



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 08:43 AM UTC

PDB ID : 7NH3 / pdb_00007nh3
EMDB ID : EMD-12319
Title : Nematocida Huwe1 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

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

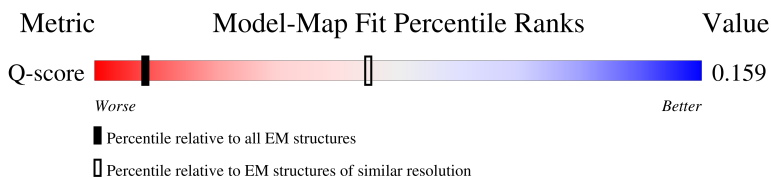
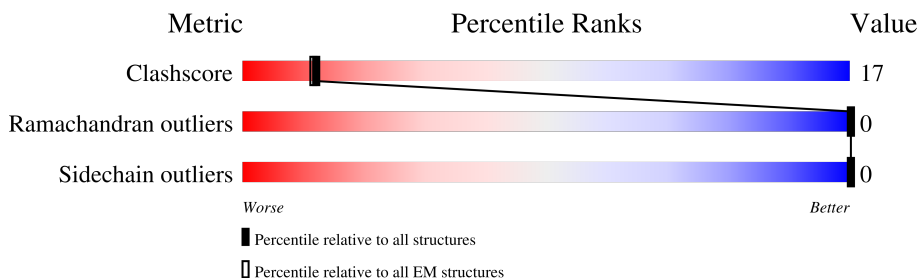
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	512 (5.87 - 6.87)

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 [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.

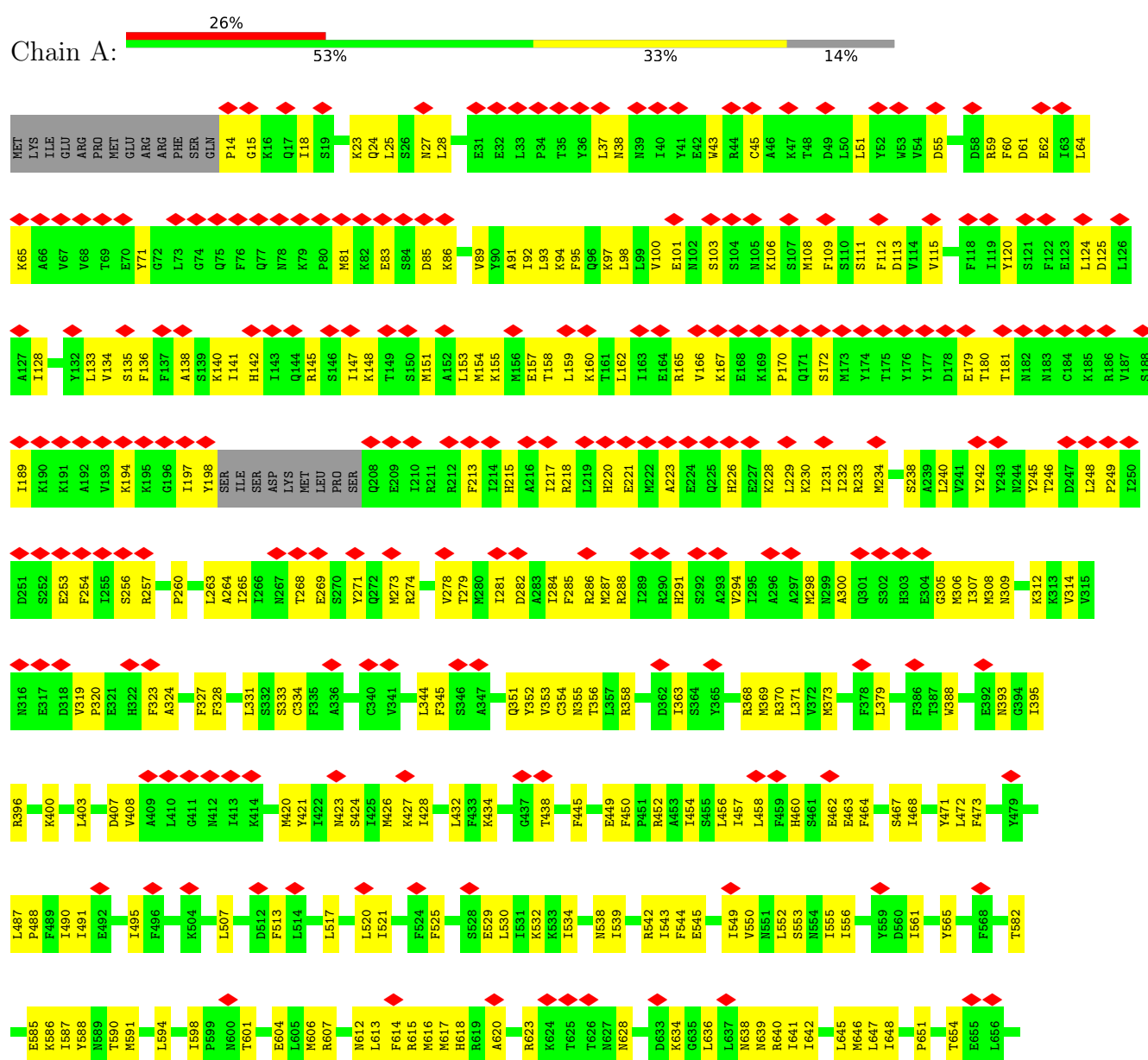
- Molecule 1 is a protein called E3 ubiquitin-protein ligase HUWE1.

