



## wwPDB EM Validation Summary Report ⓘ

Jul 21, 2025 – 04:18 pm BST

PDB ID : 9QE7 / pdb\_00009qe7  
EMDB ID : EMD-53049  
Title : Membrane-distal part of extracellular domain of the Fap2 autotransporter adhesin from *Fusobacterium nucleatum* ATCC23726  
Authors : Schoepf, F.; Marongiu, G.L.; Milaj, K.; Sprink, T.; Kikhney, J.; Moter, A.; Roderer, D.  
Deposited on : 2025-03-07  
Resolution : 4.40 Å (reported)  
Based on initial model : .

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.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

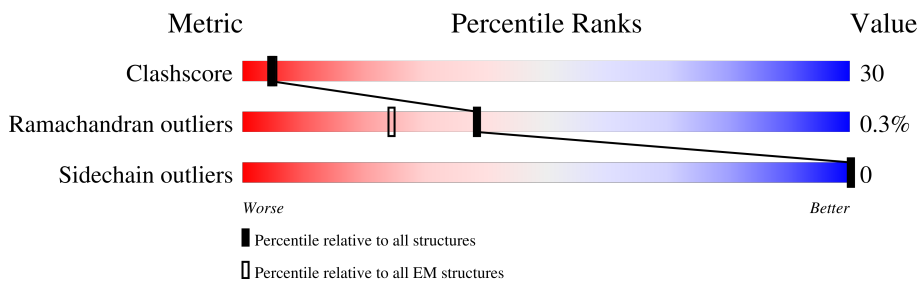
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.40 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	3250	<div> <div>17%</div> <div>22%</div> <div>24%</div> <div>54%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10826 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 Outer membrane autotransporter barrel domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1483	Total	C	N	O	S	0	0
			10826	6651	1867	2289	19		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3272	GLY	-	expression tag	UNP D5RBA4
A	3273	SER	-	expression tag	UNP D5RBA4
A	3274	ALA	-	expression tag	UNP D5RBA4
A	3275	HIS	-	expression tag	UNP D5RBA4
A	3276	HIS	-	expression tag	UNP D5RBA4
A	3277	HIS	-	expression tag	UNP D5RBA4
A	3278	HIS	-	expression tag	UNP D5RBA4
A	3279	HIS	-	expression tag	UNP D5RBA4
A	3280	HIS	-	expression tag	UNP D5RBA4
A	3281	HIS	-	expression tag	UNP D5RBA4
A	3282	HIS	-	expression tag	UNP D5RBA4
A	3283	SER	-	expression tag	UNP D5RBA4
A	3284	ALA	-	expression tag	UNP D5RBA4
A	3285	GLY	-	expression tag	UNP D5RBA4
A	3286	GLU	-	expression tag	UNP D5RBA4
A	3287	ASN	-	expression tag	UNP D5RBA4
A	3288	LEU	-	expression tag	UNP D5RBA4
A	3289	TYR	-	expression tag	UNP D5RBA4
A	3290	PHE	-	expression tag	UNP D5RBA4
A	3291	GLN	-	expression tag	UNP D5RBA4



