



wwPDB EM Validation Summary Report ⓘ

Oct 20, 2025 – 01:32 pm BST

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.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

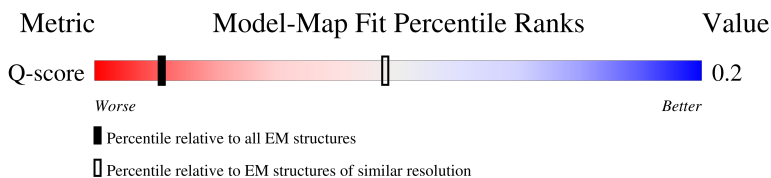
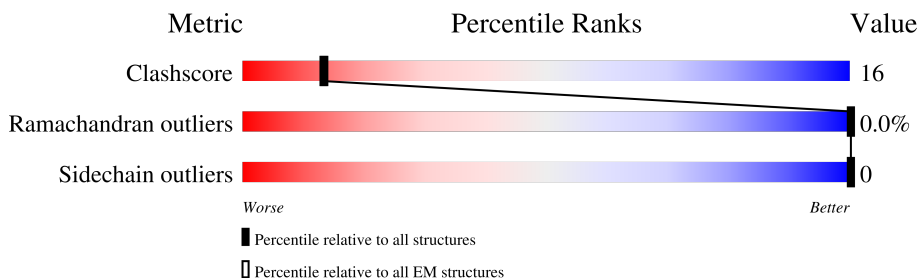
1 Overall quality at a glance

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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
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.

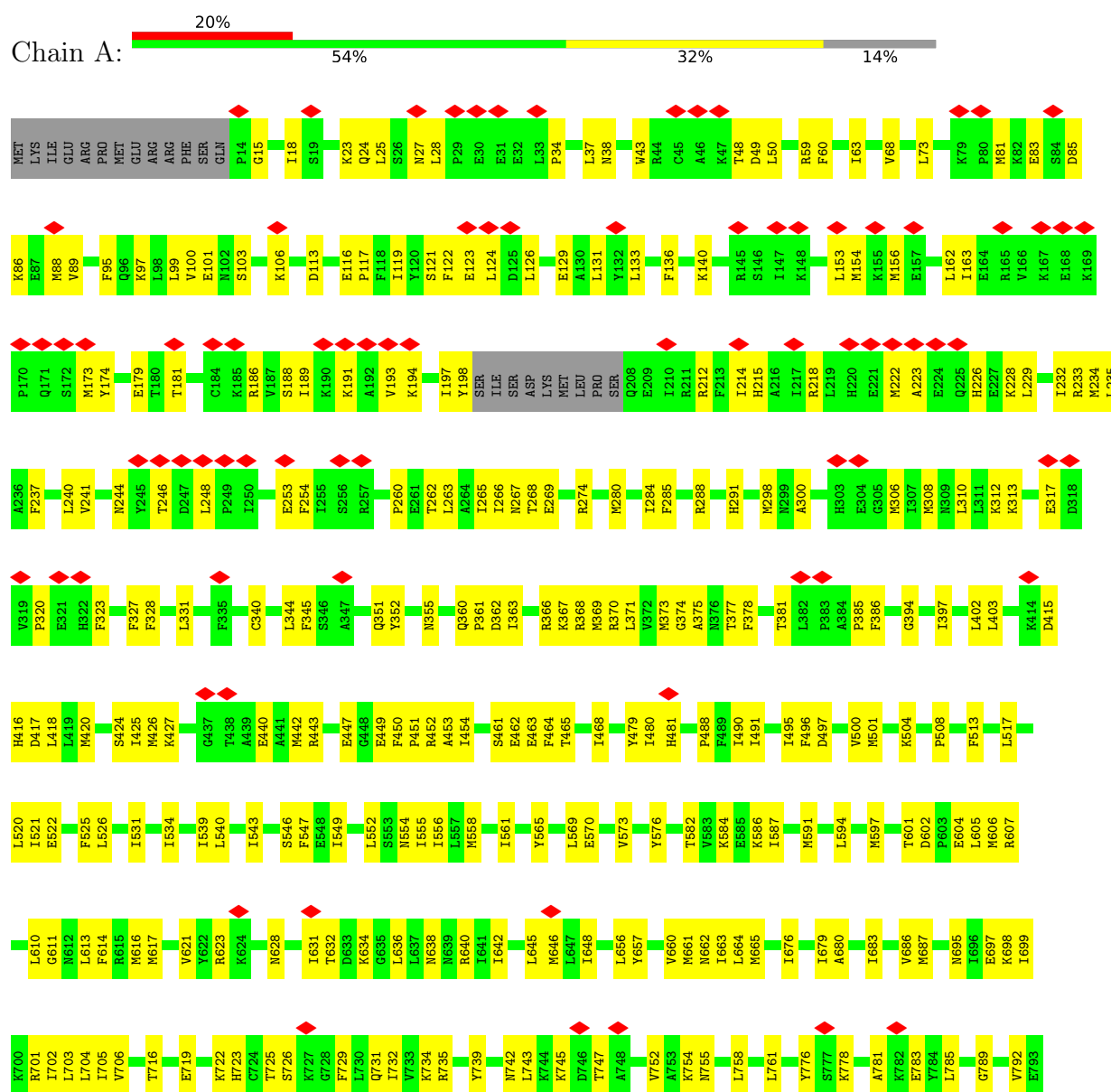
- Molecule 1 is a protein called E3 ubiquitin-protein ligase HUWE1.

