index: 195

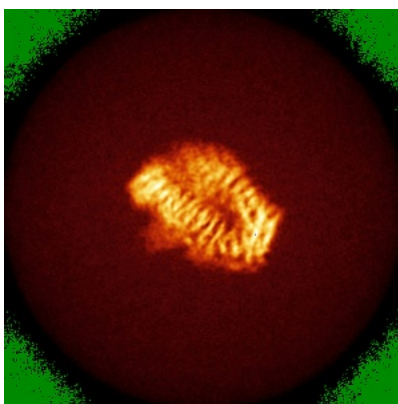
The images above show the largest variance slices of the map in three orthogonal directions.

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

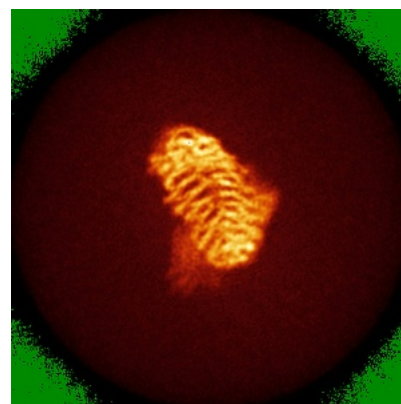
6.4.1 Primary map



X

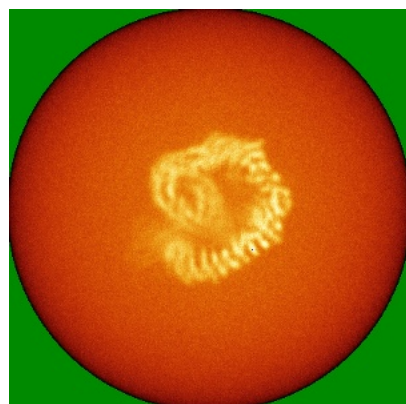


Y

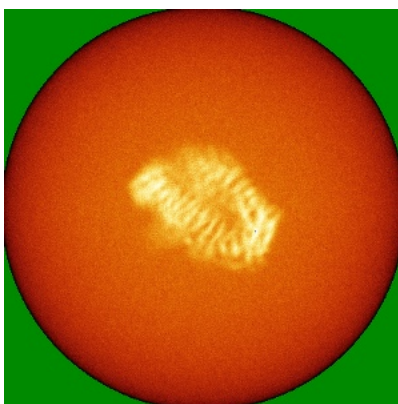


Z

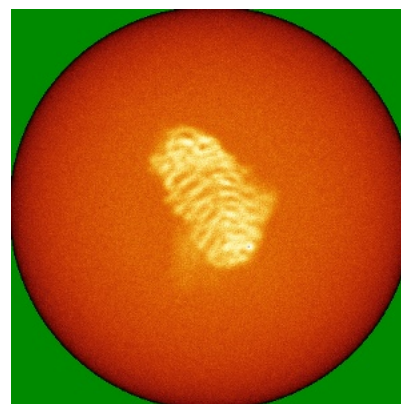
6.4.2 Raw map



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.

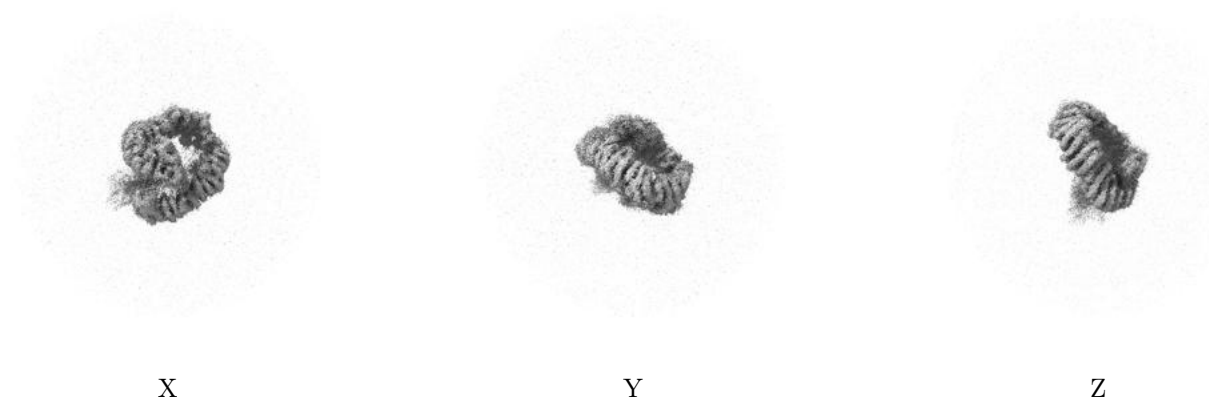
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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.