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





SER	E2425	L2363	F2297	I2230	L1256	L2089	Y2009	Y1934	V1856	G1790	PHE	
	G2426	E2364	G2298	I2231	N2157	I2090	L2013	D1936	T1857	N1791		LEU
	F2427	L2365	G2299	G2232	G2158	N2091	L2016	N1936	T1858	R1792		ASN
	A2428	L2366	T2299	K2233	E2159	Q2095	L2017	D1938	K1859	N1793		ARG
PHE	G2429	I2367	E2301	A2234	Q2160	Q2096	E2018	D1939	R1860	L1795	ARG	
	L2430	L2367	L2302	G2235	V2161	D2097	E2019	T1940	G1861	R1796	GLU	
	R2431	L2370	L2305	Y2236	R2162	D2098	R2019	F1941	F1862	R1797	GLU	
	G2432	E2371	L2306	D2237	N2163	L2100	F2020	K1942	I1798	I1798	VAL	
ALA	G2433	E2372	E2307	E2238	A2164	H2103	W2022	H1943	L1865	I1799	ARG	
	G2434	L2373	R2308	M2239	G2165	K2110	E2023	H1944	T1866	I1802	SER	
	N2435	D2374	N2308	T2240	F2166	L2113	Y2024	C1945	Y1867	I1805	PHE	
	E2436	V2375	G2309	V2241	N2167	F2105	Y2025	E1946	L1868	N1806	GLU	
THR	D2437	D2376	G2310	D2242	T2168	F2106	F2026	K1950	F1875	V1808	GLU	
	G2438	D2377	N2311	T2246	R2169	Q2109	L2030	T1951	V1878	R1809	HIS	
	F2439	Q2378	T2312	R2247	F2170	K2110	E2033	D1952	F1879	R1809	GLU	
	Q2440	A2313	A2313	A2248	A2171	K2111	K2034	R1953	S1880	F1810	ALA	
TYR	N2441	N2380	V2314	F2249	G2172	L2113	E2035	P1957	Y1881	F1811	ARG	
	H2442	N2381	T2315	L2254	E2173	L2114	S2036	R1956	T1882	E1814	TYR	
	K2443	T2382	N2316	S2255	Q2174	D2115	Y2037	Y1962	N1883	V1817	THR	
	A2444	I2383	E2317	I2256	E2175	F2115	Y2038	L1963	E1884	N1818	PHE	
GLY	S2445	Y2384	N2318	P2257	G2176	K2118	Y2039	M1964	T1886	S1819	GLY	
	G2446	F2385	N2319	V2258	V2176	R2119	A2039	G1965	N1887	I1820	GLY	
	G2447	Q2386	R2320	D2259	D2177	I2120	S2040	K1966	K1888	Q1822	ILE	
	S2448	Y2387	E2321	L2260	Q2178	Y2121	S2041	K1967	I1889	A1823	VAL	
MET	S2449	S2389	V2322	T2261	G2180	Y2123	L2043	K1968	T1893	V1824	PRO	
	R2450	D2390	G2324	D2262	L2181	K2124	P2044	K1969	T1897	A1824	ARG	
	L2451	S2391	L2325	V2263	T2182	K2125	R2047	S1970	I1897	G1827	GLU	
	F2452	Q2392	V2326	E2264	R2183	I2126	L2050	L1975	T1898	ALA	GLU	
LYS	T2453	V2393	G2327	A2265	E2184	R2127	Y2050	D1976	S1899	SER	LYS	
	A2454	L2394	R2328	P2268	W2185	E2128	T2051	K1977	E1900	SER	LYS	
	R2455	R2395	F2329	E2269	V2186	D2129	V2052	K1978	S1901	SER	LYS	
	T2456	Q2396	F2332	F2270	S2187	V2130	T2053	A1979	V1902	ALA	LYS	
GLN	E2457	Q2397	R2332	H2271	R2188	Q2131	T2055	E1980	L1905	GLY	GLN	
	F2458	L2398	R2333	R2272	L2189	L2132	Q2056	F1981	S1906	GLY	GLN	
	N2459	F2399	T2334	S2273	A2196	R2133	W2057	N1982	C1911	SER	PRO	
	Q2460	A2400	E2336	L2274	N2197	P2134	Y2058	S1983	D1915	THR	PRO	
ASN	L2461	V2401	R2337	V2275	W2198	T2135	G2060	K1988	K1916	VAL	ASN	
	D2462	R2402	Q2338	W2276	V2199	I2136	G2061	Y1917	A1918	ALA	ASN	
	L2463	N2403	S2340	W2277	A2199	G2137	W2062	K1989	E1919	GLY	ASN	
	F2464	F2404	A2341	L2278	L2200	S2137	E2063	L1997	P1920	SER	ASN	
VAL	E2465	S2405	K2343	E2279	F2201	L2138	W2064	M1996	E1921	GLY	ASN	
	Y2466	M2406	E2344	N2280	L2204	W2140	T2065	S1998	N1922	ASN	VAL	
	D2467	E2407	E2348	D2281	G2205	Q2141	E2070	L1989	R1926	GLU	VAL	
	S2468	E2408	L2349	I2282	S2206	R2142	T2071	V2000	K1927	V1851	GLU	
GLU	Y2469	R2409	L2350	E2283	G2209	G2143	F2072	N2001	Y1928	M1785	GLU	
	E2470	A2410	D2351	N2284	P2210	A2144	T2075	I2002	I1929	V1786	GLU	
	L2471	K2411	V2352	V2285	P2210	V2145	G2075	M2003	G1930	L1852	GLU	
	T2472	L2412	D2353	L2286	I2213	F2146	Y2080	G2004	F1931	A1788	GLU	
THR	V2473	L2413	D2353	D2287	G2214	E2147	Y2083	L1932	L1932	C1789	THR	
	K2414	Q2414	D2288	M2288	H2215	T2148	V2083	E1933			THR	
	F2415	A2416	T2289	I2216	S2214	D2148					THR	
	A2416	T2417	T2289	I2216	H2151	F2150					THR	
PHE	L2476	G2418	N2359	F2290	Q2152	R2155					PHE	
	L2477	G2418	E2360	I2291	L2153	M2154					PHE	
	F2478	S2479	K2361	I2292	Q2152	R2155					PHE	
	S2479	S2479	E2362	E2293	L2227	R2229					PHE	
GLU	L2480	L2422	E2481	E2293	L2227	R2229					GLU	
	E2481	L2422	E2481	E2293	L2227	R2229					GLU	
	E2482	L2422	E2481	E2293	L2227	R2229					GLU	
	CYS	TYP									CYS	

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	0.13	0/17754	0.37	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	603	0
All	All	17417	0	17695	603	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 17.

The worst 5 of 603 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%)	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 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1116	ASN
1	A	1563	GLN
1	A	1176	ASN
1	A	1891	GLN
1	A	593	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](#)

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

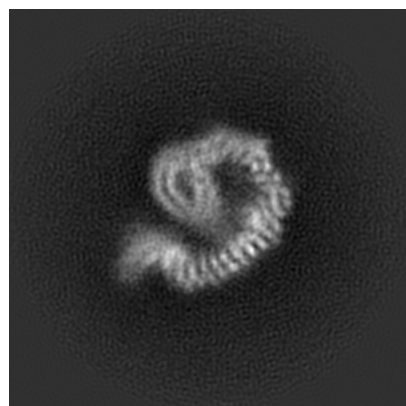
6 Map visualisation [i](#)

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.

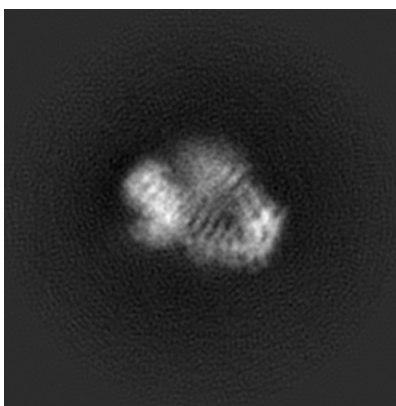
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

