



wwPDB EM Validation Summary Report

Feb 24, 2022 – 01:07 am GMT


PDB ID : 7YXY
EMDB ID : EMD-14369
Title : Cryo-EM structure of USP9X, local refinement of monomer
Authors : Deme, J.C.; Halabelian, L.; Arrowsmith, C.H.; Lea, S.M.; Structural Genomics Consortium (SGC)
Deposited on : 2022-02-16
Resolution : 3.10 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 following versions of software and data (see [references](#) ) were used in the production of this report:

EMDB validation analysis : 0.0.0.dev97
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.26

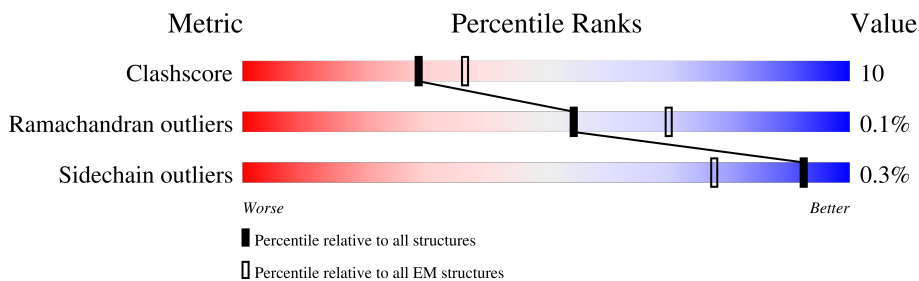
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	2579	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14031 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 Probable ubiquitin carboxyl-terminal hydrolase FAF-X.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1739	14031	8988	2403	2544	96	1	0

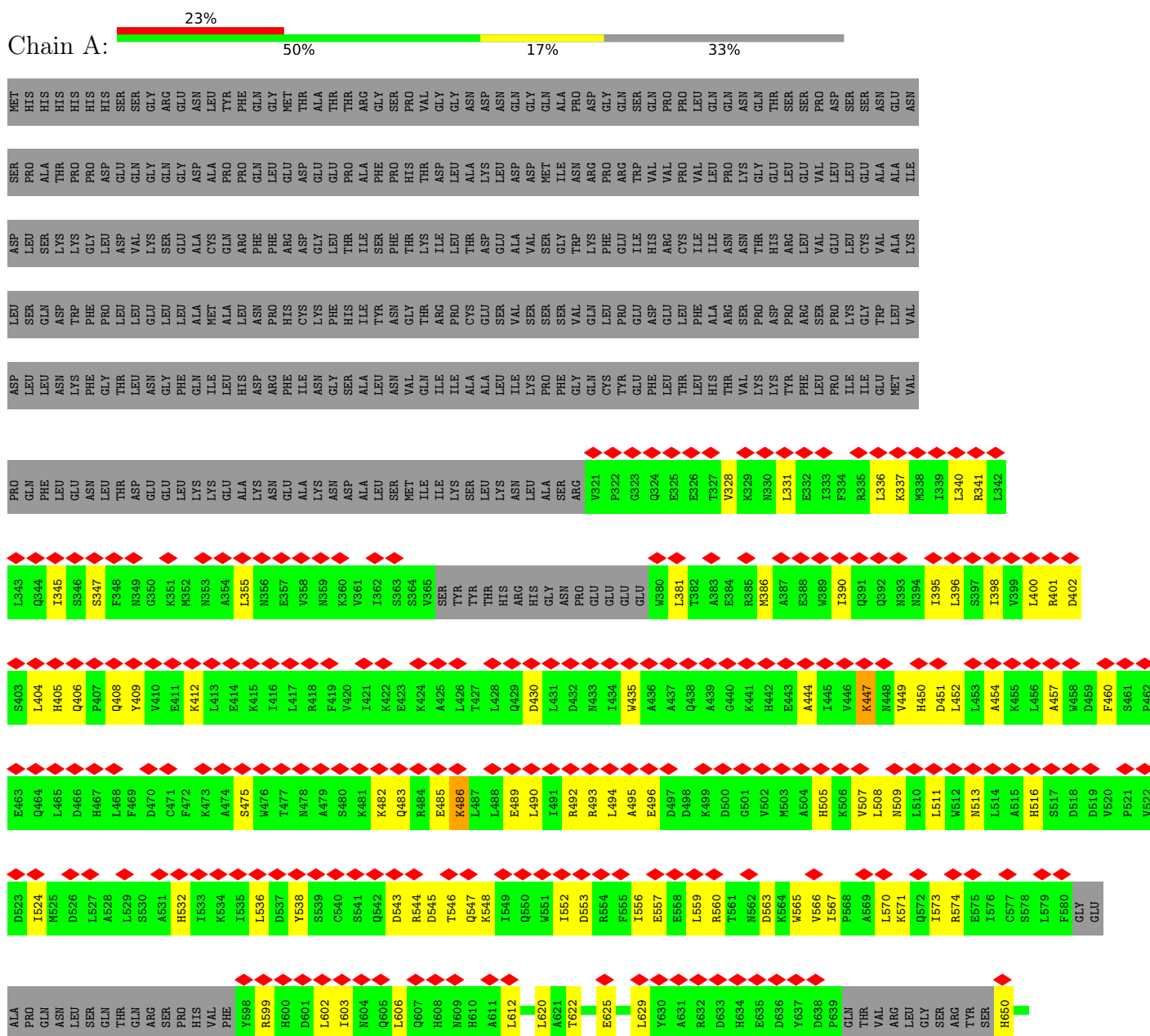
There are 25 discrepancies between the modelled and reference sequences:

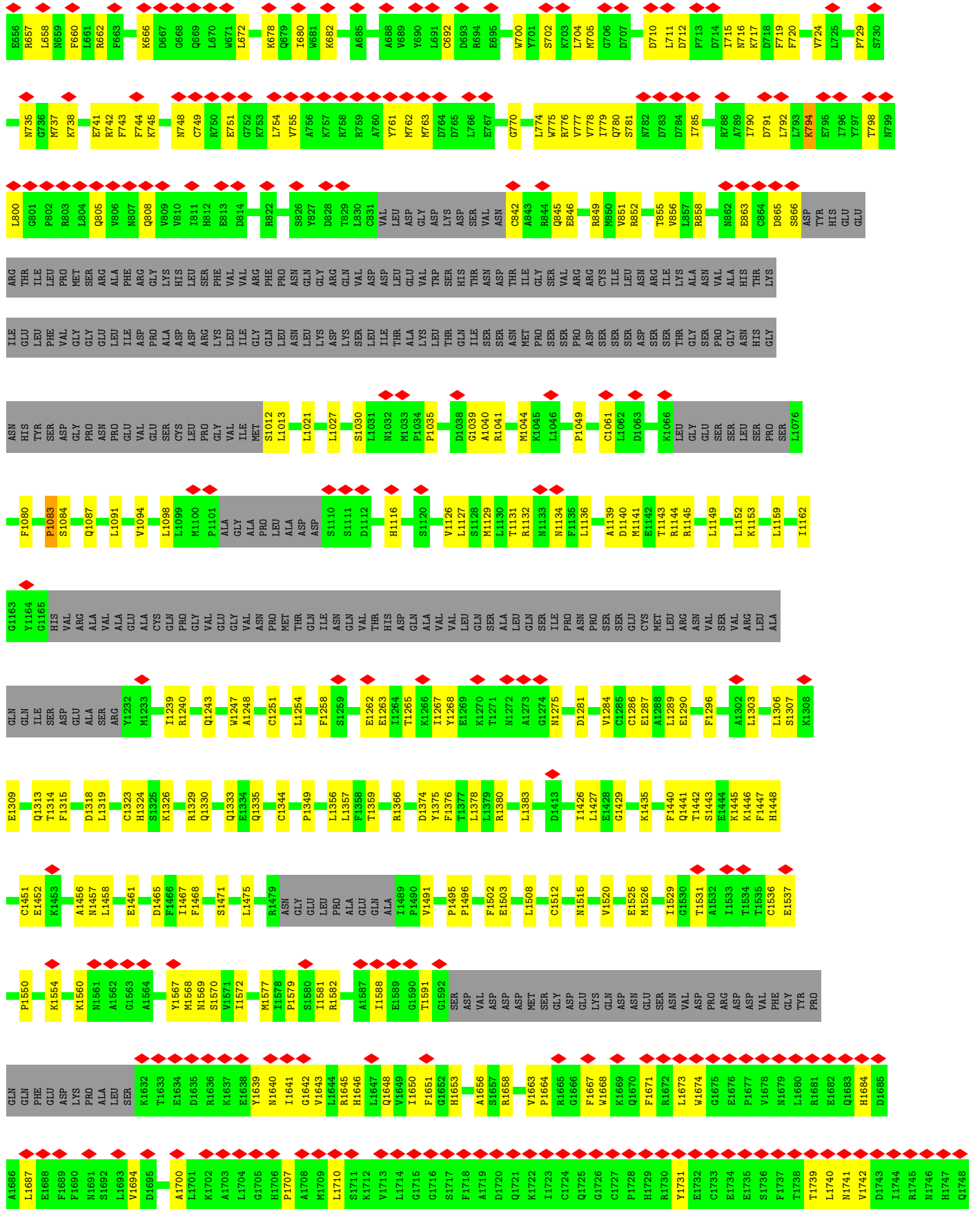
Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP Q93008
A	-16	HIS	-	expression tag	UNP Q93008
A	-15	HIS	-	expression tag	UNP Q93008
A	-14	HIS	-	expression tag	UNP Q93008
A	-13	HIS	-	expression tag	UNP Q93008
A	-12	HIS	-	expression tag	UNP Q93008
A	-11	HIS	-	expression tag	UNP Q93008
A	-10	SER	-	expression tag	UNP Q93008
A	-9	SER	-	expression tag	UNP Q93008
A	-8	GLY	-	expression tag	UNP Q93008
A	-7	ARG	-	expression tag	UNP Q93008
A	-6	GLU	-	expression tag	UNP Q93008
A	-5	ASN	-	expression tag	UNP Q93008
A	-4	LEU	-	expression tag	UNP Q93008
A	-3	TYR	-	expression tag	UNP Q93008
A	-2	PHE	-	expression tag	UNP Q93008
A	-1	GLN	-	expression tag	UNP Q93008
A	0	GLY	-	expression tag	UNP Q93008
A	2555	ASP	-	expression tag	UNP Q93008
A	2556	TYR	-	expression tag	UNP Q93008
A	2557	LYS	-	expression tag	UNP Q93008
A	2558	ASP	-	expression tag	UNP Q93008
A	2559	ASP	-	expression tag	UNP Q93008
A	2560	ASP	-	expression tag	UNP Q93008
A	2561	LYS	-	expression tag	UNP Q93008

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: Probable ubiquitin carboxyl-terminal hydrolase FAF-X