6.5.2 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.

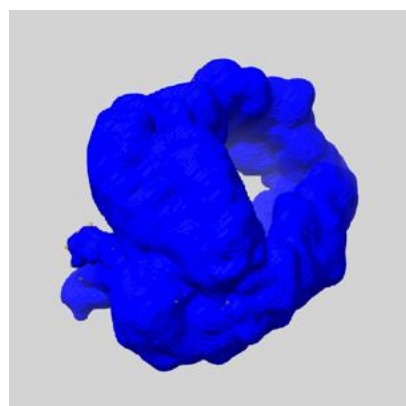
6.6 Mask visualisation [i](#)

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

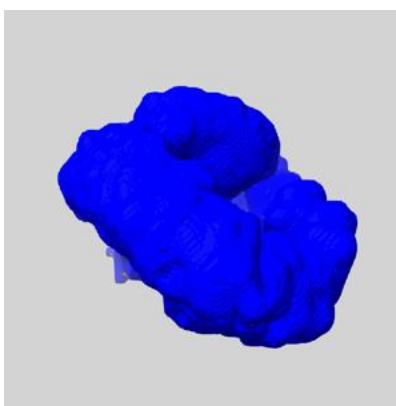
A mask typically either:

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

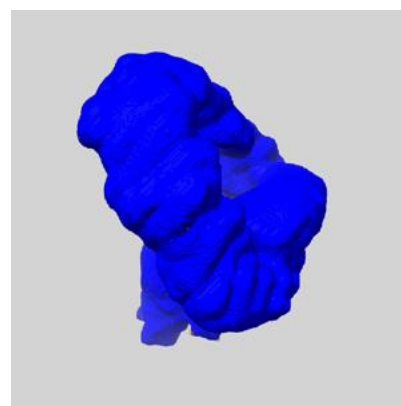
6.6.1 emd_12318_msk_1.map [i](#)