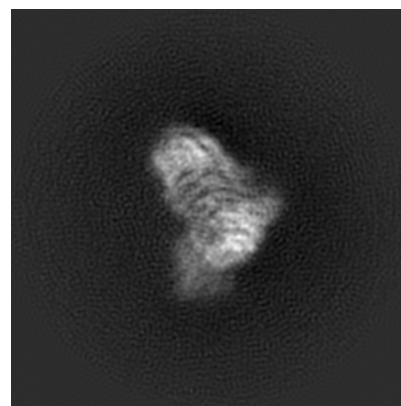
6.1.1 Primary map



X

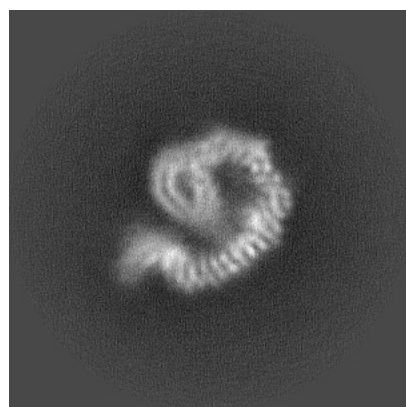


Y

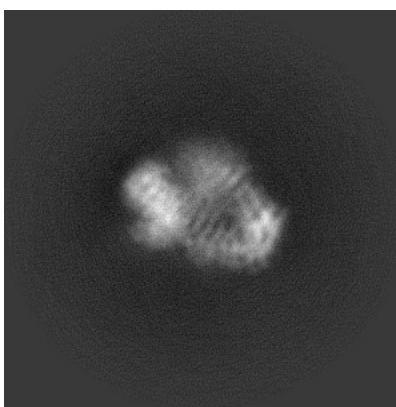


Z

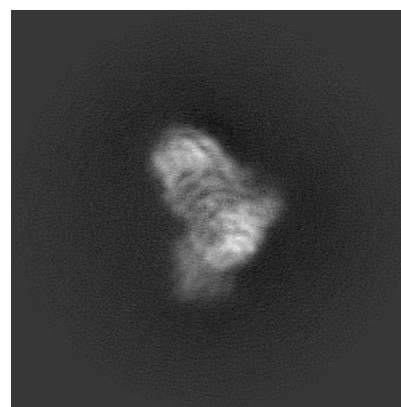
6.1.2 Raw map



X



Y

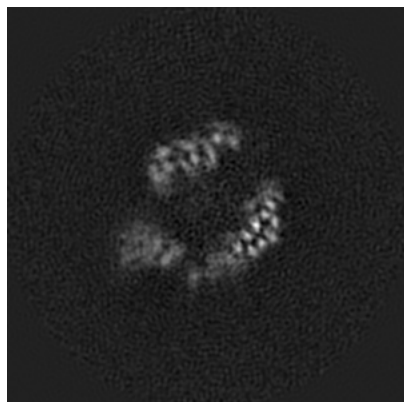


Z

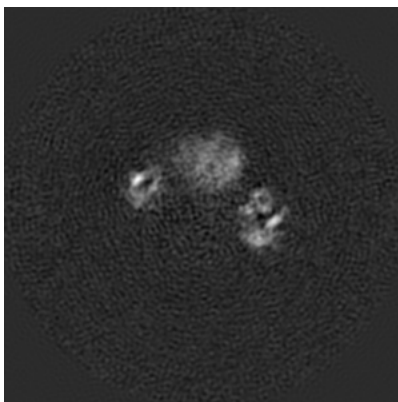
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

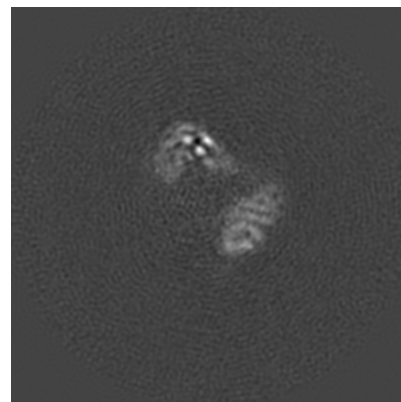
6.2.1 Primary map



X Index: 200

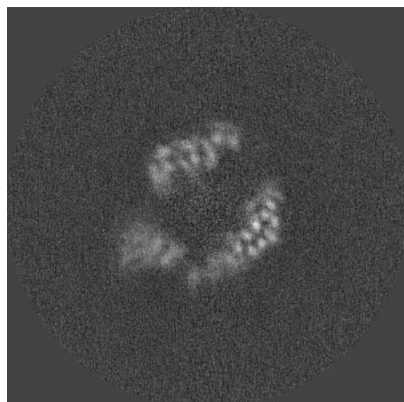


Y Index: 200

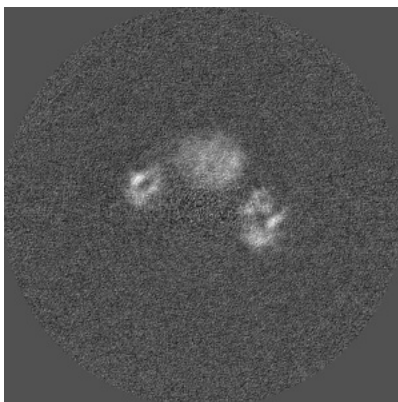


Z Index: 200

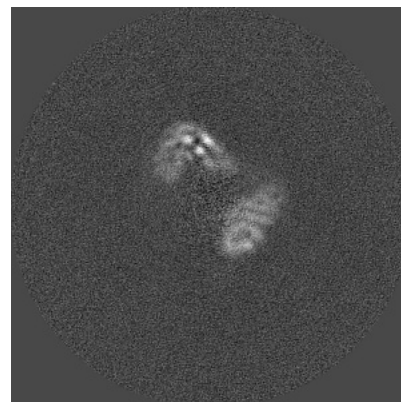
6.2.2 Raw map



X Index: 200



Y Index: 200

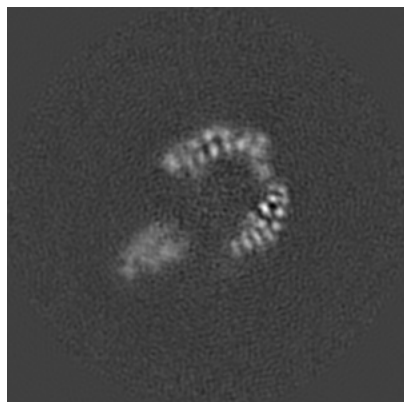


Z Index: 200

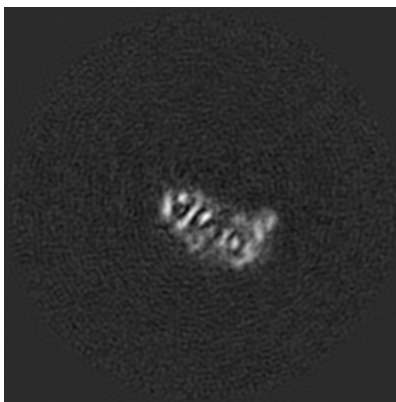
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