M1749	D1814	G1877	Y1939	F2012	ASP	D2364	PRO	GLU
L1750	Y1815	G1878	R1940	M2013	N2149	S2376	ASP	VAL
L1751	F1816	H1879	R1941	K2015	D2154	A2384	GLU	SER
D1752	E1817	Y1880	Q1942	L2034	V2150	C2387	GLU	PRO
S1753	F1818	I1884	K1943	P2035	L2164	M2391	PRO	THR
L1754	P1819	I1885	R1944	E2036	R2165	A2401	PRO	LYS
E1755	R1820	Q1886	V1945	A2037	V2168	N2408	PRO	GLN
Q1756	E1821	R1887	V1946	E2038	G2172	R2428	ASP	TYR
Y1757	L1822	N1888	M1947	E2039	R2173	PRO	ALA	LEU
V1758	D1823	G1889	I1950	I2040	H2174	ARG	PRO	ASP
K1759	M1824	G1890	L1951	K2042	L2175	PRO	LEU	ASP
G1760	E1825	GLY	F1952	S2044	Q2176	THR	TYR	ASP
D1761	P1826	GLU	Y1953	Q2046	Y2178	THR	GLY	LYS
L1762	Y1827	ARG	M1956	L2047	F2179	GLY	THR	
L1763	T1828	ASN	ASP	R2050	N2180	GLY	GLY	
E1764	V1829	R1896	THR	R2050	L2181	ASN	SER	
G1765	A1830	W1897	I1E	F2051	Q2195	PRO	GLN	
G1766	G1831	Y1898	ASP	L2052	V2208	ASN	ASN	
A1766	G1832	K1899	Q1961	F2053	S2209	ASN	ASN	
M1767	V1833	F1900	D1962	T2054	G2215	THR	VAL	
A1768	A1833	D1901	D1963	T2055	L2236	PRO	GLY	
V1769	K1834	D1902	E1964	G2056	S2247	PRO	PRO	
H1770	L1835	G1903	L1965	V2062	P2256	GLN	VAL	
C1771	E1836	D1904	I1966	V2063	N2257	ASN	GLN	
E1772	G1837	V1905	R1967	A2067	P2258	GLU	VAL	
K1773	D1838	E1907	Y1968	W2070	M2277	GLU	THR	
C1774	ASN	C1908	I1969	S2081	L2278	THR	ALA	
M1775	VAL	K1909	S1970	V2084	L2279	ASN	ALA	
K1776	ASN	K1909	GLU	R2085	F2280	ASN	HIS	
K1777	PRO	M1910	LEU	F2094	V2281	TYR	HIS	
V1778	GLU	D1911	ALA	R2099	K2288	ASN	ASN	
D1779	SER	D1912	ILE	A2117	S2296	LEU	ASN	
D1780	GLN	D1913	THR	D2130	T2299	GLU	PRO	
T1780	LEU	E1914	THR	P2136	E2309	GLU	ALA	
V1781	ILE	E1915	ARG	F2137	L2321	GLU	ALA	
K1782	GLN	E1916	PRO	ALA	L2339	GLU	GLN	
R1783	SER	K1917	HIS	PRO	T2355	PRO	ASN	
L1784	GLN	M1918	GLN	ALA	L2359	ASP	TYR	
L1785	SER	Q1919	ILE	I1987		GLU	GLU	
I1786	GLU	C1920	ILE	E1988		GLU	GLU	
K1787	SER	F1921	MET	V1991		PRO	PRO	
K1788	THR	G1922	PRO	M1995		ASP	ASP	
L1789	ALA	G1923	SER	R2002		GLN	GLN	
I1795	G1859	E1924	ALA	M2007		ARG	ARG	
K1798	S1860	Y1925	E1988	E2008		ALA	ALA	
R1799	T1861	M1926	V1991	Y2009		GLN	GLN	
F1800	Y1863	G1927	M1995	F2010		GLU	GLU	
D1801	R1864	E1928	R2002	Q2011		PRO	PRO	
D1802	L1869	F1930	M2007			TYR	TYR	
Y1802	V1870	D1931	E2008			GLU	GLU	
D1803	H1871	H1932	Y2009			GLU	GLU	
W1804	S1872	M1933	F2010			ASP	ASP	
E1805	G1873	M1934	Q2011			GLY	GLY	
R1806	Q1874	K1935				SER	SER	
E1807	A1875	R1936				ALA	ALA	
C1808	S1876	M1937						
A1809		S1938						
I1810								
K1811								
F1812								
M1813								

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	330000	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 ($e^-/\text{\AA}^2$)	56.7	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.402	Depositor
Minimum map value	-1.221	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.323	Depositor
Map size (\AA)	372.73602, 372.73602, 372.73602	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.8320001, 0.8320001, 0.8320001	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	0/14334	0.48	1/19388 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1083	PRO	CA-N-CD	-5.58	103.69	111.50

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	14031	0	13943	288	0
All	All	14031	0	13943	288	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 10.

The worst 5 of 288 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:2007:MET:HG2	1:A:2011:GLN:HE22	1.44	0.82
1:A:2054:THR:HG22	1:A:2055:THR:HG23	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:842:CYS:SG	1:A:845:GLN:NE2	2.61	0.74
1:A:658:LEU:HD11	1:A:700:TRP:HB2	1.69	0.73
1:A:543:ASP:O	1:A:547:GLN:NE2	2.22	0.72

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	1706/2579 (66%)	1621 (95%)	84 (5%)	1 (0%)	51 83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	712	ASP

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	1530/2286 (67%)	1526 (100%)	4 (0%)	92 96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	447	LYS
1	A	486	LYS
1	A	794	LYS
1	A	2408	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1653	HIS
1	A	1994	GLN
1	A	2408	ASN
1	A	2011	GLN
1	A	845	GLN

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 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.

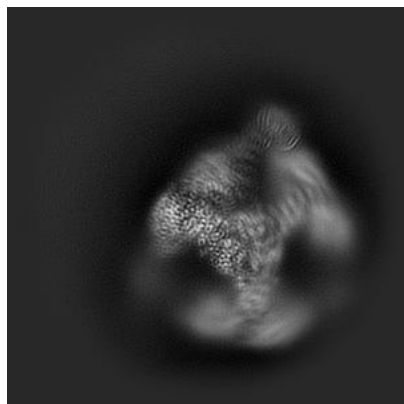
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14369. These allow visual inspection of the internal detail of the map and identification of artifacts.

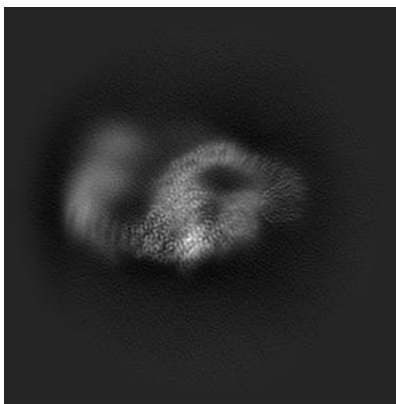
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