X



Y

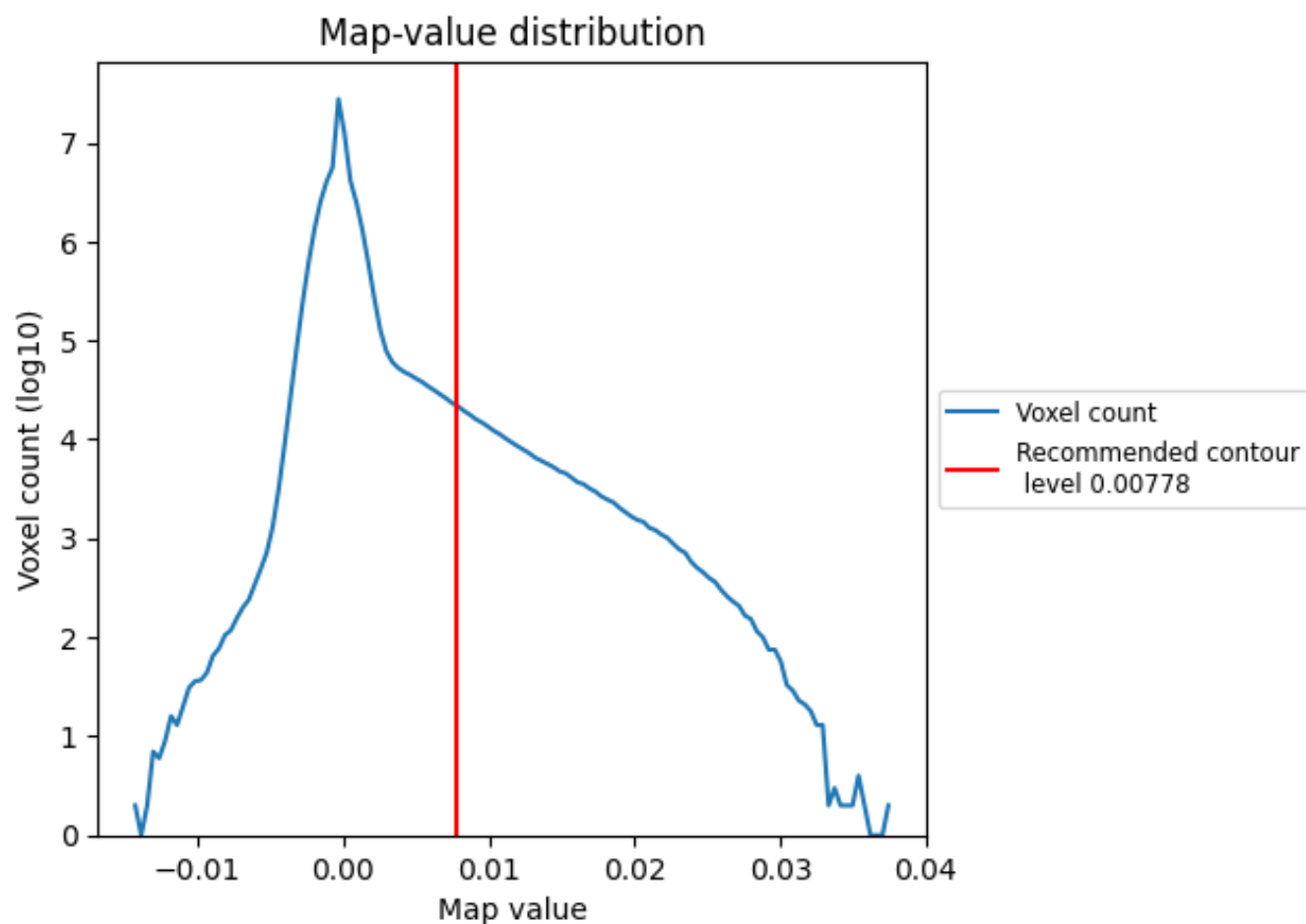


Z

7 Map analysis [i](#)

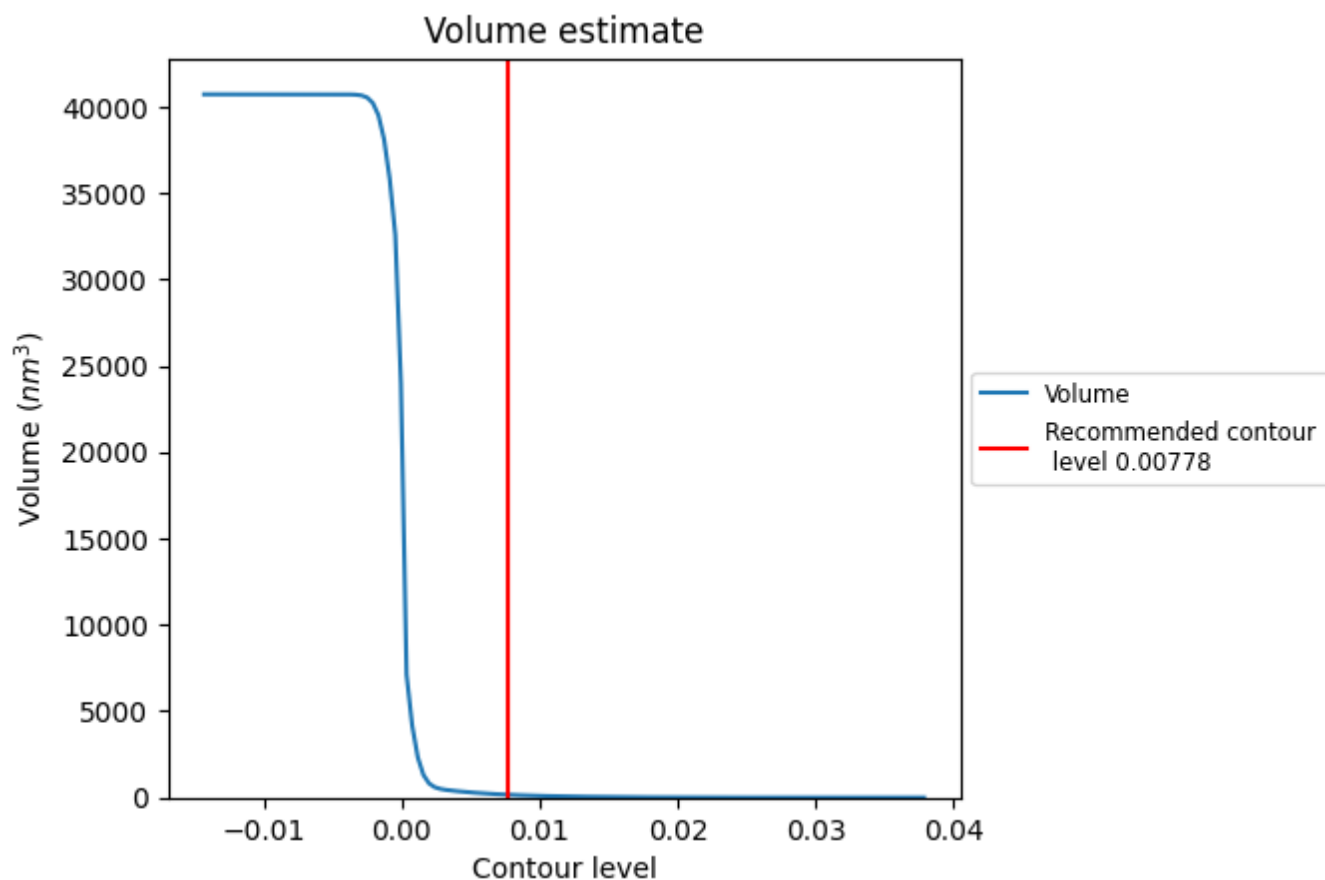
This section contains the results of statistical analysis of the map.