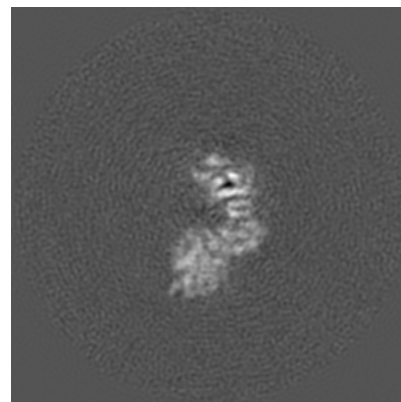
6.3.1 Primary map



X Index: 187

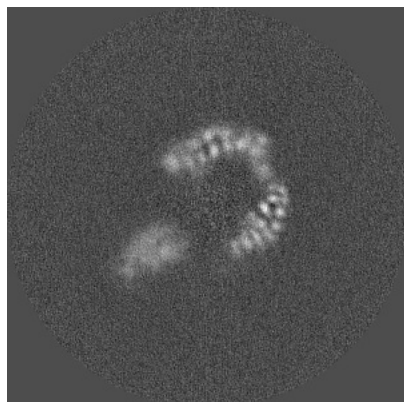


Y Index: 255

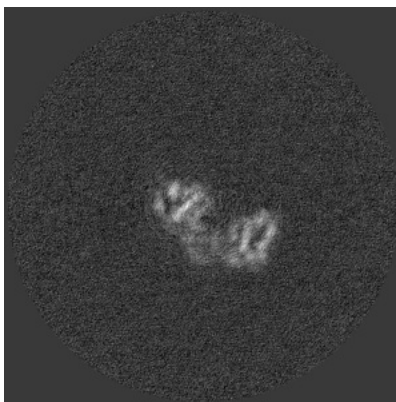


Z Index: 152

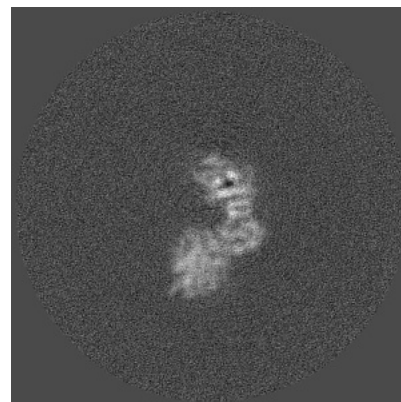
6.3.2 Raw map



X Index: 187



Y Index: 247

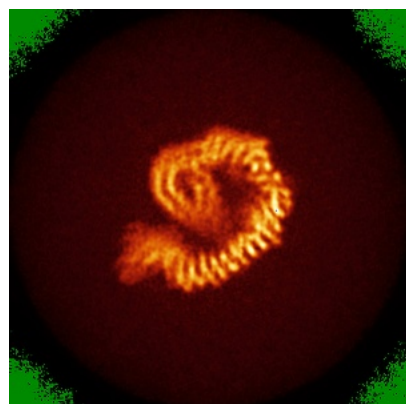


Z Index: 151

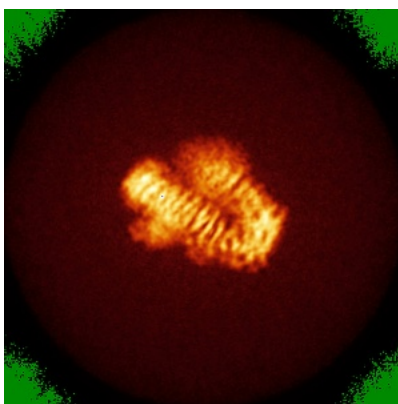
The images above show the largest variance slices of the map in three orthogonal directions.

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

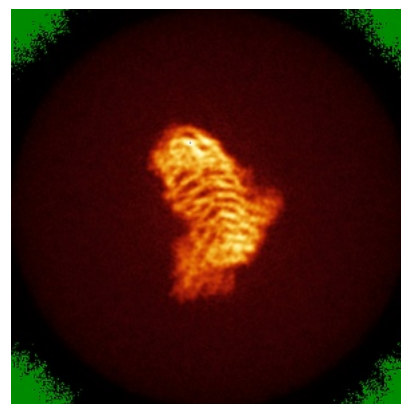
6.4.1 Primary map



X

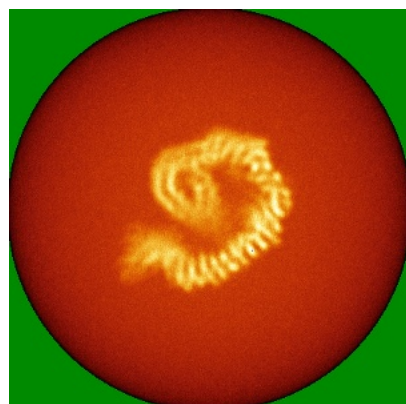


Y

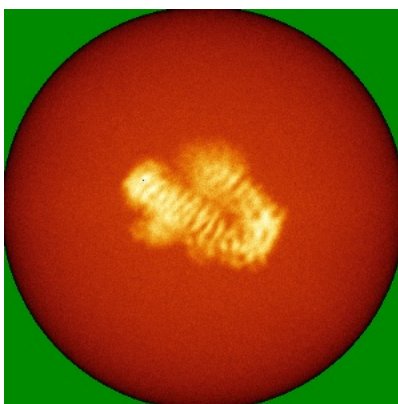


Z

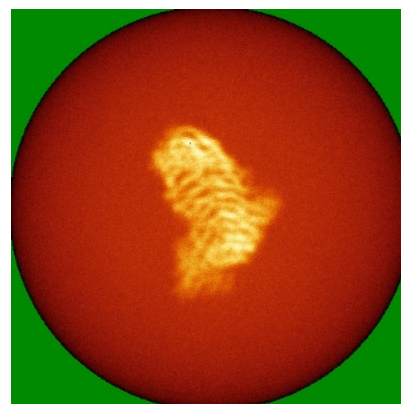
6.4.2 Raw map



X



Y

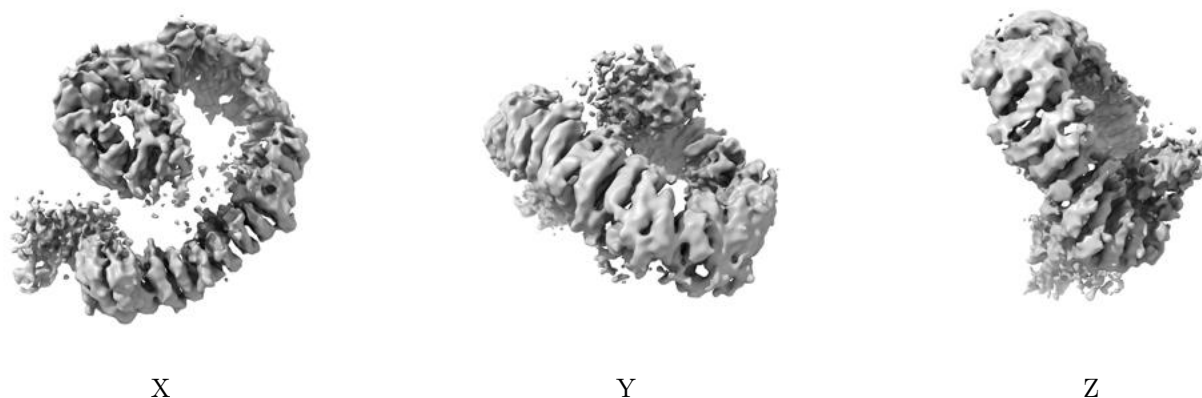


Z

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.