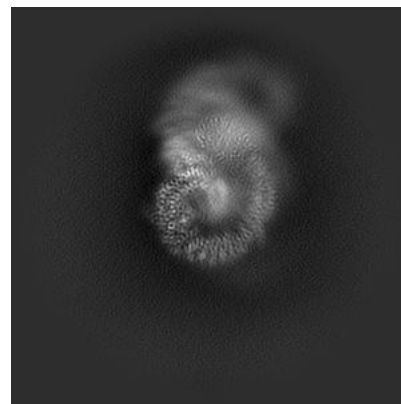
6.1.1 Primary map



X

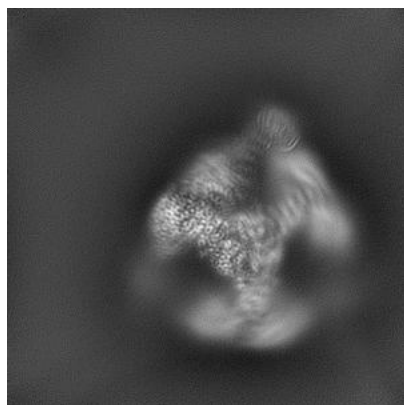


Y

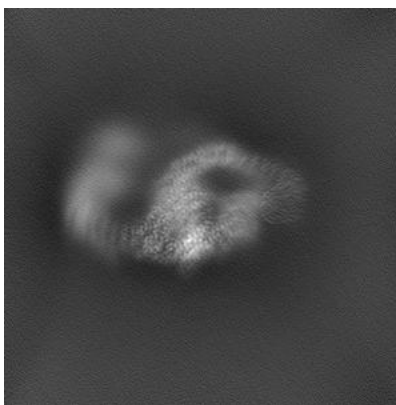


Z

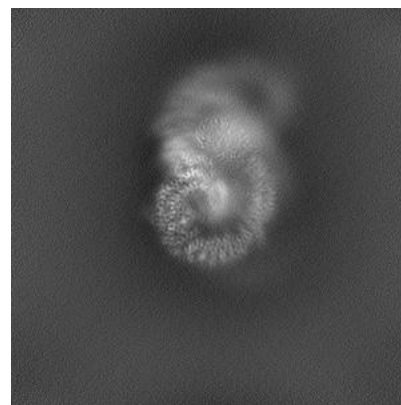
6.1.2 Raw map



X



Y

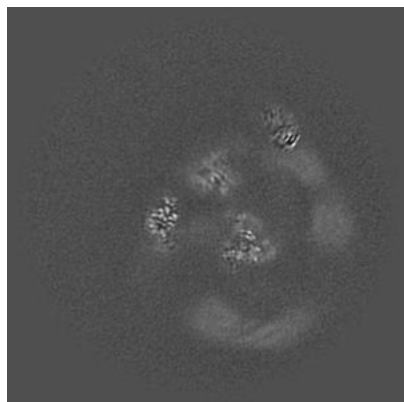


Z

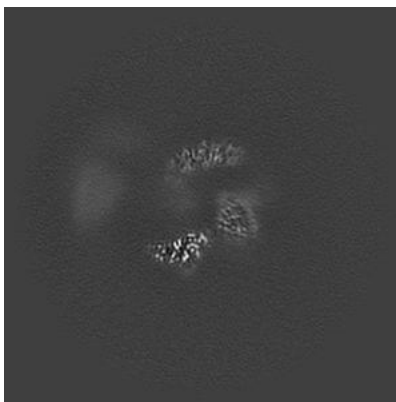
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

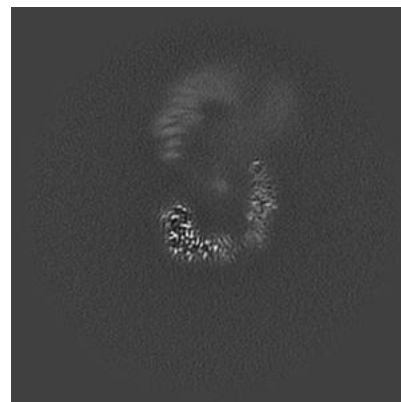
6.2.1 Primary map



X Index: 224

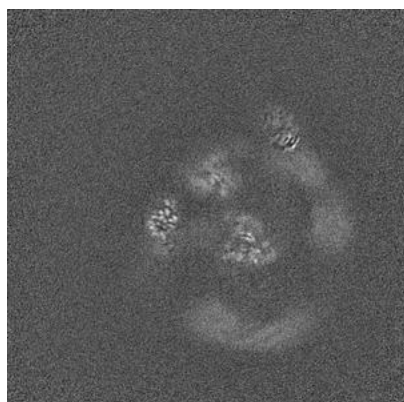


Y Index: 224

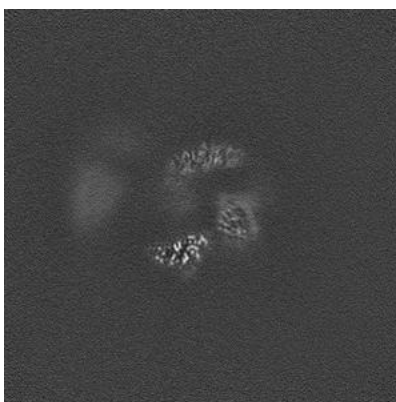


Z Index: 224

6.2.2 Raw map



X Index: 224



Y Index: 224

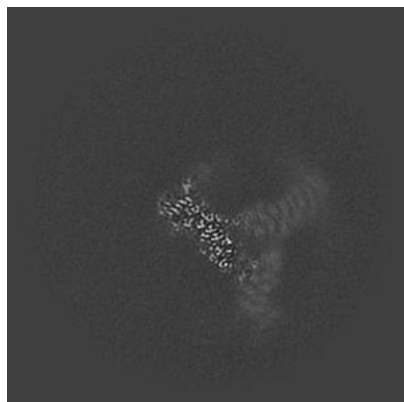


Z Index: 224

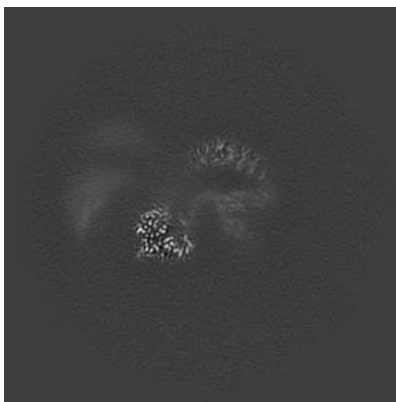
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