N1480	K1481	N1485	S1486	G1487	M1413	L1420	S1421	D1490	I1491	A1492	G1493	T1494	S1495	K1496	T1497	G1498	I1502	Y1503	E1507	S1508	G1509	A1510	T1511	K1512	K1513	L1514	S1515	V1516	N1517	N1518	N1519	G1520	T1523	N1524	N1525	Q1526	K1527	V1530	G1531	I1532	Y1533	N1536	E1537	S1538	N1539	H1540	A1541	N1542	T1543	E1544	S1545	D1546	V1547	T1548																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
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T1204	G1205	I1206	I1207	E1208	L1209	E1210	V1217	I1218	A1219	M1224	I1225	N1226	S1227	G1228	T1229	E1232	V1235	N1236	K1237	E1238	T1239	S1240	V1241	G1242	I1243	Y1244	T1248	S1249	I1250	S1251	S1252	V1253	S1254	K1255	N1256	K1258	N1259	E1260	G1261	T1262	I1263	E1264	I1265	K1266	A1267	D1268	G1269	D1270	L1271	K1272	S1273	A1274	G1275																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
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L1755	V1756	G1757	D1758	T1759	E1760	D1762	L1763	N1764	K1765	G1766	G1767	L1768	T1769	E1770	K1775	G1776	S1777	N1778	V1779	D1780	E1781	K1782	L1783	R1784	S1785	S1786	I1789	T1790	A1791	K1792	S1793	N1794	S1795	V1796	I1797	N1798	V1799	G1800	G1801	K1802	K1803	N1804	E1805	G1806	F1807	G1808	N1811	S1812	A1813	H1814	S1815	S1816	K1817	F1818	G1819																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
T1920	T1921	V1922	D1923	S1924	E1926	Y1927	D1930	K1931	T1932	H1933	H1934	G1935	K1936	N1939	E1940	G1941	I1942	I1943	N1944	S1945	G1946	S1947	D1948	E1949	S1950	K1951	G1952	F1953	A1954	M1955	N1956	K1957	G1958	N1959	S1960	S1961	K1962	S1963	G1964	V1969	K1970	K1971	G1972	I1973	N1974	S1975	G1976	H1977	S1978	S1979	G1980	S1981	S1982	S1983	S1984	S1985	S1986	S1987	S1988	S1989	S1990	S1991	S1992	S1993	S1994	S1995	S1996	S1997	S1998	S1999	S2000	S2001	S2002	S2003	S2004	S2005	S2006	S2007	S2008	S2009	S2010	S2011	S2012	S2013	S2014	S2015	S2016	S2017	S2018	S2019	S2020	S2021	S2022	S2023	S2024	S2025	S2026	S2027	S2028	S2029	S2030	S2031	S2032	S2033	S2034	S2035	S2036	S2037	S2038	S2039	S2040	S2041	S2042	S2043	S2044	S2045	S2046	S2047	S2048	S2049	S2050	S2051	S2052	S2053	S2054	S2055	S2056	S2057	S2058	S2059	S2060	S2061	S2062	S2063	S2064	S2065	S2066	S2067	S2068	S2069	S2070	S2071	S2072	S2073	S2074	S2075	S2076	S2077	S2078	S2079	S2080	S2081	S2082	S2083	S2084	S2085	S2086	S2087	S2088	S2089	S2090	S2091	S2092	S2093	S2094	S2095	S2096	S2097	S2098	S2099	S2100	S2101	S2102	S2103	S2104	S2105	S2106	S2107	S2108	S2109	S2110	S2111	S2112	S2113	S2114	S2115	S2116	S2117	S2118	S2119	S2120	S2121	S2122	S2123	S2124	S2125	S2126	S2127	S2128	S2129	S2130	S2131	S2132	S2133	S2134	S2135	S2136	S2137	S2138	S2139	S2140	S2141	S2142	S2143	S2144	S2145	S2146	S2147	S2148	S2149	S2150	S2151	S2152	S2153	S2154	S2155	S2156	S2157	S2158	S2159	S2160	S2161	S2162	S2163	S2164	S2165	S2166	S2167	S2168	S2169	S2170	S2171	S2172	S2173	S2174	S2175	S2176	S2177	S2178	S2179	S2180	S2181	S2182	S2183	S2184	S2185	S2186	S2187	S2188	S2189	S2190	S2191	S2192	S2193	S2194	S2195	S2196	S2197	S2198	S2199	S2200	S2201	S2202	S2203	S2204	S2205	S2206	S2207	S2208	S2209	S2210	S2211	S2212	S2213	S2214	S2215	S2216	S2217	S2218	S2219	S2220	S2221	S2222	S2223	S2224	S2225	S2226	S2227	S2228	S2229	S2230	S2231	S2232	S2233	S2234	S2235	S2236	S2237	S2238	S2239	S2240	S2241	S2242	S2243	S2244	S2245	S2246	S2247	S2248	S2249	S2250	S2251	S2252	S2253	S2254	S2255	S2256	S2257	S2258	S2259	S2260	S2261	S2262	S2263	S2264	S2265	S2266	S2267	S2268	S2269	S2270	S2271	S2272	S2273	S2274	S2275	S2276	S2277	S2278	S2279	S2280	S2281	S2282	S2283	S2284	S2285	S2286	S2287	S2288	S2289	S2290	S2291	S2292	S2293	S2294	S2295	S2296	S2297	S2298	S2299	S2300	S2301	S2302	S2303	S2304	S2305	S2306	S2307	S2308	S2309	S2310	S2311	S2312	S2313	S2314	S2315	S2316	S2317	S2318	S2319	S2320	S2321	S2322	S2323	S2324	S2325	S2326	S2327	S2328	S2329	S2330	S2331	S2332	S2333	S2334	S2335	S2336	S2337	S2338	S2339	S2340	S2341	S2342	S2343	S2344	S2345	S2346	S2347	S2348	S2349	S2350	S2351	S2352	S2353	S2354	S2355	S2356	S2357	S2358	S2359	S2360	S2361	S2362	S2363	S2364	S2365	S2366	S2367	S2368	S2369	S2370	S2371	S2372	S2373	S2374	S2375	S2376	S2377	S2378	S2379	S2380	S2381	S2382	S2383	S2384	S2385	S2386	S2387	S2388	S2389	S2390	S2391	S2392	S2393	S2394	S2395	S2396	S2397	S2398	S2399	S2400	S2401	S2402	S2403	S2404	S2405	S2406	S2407	S2408	S2409	S2410	S2411	S2412	S2413	S2414	S2415	S2416	S2417	S2418	S2419	S2420	S2421	S2422	S2423	S2424	S2425	S2426	S2427	S2428	S2429	S2430	S2431	S2432	S2433	S2434	S2435	S2436	S2437	S2438	S2439	S2440	S2441	S2442	S2443	S2444	S2445	S2446	S2447	S2448	S2449	S2450	S2451	S2452	S2453	S2454	S2455	S2456	S2457	S2458	S2459	S2460	S2461	S2462	S2463	S2464	S2465	S2466	S2467	S2468	S2469	S2470	S2471	S2472	S2473	S2474	S2475	S2476	S2477	S2478	S2479	S2480	S2481	S2482	S2483	S2484	S2485	S2486	S2487	S2488	S2489	S2490	S2491	S2492	S2493	S2494	S2495	S2496	S2497	S2498	S2499	S2500	S2501	S2502	S2503	S2504	S2505	S2506	S2507	S2508	S2509	S2510	S2511	S2512	S2513	S2514	S2515





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	151825	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	58.8	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.460	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	407.03998, 407.03998, 407.03998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	0.19	0/10944	0.53	2/14805 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	1376	ILE	N-CA-C	-5.26	106.30	111.88
1	A	678	ILE	N-CA-C	-5.09	106.70	111.48

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1102	ASP	Peptide

### 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	10826	0	10829	644	0
All	All	10826	0	10829	644	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 30.

The worst 5 of 644 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:1126:ILE:HB	1:A:1155:ASN:HA	1.61	0.83
1:A:1235:VAL:HB	1:A:1265:ILE:HG23	1.59	0.82
1:A:882:LYS:HB3	1:A:909:THR:HA	1.62	0.81
1:A:1238:GLU:HB2	1:A:1272:LYS:HB3	1.64	0.78
1:A:439:ILE:HB	1:A:473:ILE:HG22	1.65	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	1481/3250 (46%)	1316 (89%)	160 (11%)	5 (0%)	37	72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1383	ILE
1	A	319	ASN
1	A	778	ASN
1	A	1667	TYR
1	A	915	ILE

### 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	1208/2632 (46%)	1208 (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 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1664	ASN
1	A	1600	ASN
1	A	1047	ASN
1	A	1572	ASN
1	A	986	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-53049. These allow visual inspection of the internal detail of the map and identification of artifacts.