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 GLY PHE ALA	F2427	A2428	G2429	L2430	R2431	C2432	Q2433	N2434	G2435	N2436	Q2437	K2438	F2439	Q2440	T2441	H2442	K2443	A2444	S2445	G2446	G2447	S2448	S2449	R2450	L2451	P2452	T2453	A2454	H2455	T2456	C2457	F2458	N2459	Q2460	L2461	D2462	L2463	L2464	E2465	Y2466	D2467	S2468	Y2469	E2470	Q2471	L2472	V2473	K2474	A2475	L2476	L2477	F2478	S2479	L2480	E2481	E2482	CYS	THR	SER	GLY
	I2367	S2368	G2369	L2370	P2371	E2372	L2373	D2374	V2375	D2376	D2377	W2378	R2379	N2380	W2381	T2382	L2383	Y2384	F2385	G2386	Y2387	T2388	S2389	D2390	S2391	Q2392	V2393	L2394	R2395	W2396	Y2397	W2398	R2399	A2400	V2401	R2402	N2403	F2404	S2405	N2406	E2407	E2408	R2409	A2410	K2411	L2412	L2413	Q2414	F2415	A2416	T2417	G2418	T2419	S2420	K2421	L2422	P2423	L2424	E2425	G2426
	K2306	E2307	N2308	G2309	R2310	N2311	L2312	A2313	V2314	T2315	N2316	E2317	N2318	K2319	R2320	E2321	Y2322	V2323	E2324	L2325	V2326	C2327	R2328	F2329	K2330	R2331	V2332	R2333	V2334	I2335	E2336	R2337	Q2338	L2339	S2340	F2341	A2342	A2343	E2344	G2345	F2346	F2347	E2348	I2349	L2350	D2351	V2352	D2353	M2354	L2355	K2356	N2359	E2360	K2361	E2362	L2363	E2364	L2365	L2366	
	T2246	R2247	A2248	F2249	Y2250	K2251	R2252	V2253	L2254	S2255	T2256	P2257	V2258	D2259	L2260	T2261	D2262	V2263	E2264	A2265	L2266	D2267	P2268	E2269	F2270	H2271	R2272	S2273	L2274	V2275	W2276	L2277	L2278	E2279	W2280	T2281	L2282	E2283	W2284	V2285	L2286	D2287	W2288	T2289	F2290	S2291	L2292	E2293	Q2294	D2295	R2296	F2297	G2298	T2299	T2300	E2301	T2302	T2303	D2304	L2305
PHE GLY PHE ALA	W2185	Y2186	S2187	E2188	L2189	K2191	E2192	M2193	F2194	N2195	A2196	N2197	Y2198	A2199	L2200	F2201	T2202	P2203	I2204	G2205	S2206	S2207	Q2208	P2210	N2211	H2212	I2213	S2214	H2215	I2216	N2217	P2218	E2219	H2220	L2221	Y2222	Y2223	F2224	K2225	F2226	I2227	G2228	R2229	I2230	I2231	G2232	K2233	A2234	V2235	Y2236	D2237	E2238	M2239	T2240	V2241	D2242	F2245			
	K2124	K2125	I2126	R2127	E2128	D2129	V2130	Q2131	L2132	R2133	P2134	T2135	I2136	S2137	L2138	M2139	V2140	Q2141	R2142	G2143	A2144	E2147	D2148	T2149	F2150	H2151	Q2152	L2153	M2154	R2155	L2156	N2157	G2158	E2159	Q2160	V2161	R2162	N2163	A2164	K2165	F2166	M2167	L2168	K2169	F2170	A2171	G2172	E2173	E2174	G2175	V2176	D2177	A2178	G2179	G2180	L2181	T2182	R2183	E2184	
	S2036	A2039	S2040	S2041	L2042	L2043	P2044	L2045	F2046	K2047	V2050	L2051	T2054	I2055	Q2056	M2057	V2058	I2059	G2060	S2061	N2062	E2063	N2064	I2065	E2066	E2067	S2069	E2070	I2071	P2072	D2075	S2076	I2090	I2094	Q2095	F2105	G2107	L2108	Q2109	K2110	K2111	F2115	D2116	M2117	K2118	R2119	I2120	Y2121	F2122	Y2123										
	L1932	E1933	M1936	T1937	D1938	L1939	T1940	F1941	K1942	H1943	K1950	T1951	D1952	R1953	F1954	Y1955	R1956	M1964	G1965	G1966	S1967	K1968	K1969	L1970	L1971	D1976	K1977	K1978	F1981	N1982	S1983	H1987	I1990	R1995	M2003	D2011	M2014	E2015	L2016	F2026	N2027	I2028	I2029	L2030	P2031	K2032	E2033													
PHE GLY PHE ALA	I1852	A1853	V1856	T1857	T1858	K1859	R1860	F1861	F1862	T1866	Y1867	L1868	G1869	T1870	F1875	V1878	F1879	S1880	Y1881	N1882	T1883	E1884	L1885	T1886	H1887	K1888	T1897	I1898	S1899	E1900	L1901	V1902	K1903	L1904	L1905	S1906	T1907	V1908	G1909	D1910	C1911	F1912	V1917	A1918	E1919	P1920	E1924	V1925	R1926	I1929										
	L1852	A1853	V1856	T1857	T1858	K1859	R1860	F1861	F1862	T1866	Y1867	L1868	G1869	T1870	F1875	V1878	F1879	S1880	Y1881	N1882	T1883	E1884	L1885	T1886	H1887	K1888	T1897	I1898	S1899	E1900	L1901	V1902	K1903	L1904	L1905	S1906	T1907	V1908	G1909	D1910	C1911	F1912	V1917	A1918	E1919	P1920	E1924	V1925	R1926	I1929										
	L1852	A1853	V1856	T1857	T1858	K1859	R1860	F1861	F1862	T1866	Y1867	L1868	G1869	T1870	F1875	V1878	F1879	S1880	Y1881	N1882	T1883	E1884	L1885	T1886	H1887	K1888	T1897	I1898	S1899	E1900	L1901	V1902	K1903	L1904	L1905	S1906	T1907	V1908	G1909	D1910	C1911	F1912	V1917	A1918	E1919	P1920	E1924	V1925	R1926	I1929										
	L1852	A1853	V1856	T1857	T1858	K1859	R1860	F1861	F1862	T1866	Y1867	L1868	G1869	T1870	F1875	V1878	F1879	S1880	Y1881	N1882	T1883	E1884	L1885	T1886	H1887	K1888	T1897	I1898	S1899	E1900	L1901	V1902	K1903	L1904	L1905	S1906	T1907	V1908	G1909	D1910	C1911	F1912	V1917	A1918	E1919	P1920	E1924	V1925	R1926	I1929										

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.

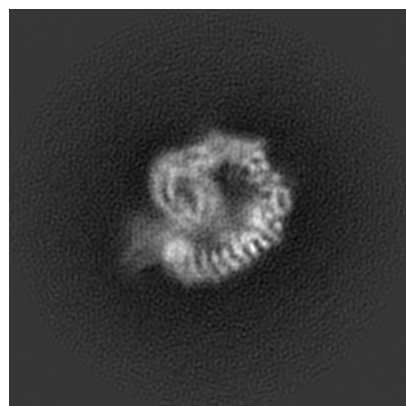
6 Map visualisation [i](#)

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.