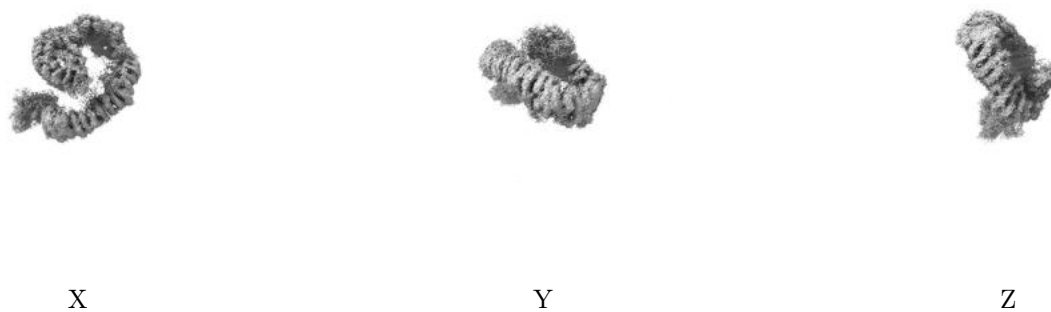
6.5 Orthogonal surface views [i](#)

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.

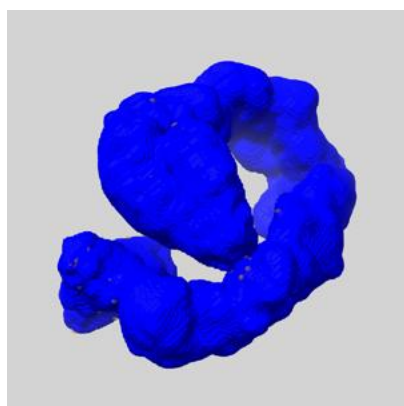
6.6 Mask visualisation [i](#)

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

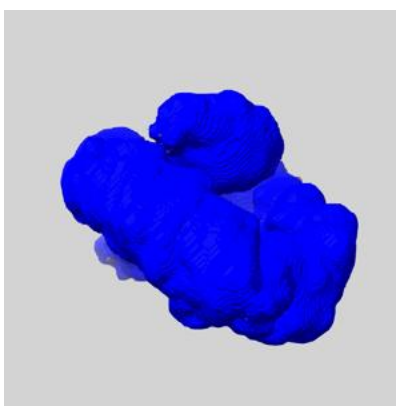
A mask typically either:

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

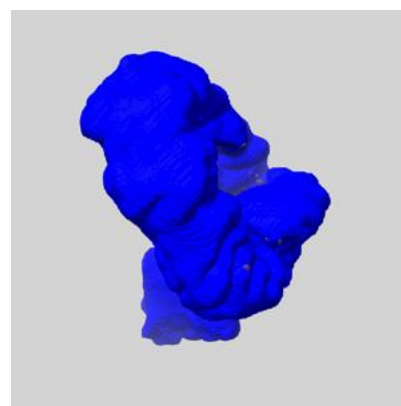
6.6.1 emd_12319_msk_1.map [i](#)



