



wwPDB EM Validation Summary Report ⓘ

Jun 20, 2024 – 05:39 AM JST

PDB ID : 7WJI
EMDB ID : EMD-32544
Title : Architecture of the human NALCN channelosome
Authors : Wu, J.P.; Yan, Z.; Zhou, L.; Liu, H.; Zhao, Q.
Deposited on : 2022-01-06
Resolution : 4.50 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.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

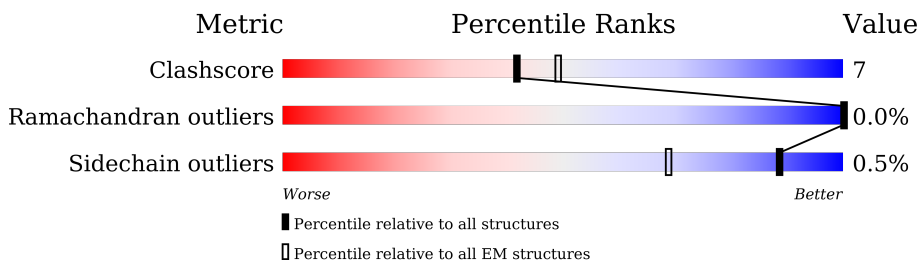
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	3258	
2	B	2658	
3	E	149	
4	C	1992	
5	D	458	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 41173 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 Protein unc-80 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1763	Total	C	N	O	S	0	0
			14143	9070	2451	2525	97		

- Molecule 2 is a protein called Protein unc-79 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1663	Total	C	N	O	S	0	0
			13146	8488	2188	2355	115		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2636	ASP	-	expression tag	UNP Q9P2D8
B	2637	GLU	-	expression tag	UNP Q9P2D8
B	2638	VAL	-	expression tag	UNP Q9P2D8
B	2639	ASP	-	expression tag	UNP Q9P2D8
B	2640	ALA	-	expression tag	UNP Q9P2D8
B	2641	GLY	-	expression tag	UNP Q9P2D8
B	2642	SER	-	expression tag	UNP Q9P2D8
B	2643	ASP	-	expression tag	UNP Q9P2D8
B	2644	TYR	-	expression tag	UNP Q9P2D8
B	2645	LYS	-	expression tag	UNP Q9P2D8
B	2646	ASP	-	expression tag	UNP Q9P2D8
B	2647	ASP	-	expression tag	UNP Q9P2D8
B	2648	ASP	-	expression tag	UNP Q9P2D8
B	2649	LYS	-	expression tag	UNP Q9P2D8
B	2650	GLY	-	expression tag	UNP Q9P2D8
B	2651	SER	-	expression tag	UNP Q9P2D8
B	2652	ASP	-	expression tag	UNP Q9P2D8
B	2653	TYR	-	expression tag	UNP Q9P2D8
B	2654	LYS	-	expression tag	UNP Q9P2D8
B	2655	ASP	-	expression tag	UNP Q9P2D8
B	2656	ASP	-	expression tag	UNP Q9P2D8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2657	ASP	-	expression tag	UNP Q9P2D8
B	2658	LYS	-	expression tag	UNP Q9P2D8

- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	126	Total	C	N	O	S	0	0
			988	615	160	204	9		

- Molecule 4 is a protein called Sodium leak channel non-selective protein,Extended tegument protein pp150.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	1394	Total	C	N	O	S	0	0
			11413	7523	1877	1926	87		

There are 15 discrepancies between the modelled and reference sequences:

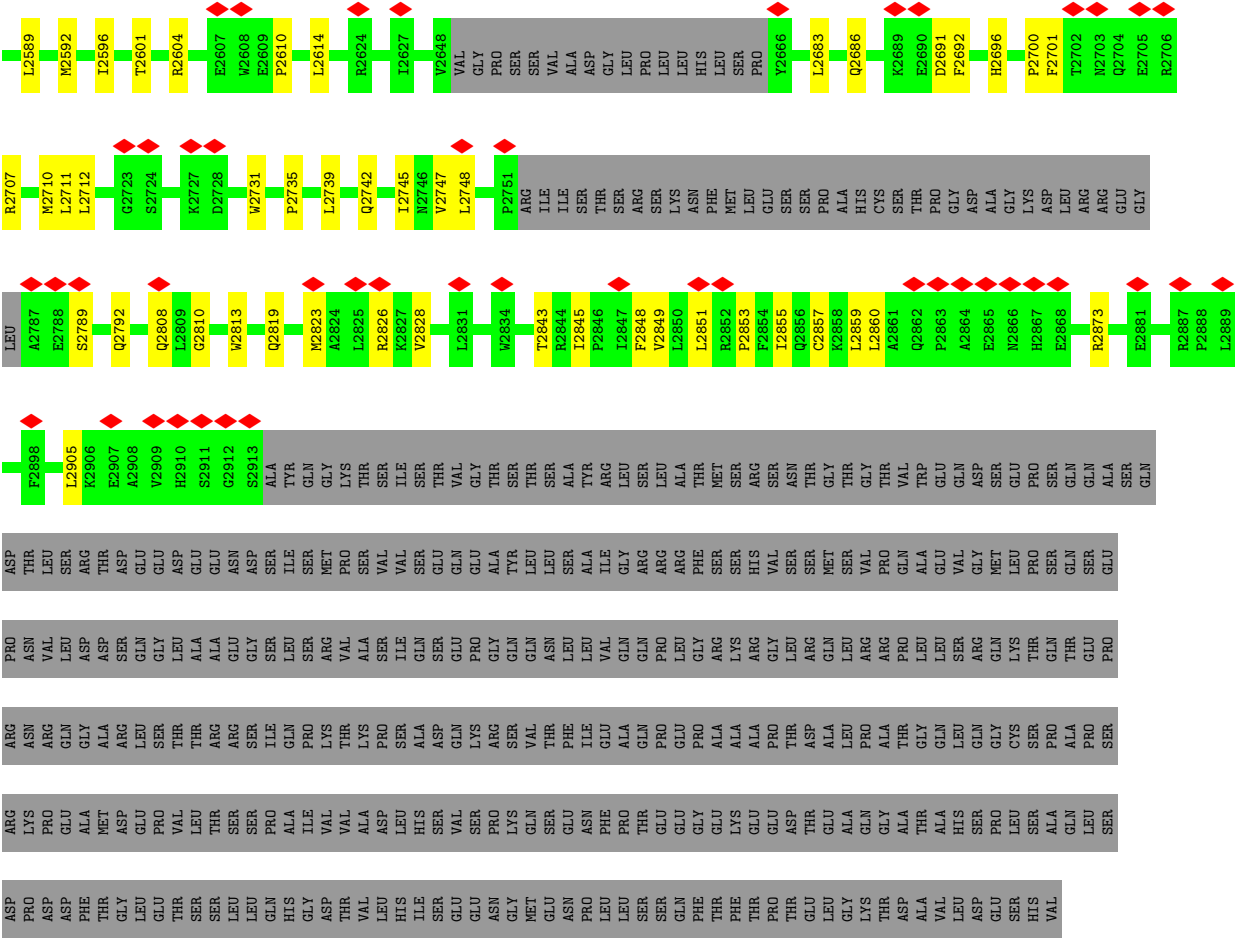
Chain	Residue	Modelled	Actual	Comment	Reference
C	1739	LEU	-	linker	UNP Q8IZF0
C	1740	GLU	-	linker	UNP Q8IZF0
C	1741	GLY	-	linker	UNP Q8IZF0
C	1742	SER	-	linker	UNP Q8IZF0
C	1743	GLU	-	linker	UNP Q8IZF0
C	1744	ASN	-	linker	UNP Q8IZF0
C	1745	LEU	-	linker	UNP Q8IZF0
C	1746	TYR	-	linker	UNP Q8IZF0
C	1747	PHE	-	linker	UNP Q8IZF0
C	1748	GLN	-	linker	UNP Q8IZF0
C	1749	GLY	-	linker	UNP Q8IZF0
C	1750	GLY	-	linker	UNP Q8IZF0
C	1751	GLY	-	linker	UNP Q8IZF0
C	1752	GLY	-	linker	UNP Q8IZF0
C	1753	SER	-	linker	UNP Q8IZF0

- Molecule 5 is a protein called Transmembrane protein FAM155A.