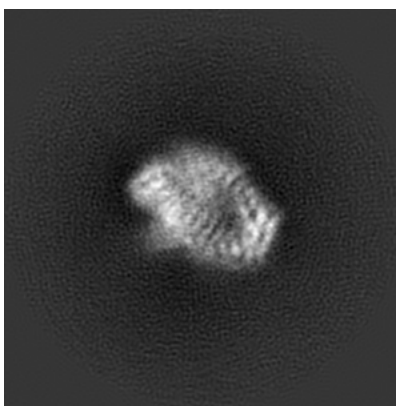
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

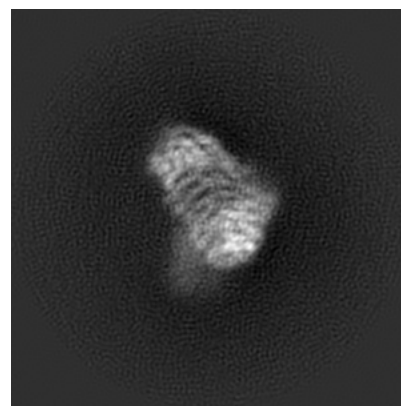
6.1.1 Primary map



X

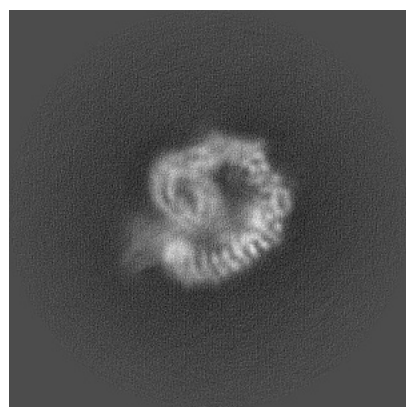


Y

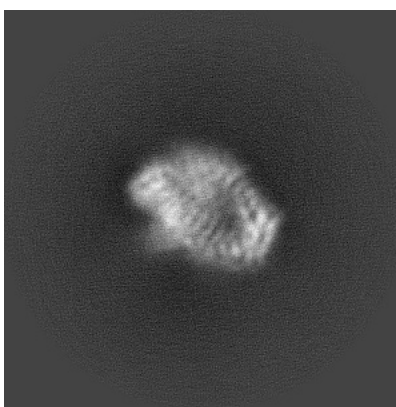


Z

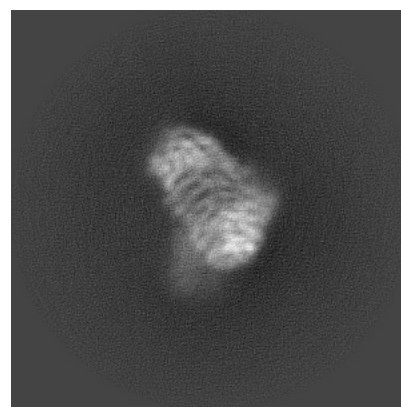
6.1.2 Raw map



X



Y



Z

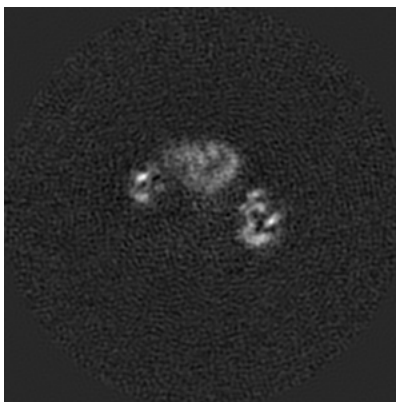
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

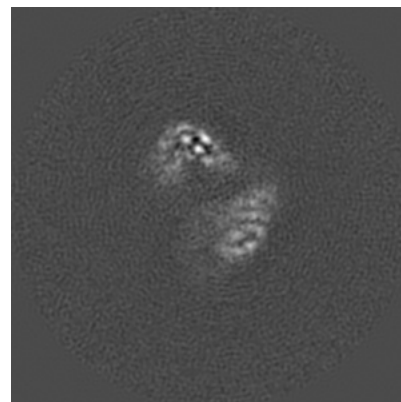
6.2.1 Primary map



X Index: 200

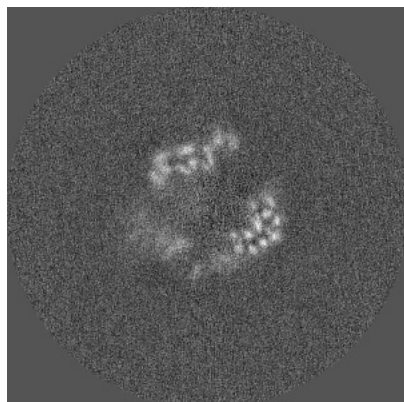


Y Index: 200

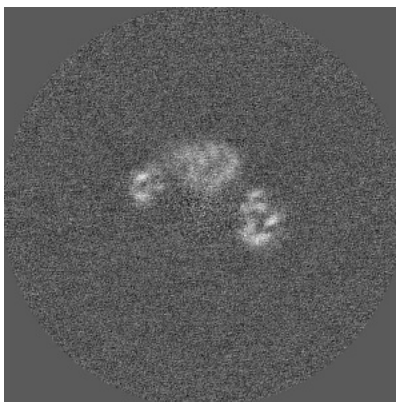


Z Index: 200

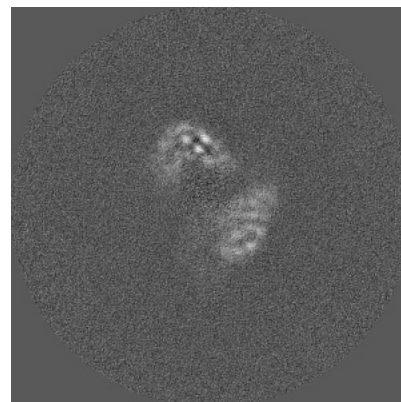
6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

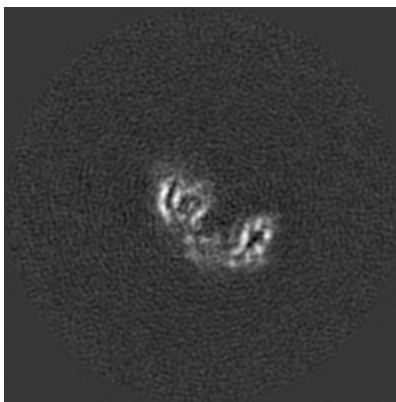
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 216