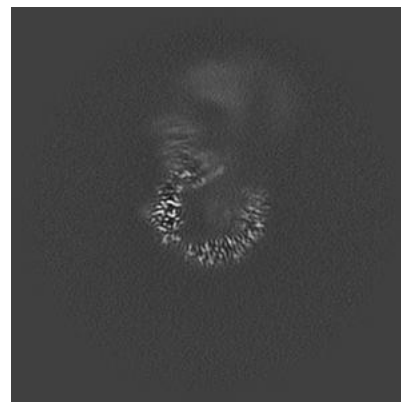
6.3.1 Primary map



X Index: 182

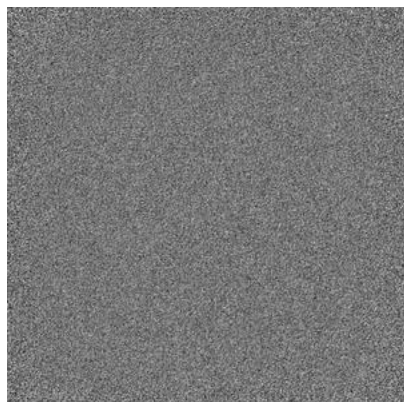


Y Index: 246

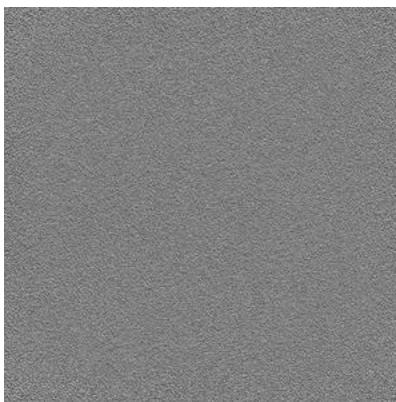


Z Index: 202

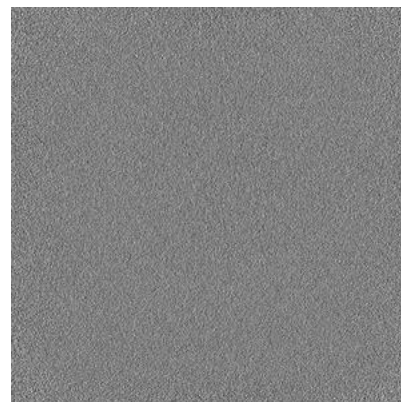
6.3.2 Raw map



X Index: 0



Y Index: 0



Z Index: 0

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

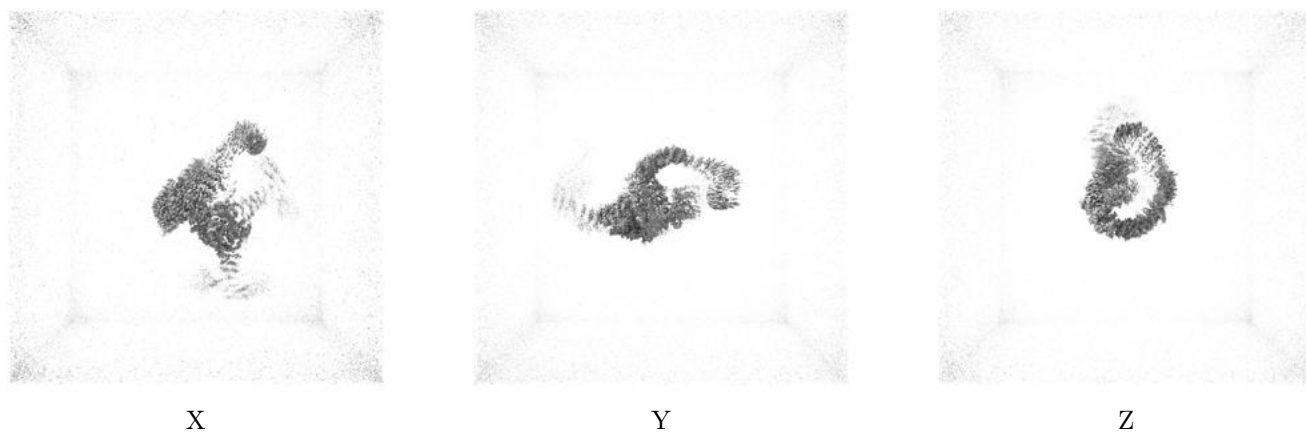
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.323. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

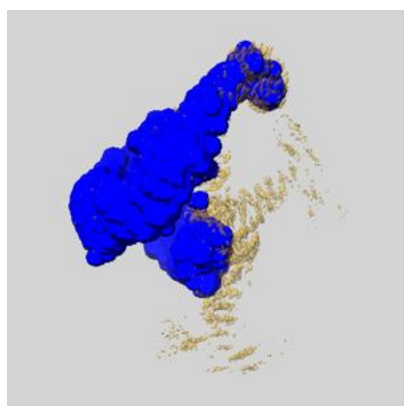
6.5 Mask visualisation [i](#)

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

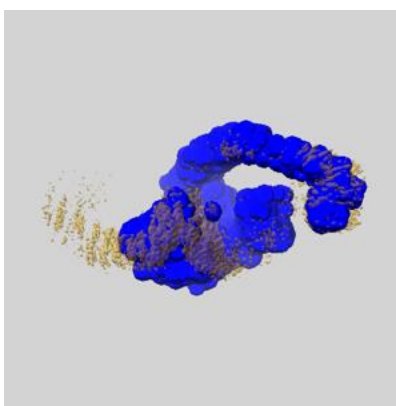
A mask typically either:

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

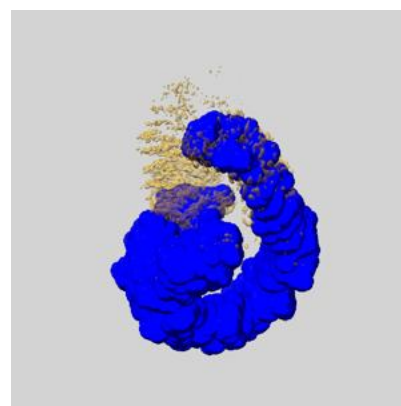
6.5.1 emd_14369_msk_1.map [i](#)