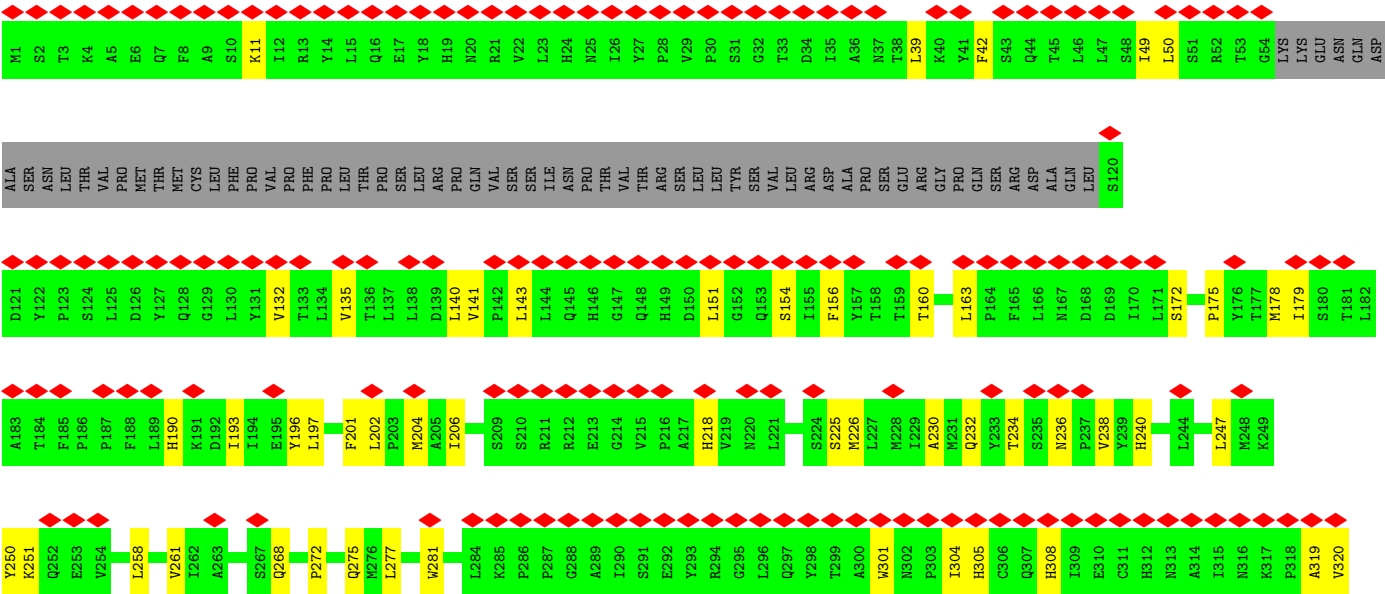
Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	182	Total	C	N	O	S	0	0
			1483	934	243	292	14		