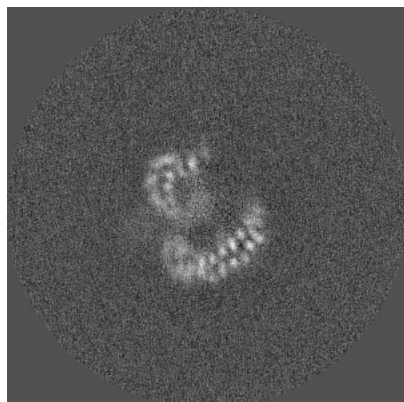


Y Index: 244

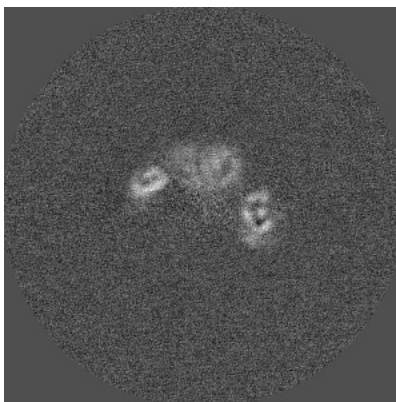


Z Index: 244

6.3.2 Raw map



X Index: 216



Y Index: 194

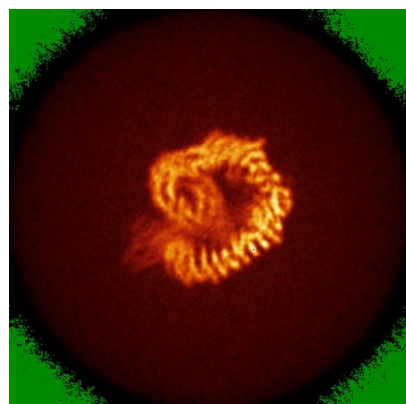


Z Index: 195

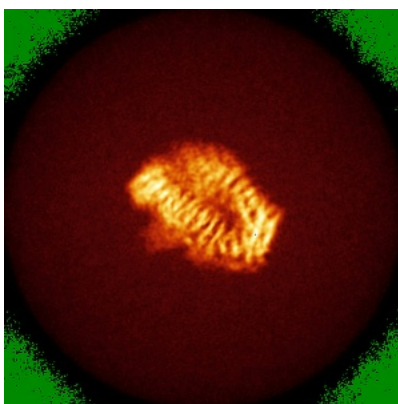
The images above show the largest variance slices of the map in three orthogonal directions.

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

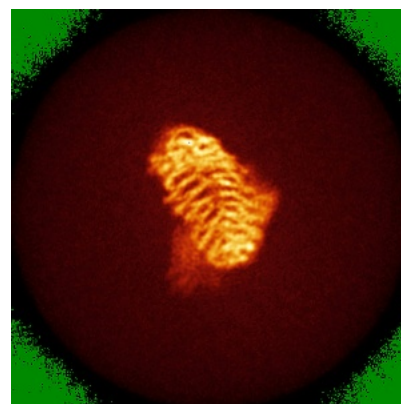
6.4.1 Primary map



X

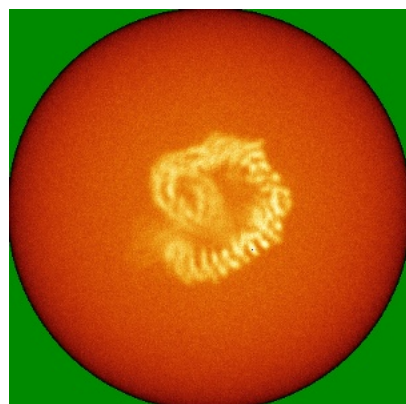


Y

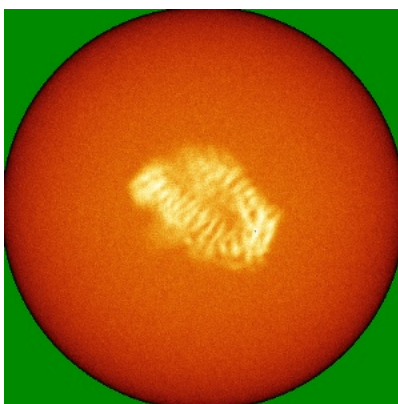


Z

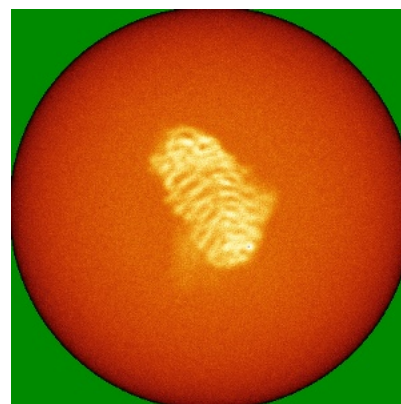
6.4.2 Raw map



X



Y

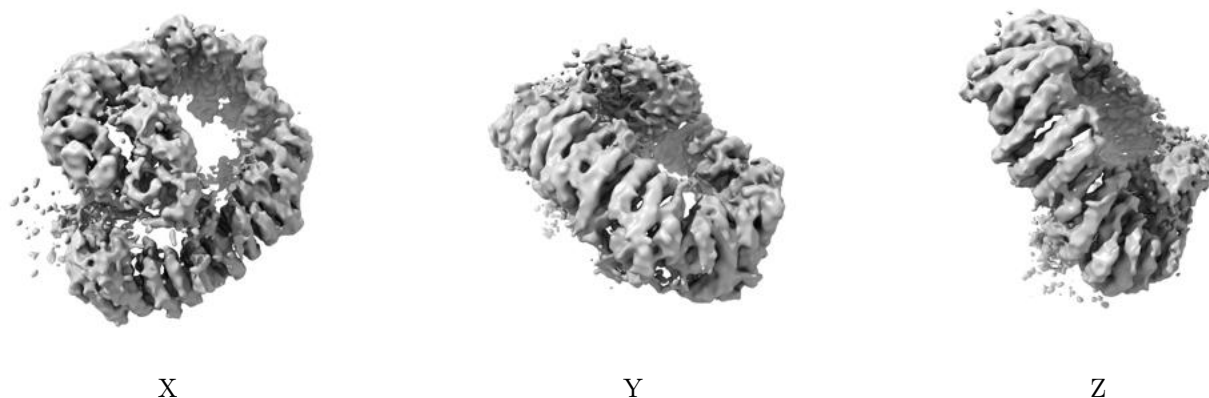


Z

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.

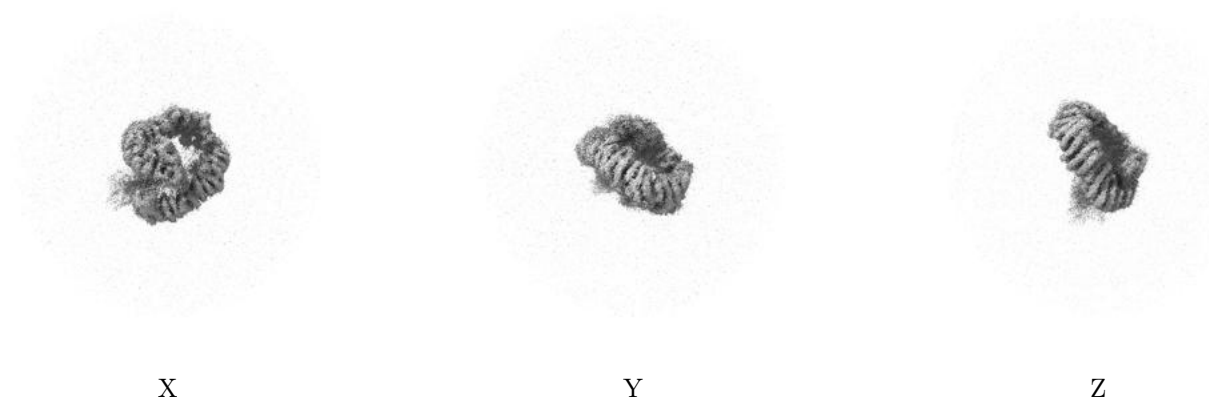
6.5 Orthogonal surface views [i](#)

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.