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.

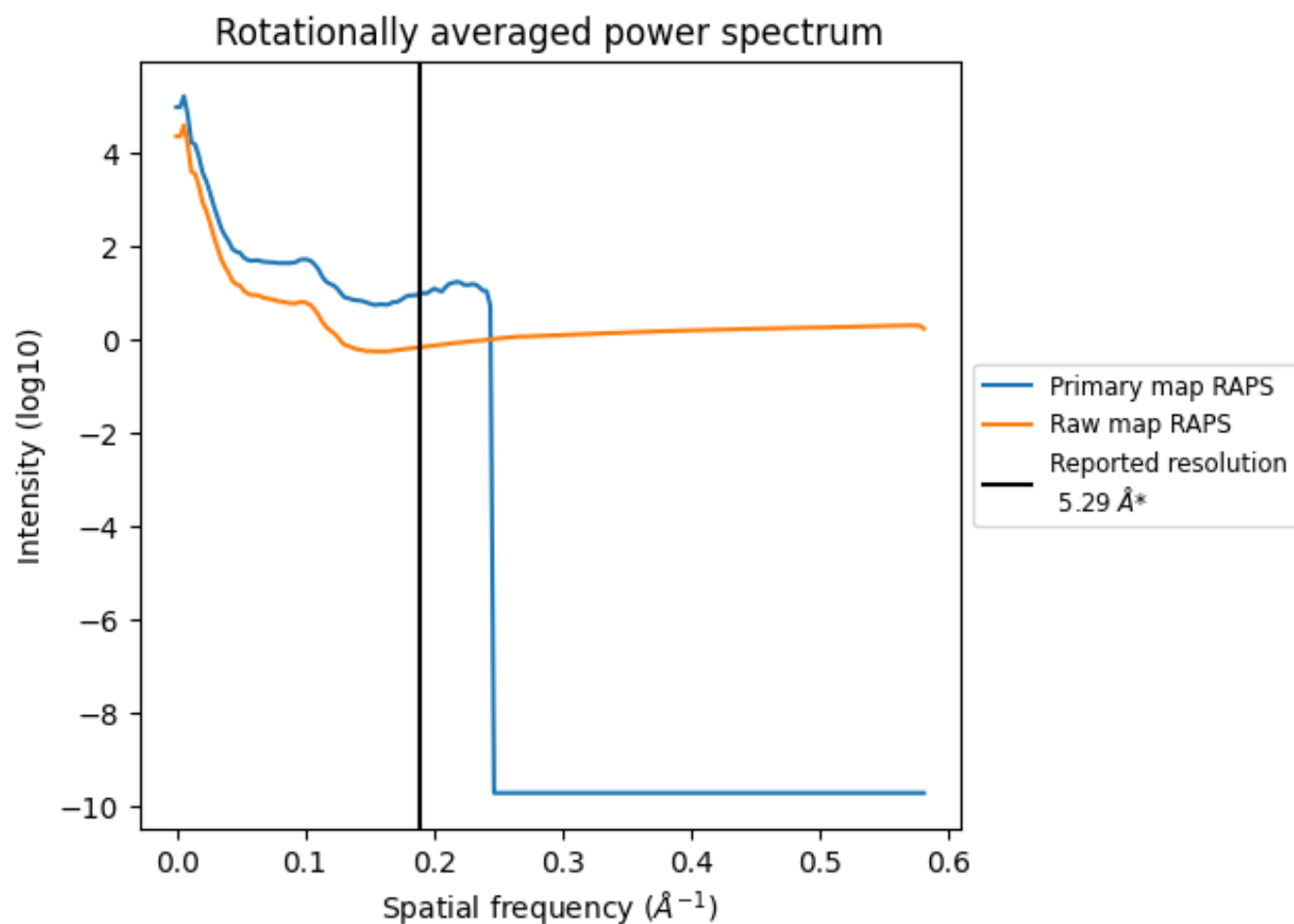
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 161 nm^3 ; this corresponds to an approximate mass of 145 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 ⓘ