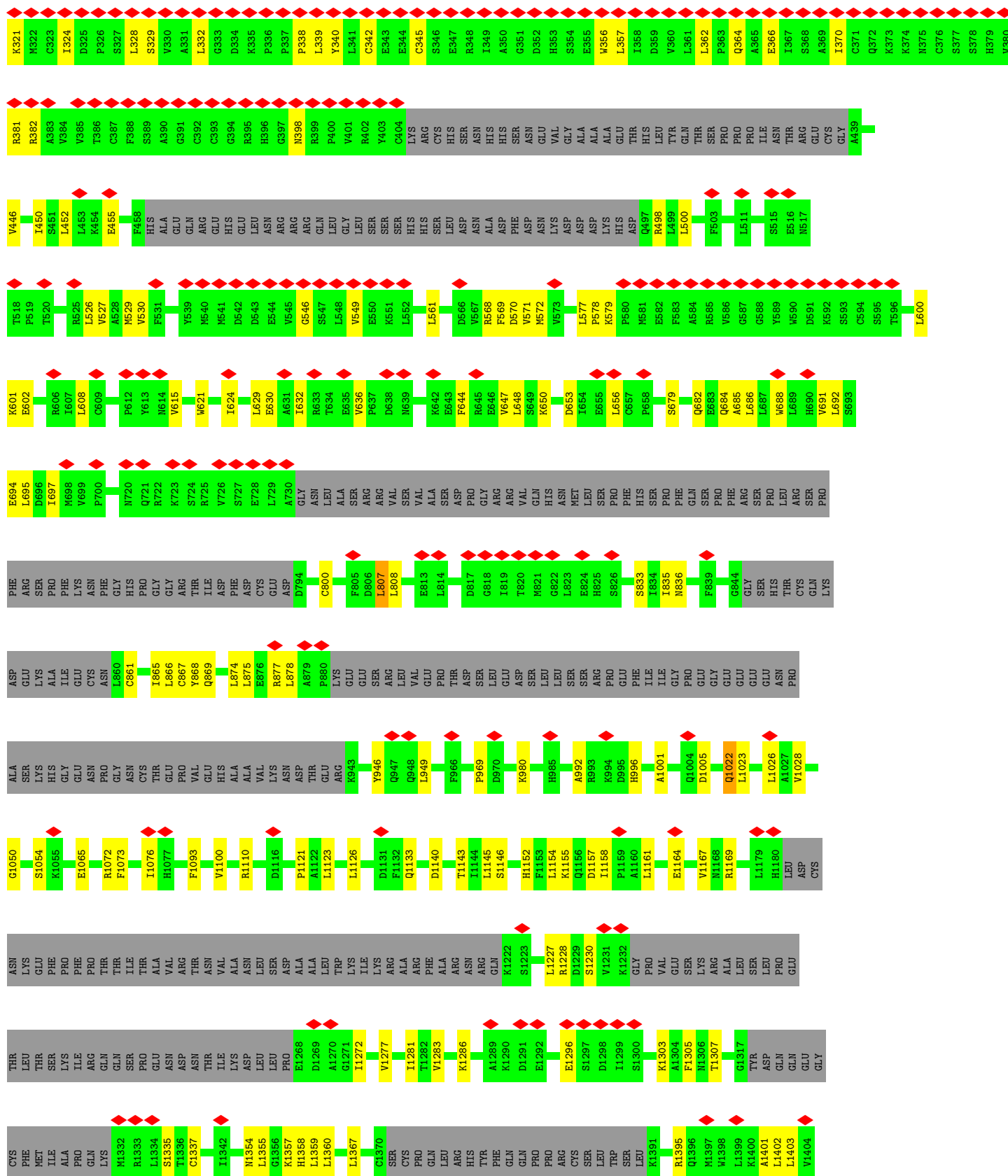


HIS	LEU	LEU	GLU	GLY	GLN	GLY	ILE	PRO	ARG	E2478	E2479	E2480	D2481	E2487	E2488	F2489	R2490	R2491	P2492	R2493	L2496	L2517	A2518	Q2519	E2520	P2521	R2522	A2525	R2536	I2540	L2545	R2546	L2547	Y2550	Q2553	T2554	R2555	R2558	R2562	T2563	I2564	P2560	I2563	L2586															
E2389	T2390	V2391	P2392	R2395	E2396	L2404	A2405	L2408	R2420	P2421	M2422	T2423	ALA	PRO	GLN	MET	SER	ARG	ARG	CYS	ASP	L2496	L2517	A2518	Q2519	E2520	P2521	R2522	A2525	R2536	I2540	L2545	R2546	L2547	Y2550	Q2553	T2554	R2555	R2558	R2562	T2563	I2564	P2560	I2563	L2586														
F2142	S2143	L2144	F2145	S2146	A2150	L2157	L2160	Q2161	S2162	S2163	L2164	L2169	F2173	L2174	Q2175	E2179	T2186	L2187	L2188	F2189	L2190	N2191	V2192	F2193	L2199	H2200	A2205	L2206	Y2210	V2214	T2217	H2223	L2224	F2225	S2226	L2227	Y2241	E2245	R2251	Q2252	A2253	Y2277																	
D2045	K2046	R2047	W2048	N2049	L2050	T2056	R2059	D2060	P2063	F2064	R2065	R2066	S2067	V2068	S2069	L2072	N2073	L2074	I2086	Q2087	K2088	K2094	L2095	E2096	G2099	L2102	F2103	L2107	K2110	I2111	P2112	T2113	A2114	H2119	E2125	D2126	L2127	L2128	R2129	L2130	F2133	P2134	R2136	A2140	E2141														
F1970	K1971	D1972	L1973	K1974	Q1975	T1976	M1977	K1978	E1980	Q1981	C1982	E1983	V1984	K1985	L1986	L1987	V1988	T1989	M1992	F1993	G1994	V2000	H2001	Q2002	Q2003	N2004	E2005	C2006	P2009	L2012	P2013	V2014	D2017	K2025	E2026	C2027	L2028	E2029	F2030	L2033	P2034	E2035	Q2036	Q2037	W1959	E1960	V1961	V1962	G1963	Y1964	V1965	E1966	G1967	L1968	F1969				
PRO	PRO	GLN	ALA	VAL	PHE	PRO	A1845	C1846	I1847	C1848	A1849	A1850	V1851	L1852	P1853	I1854	V1855	H1856	L1857	M1858	E1859	D1860	G1861	E1862	I1863	R1864	E1865	D1866	G1867	V1868	A1869	V1870	V1873	A1874	Q1875	Q1876	V1877	L1878	W1879	N1880	I1883	E1884	D1885	P1886	S1887	T1888	V1889	L1890	R1891	H1892	L1893	L1894	E1895	K1896	L1897	T1898	I1899		
VAL	GLU	GLU	VAL	VAL	THR	ASN	LEU	ALA	ALA	SER	ARG	ARG	LEU	SER	VAL	VAL	PRO	LEU	GLN	THR	GLU	HIS	ARG	GLU	GLY	GLY	VAL	VAL	THR	VAL	ARG	SER	ALA	VAL	ALA	VAL	ILE	PRO	PHE	ASP	PRO	GLN	VAL	THR	GLY	SER	SER	VAL	GLN	ASN	PRO	ASP	PRO	ILE	ASN	GLU	PRO	GLU	GLN
PHE	SER	ALA	ARG	ALA	VAL	SER	ARG	ARG	HIS	GLN	ARG	GLN	ARG	VAL	GLU	HIS	ILE	LEU	ASN	THR	LEU	SER	GLN	THR	SER	GLY	GLU	VAL	ALA	ALA	ILE	PRO	PHE	ASP	PRO	GLN	VAL	THR	GLY	SER	SER	VAL	GLN	ASN	PRO	ASP	PRO	ILE	ASN	GLU	PRO	GLU	GLN	GLU	GLN				
V1658	W1659	P1660	R1661	A1662	E1663	E1664	E1665	A1666	Q1667	Q1668	I1669	PHE	LYS	LYS	ILE	PRO	PRO	PRO	GLN	GLN	PRO	ILE	ASN	THR	PHE	LYS	THR	LEU	GLY	MET	SER	PRO	SER	VAL	VAL	PRO	ILE	PRO	PHE	ASP	PRO	GLN	TRP	TRP	VAL	VAL	GLY	CYS	PRO	GLN	GLY	THR	THR	VAL	VAL	GLU	GLU	GLU	
Q1592	P1593	W1596	L1599	L1600	S1601	M1602	D1603	E1604	H1605	M1606	A1607	G1608	A1609	A1610	A1611	A1612	M1613	F1614	G1615	L1616	C1617	A1618	V1619	K1620	L1621	P1622	E1623	A1624	V1625	S1626	D1627	M1628	L1629	M1630	F1633	H1634	T1638	V1639	L1642	P1643	I1644	V1645	L1646	K1647	F1648	H1649	T1650	L1651	W1652	R1653	F1654	R1655	Y1656	Q1657					



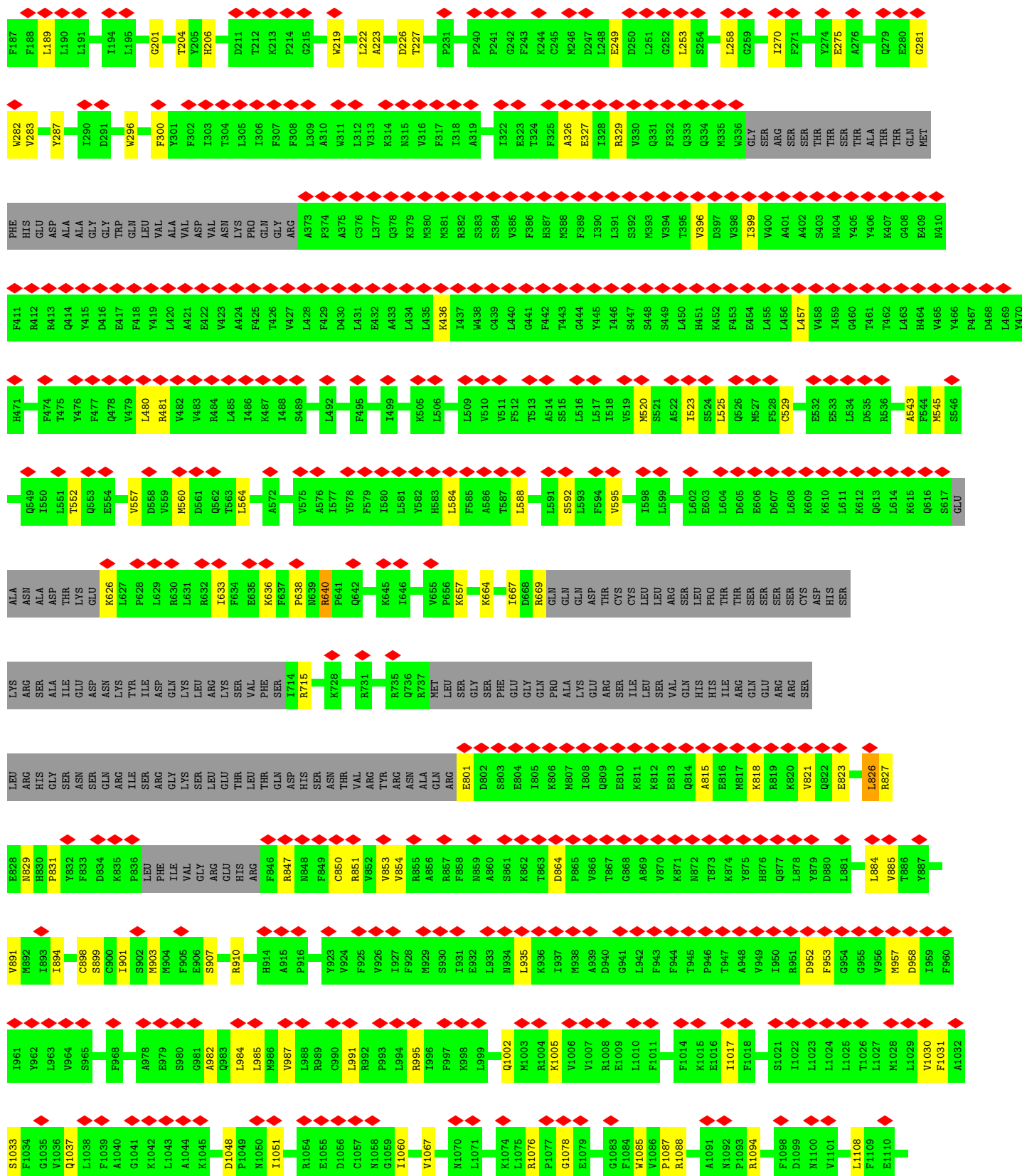
● Molecule 2: Protein unc-79 homolog













[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	174294	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.947	Depositor
Minimum map value	-1.055	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.4	Depositor
Map size (\AA)	556.544, 556.544, 556.544	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.087, 1.087, 1.087	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	0.33	0/14450	0.69	0/19574
2	B	0.32	0/13441	0.68	0/18238
3	E	0.33	0/997	0.67	0/1335
4	C	0.34	0/11701	0.72	0/15843
5	D	0.38	0/1522	0.73	0/2065
All	All	0.33	0/42111	0.69	0/57055

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	14143	0	14323	208	0
2	B	13146	0	13362	207	0
3	E	988	0	920	12	0
4	C	11413	0	11682	157	0
5	D	1483	0	1374	30	0
All	All	41173	0	41661	601	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 7.

The worst 5 of 601 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)
2:B:178:MET:SD	2:B:197:LEU:HD22	1.47	1.53
1:A:1460:LEU:HD22	1:A:1463:MET:CE	1.47	1.40
2:B:178:MET:SD	2:B:197:LEU:CD2	2.34	1.15
1:A:1460:LEU:HD22	1:A:1463:MET:HE2	1.31	1.13
3:E:110:MET:HG3	4:C:1576:LEU:HD11	1.30	1.11

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	1739/3258 (53%)	1635 (94%)	104 (6%)	0	100	100
2	B	1639/2658 (62%)	1527 (93%)	112 (7%)	0	100	100
3	E	118/149 (79%)	111 (94%)	7 (6%)	0	100	100
4	C	1382/1992 (69%)	1311 (95%)	71 (5%)	0	100	100
5	D	178/458 (39%)	162 (91%)	15 (8%)	1 (1%)	25	65
All	All	5056/8515 (59%)	4746 (94%)	309 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	214	PRO

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	1563/2853 (55%)	1554 (99%)	9 (1%)	86	92
2	B	1486/2380 (62%)	1477 (99%)	9 (1%)	86	92
3	E	103/127 (81%)	103 (100%)	0	100	100
4	C	1261/1787 (71%)	1255 (100%)	6 (0%)	88	93
5	D	168/397 (42%)	168 (100%)	0	100	100
All	All	4581/7544 (61%)	4557 (100%)	24 (0%)	89	93

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	2110	ARG
2	B	2153	ASN
2	B	2139	LYS
4	C	640	ARG
1	A	2187	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
5	D	269	GLN
4	C	1318	HIS
2	B	2425	HIS
2	B	1022	GLN
4	C	1274	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

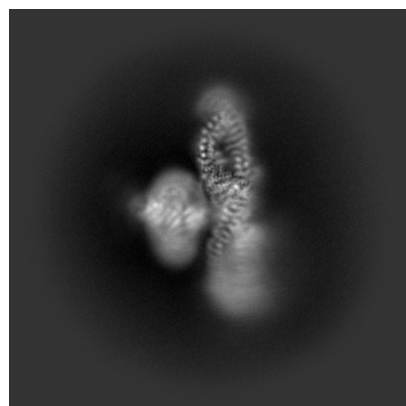
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32544. These allow visual inspection of the internal detail of the map and identification of artifacts.