X



Y

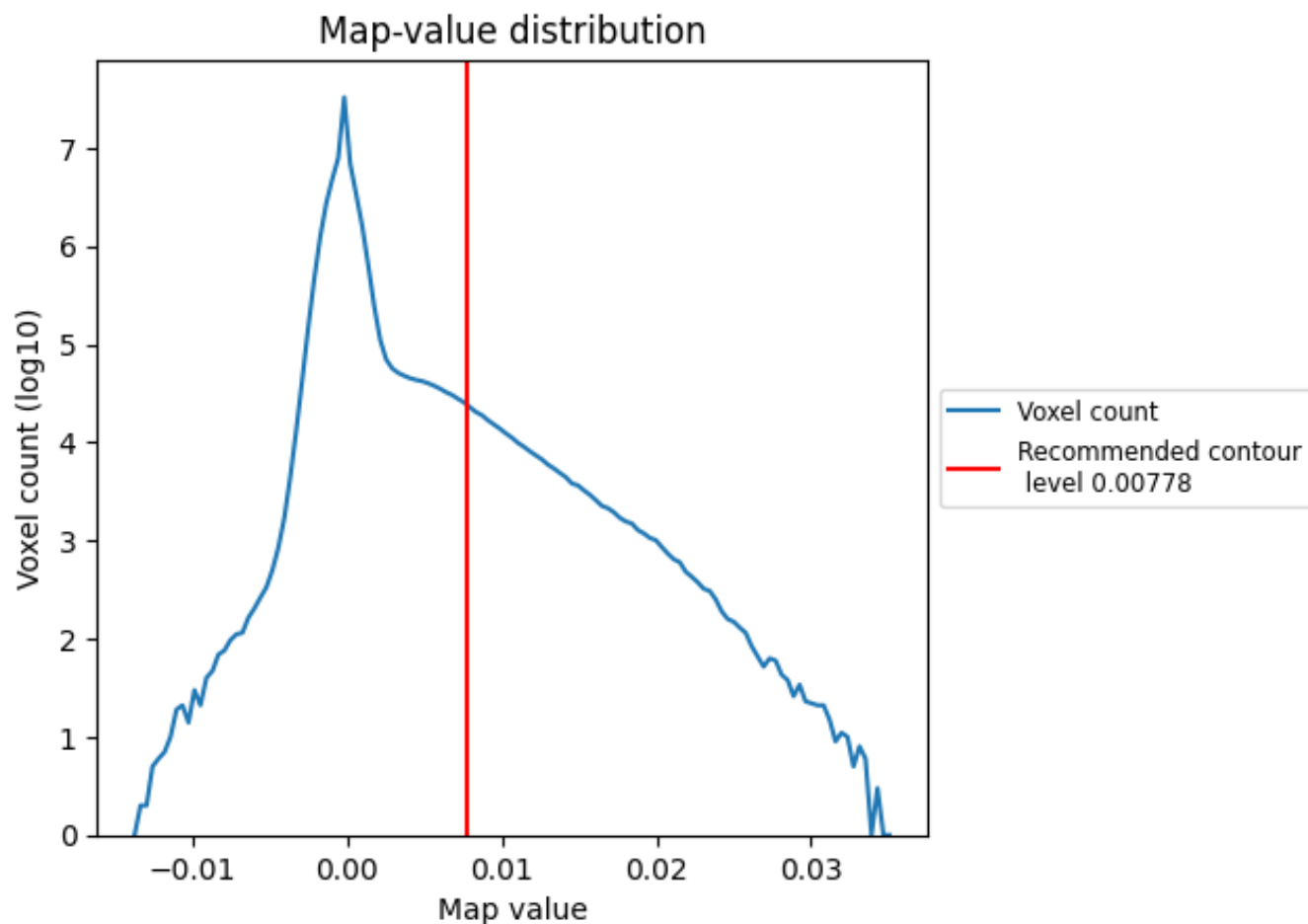


Z

7 Map analysis [i](#)

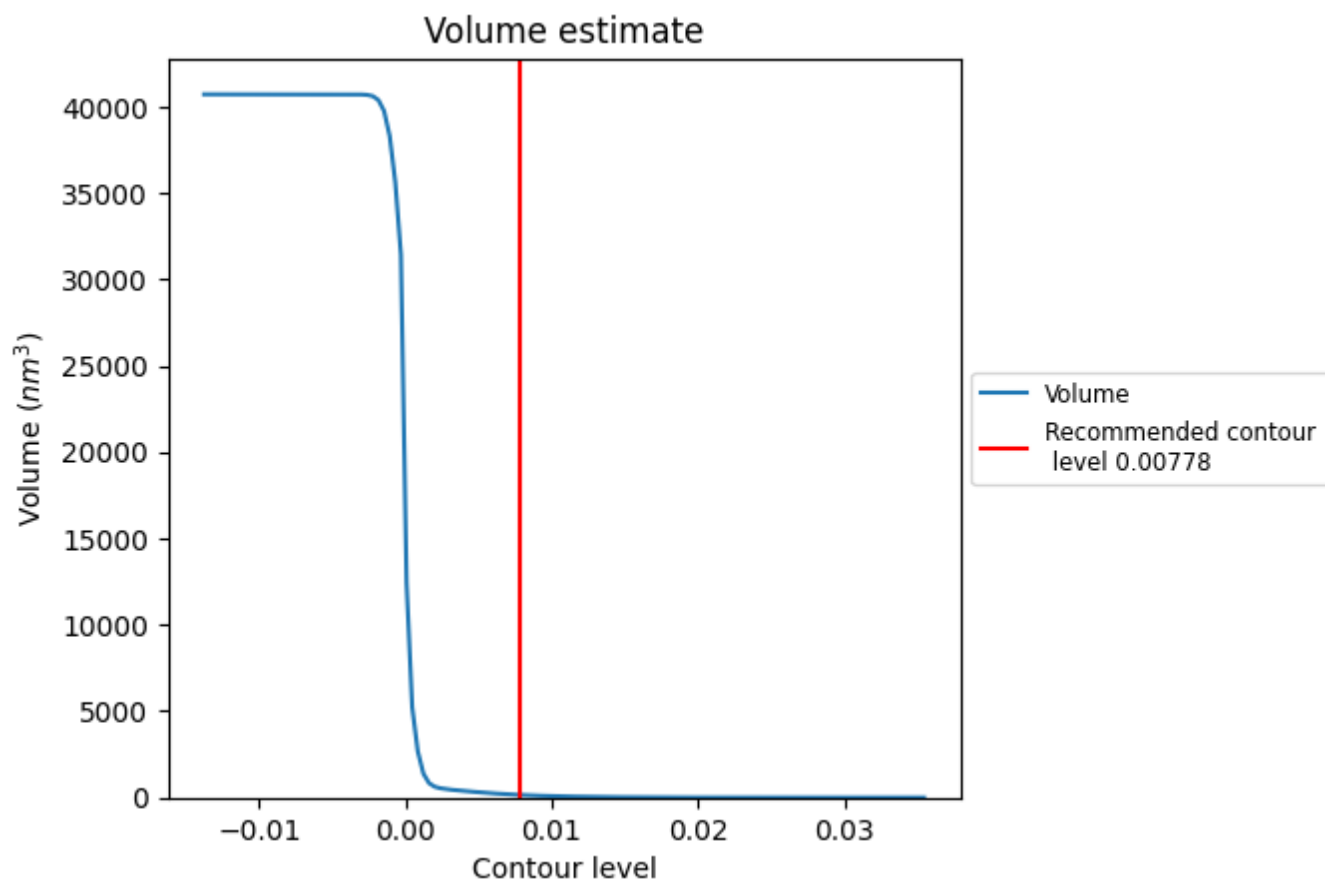
This section contains the results of statistical analysis of the map.

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.

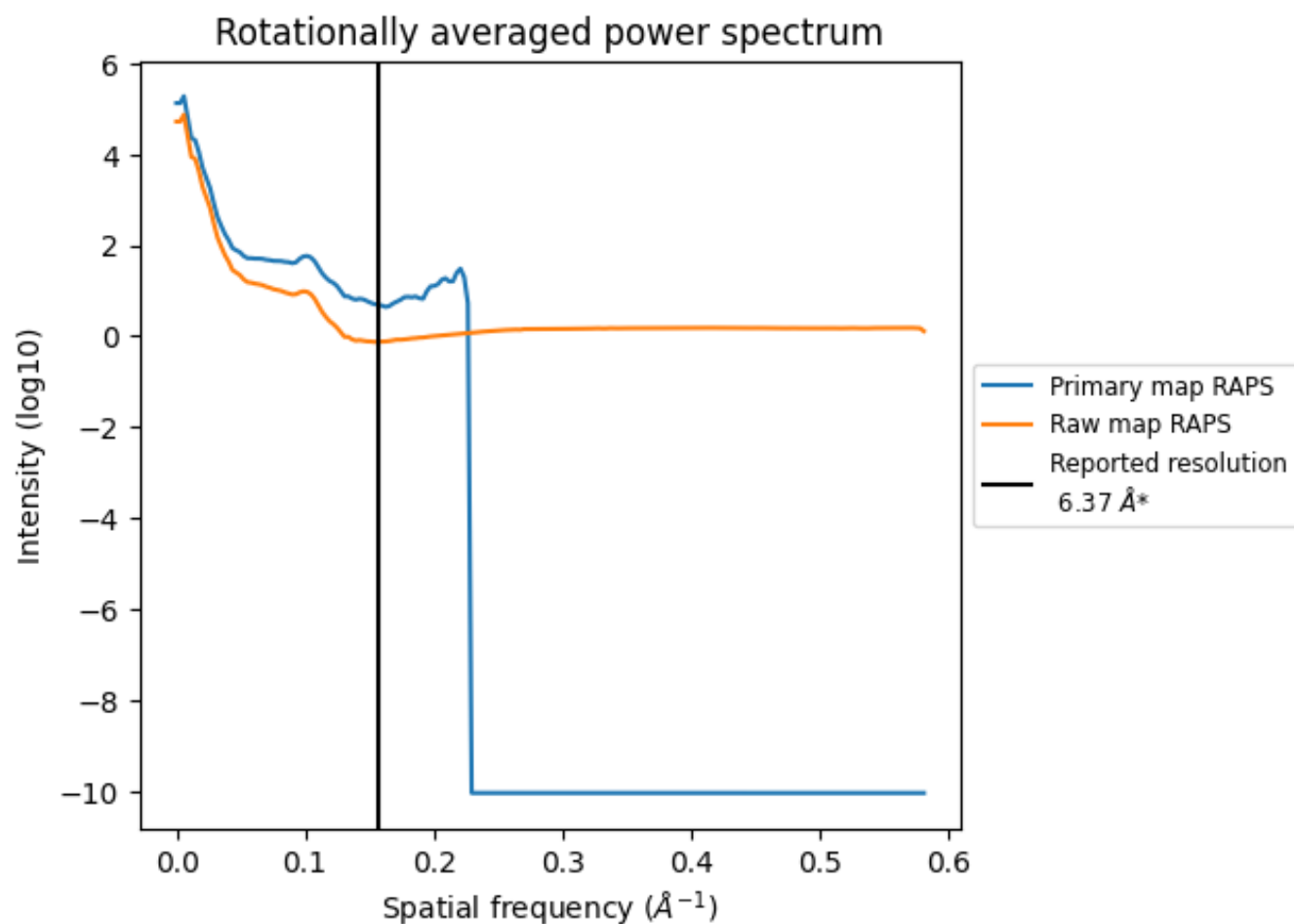
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 154 nm³; 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 ⓘ