X



Y

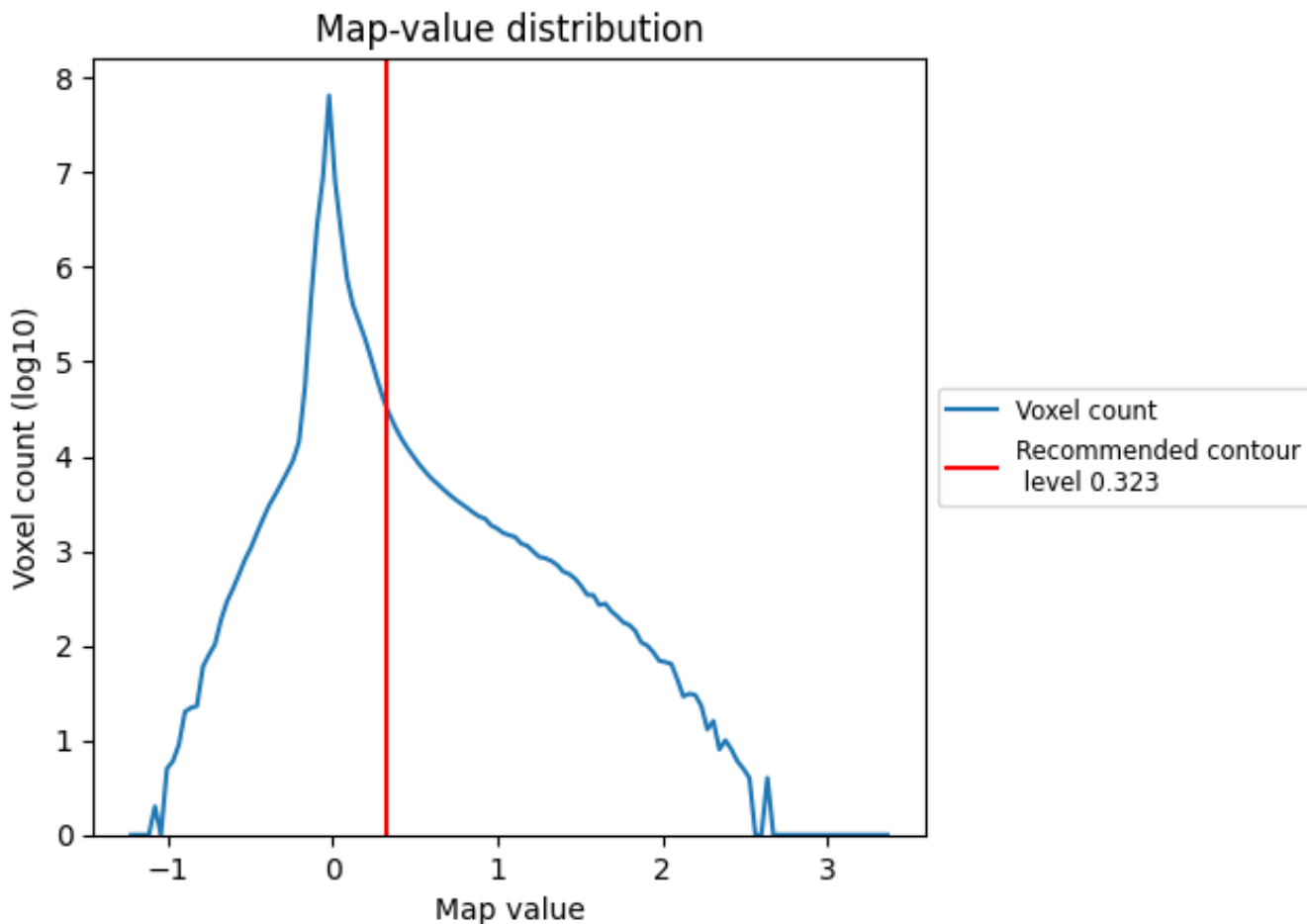


Z

7 Map analysis [i](#)

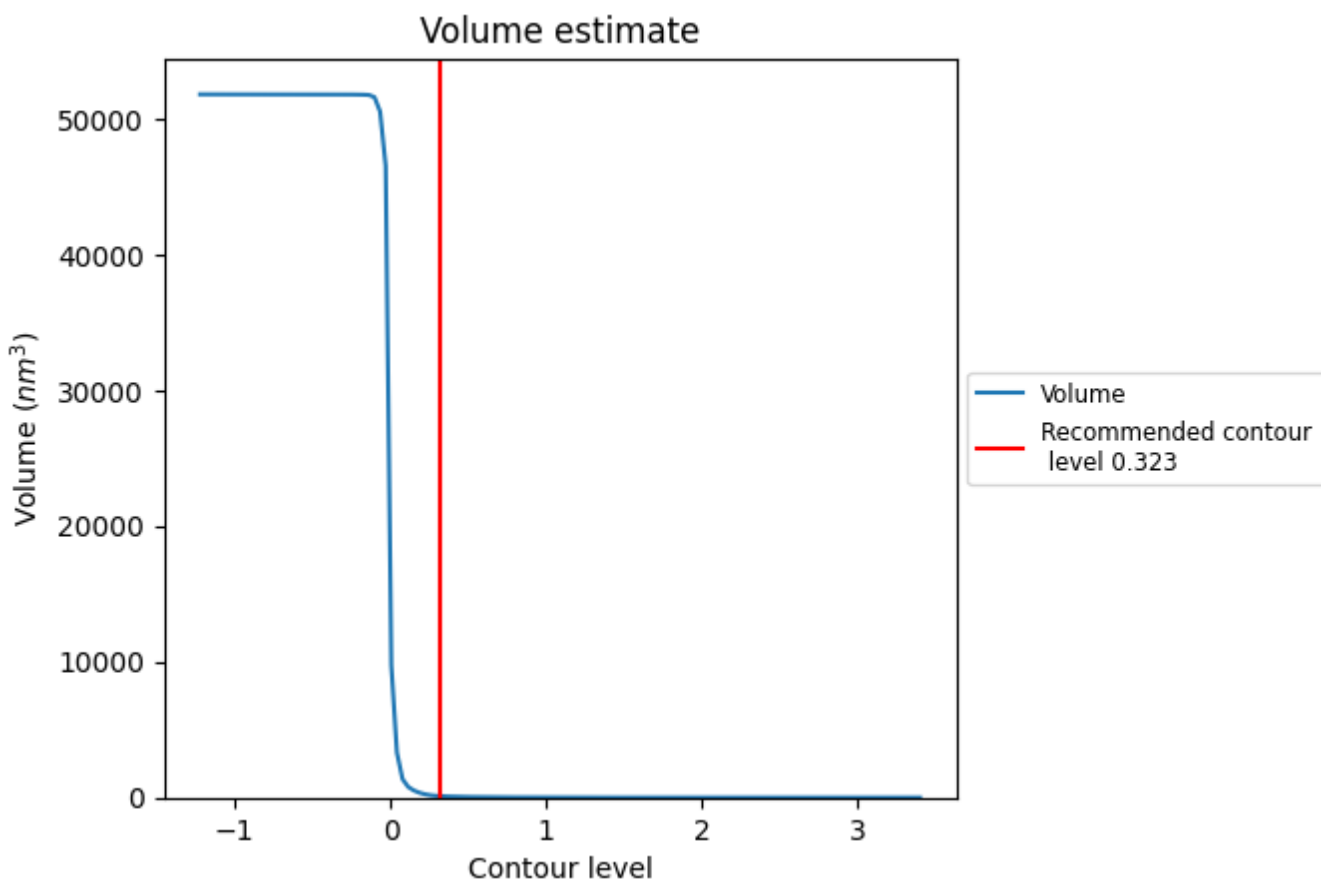
This section contains the results of statistical analysis of the map.

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.