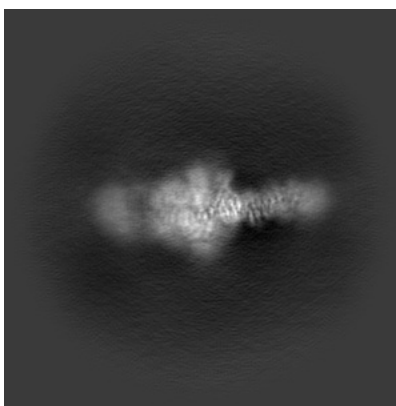
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

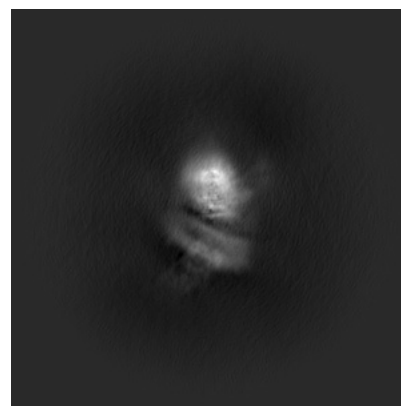
6.1.1 Primary map



X

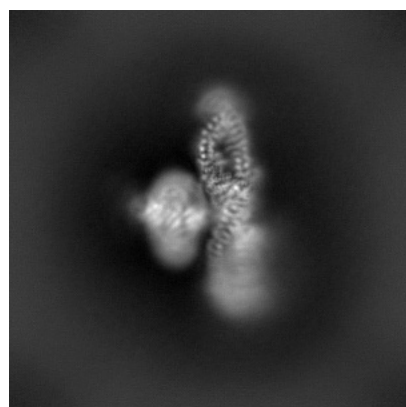


Y

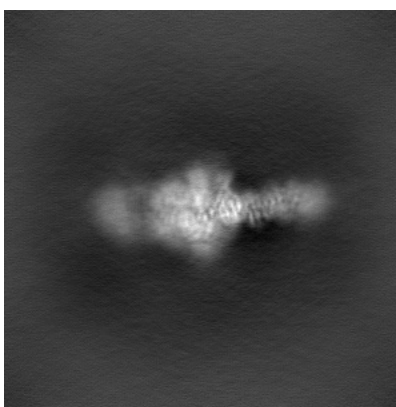


Z

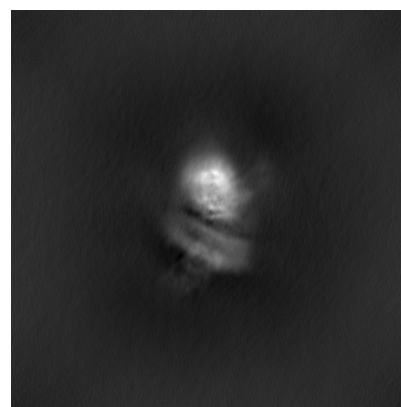
6.1.2 Raw map



X



Y

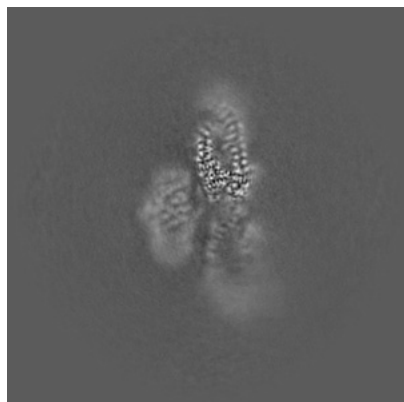


Z

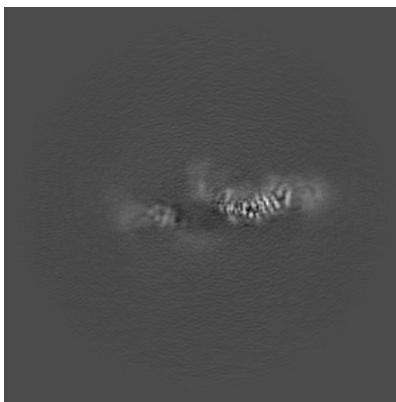
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

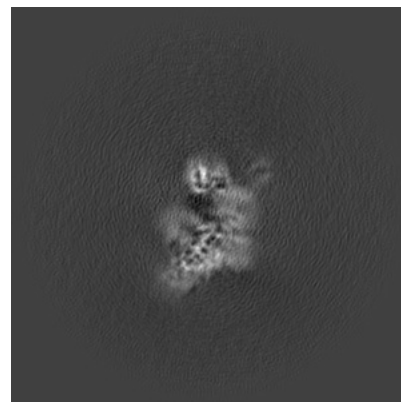
6.2.1 Primary map



X Index: 256

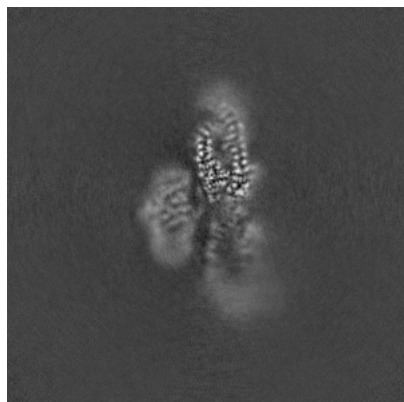


Y Index: 256

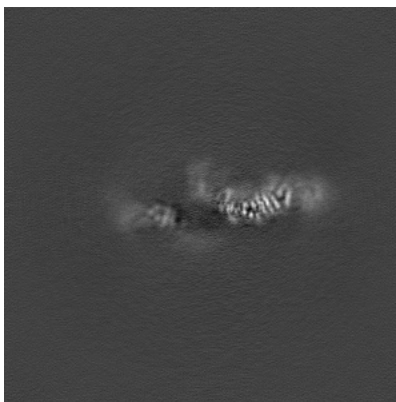


Z Index: 256

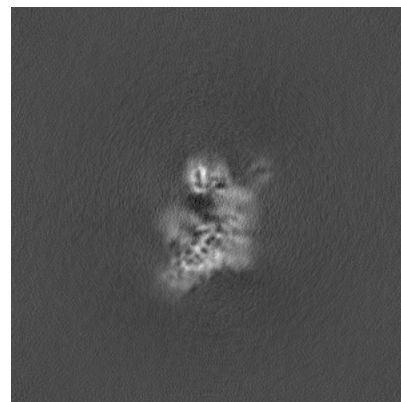
6.2.2 Raw map



X Index: 256



Y Index: 256

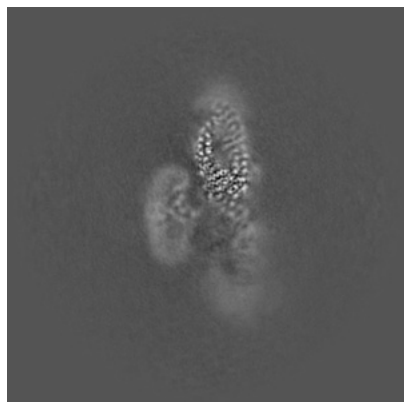


Z Index: 256

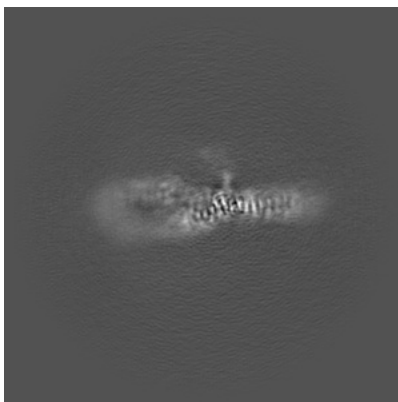
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

