



wwPDB EM Validation Summary Report ⓘ

Jan 2, 2025 – 03:16 pm GMT

PDB ID : 8P1L
EMDB ID : EMD-17353
Title : Structure of hantaan orthohantavirus (HTNV) polymerase - Apo full length
Authors : Keown, J.R.; Carrique, L.; Grimes, J.M.
Deposited on : 2023-05-12
Resolution : 3.30 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

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.dev113
MolProbity : 4.02b-467
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) : 2.40

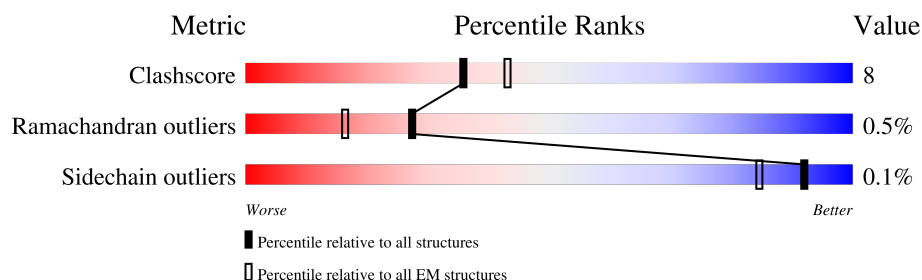
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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 ≥ 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	2196	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 32936 atoms, of which 16512 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 RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2036	Total	C	H	N	O	S	0	0
			32936	10567	16512	2770	3000	87		

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-44	MET	-	initiating methionine	UNP P23456
A	-43	TRP	-	expression tag	UNP P23456
A	-42	SER	-	expression tag	UNP P23456
A	-41	HIS	-	expression tag	UNP P23456
A	-40	PRO	-	expression tag	UNP P23456
A	-39	GLN	-	expression tag	UNP P23456
A	-38	PHE	-	expression tag	UNP P23456
A	-37	GLU	-	expression tag	UNP P23456
A	-36	LYS	-	expression tag	UNP P23456
A	-35	GLY	-	expression tag	UNP P23456
A	-34	GLY	-	expression tag	UNP P23456
A	-33	GLY	-	expression tag	UNP P23456
A	-32	SER	-	expression tag	UNP P23456
A	-31	GLY	-	expression tag	UNP P23456
A	-30	GLY	-	expression tag	UNP P23456
A	-29	GLY	-	expression tag	UNP P23456
A	-28	SER	-	expression tag	UNP P23456
A	-27	GLY	-	expression tag	UNP P23456
A	-26	GLY	-	expression tag	UNP P23456
A	-25	SER	-	expression tag	UNP P23456
A	-24	SER	-	expression tag	UNP P23456
A	-23	ALA	-	expression tag	UNP P23456
A	-22	TRP	-	expression tag	UNP P23456
A	-21	SER	-	expression tag	UNP P23456
A	-20	HIS	-	expression tag	UNP P23456
A	-19	PRO	-	expression tag	UNP P23456
A	-18	GLN	-	expression tag	UNP P23456
A	-17	PHE	-	expression tag	UNP P23456

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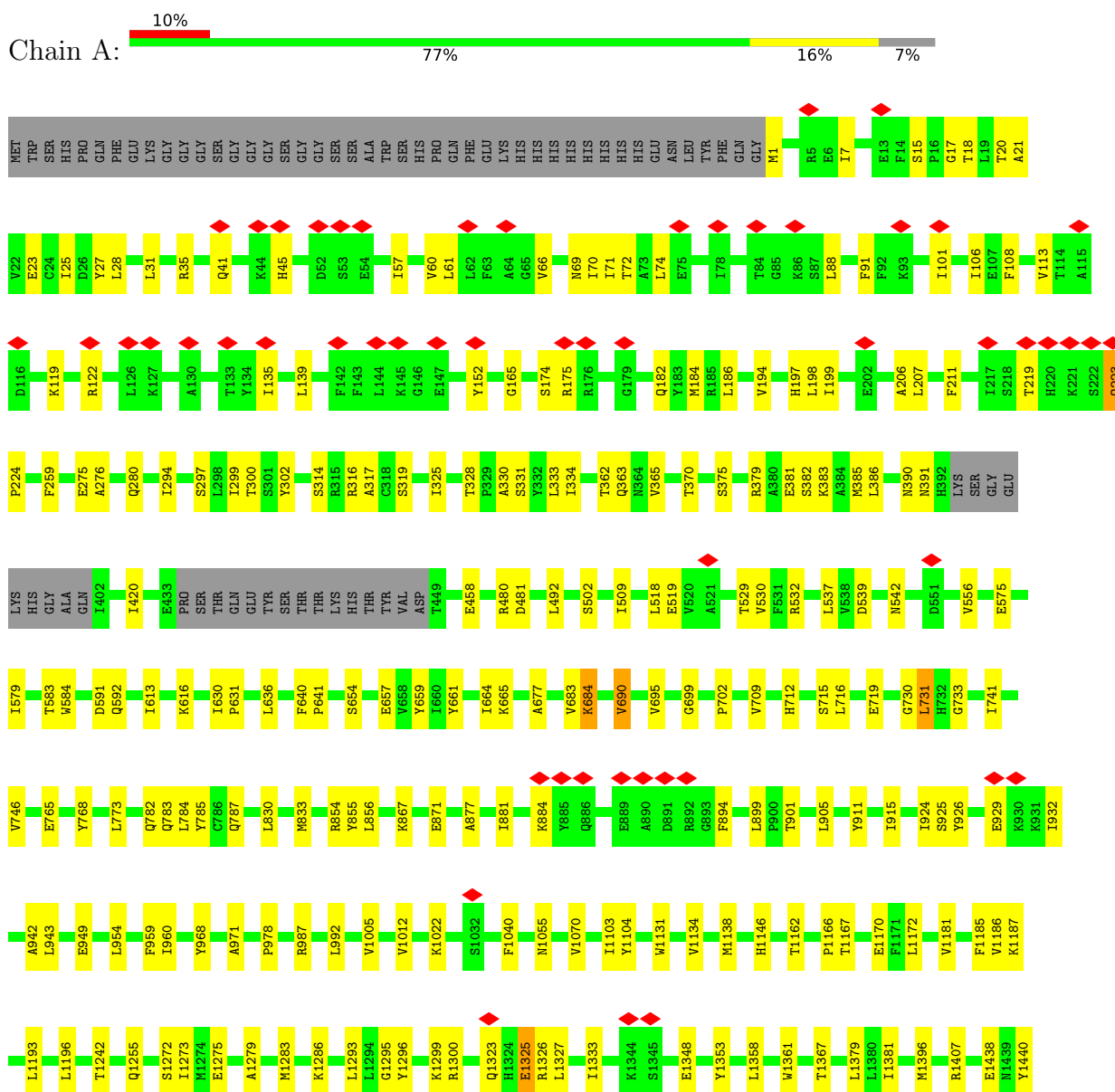
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	GLU	-	expression tag	UNP P23456
A	-15	LYS	-	expression tag	UNP P23456
A	-14	HIS	-	expression tag	UNP P23456
A	-13	HIS	-	expression tag	UNP P23456
A	-12	HIS	-	expression tag	UNP P23456
A	-11	HIS	-	expression tag	UNP P23456
A	-10	HIS	-	expression tag	UNP P23456
A	-9	HIS	-	expression tag	UNP P23456
A	-8	HIS	-	expression tag	UNP P23456
A	-7	HIS	-	expression tag	UNP P23456
A	-6	GLU	-	expression tag	UNP P23456
A	-5	ASN	-	expression tag	UNP P23456
A	-4	LEU	-	expression tag	UNP P23456
A	-3	TYR	-	expression tag	UNP P23456
A	-2	PHE	-	expression tag	UNP P23456
A	-1	GLN	-	expression tag	UNP P23456
A	0	GLY	-	expression tag	UNP P23456
A	97	ALA	ASP	engineered mutation	UNP P23456