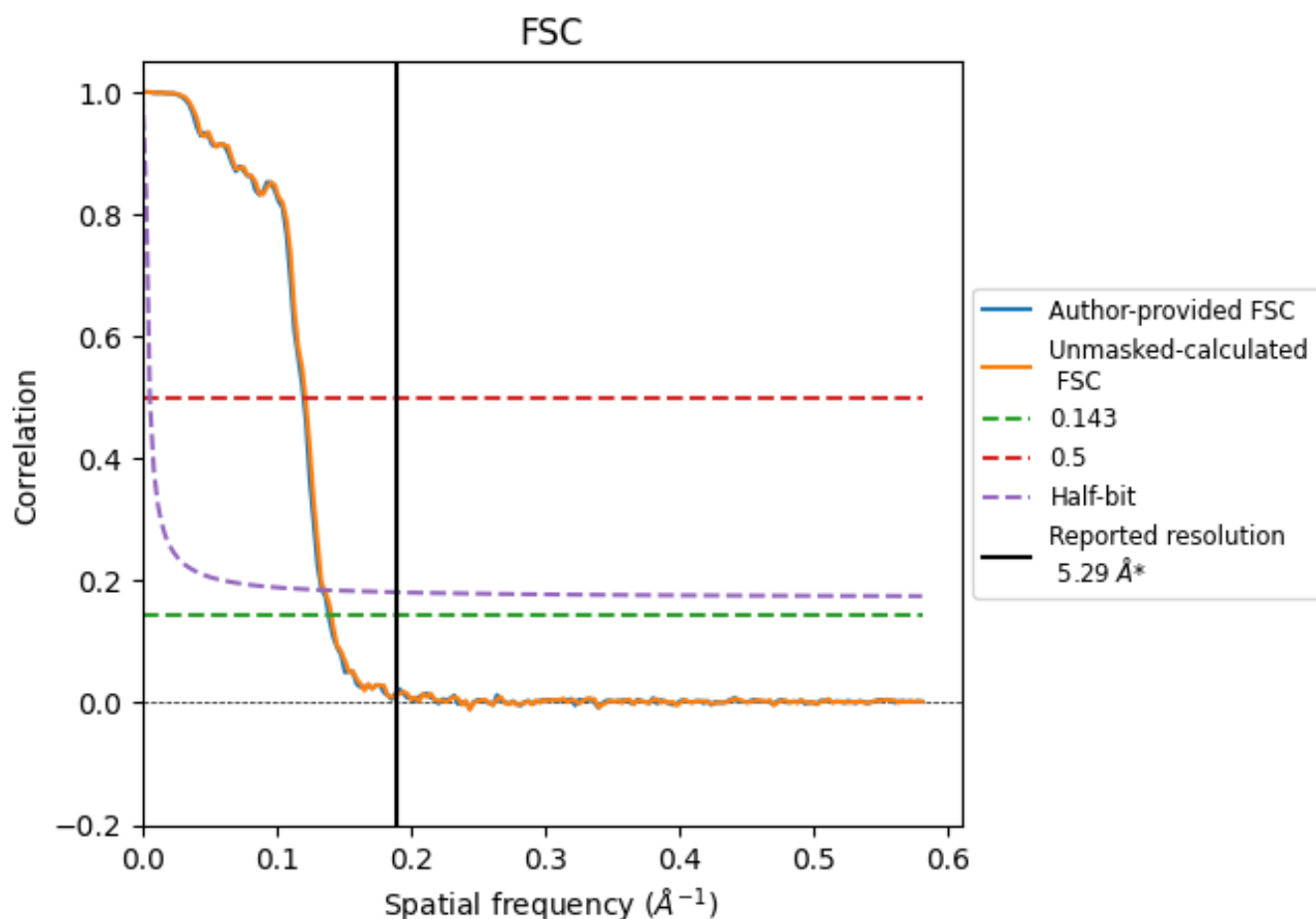


*Reported resolution corresponds to spatial frequency of 0.189 $\text{\AA}^{-1}$

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 0.189 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.29	-	-
Author-provided FSC curve	7.19	8.32	7.46
Unmasked-calculated*	7.09	8.22	7.35

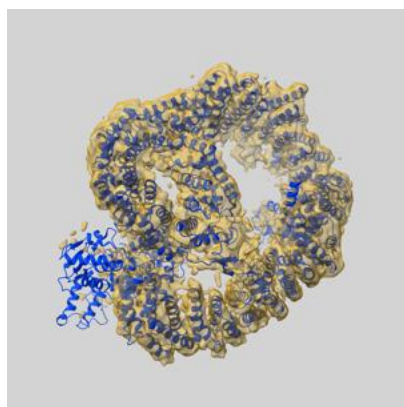
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 7.19 differs from the reported value 5.29 