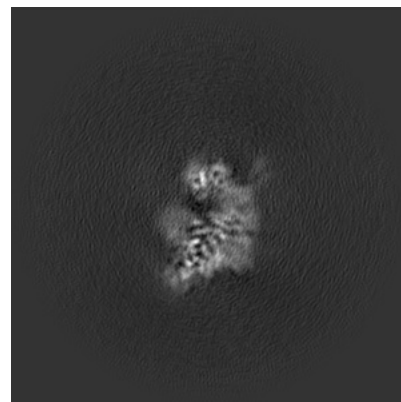
6.3.1 Primary map



X Index: 261

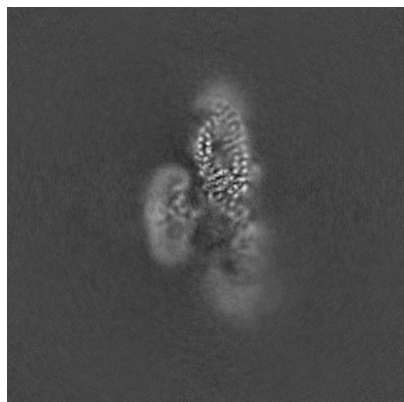


Y Index: 293

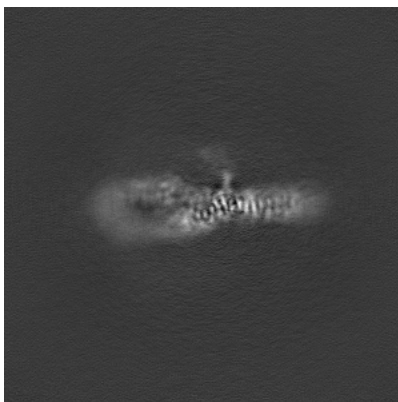


Z Index: 249

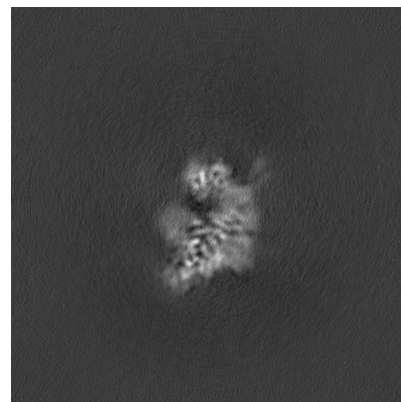
6.3.2 Raw map



X Index: 261



Y Index: 293

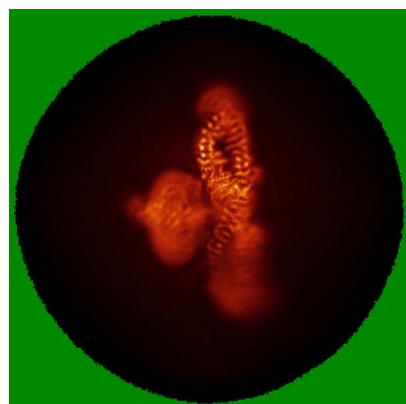


Z Index: 249

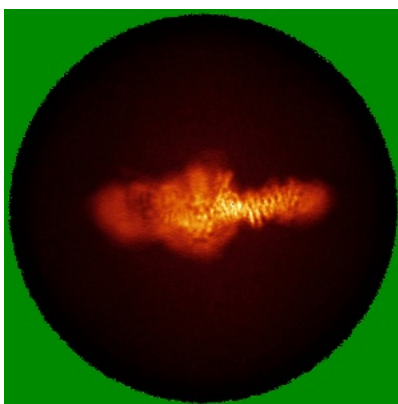
The images above show the largest variance slices of the map in three orthogonal directions.

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

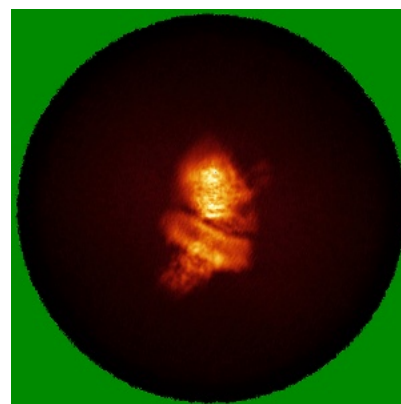
6.4.1 Primary map



X

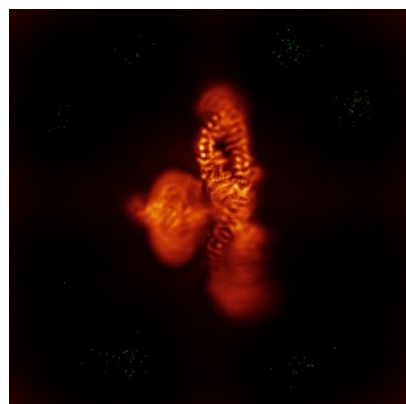


Y

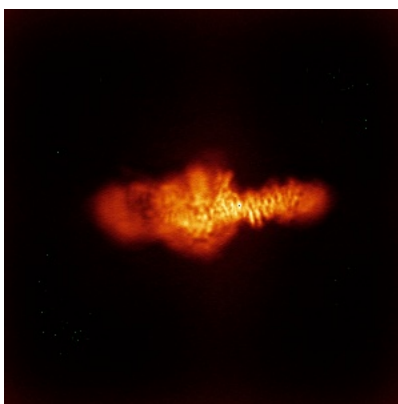


Z

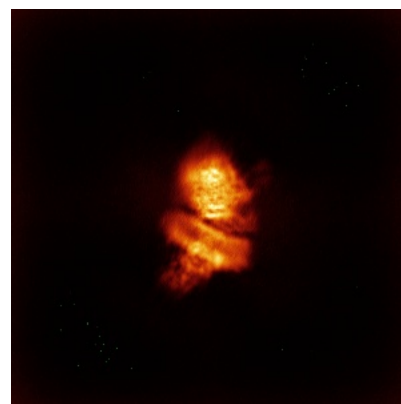
6.4.2 Raw map



X



Y

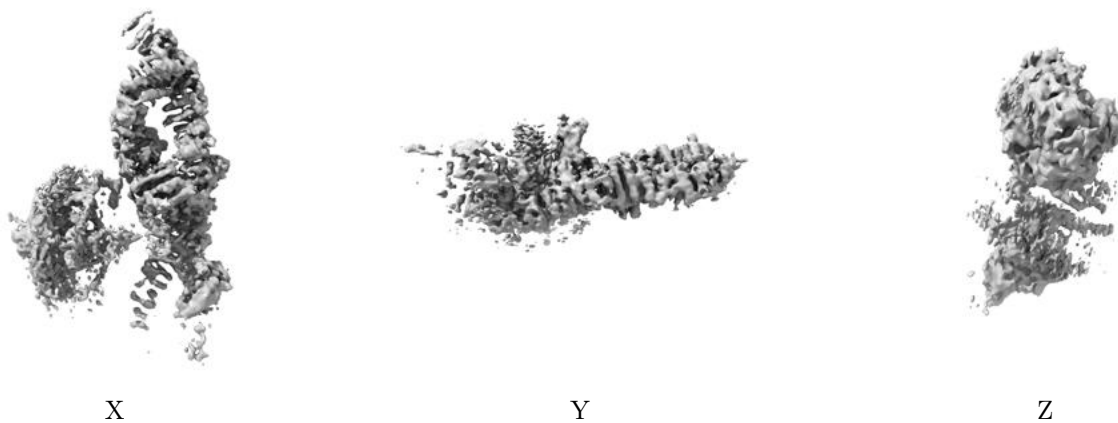


Z

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.

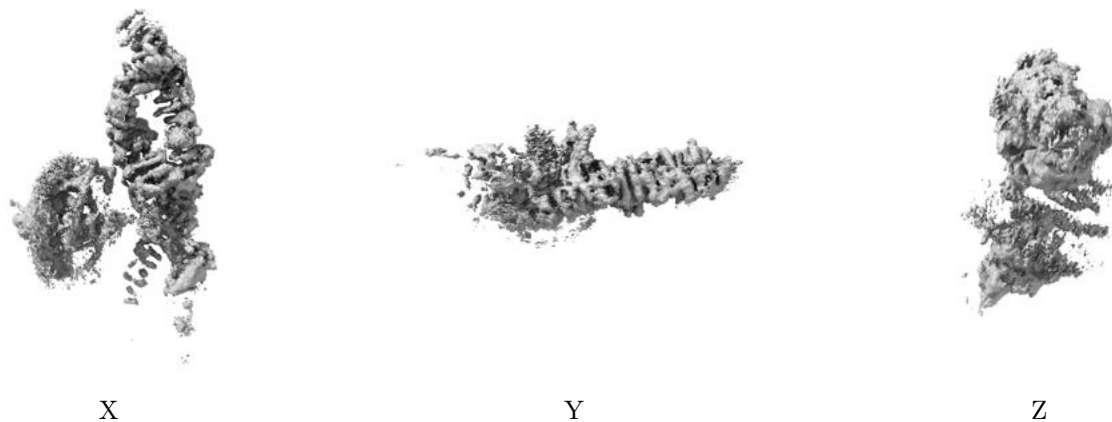
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. 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.