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: RNA-directed RNA polymerase L



L2105	D2106	R2107	E2108	A2109	Q2110	N2111	M2112	V2113	V2114	N2115	K2116	G2117	T2118	C2119	P2120	E2121	D2122	V2123	T2124	P2125	D2126	S2127	L2128	F2129	S2130	F2131	R2132	H2133	T2134	M2135	V2136	L2137	L2138	R2139	R2140	L2141	F2142	P2143	Q2144	D2145	S2146	I2147	S2148	S2149	F2150	Y2151														
S2041	S2044	R2045	G2046	L2047	S2048	I2049	E2050	K2051	V2052	Y2053	S2054	P2055	V2056	N2057	I2058	I2059	L2060	M2061	S2062	R2063	Y2064	I2065	S2066	K2067	T2068	F2069	N2070	L2071	S2072	T2073	K2074	Q2075	V2076	S2077	L2078	L2079	D2083	L2084	T2085	E2086	L2087	I2090	V2091	R2092	G2093	M2094	G2095	E2096	C2097	V2098	I2099	D2100	Q2101	F2102	E2103	S2104				
GLU	GLU	LEU	ASP	ASP	GLU	PHE	THR	THR	ASP	GLN	VAL	ASP	PHE	GLU	ASN	ILE	ASP	ALA	ASP	ILE	GLU	GLU	ASP	GLU	GLU	GLU	THR	GLY	ASP	LEU	ILE	THR	GLU	GLU	THR	GLU	THR	LYS	LYS	MET	R2027	V2030	K2031	L2032	L2033	E2034	K2040													
I1916	M1917	N1918	R1919	A1920	K1921	I1922	S1923	V1924	D1925	L1926	F1927	M1928	F1929	M1930	D1931	L1932	L1933	K1934	L1935	I1936	N1937	P1938	R1939	M1940	T1941	L1942	D1943	L1944	S1945	G1946	L1947	GLU	THR	THR	GLY	ASP	GLU	THR	PHE	SER	THR	VAL	SER	SER	MET	SER	SER	ARG	LEU	TRP	SER	GLU	GLU	MET	SER	SER	LEU	VAL	ASP	ASP
S1799	G1800	F1801	E1802	I1808	P1809	C1810	I1811	V1812	R1819	I1828	M1829	H1830	M1833	I1836	A1843	I1844	D1848	E1849	D1850	S1851	P1852	R1853	F1854	L1855	D1865	I1866	R1867	Y1868	Q1869	D1872	A1873	V1874	F1879	I1880	G1883	N1889	F1900	N1903	A1906	A1911	A1912	Y1913	S1914	L1915																
K1568	M1447	F1450	T1454	S1455	C1456	T1457	F1458	Y1462	K1465	G1470	I1471	P1477	T1478	K1479	Q1480	T1491	V1492	R1493	E1494	K1495	D1496	M1501	S1502	I1507	F1511	A1512	V1513	T1514	M1518	D1534	M1538	L1546	D1549	I1550	V1555	M1556	I1559	Y1564	S1567																					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	25000	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.910	Depositor
Minimum map value	-0.526	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	279.6, 279.6, 279.6	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93200004, 0.93200004, 0.93200004	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	0.25	0/16793	0.47	0/22702

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	16424	16512	16512	249	0
All	All	16424	16512	16512	249	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 8.

The worst 5 of 249 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:1659:THR:OG1	1:A:1662:GLU:OE1	1.88	0.91
1:A:733:GLY:O	1:A:884:LYS:NZ	2.04	0.91
1:A:1367:THR:OG1	1:A:1511:PHE:O	1.99	0.79
1:A:1440:TYR:OH	1:A:1446:ASP:OD2	2.00	0.79
1:A:616:LYS:NZ	1:A:654:SER:OG	2.14	0.79

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	2026/2196 (92%)	1875 (92%)	140 (7%)	11 (0%)	25 56

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	677	ALA
1	A	684	LYS
1	A	1606	GLU
1	A	1830	HIS
1	A	223	GLN

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	1809/1955 (92%)	1808 (100%)	1 (0%)	92 96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1939	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	542	ASN
1	A	692	GLN
1	A	842	HIS
1	A	918	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.

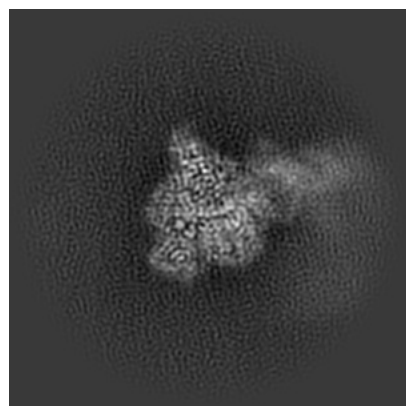
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17353. These allow visual inspection of the internal detail of the map and identification of artifacts.

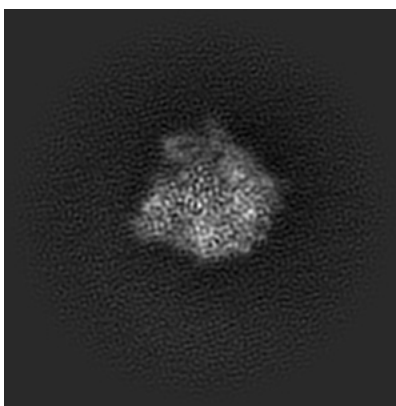
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