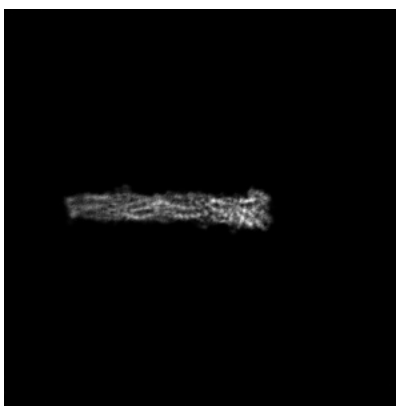
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



X

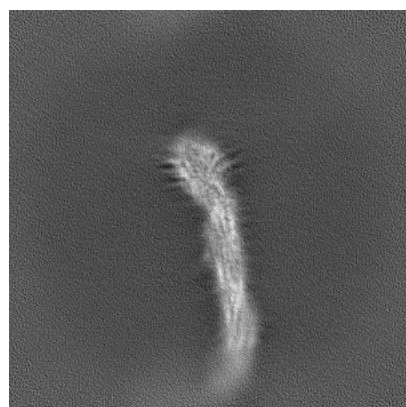


Y

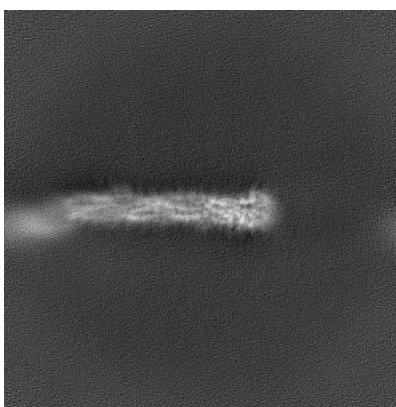


Z

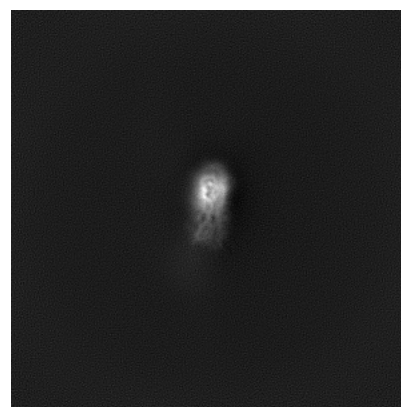
#### 6.1.2 Raw map



X



Y

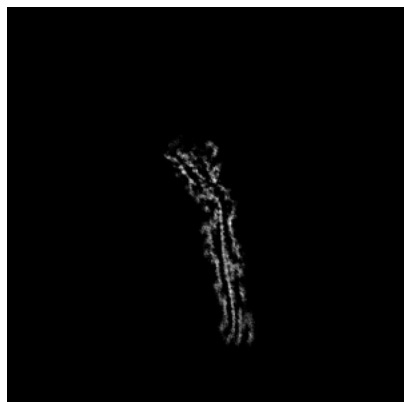


Z

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

## 6.2 Central slices [i](#)

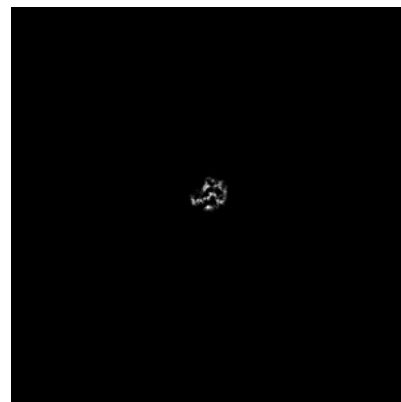
### 6.2.1 Primary map



X Index: 192

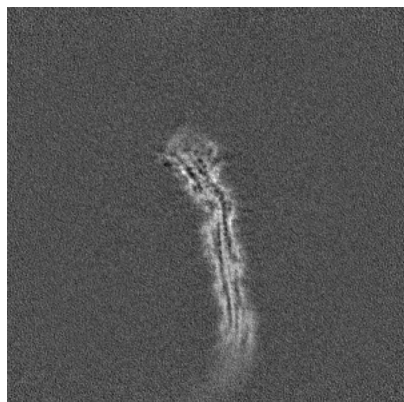


Y Index: 192



Z Index: 192

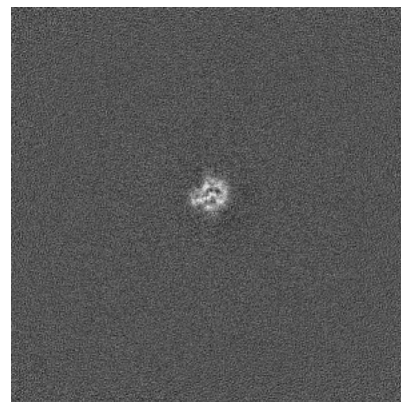
### 6.2.2 Raw map



X Index: 192



Y Index: 192



Z Index: 192

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

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

### 6.3.1 Primary map



X Index: 185



Y Index: 213

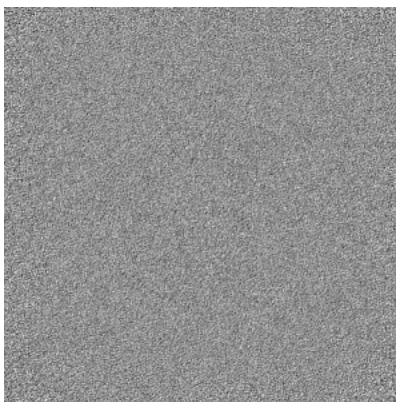


Z Index: 236