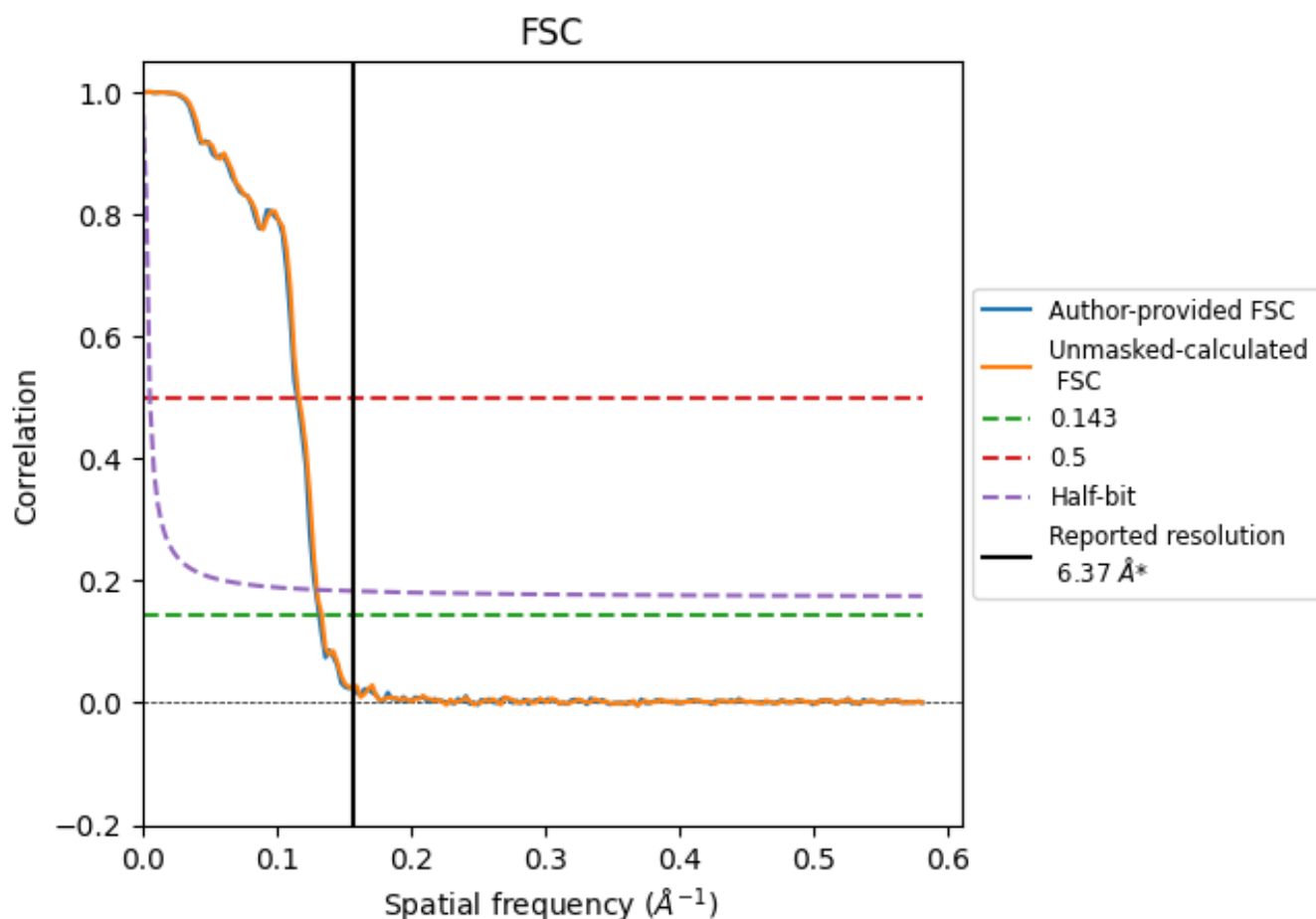


*Reported resolution corresponds to spatial frequency of 0.157 Å⁻¹

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 0.157 Å⁻¹

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

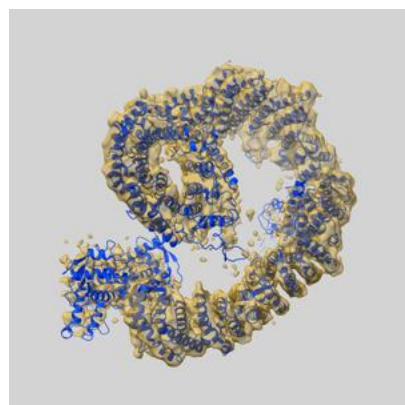
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 7.58 differs from the reported value 6.37 by more than 10 %

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 %

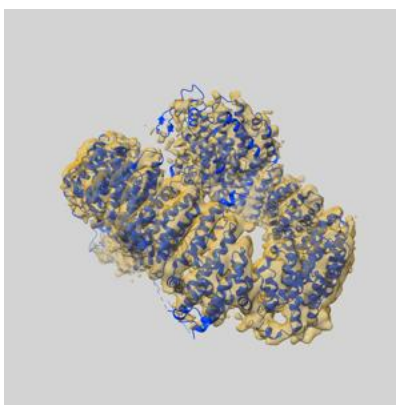
9 Map-model fit [i](#)

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](#).

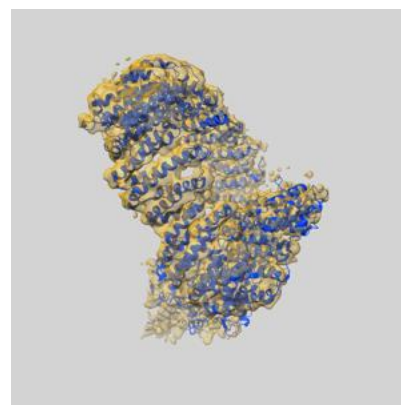
9.1 Map-model overlay [i](#)