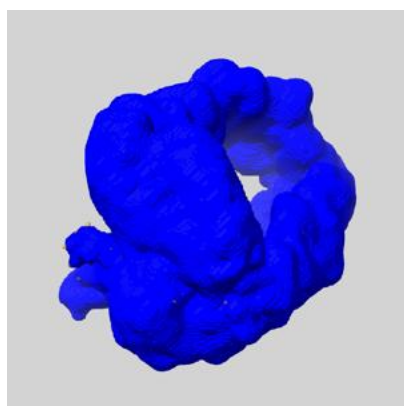
6.6 Mask visualisation [i](#)

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

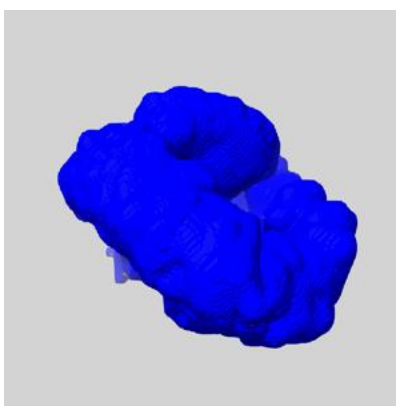
A mask typically either:

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

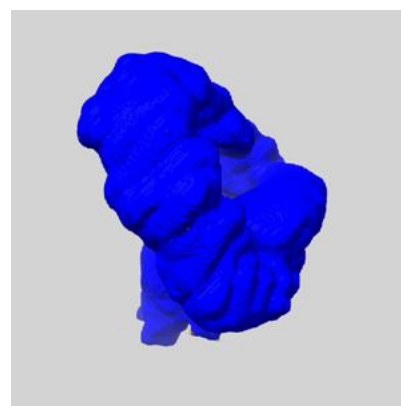
6.6.1 emd_12318_msk_1.map [i](#)