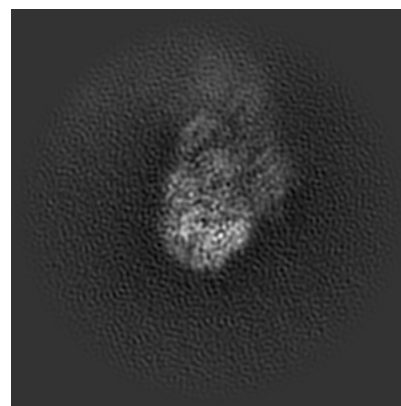
6.1.1 Primary map



X

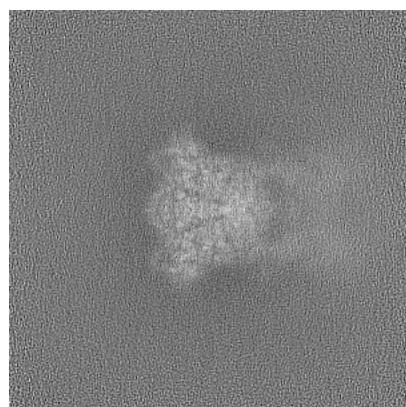


Y

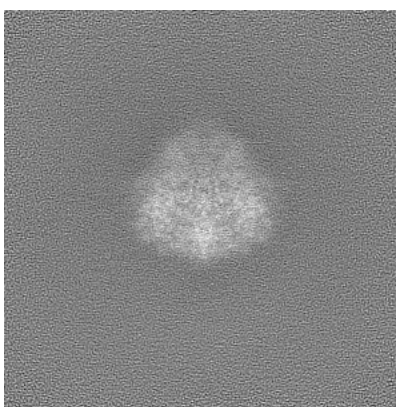


Z

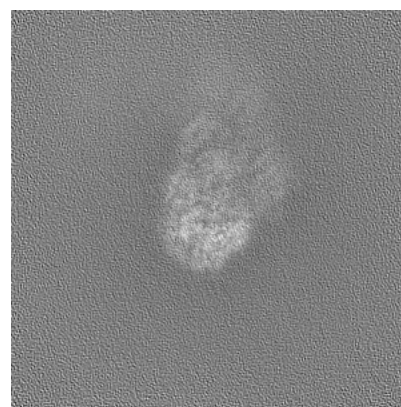
6.1.2 Raw map



X



Y

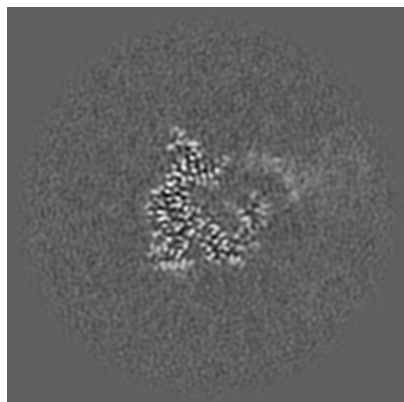


Z

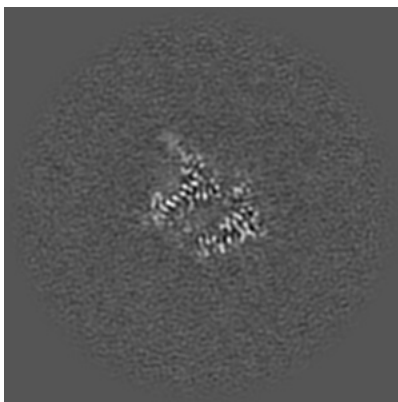
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

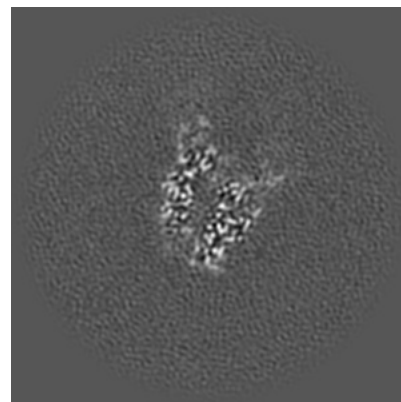
6.2.1 Primary map



X Index: 150

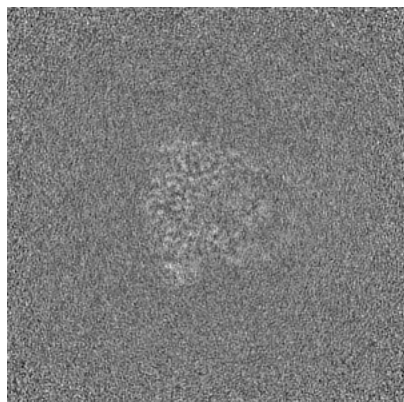


Y Index: 150

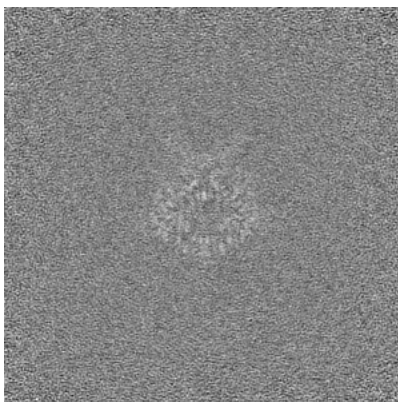


Z Index: 150

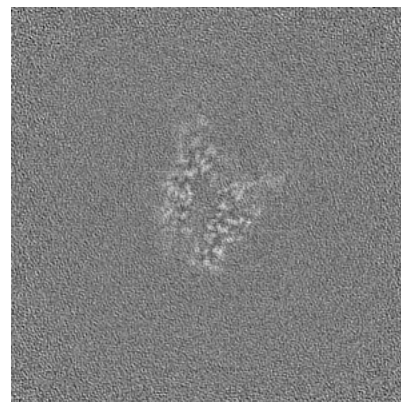
6.2.2 Raw map



X Index: 150



Y Index: 150

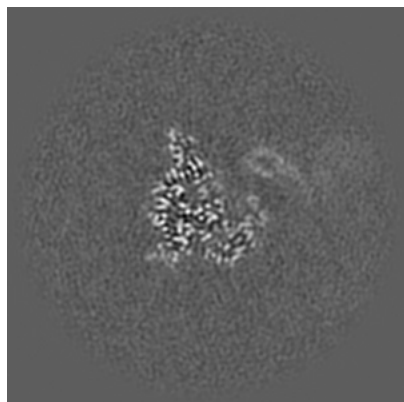


Z Index: 150

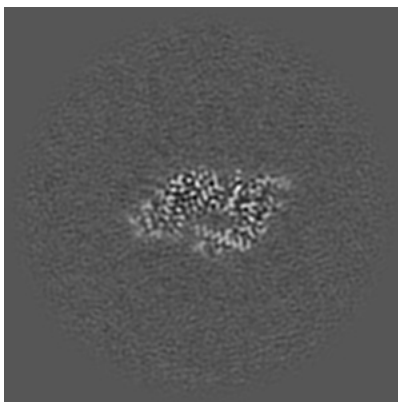
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