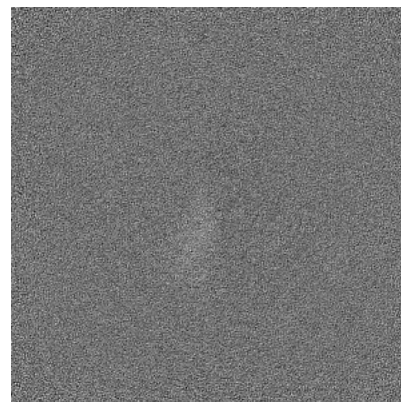
### 6.3.2 Raw map



X Index: 185



Y Index: 0

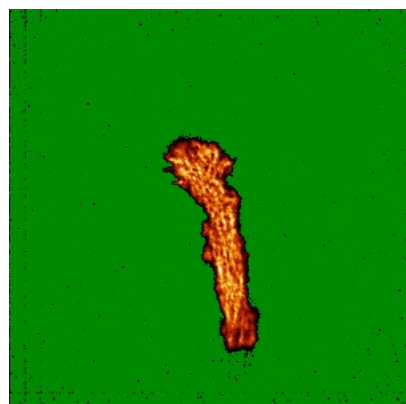


Z Index: 0

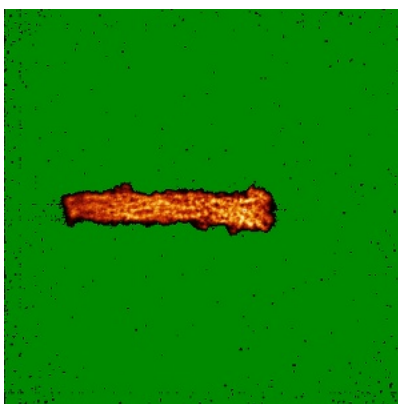
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X

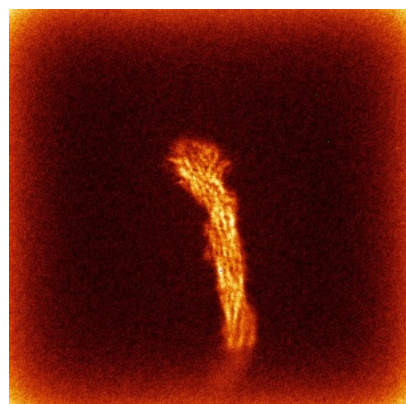


Y

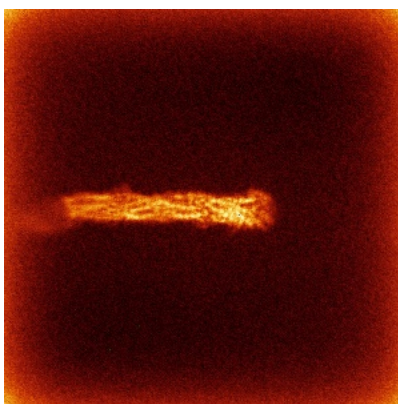


Z

### 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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. 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



X



Y



Z

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.

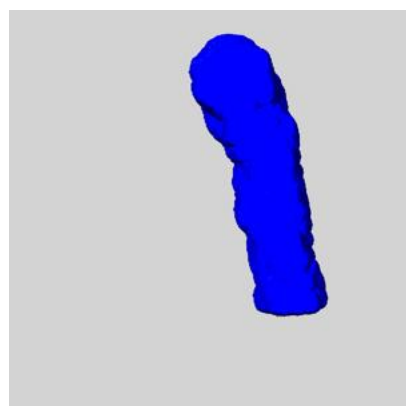
## 6.6 Mask visualisation [i](#)

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

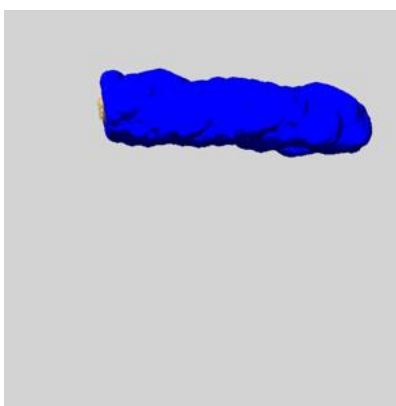
A mask typically either:

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

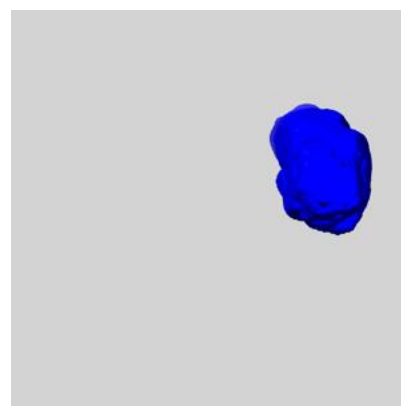
### 6.6.1 emd\_53049\_msk\_1.map [i](#)