X



Y

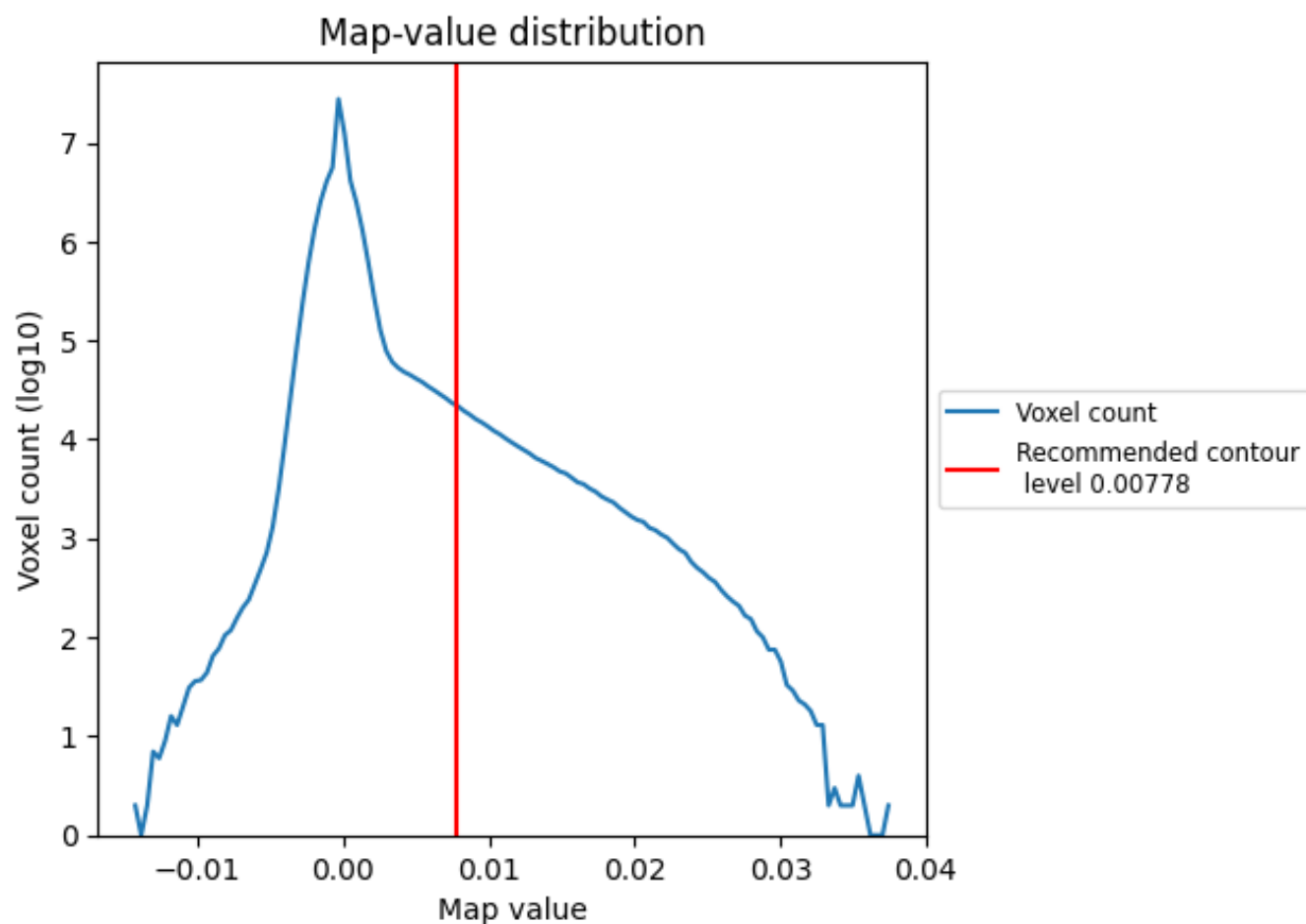


Z

7 Map analysis [i](#)

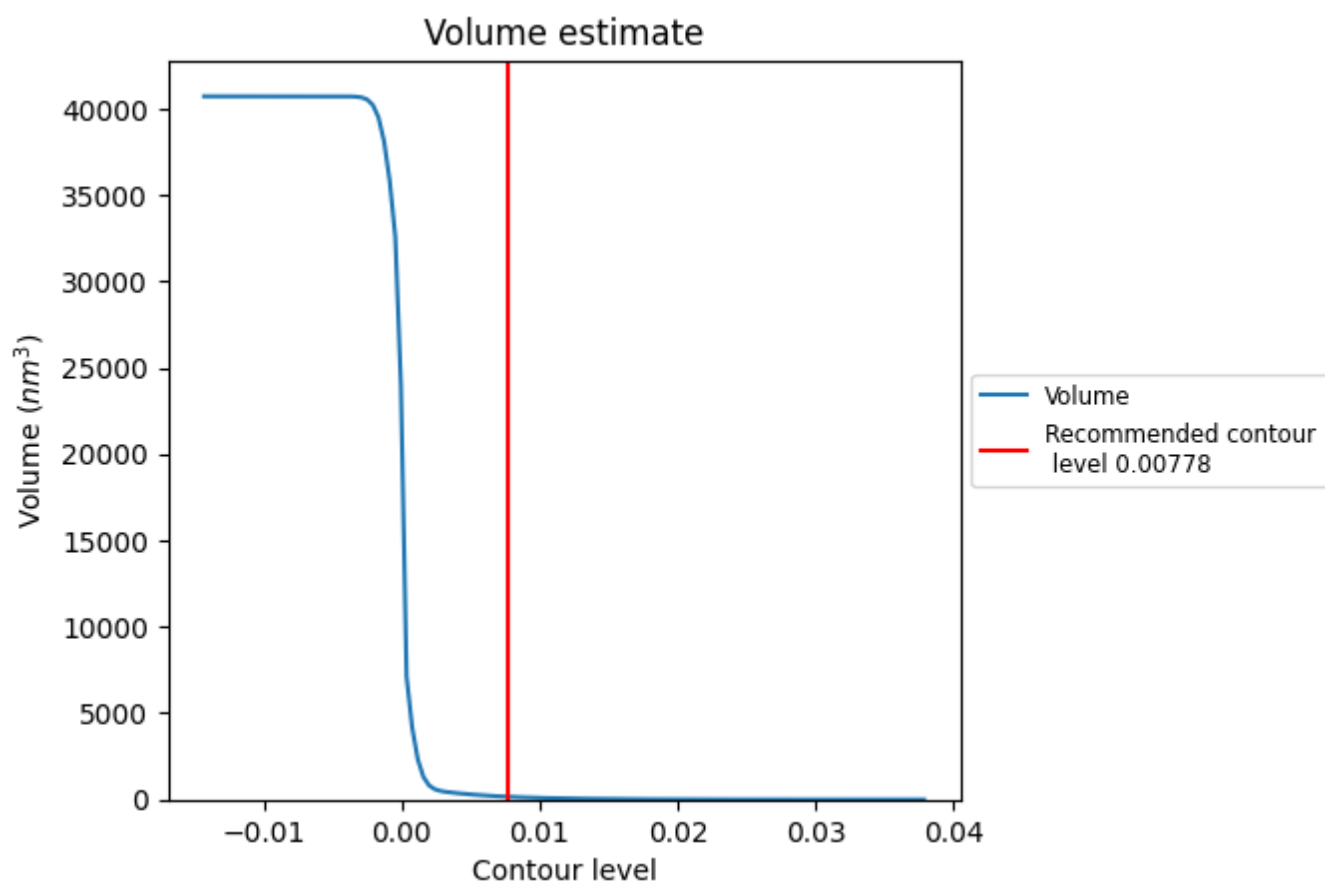
This section contains the results of statistical analysis of the map.

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.

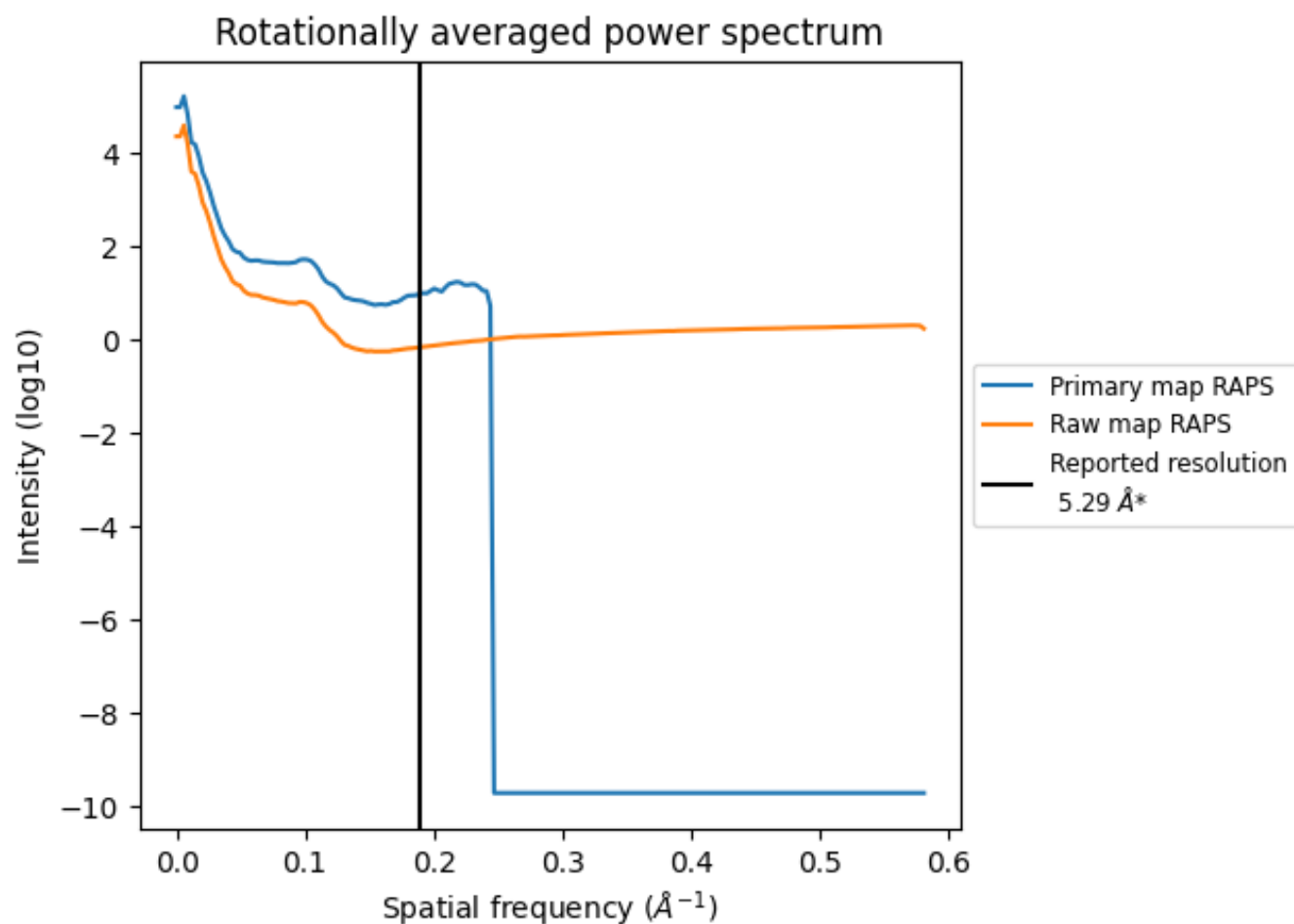
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 161 nm³; 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 ⓘ