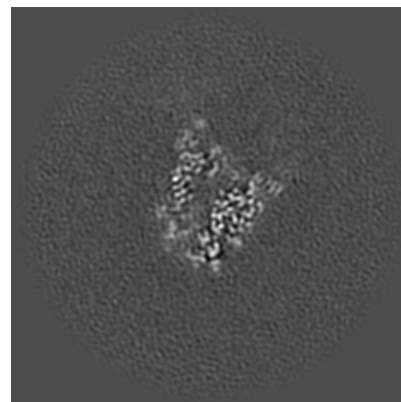
6.3.1 Primary map



X Index: 157

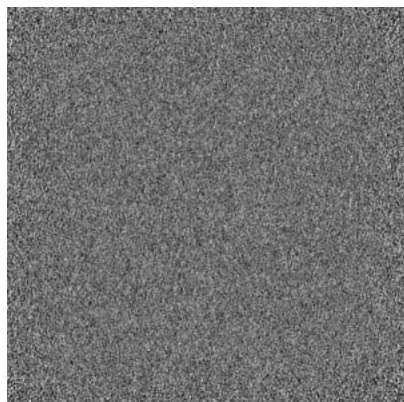


Y Index: 132

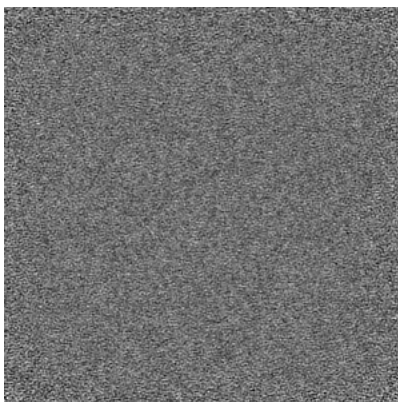


Z Index: 146

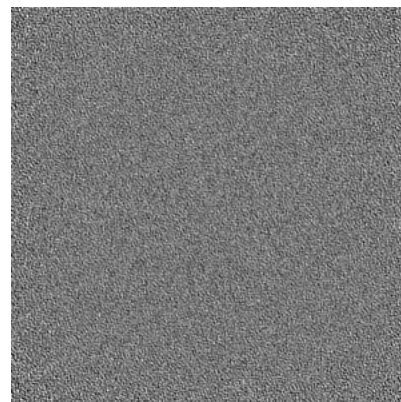
6.3.2 Raw map



X Index: 0



Y Index: 0

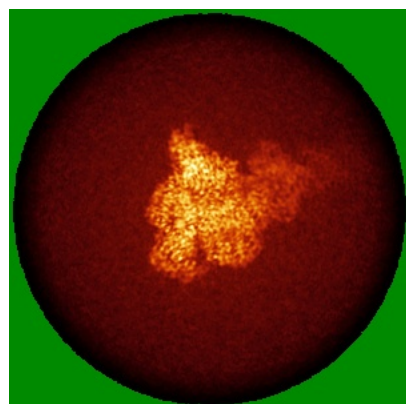


Z Index: 0

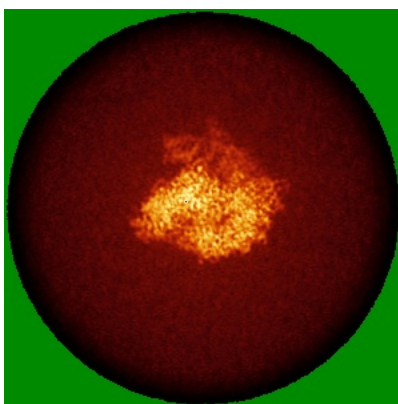
The images above show the largest variance slices of the map in three orthogonal directions.

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

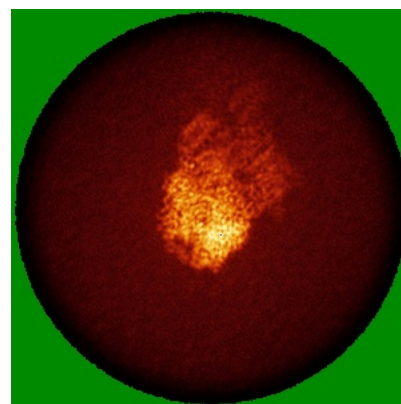
6.4.1 Primary map



X

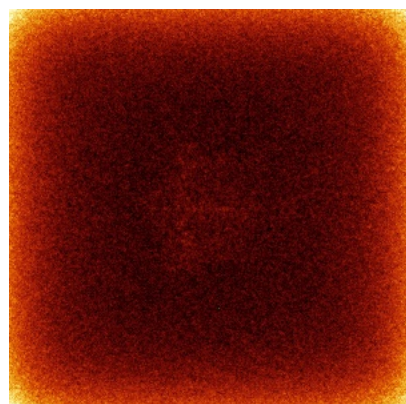


Y

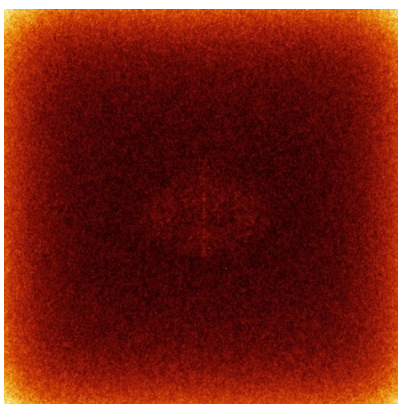


Z

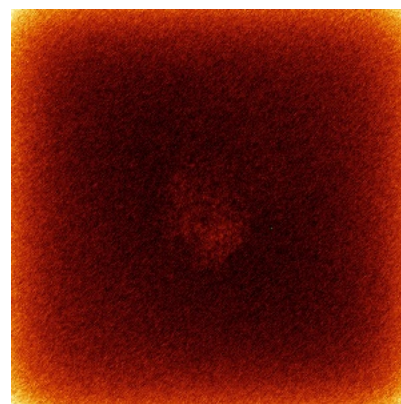
6.4.2 Raw map



X



Y

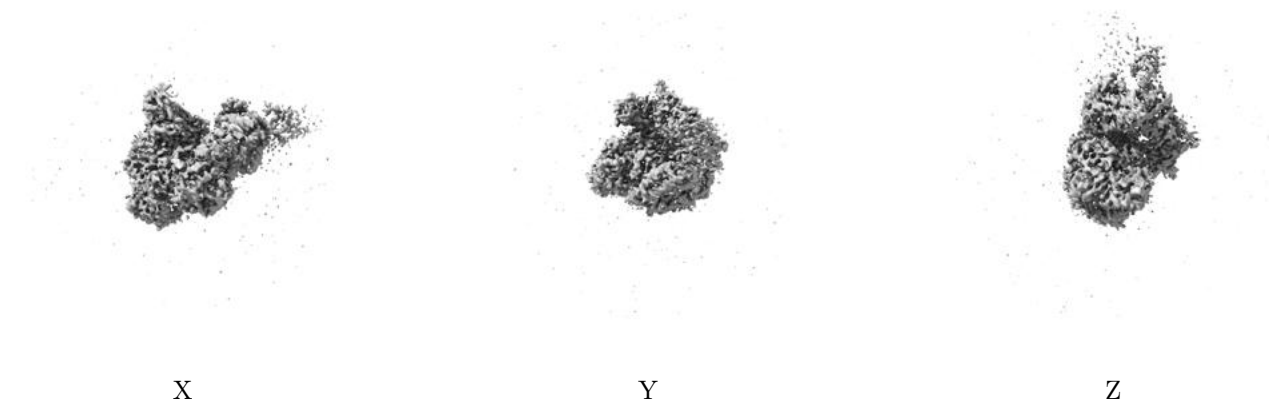


Z

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.