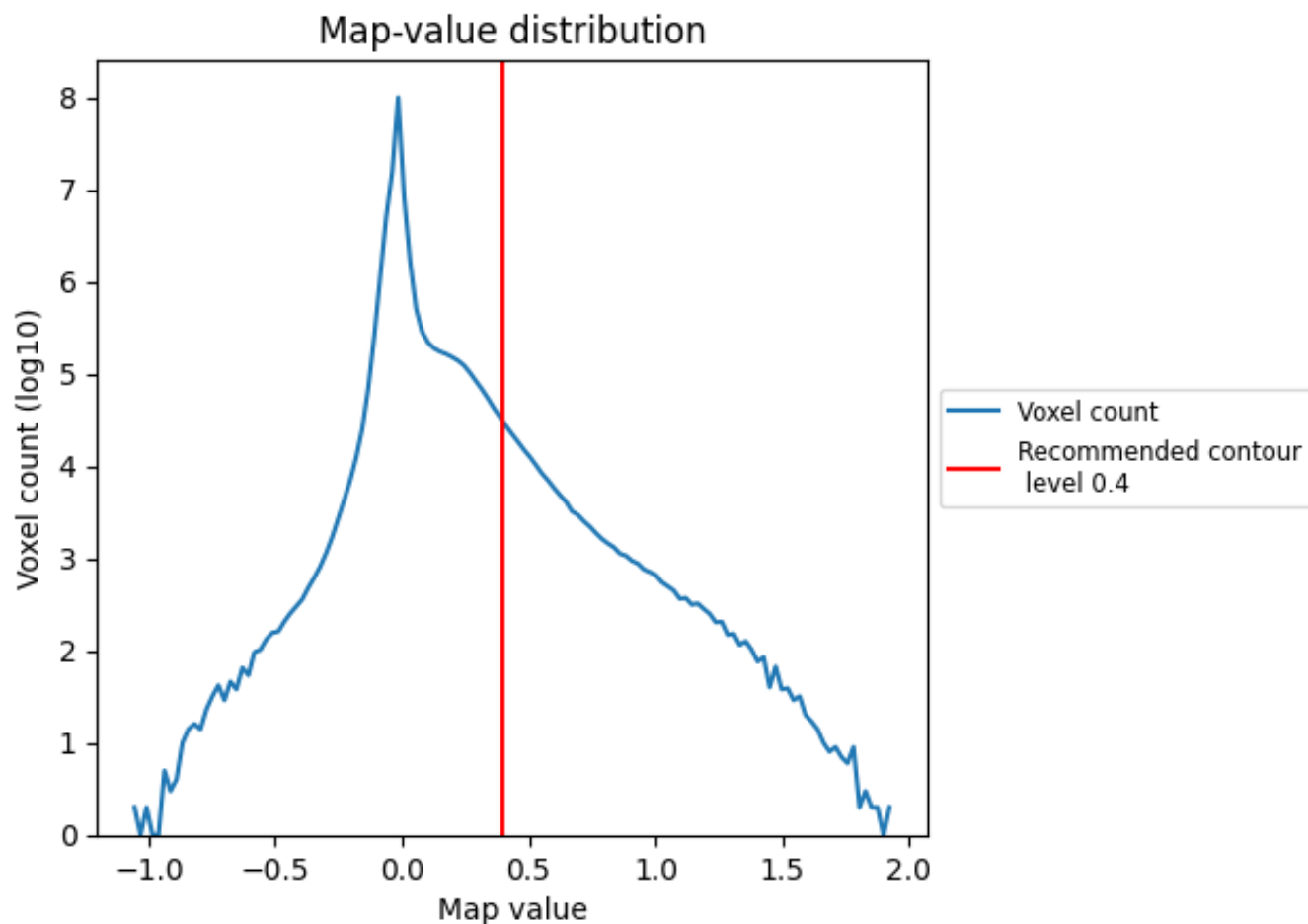
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

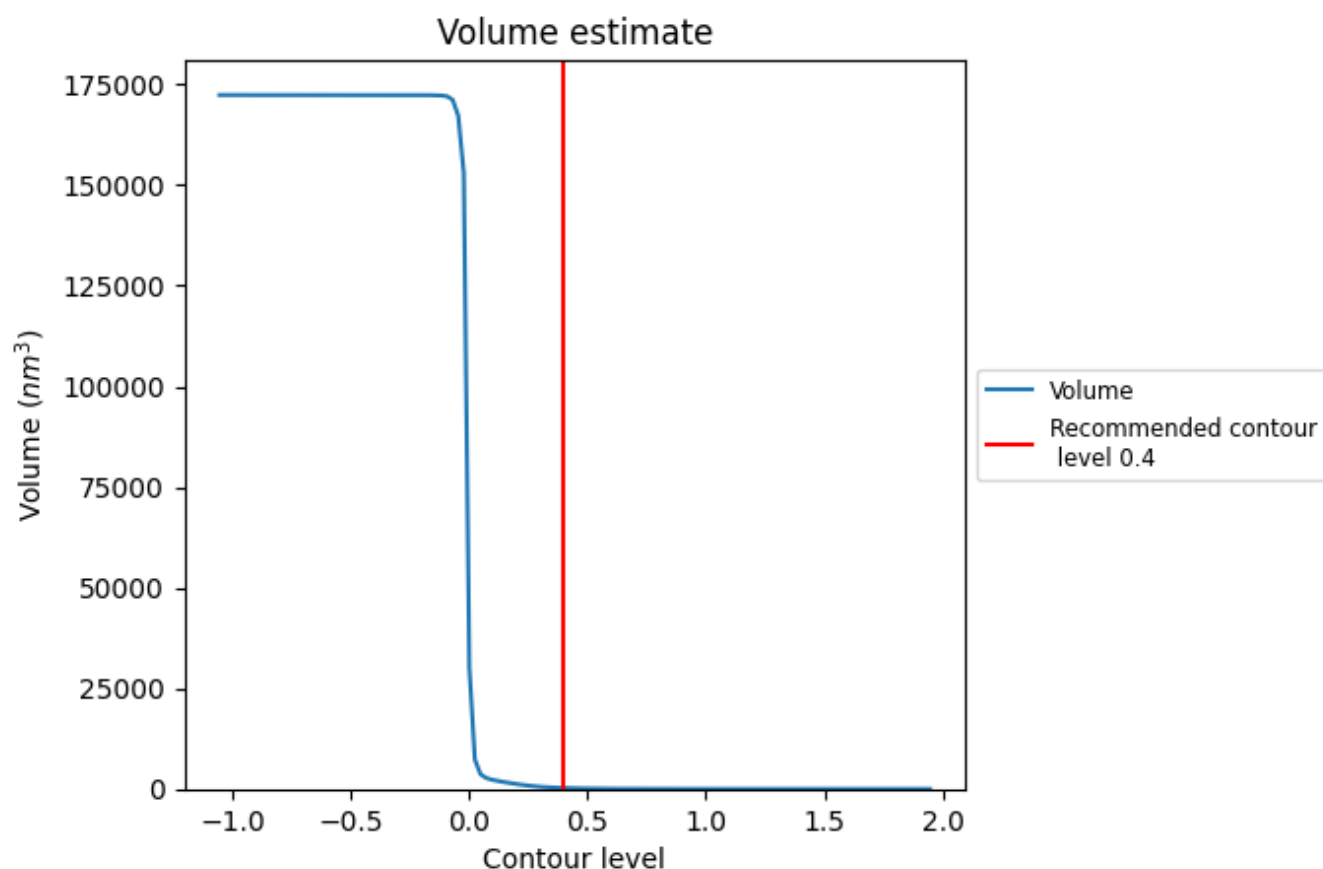
This section contains the results of statistical analysis of the map.

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.