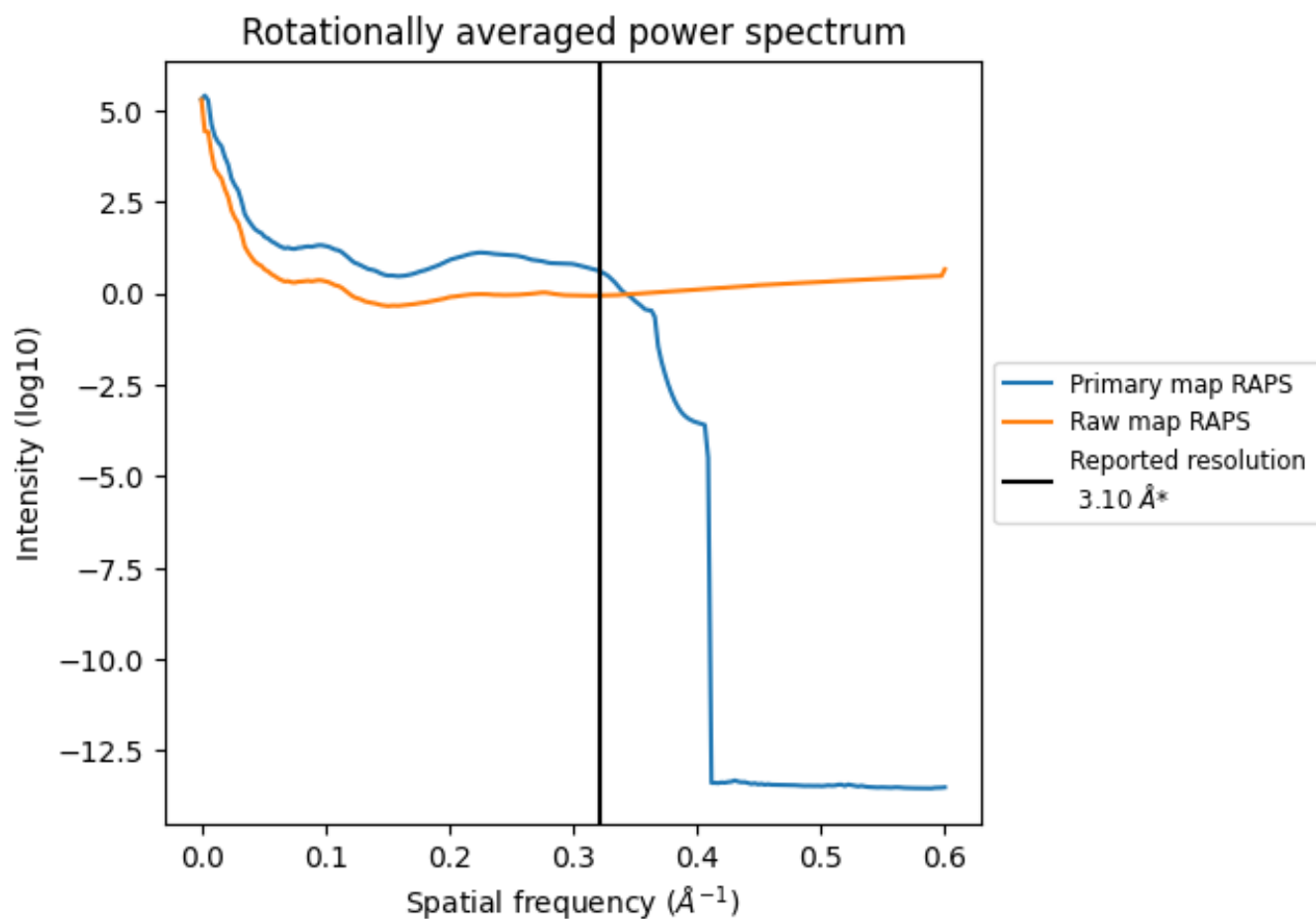
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 104 nm³; this corresponds to an approximate mass of 94 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 [i](#)