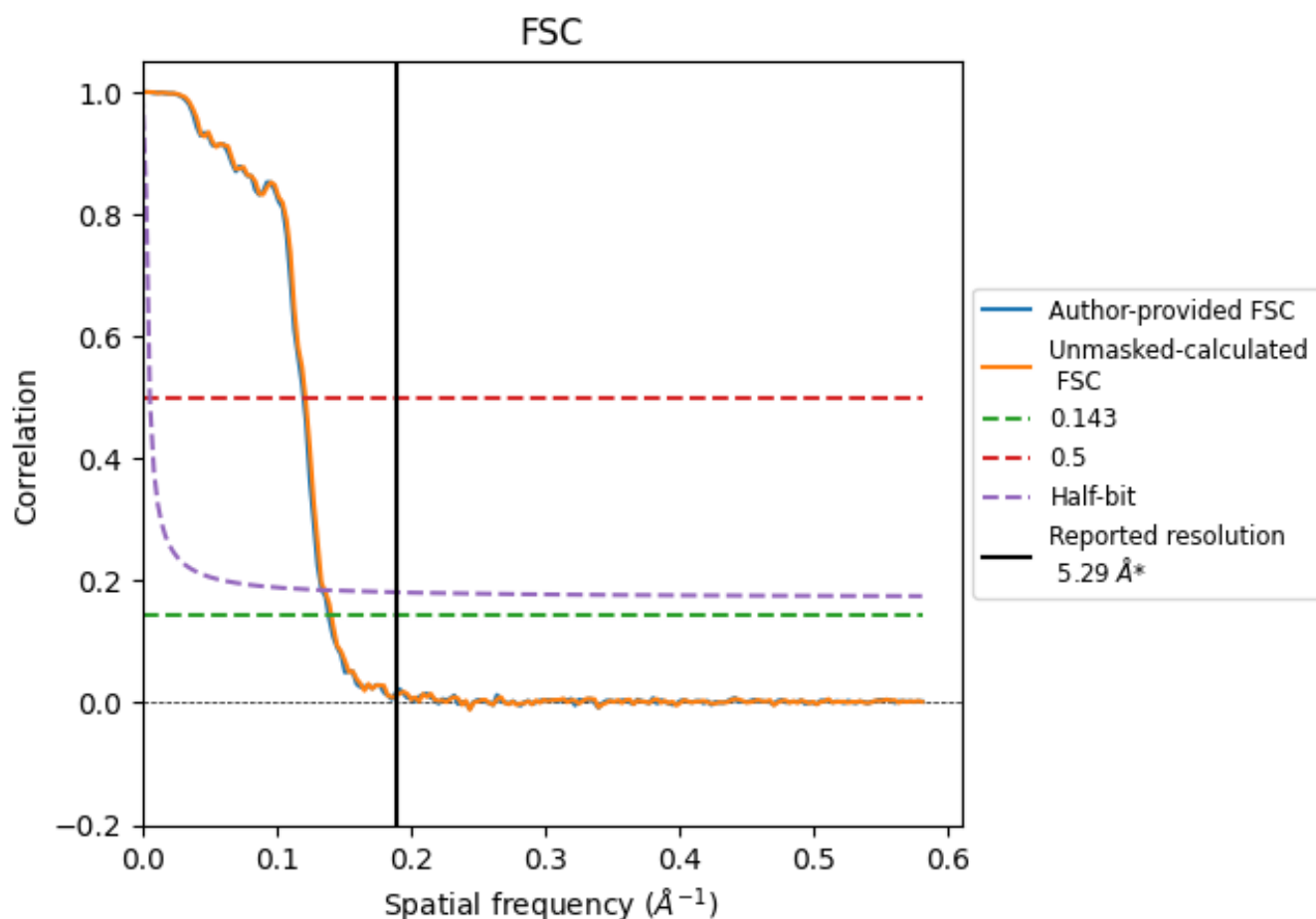


*Reported resolution corresponds to spatial frequency of 0.189 \AA^{-1}

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 \AA^{-1}

8.2 Resolution estimates

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

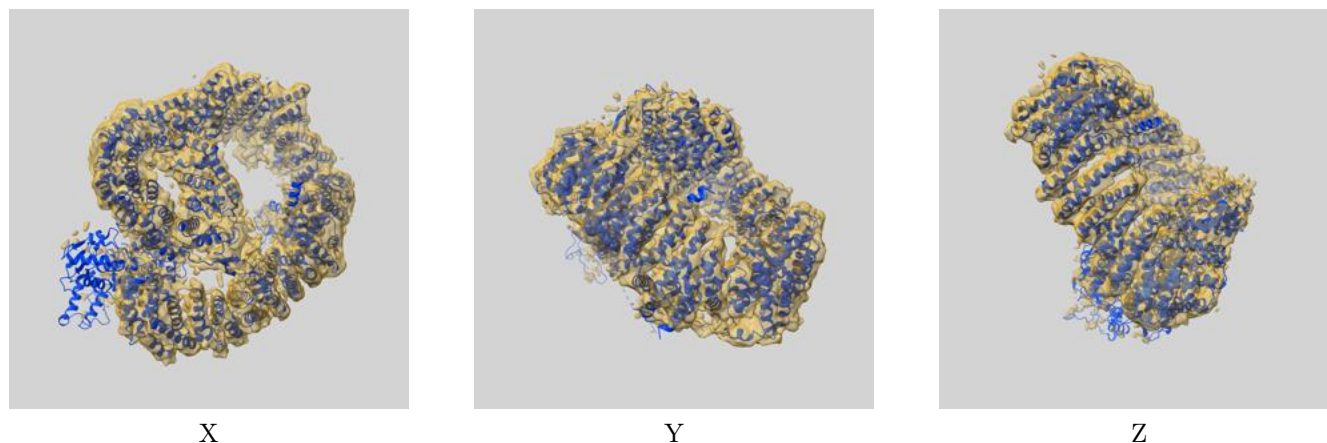
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 7.19 differs from the reported value 5.29 by more than 10 %

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](#)