X



Y

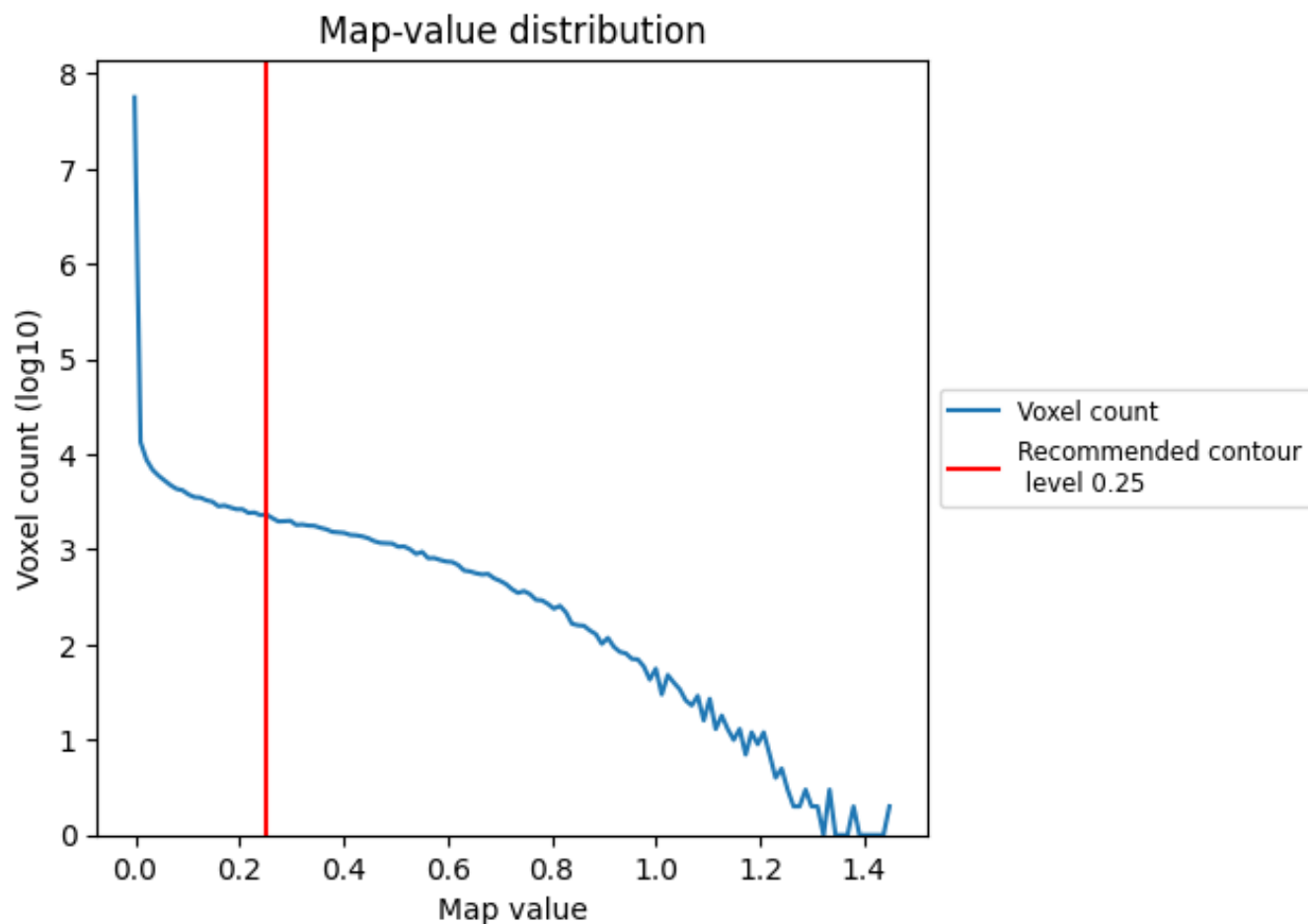


Z

## 7 Map analysis [i](#)

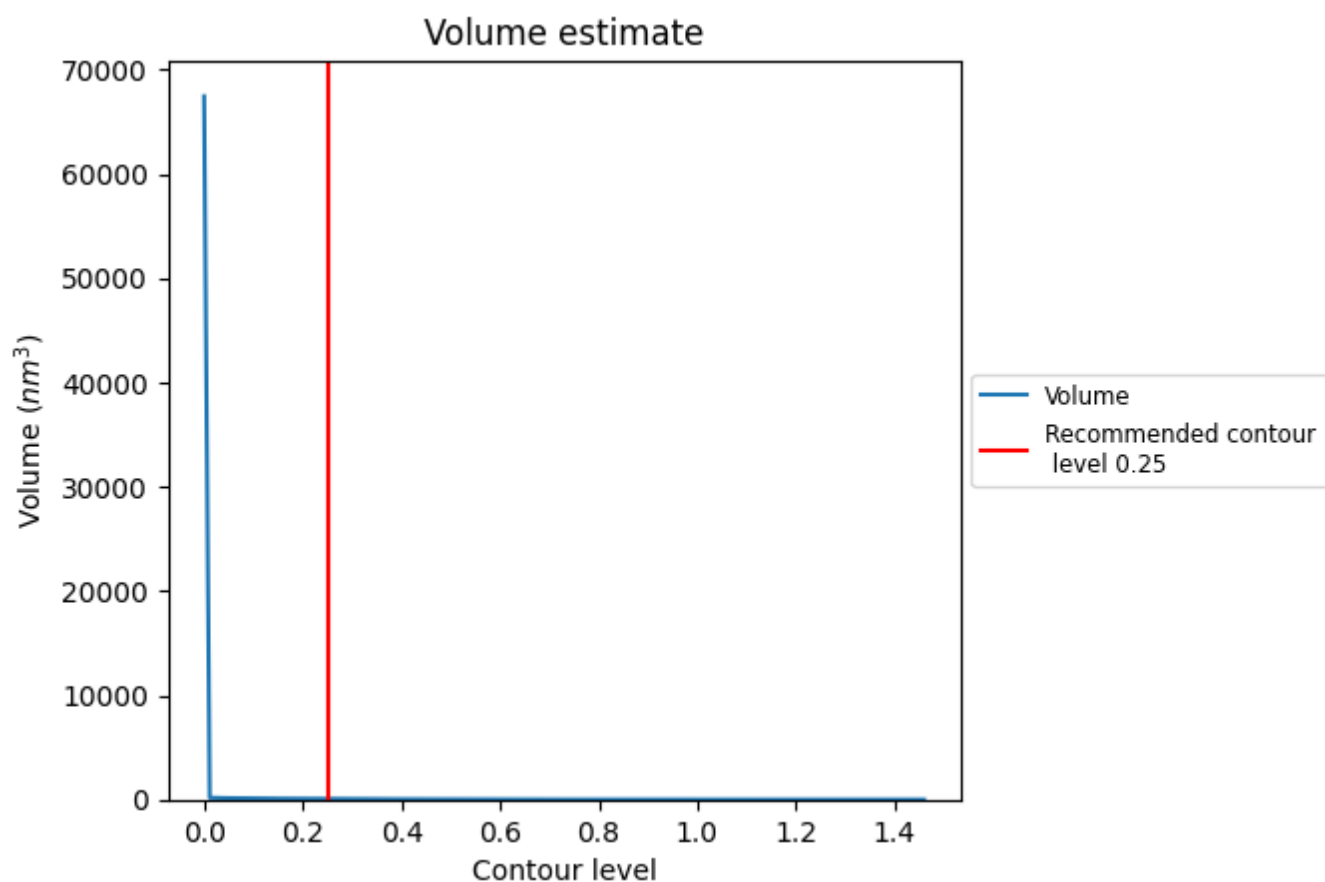
This section contains the results of statistical analysis of the map.