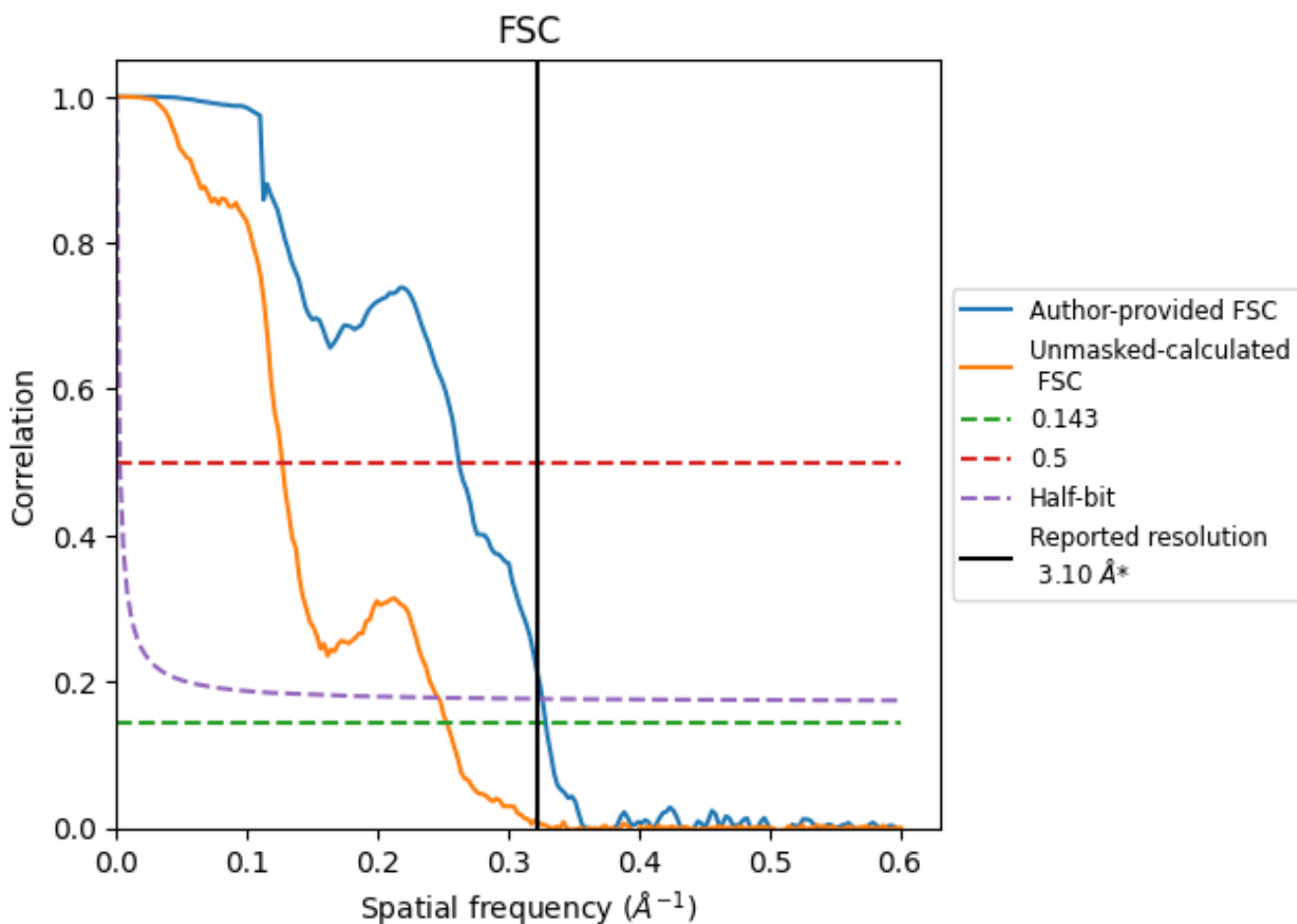


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

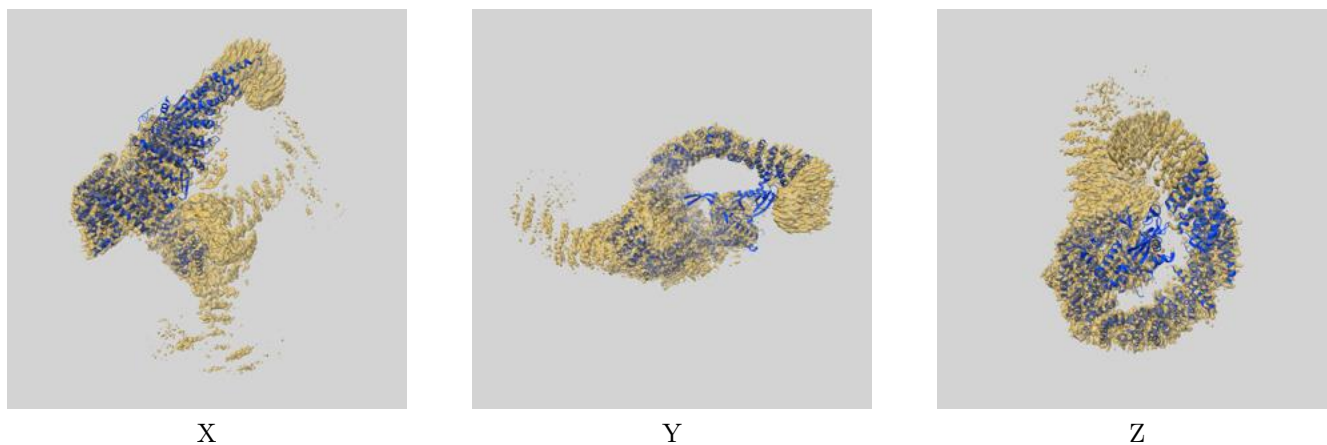
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.04	3.81	3.07
Unmasked-calculated*	3.95	7.88	4.06

*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 3.95 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

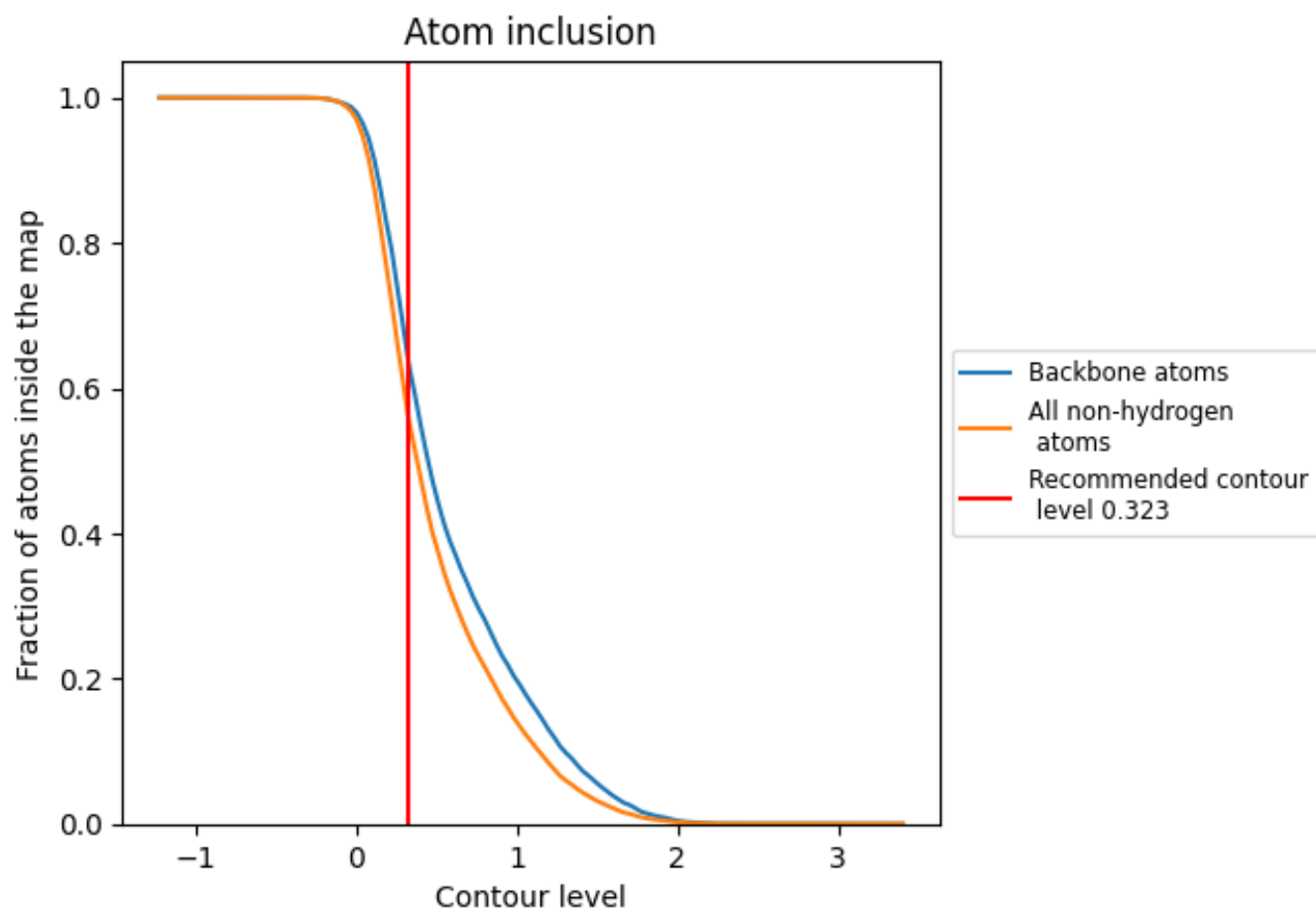
This section contains information regarding the fit between EMDB map EMD-14369 and PDB model 7YXY. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.323 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 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.