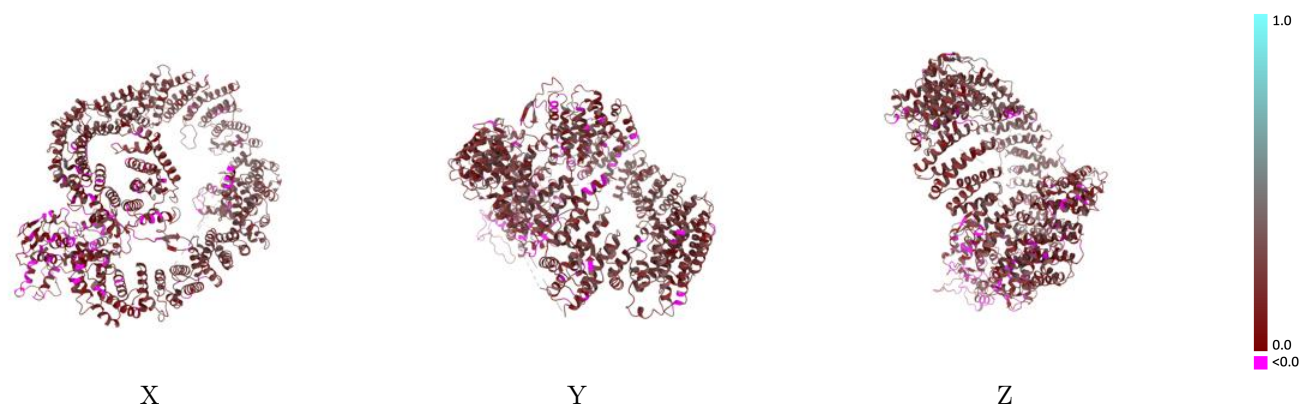
This section contains information regarding the fit between EMDB map EMD-12318 and PDB model 7NH1. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



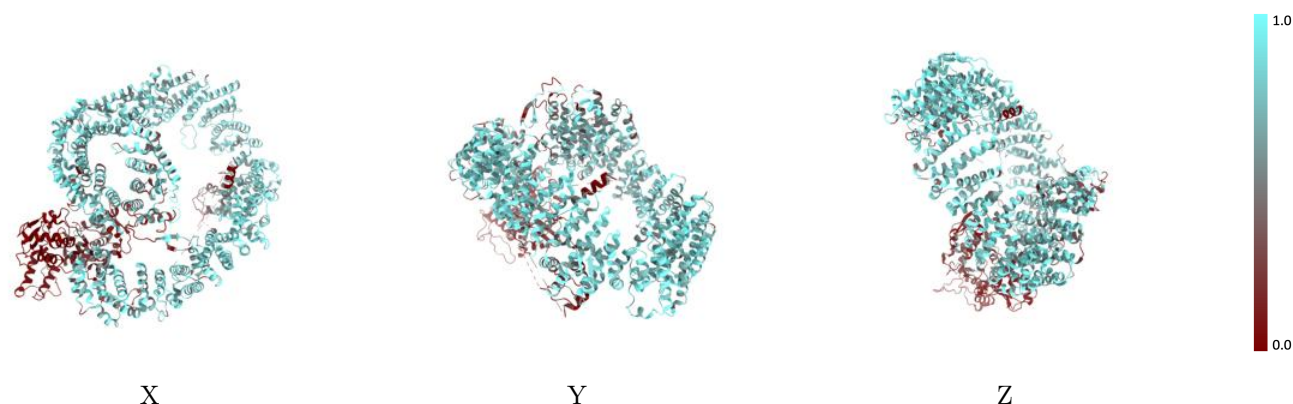
The images above show the 3D surface view of the map at the recommended contour level 0.00778 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



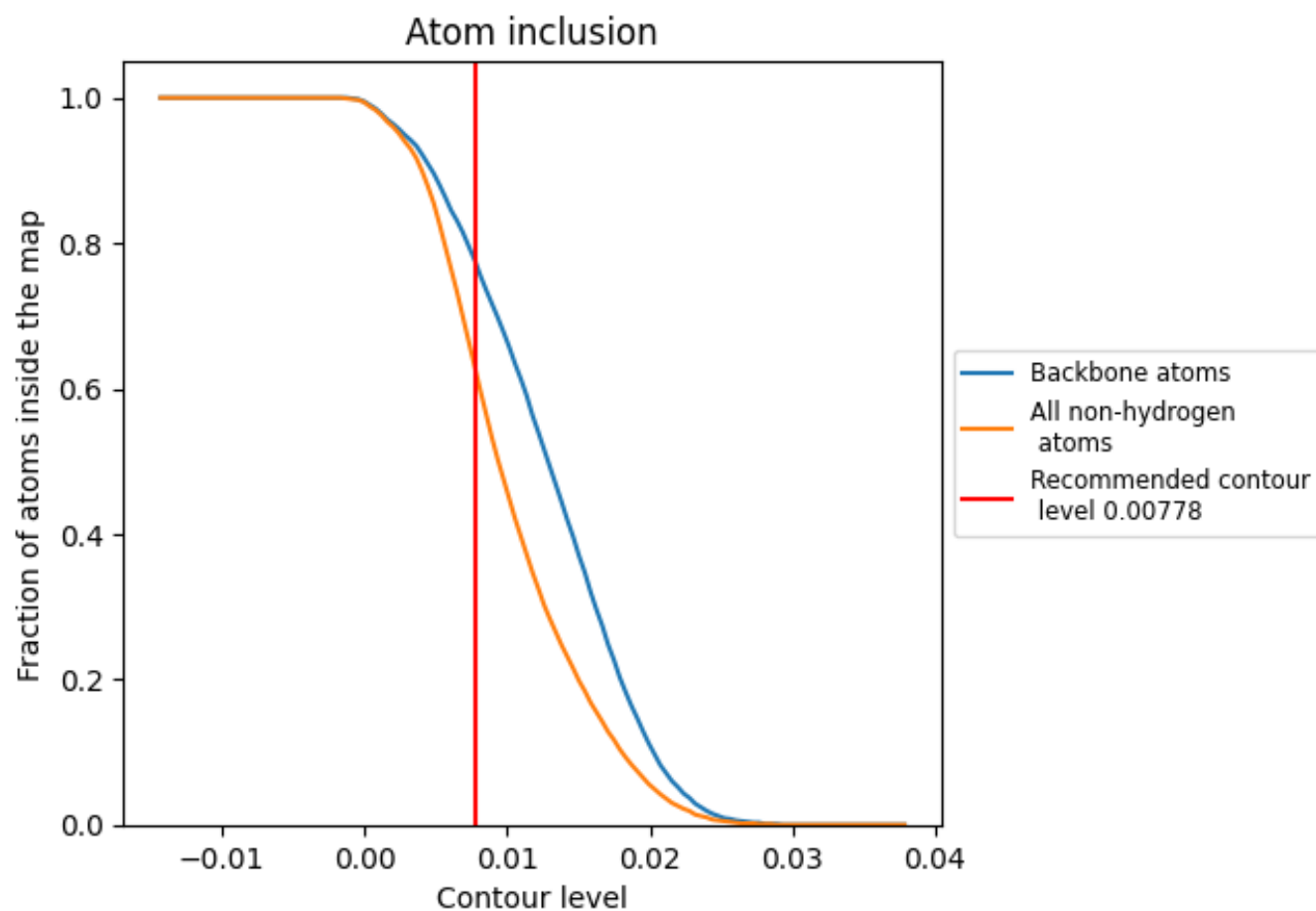
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 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	<div></div> 0.6260	<div></div> 0.2000
A	<div></div> 0.6260	<div></div> 0.2000