X



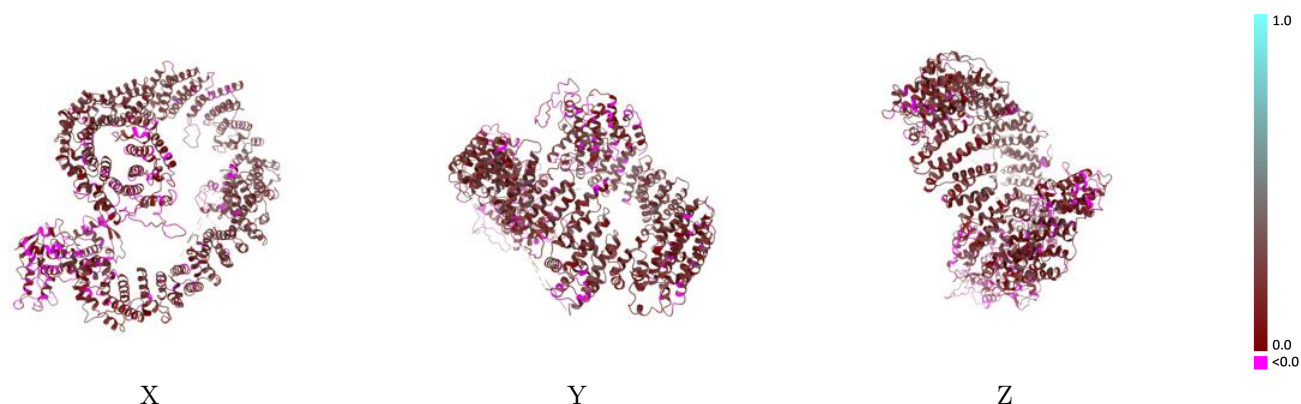
Y



Z

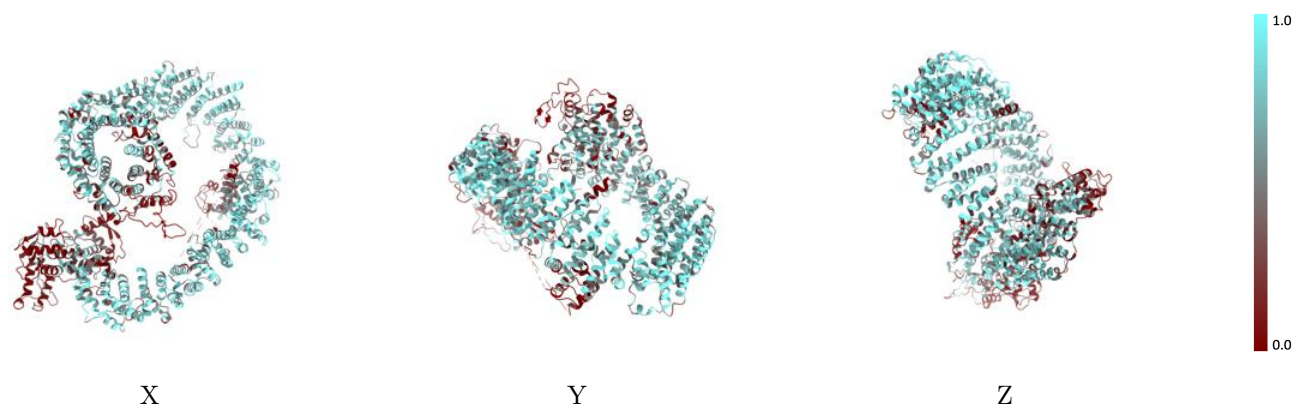
The images above show the 3D surface view of the map at the recommended contour level 0.00778 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



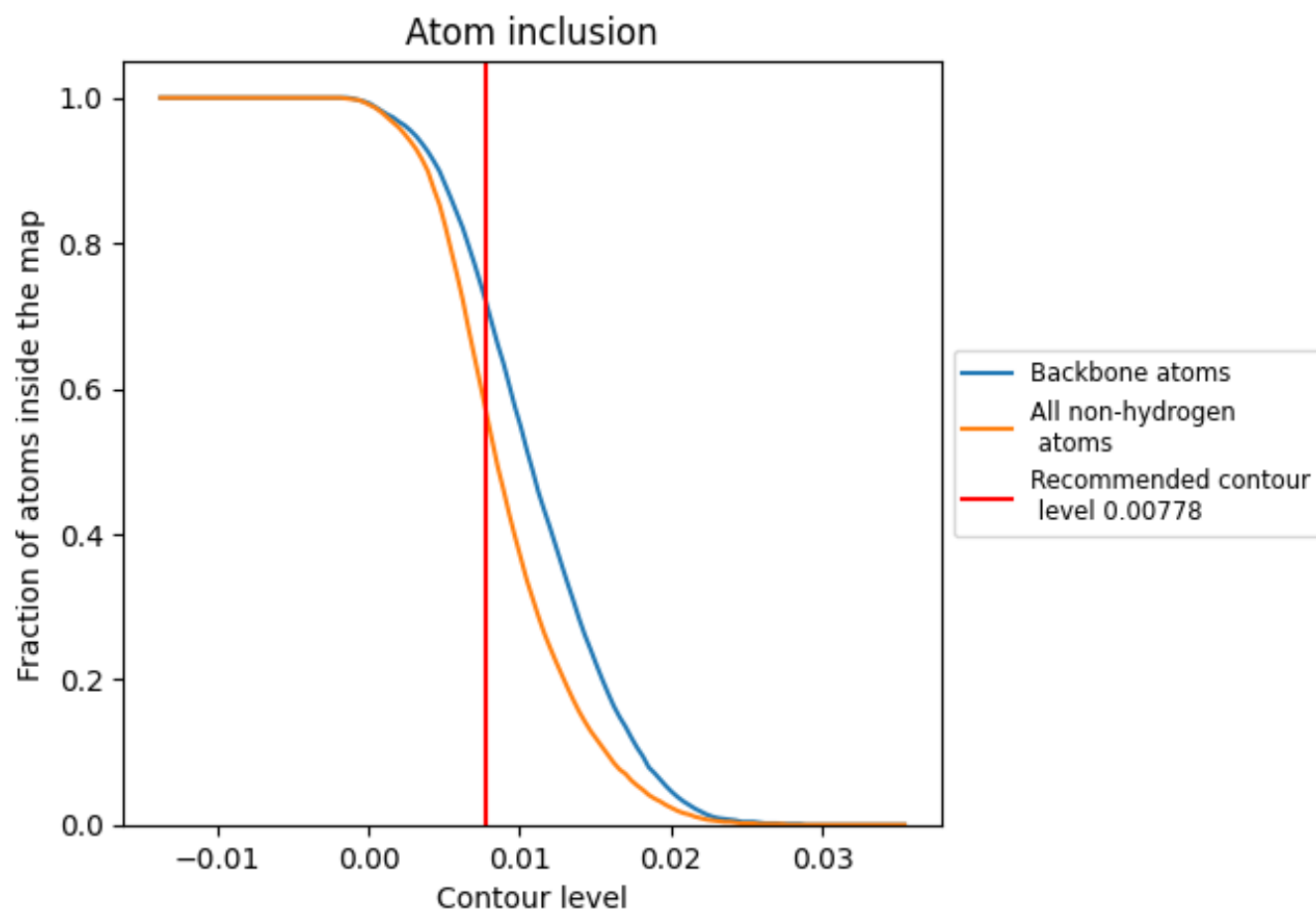
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.5670	0.1590
A	0.5670	0.1590