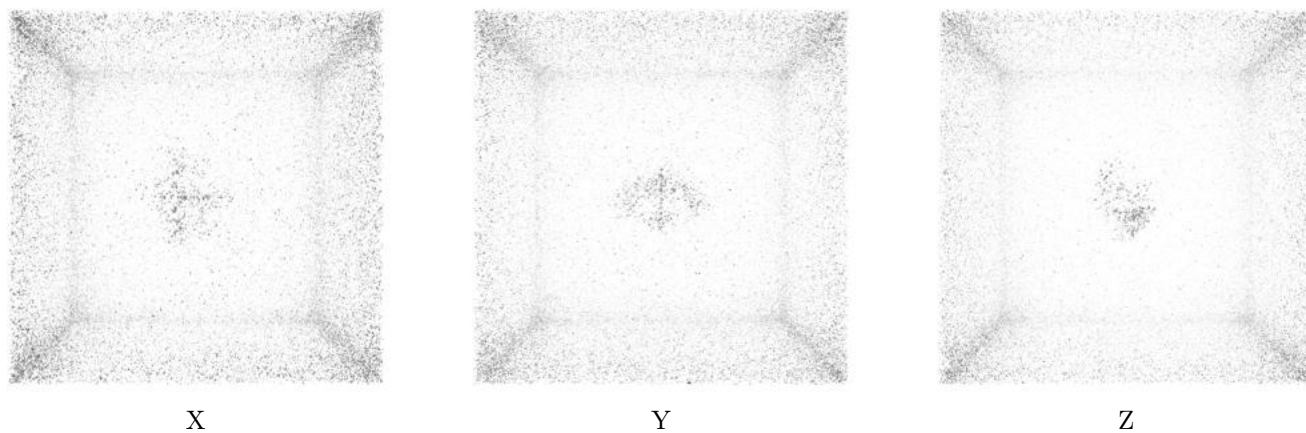
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.11. 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.

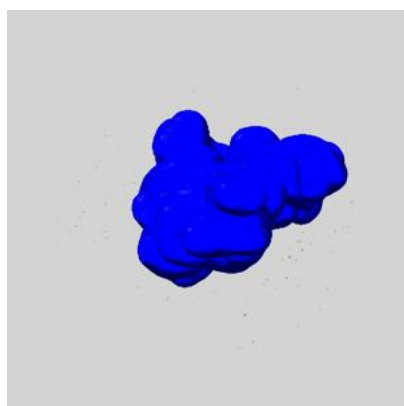
6.6 Mask visualisation [i](#)

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

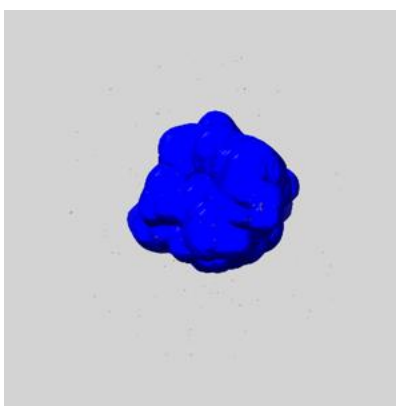
A mask typically either:

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

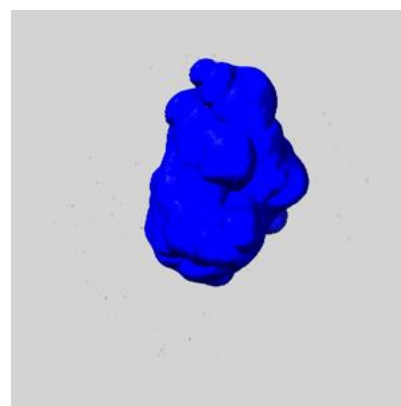
6.6.1 emd_17353_msk_1.map [i](#)