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.09 differs from the reported value 5.29 by more than 10 %

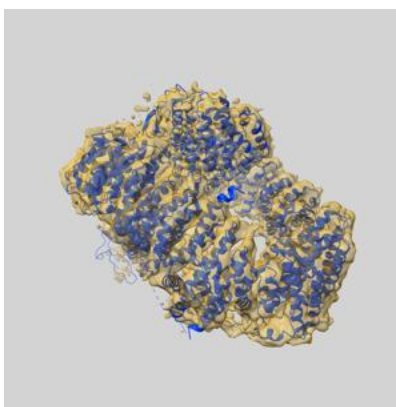
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12318 and PDB model 7NH1. Per-residue inclusion information can be found in section [3](#) on page [4](#).

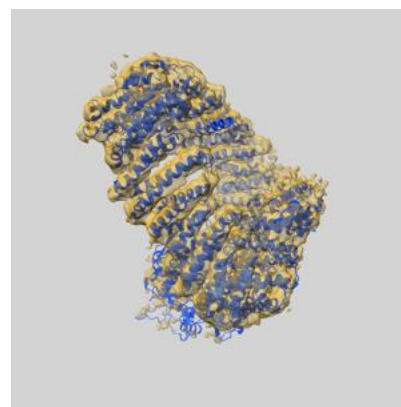
9.1 Map-model overlay [i](#)



X



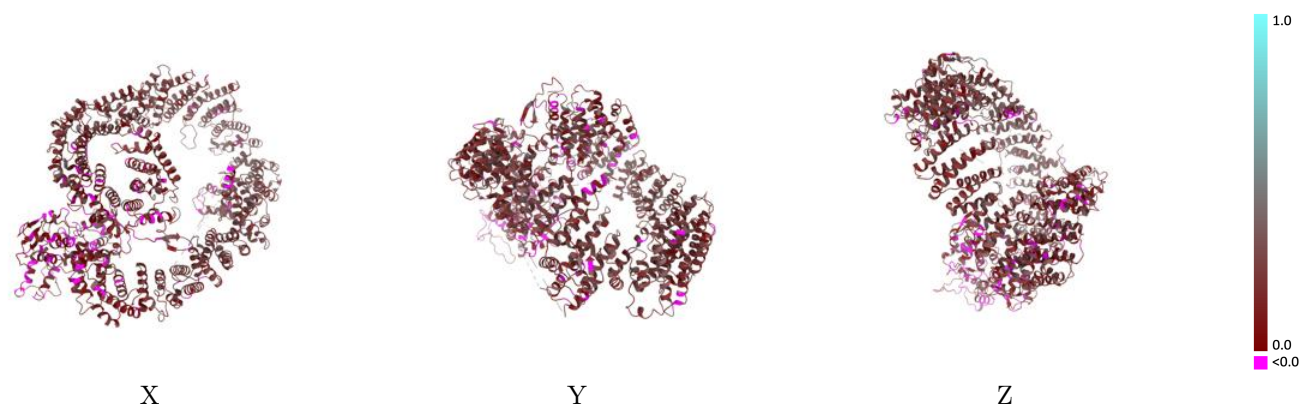
Y



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](#)