### 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.

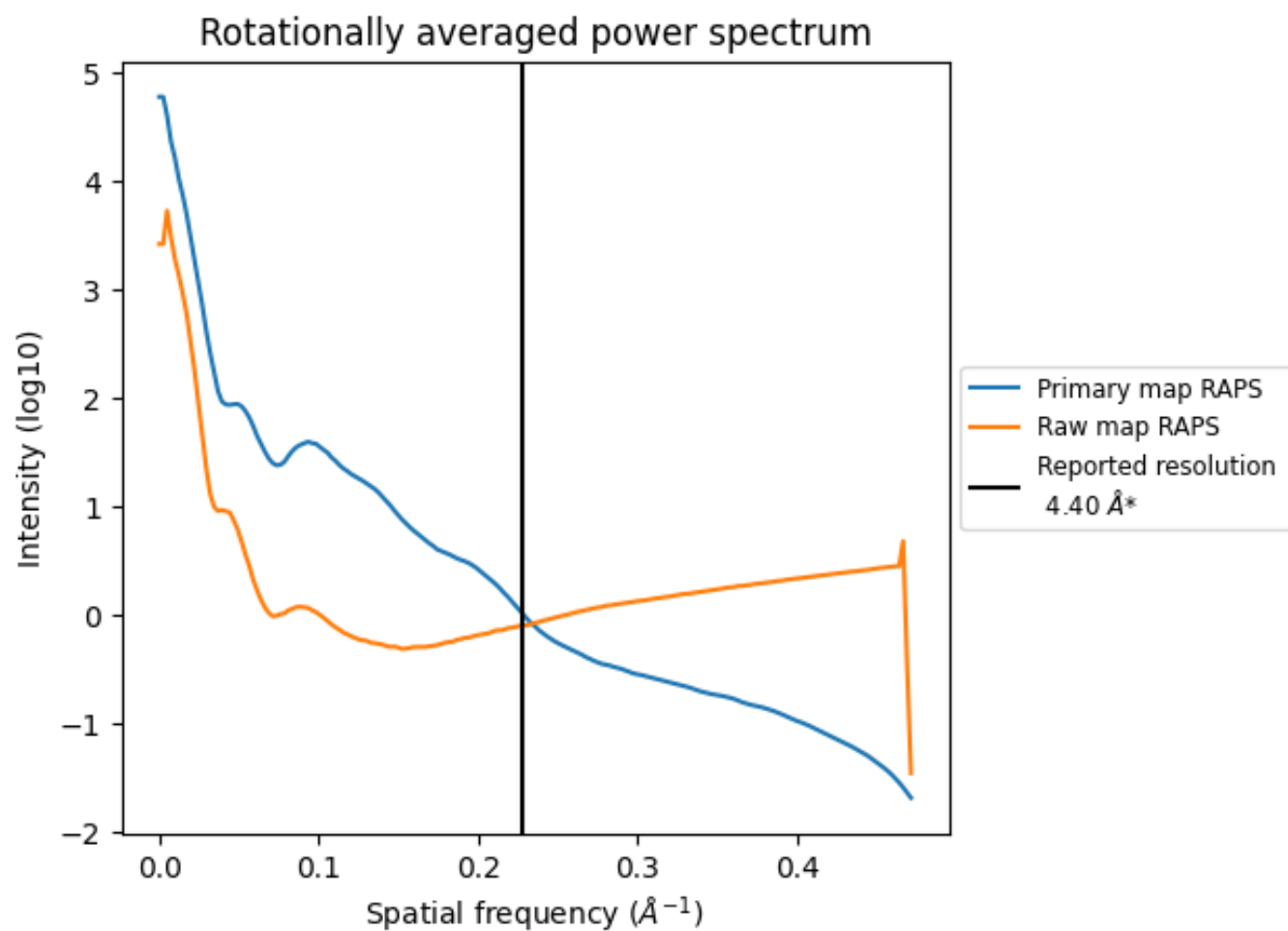
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 65  $\text{nm}^3$ ; this corresponds to an approximate mass of 59 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 ⓘ