X



Y

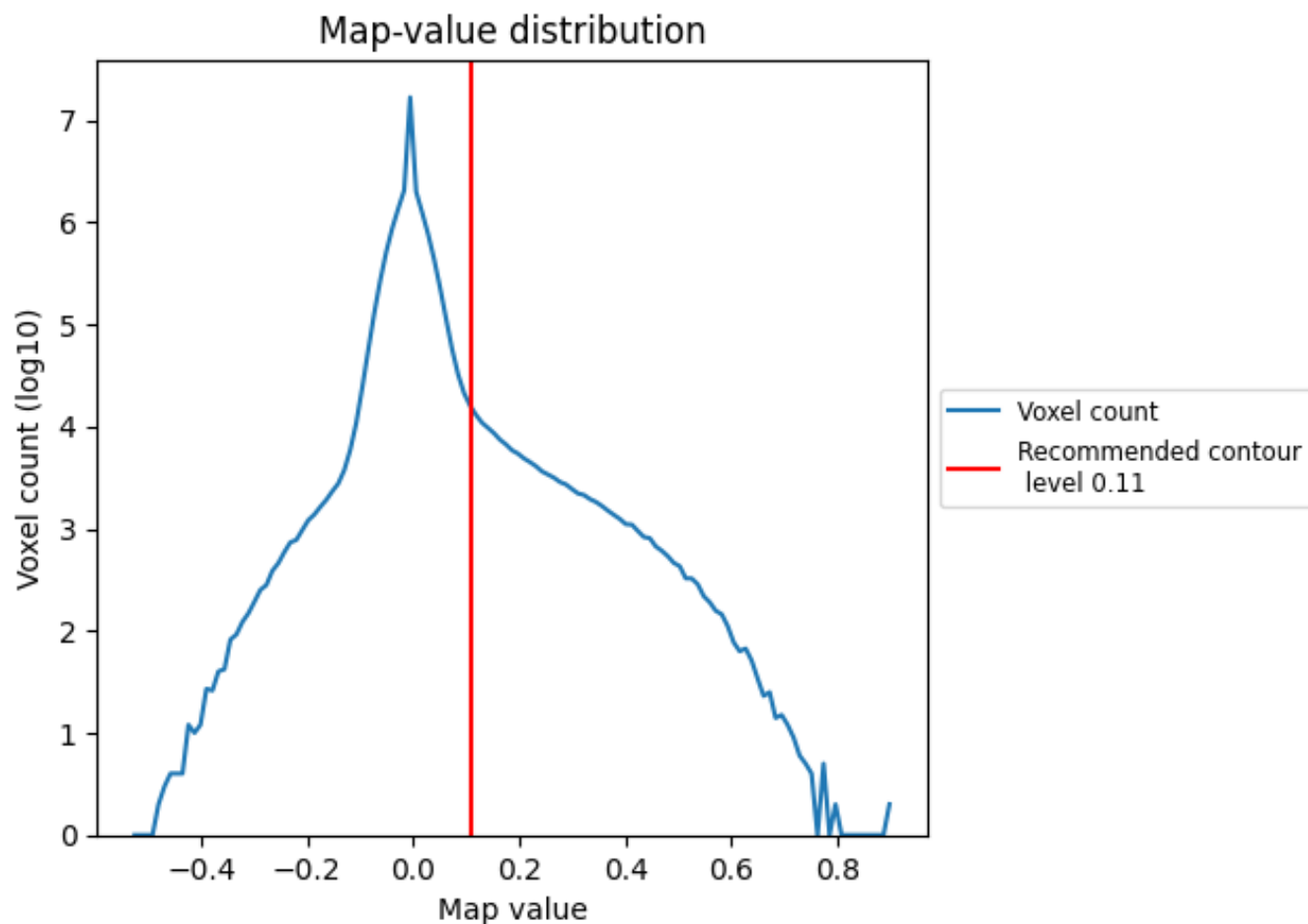


Z

7 Map analysis [i](#)

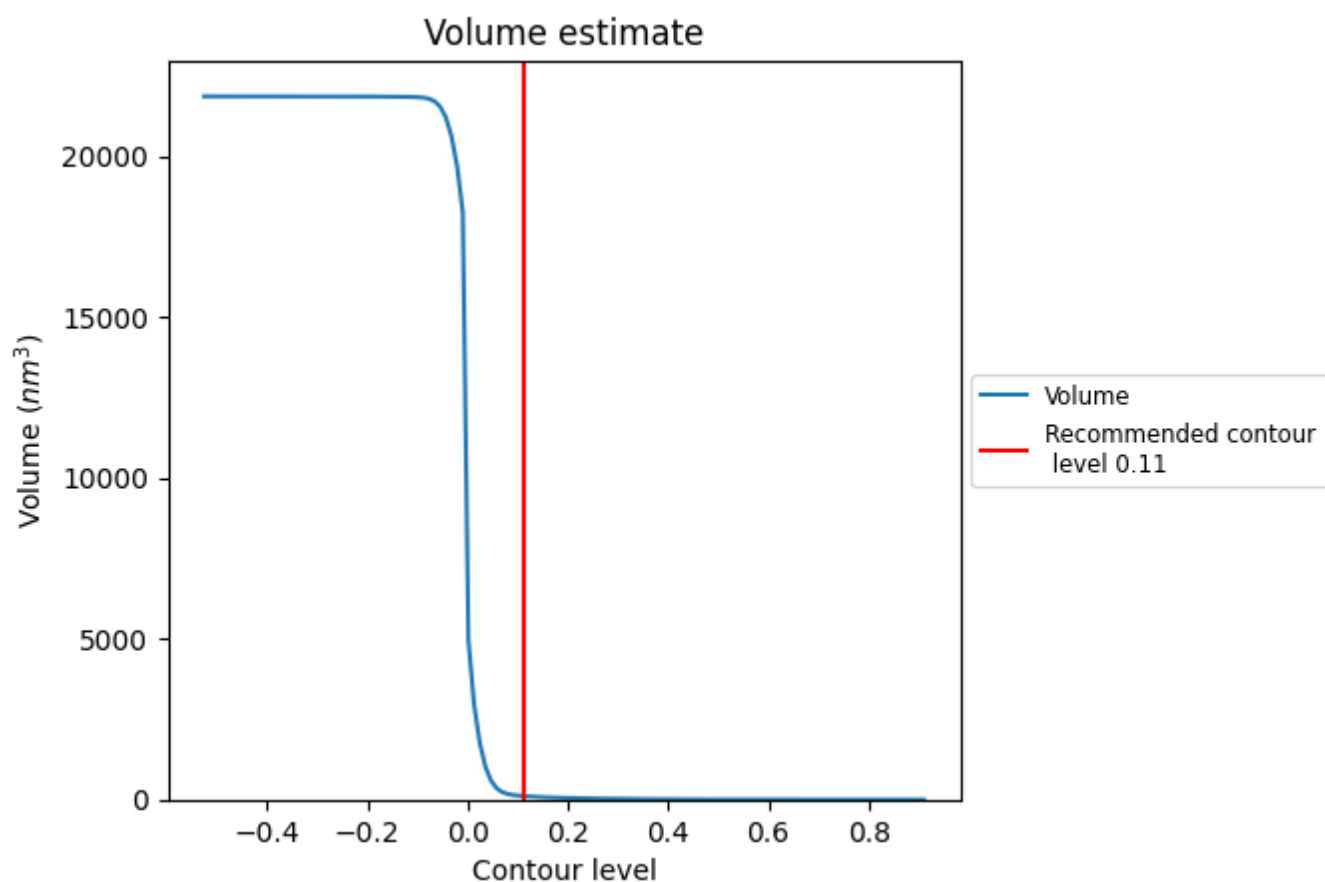
This section contains the results of statistical analysis of the map.

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.

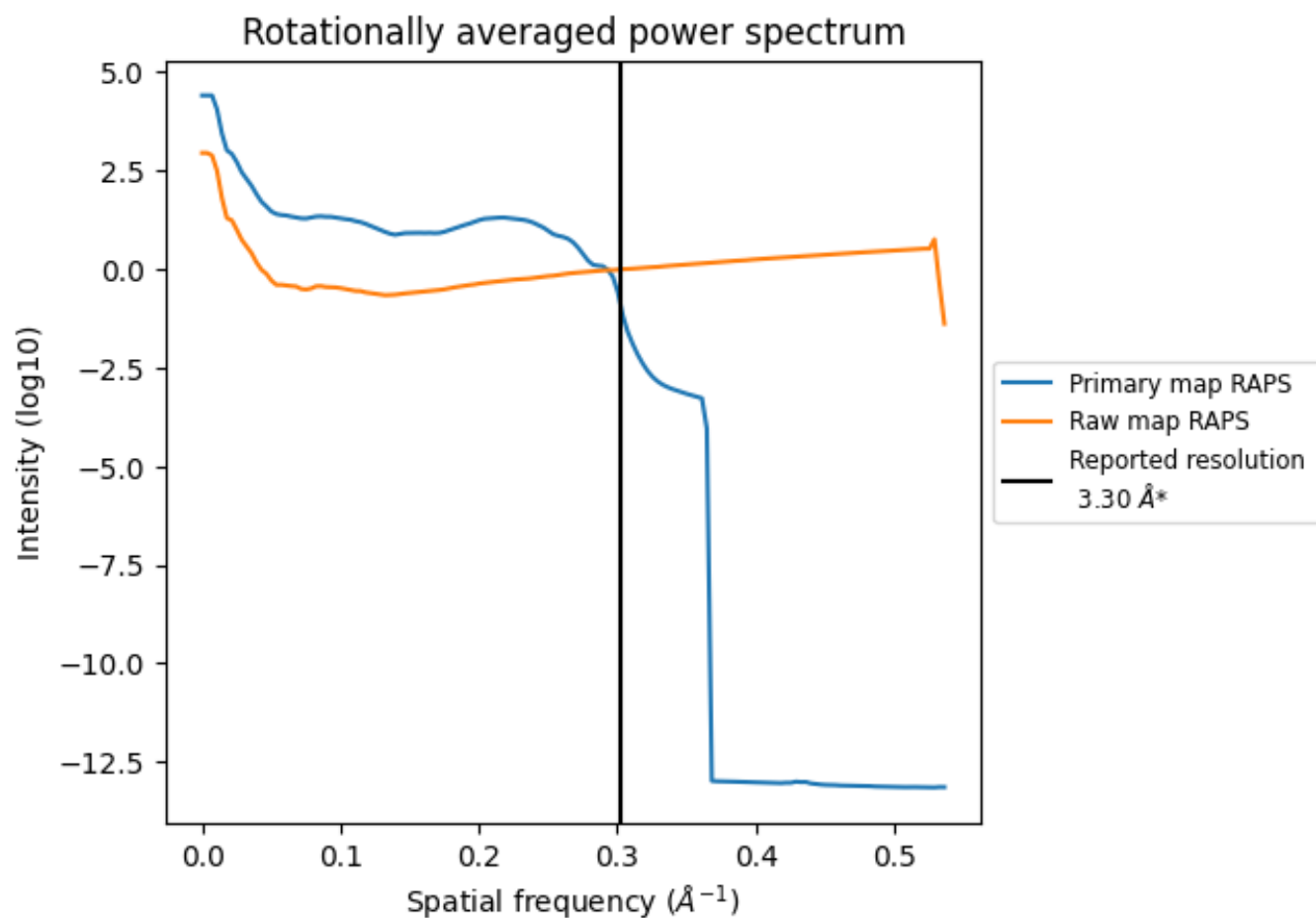
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 109 nm^3 ; this corresponds to an approximate mass of 99 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 ⓘ