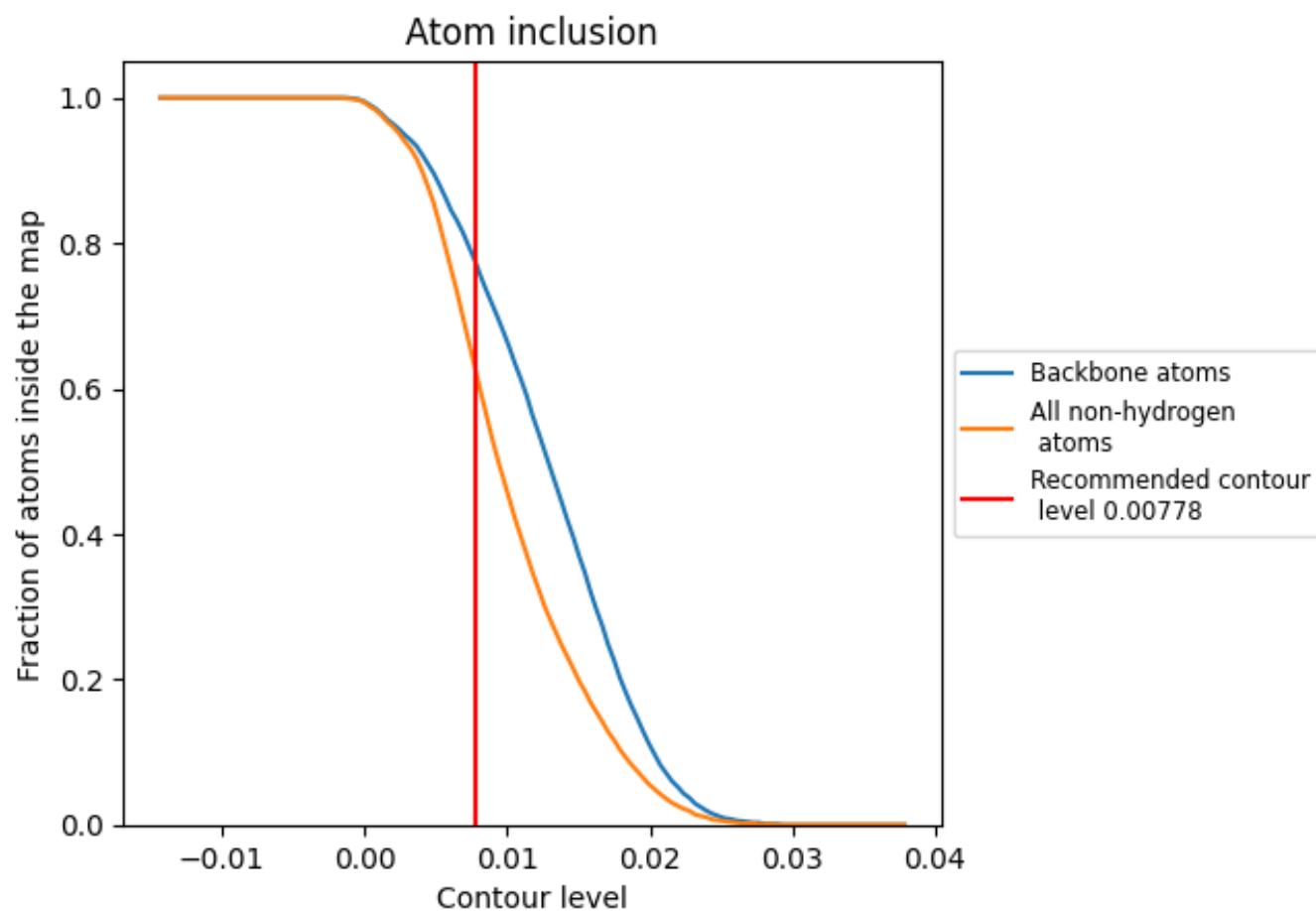


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 63% 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	0.6260	0.2000
A	0.6260	0.2000