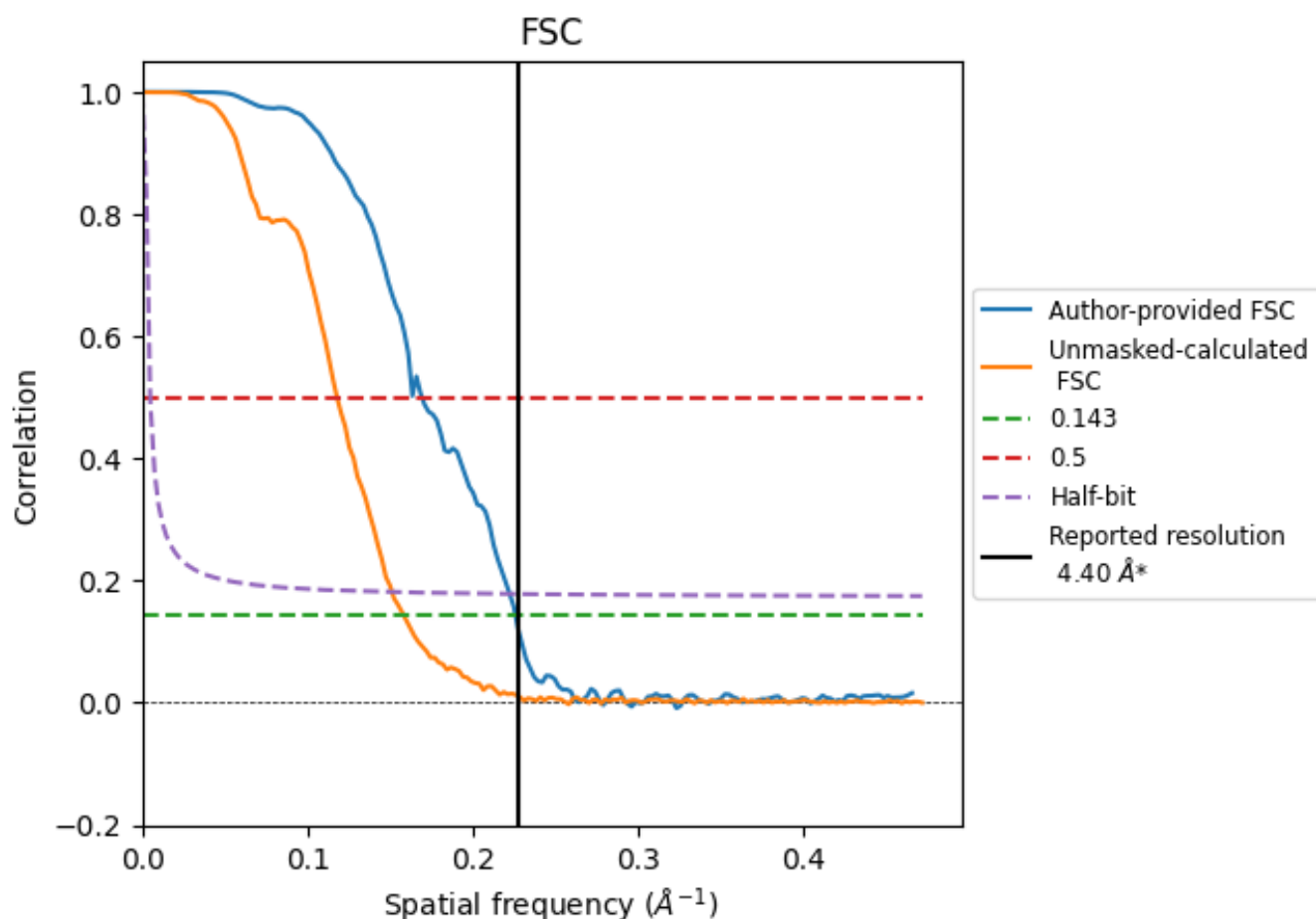


\*Reported resolution corresponds to spatial frequency of 0.227  $\text{\AA}^{-1}$

## 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  $0.227 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

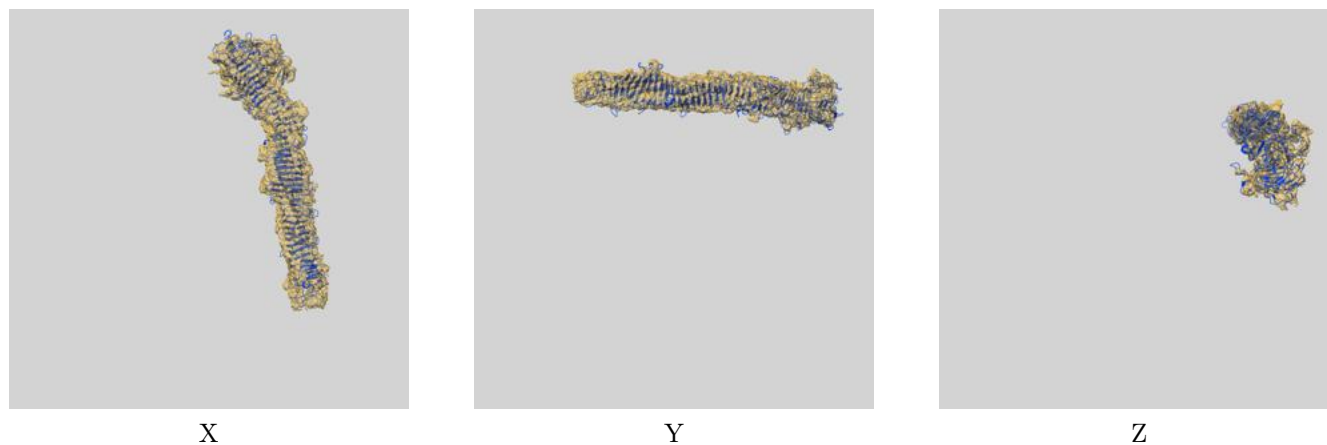
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.43	5.91	4.50
Unmasked-calculated*	6.33	8.49	6.62

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.33 differs from the reported value 4.4 by more than 10 %

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

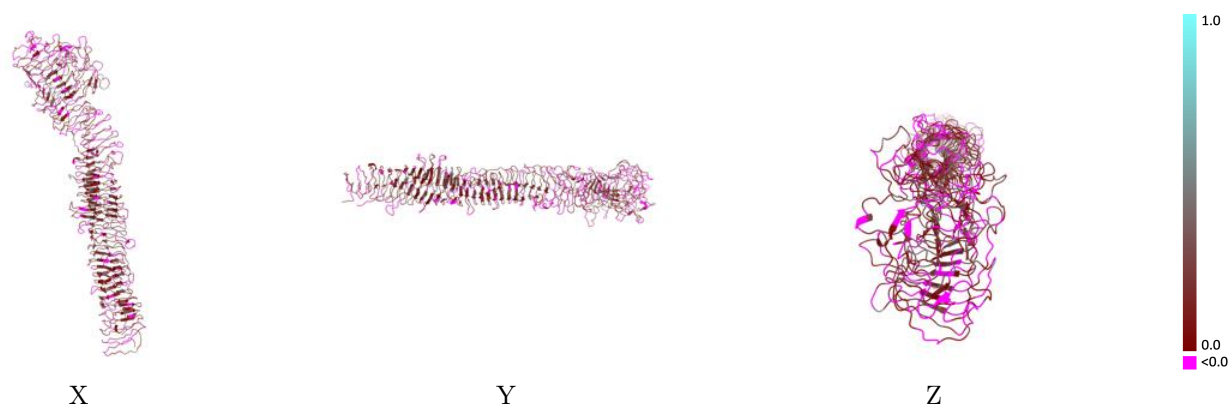
This section contains information regarding the fit between EMDB map EMD-53049 and PDB model 9QE7. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