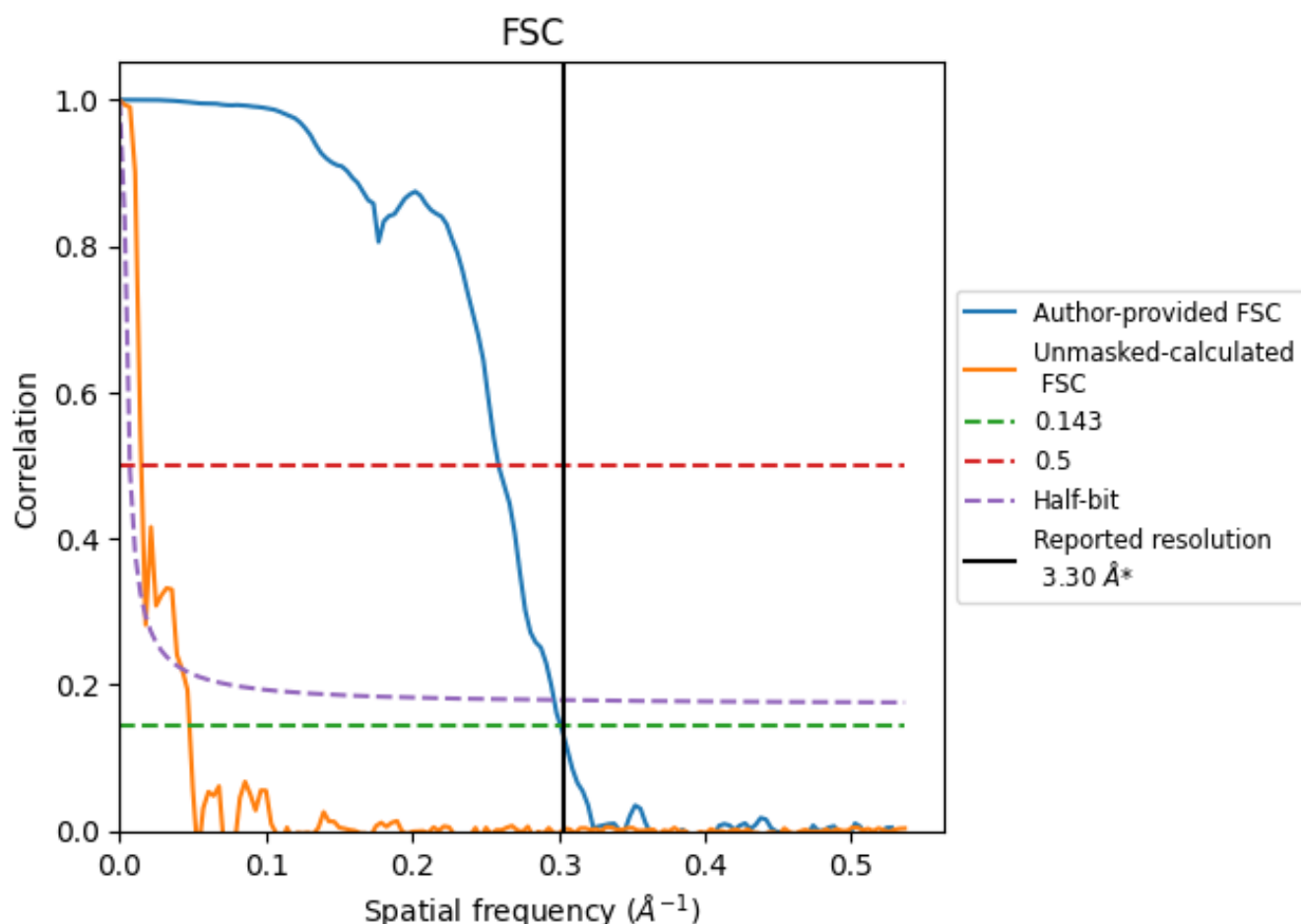


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

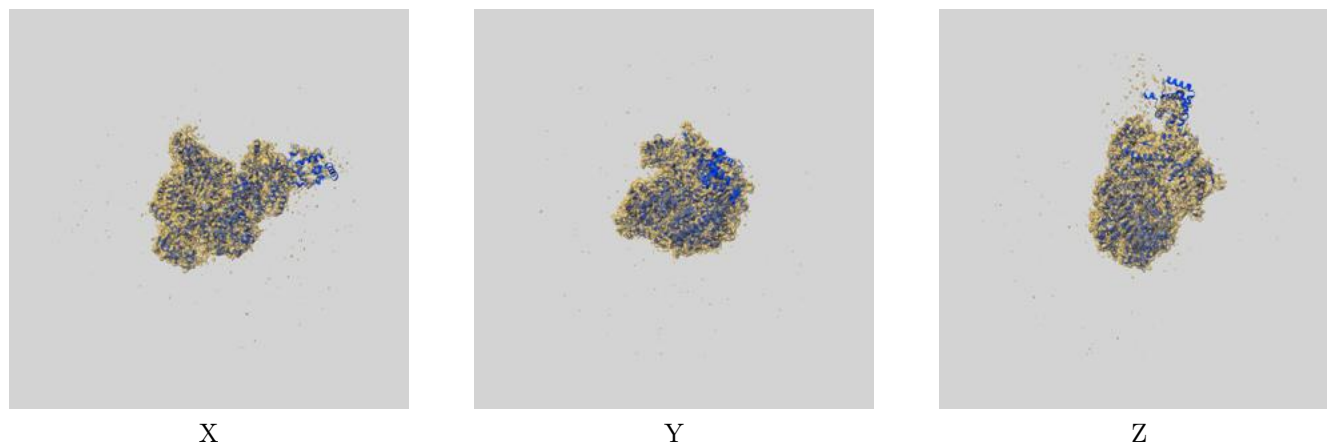
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.86	3.37
Unmasked-calculated*	20.92	67.11	56.50

*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 20.92 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