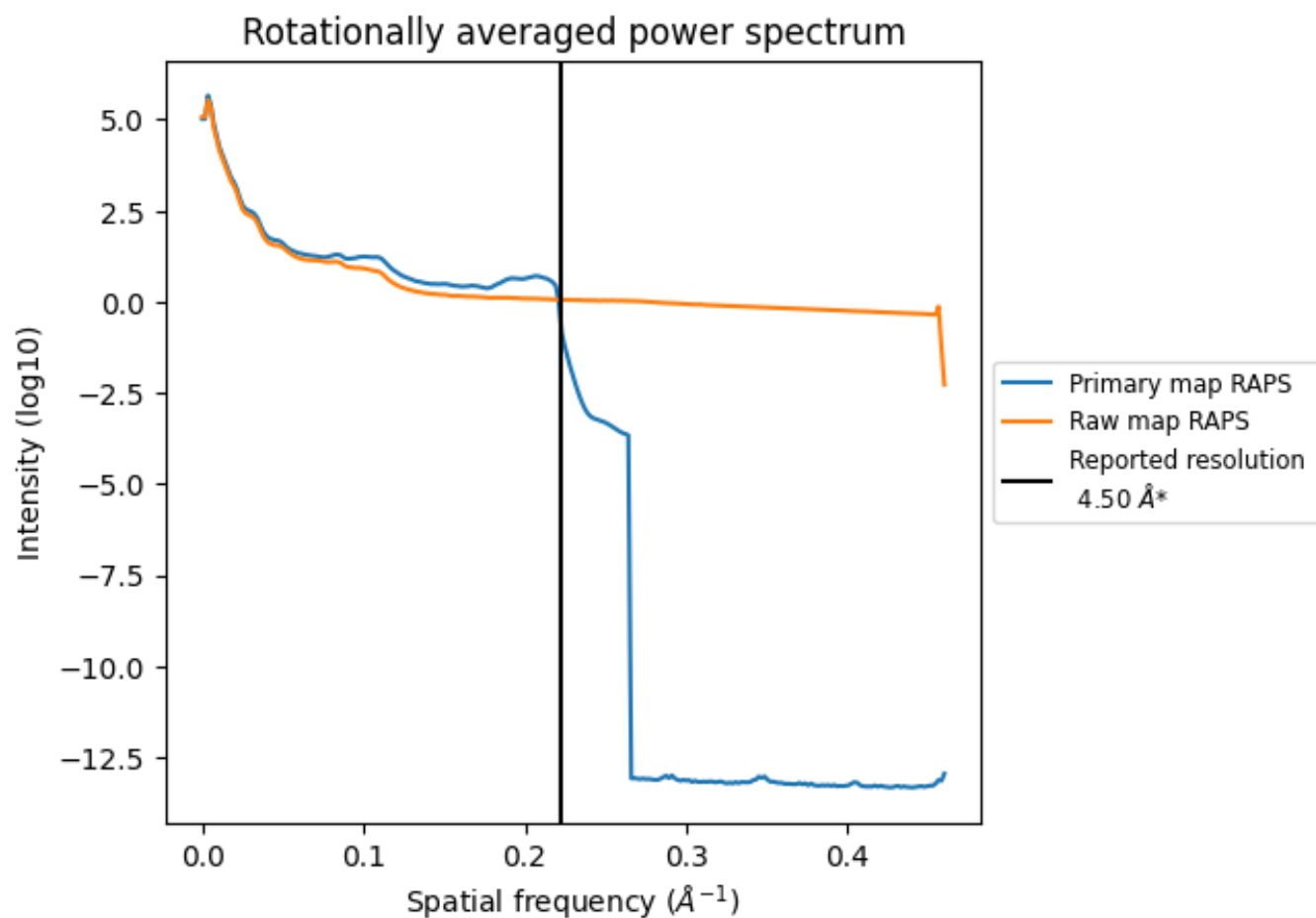
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 230 nm³; this corresponds to an approximate mass of 207 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 ⓘ

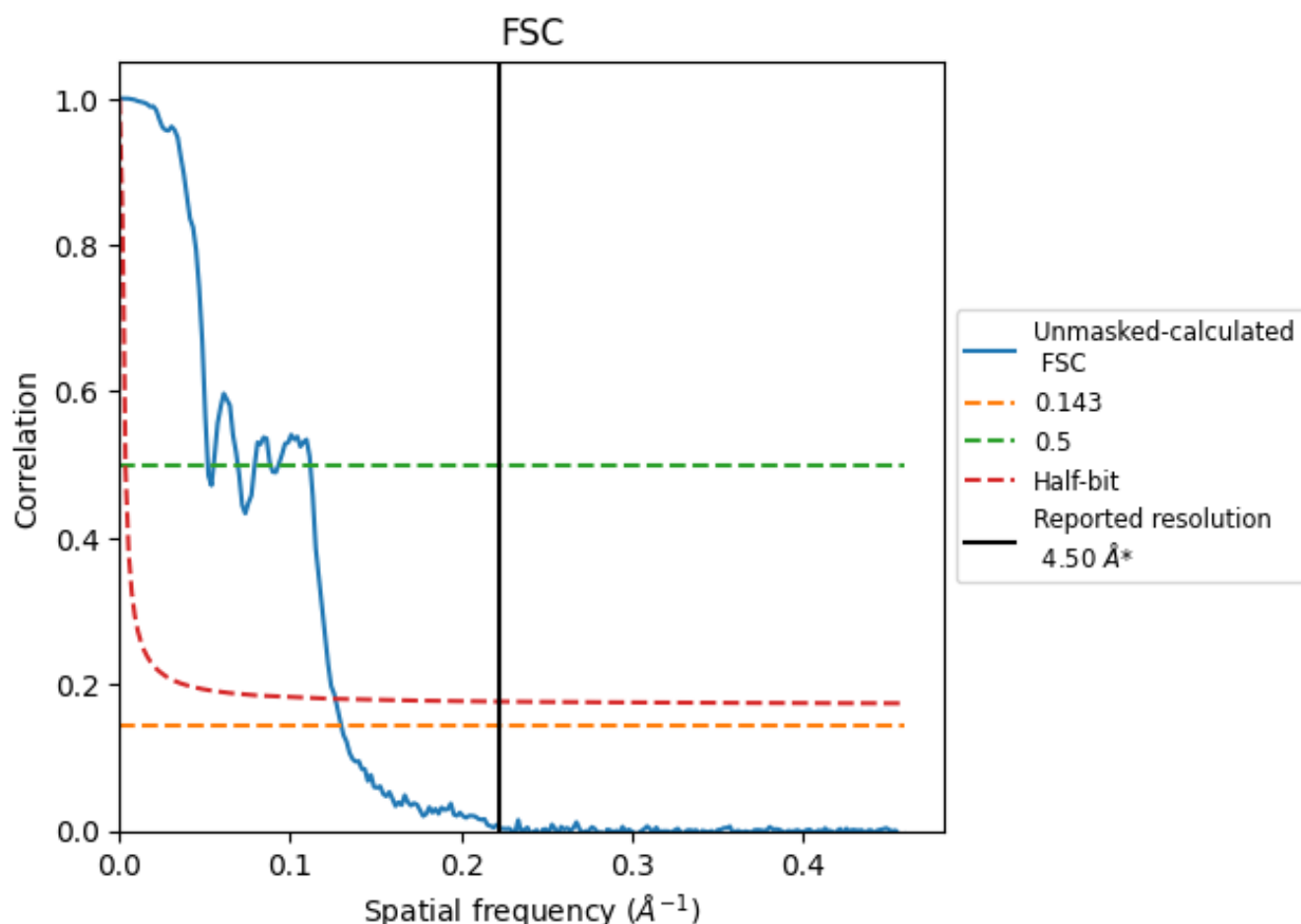


*Reported resolution corresponds to spatial frequency of 0.222 \AA^{-1}

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 0.222 \AA^{-1}

8.2 Resolution estimates [i](#)

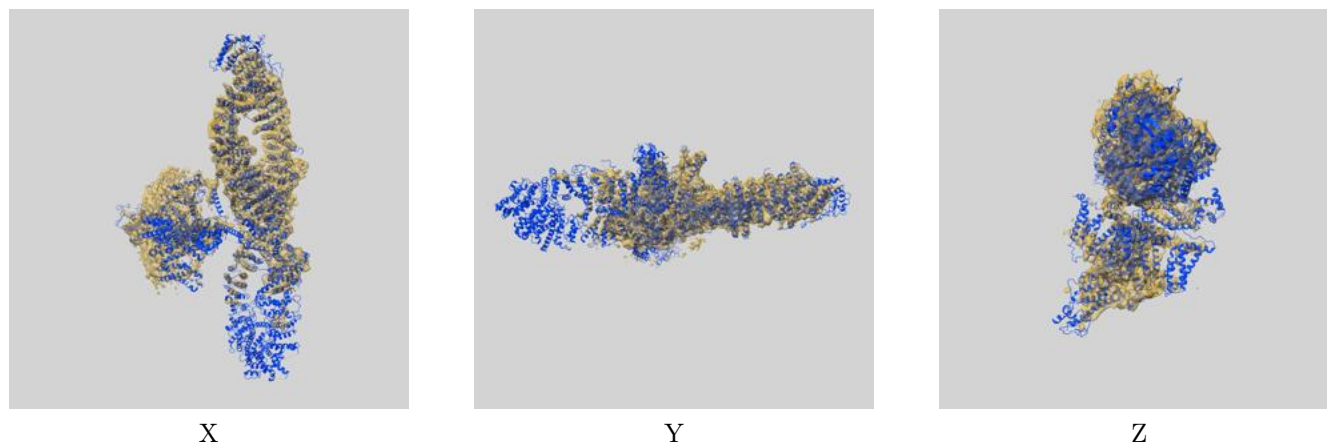
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.70	19.31	7.91