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



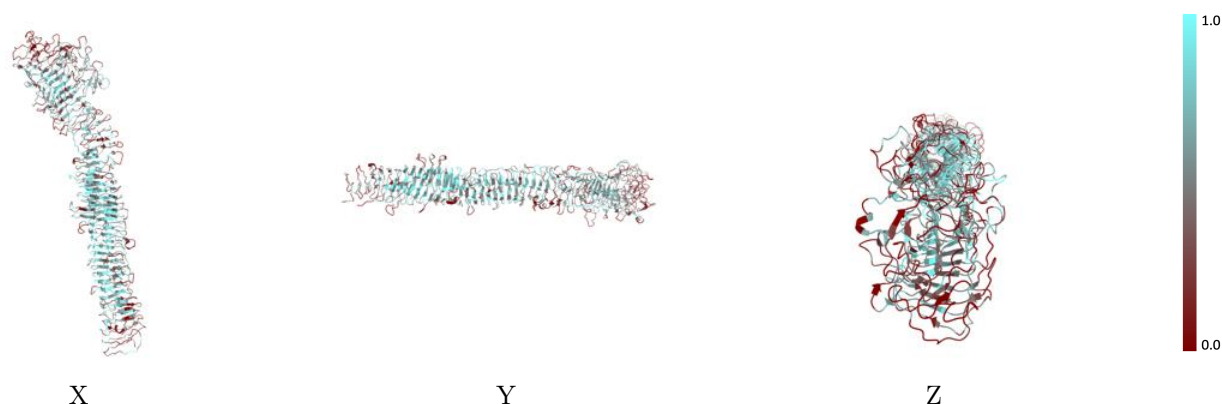
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



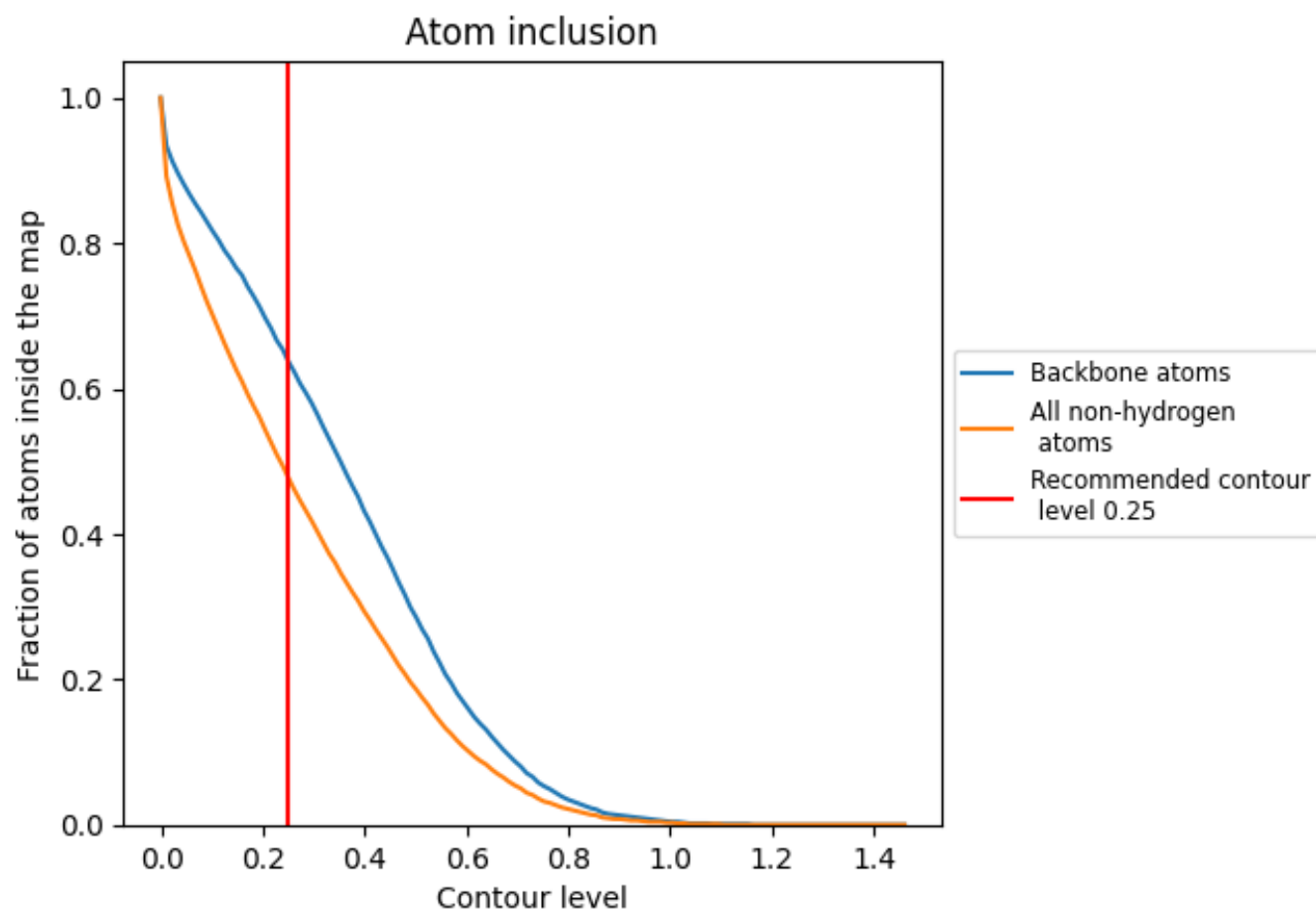
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 64% of all backbone atoms, 48% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4770	<div></div> 0.1180
A	<div></div> 0.4770	<div></div> 0.1180