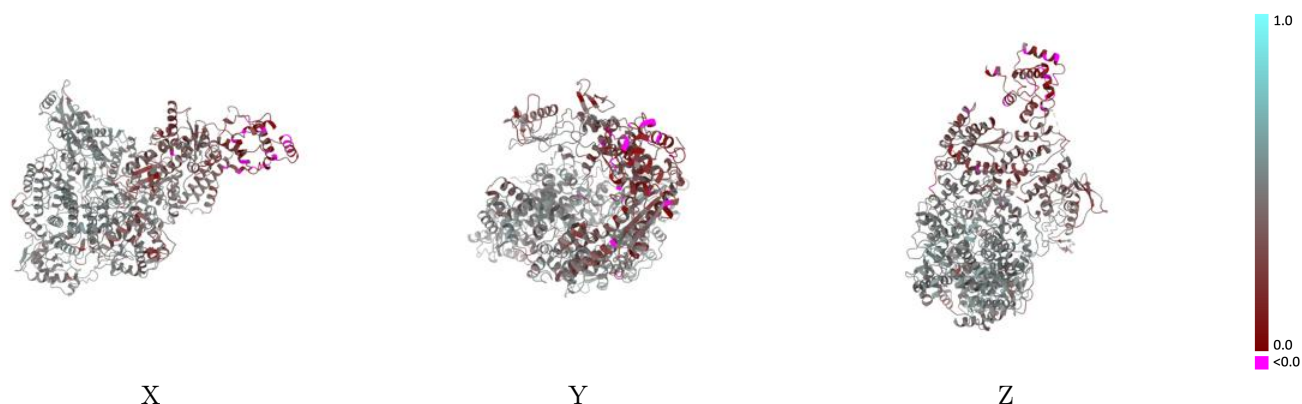
This section contains information regarding the fit between EMDB map EMD-17353 and PDB model 8P1L. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



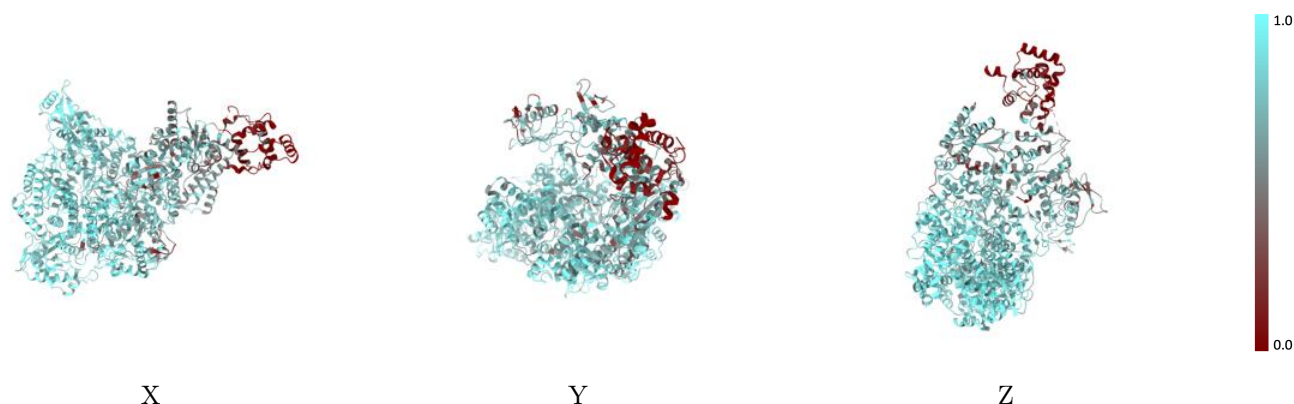
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



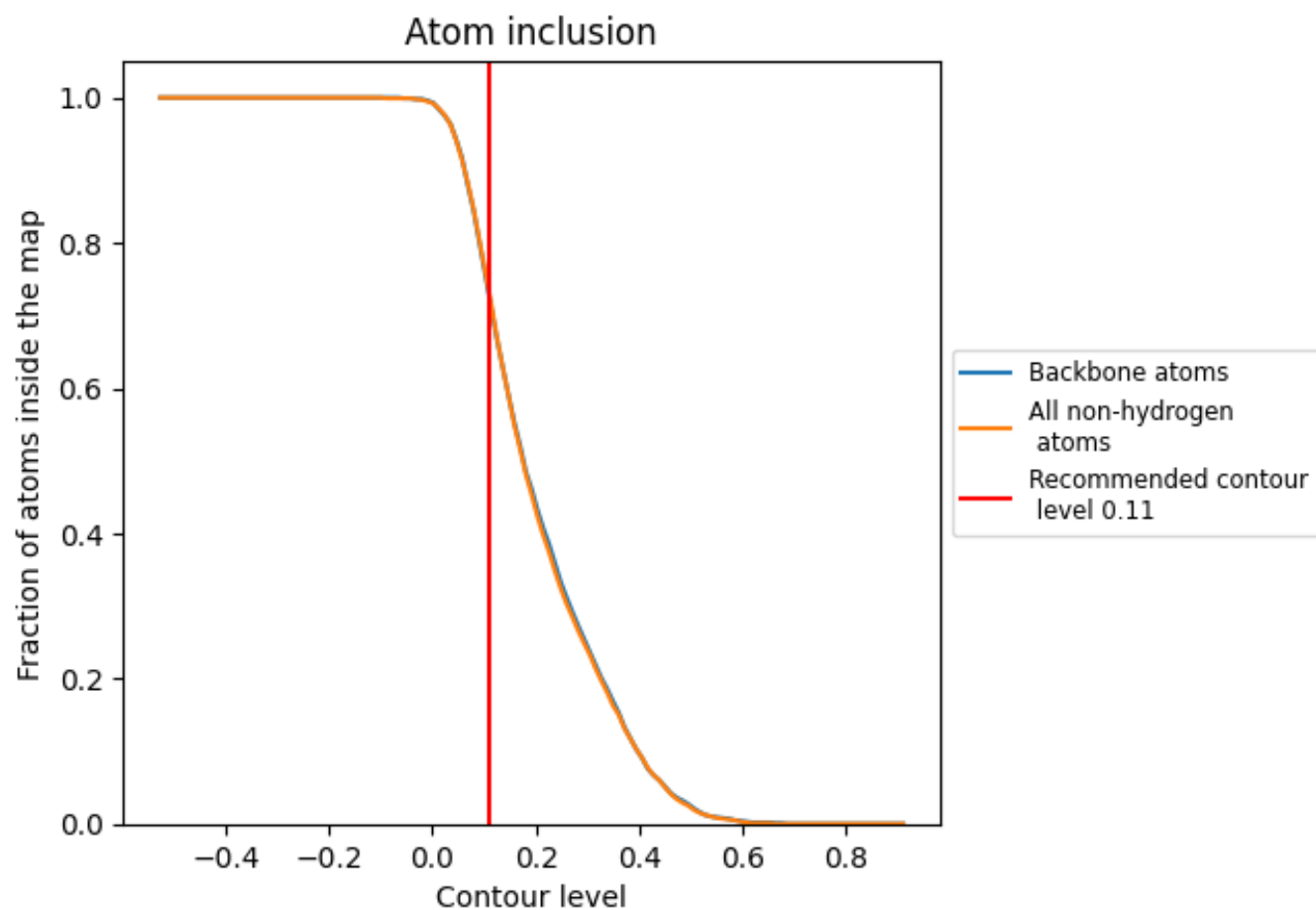
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.11).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 73% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7320	<div></div> 0.4320
A	<div></div> 0.7360	<div></div> 0.4320