*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 7.70 differs from the reported value 4.5 by more than 10 %

9 Map-model fit [i](#)

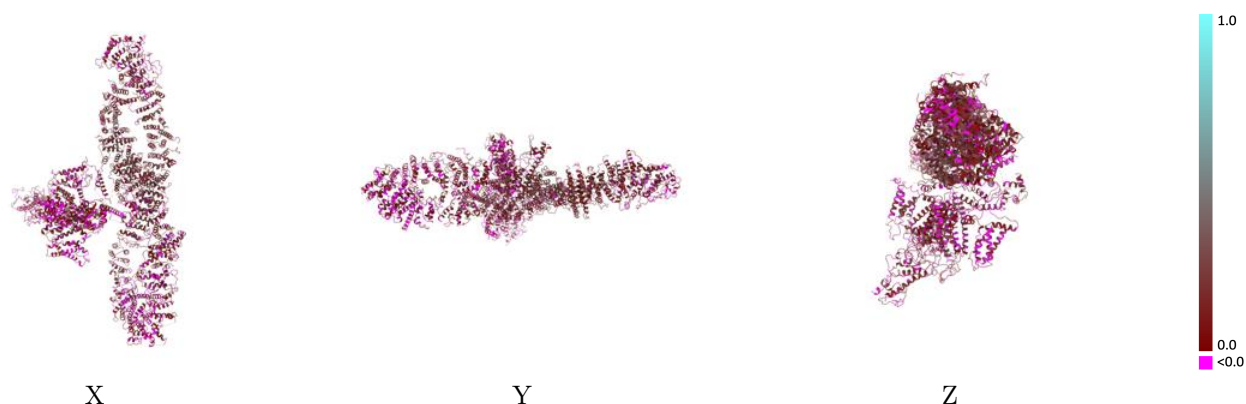
This section contains information regarding the fit between EMDB map EMD-32544 and PDB model 7WJI. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



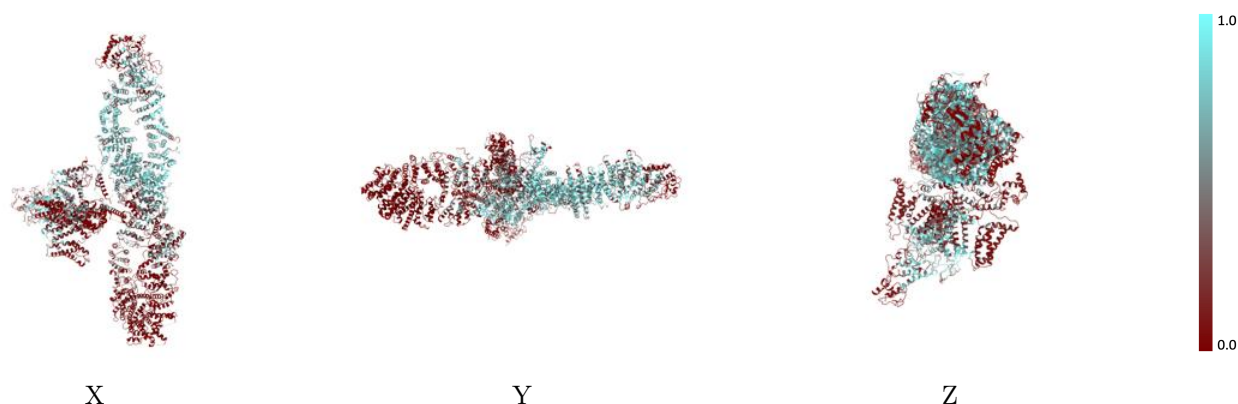
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



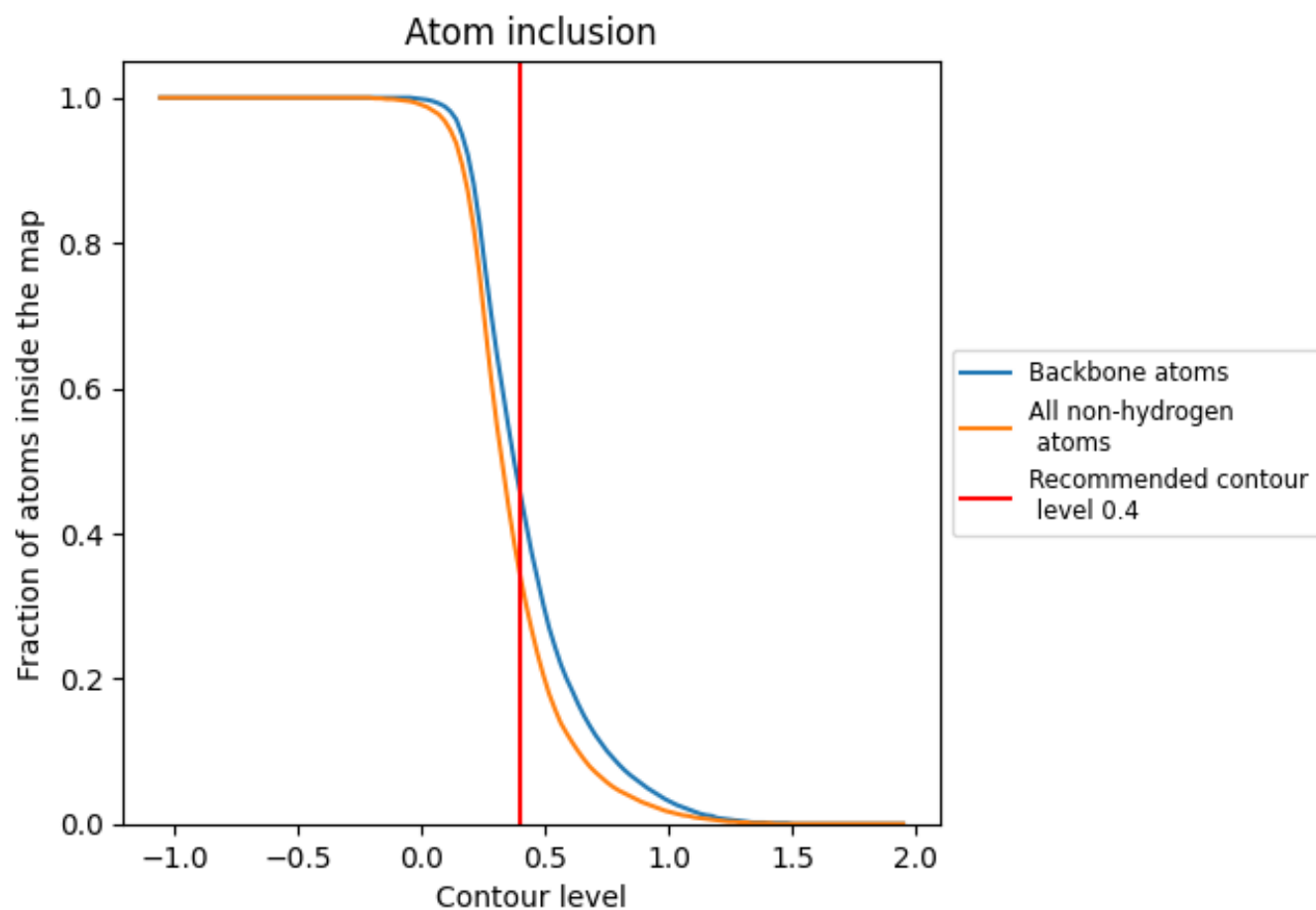
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 46% of all backbone atoms, 34% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.3410	<div></div> 0.1390
A	<div></div> 0.3790	<div></div> 0.1700
B	<div></div> 0.3520	<div></div> 0.1440
C	<div></div> 0.3140	<div></div> 0.0990
D	<div></div> 0.2650	<div></div> 0.1070
E	<div></div> 0.0530	<div></div> 0.1160

