



## Full wwPDB EM Validation 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 Full wwPDB EM Validation 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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.0.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

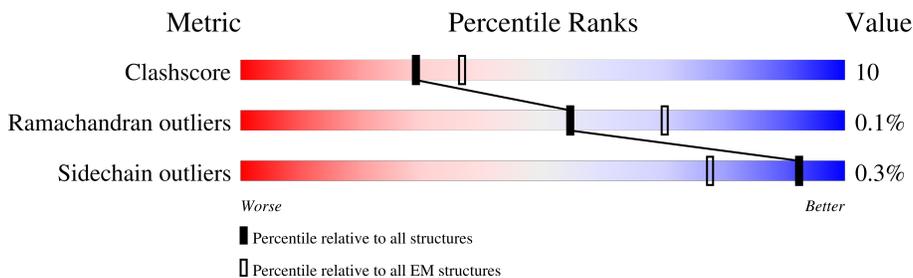
# 1 Overall quality at a glance

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  $\geq 3$ , 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	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





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	HIS	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	THR
Y1757	L1822	N1888	M1947	E2039	R2173	PRO	ALA	ASP
V1758	D1823	G1889	I1950	I2040	H2174	ARG	PRO	LEU
K1759	M1824	G1890	L1951	T2041	L2175	PRO	TYR	ASP
G1760	E1825	GLY	F1952	S2044	Q2176	HIS	HIS	ASP
D1761	P1826	GLU	Y1953	Q2046	Q2177	SER	SER	LYS
L1762	Y1827	ARG	M1956	L2047	Y2178	THR	THR	ASP
L1763	T1828	ASN	ASP	R2050	F2179	GLY	GLY	ASP
E1764	V1829	R1896	THR	R2050	N2180	GLY	SER	ASP
G1765	A1830	W1897	I1986	F2051	L2181	ASN	ASN	GLN
A1766	G1831	Y1898	ASP	L2052	Q2195	TYR	TYR	GLN
M1767	V1832	K1899	Q1961	F2053	V2208	THR	GLN	ASN
A1768	A1833	D1901	D1962	T2054	S2209	ASN	ASN	ASN
V1769	K1834	G1903	D1963	T2055	G2215	HIS	HIS	VAL
H1770	L1835	D1902	E1964	G2056	L2236	SER	SER	GLY
C1771	L1836	V1904	L1965	V2062	S2247	PRO	PRO	GLN
E1772	E1837	V1905	I1966	A2067	P2256	VAL	VAL	THR
K1773	D1838	E1907	R1967	W2070	N2257	GLN	GLN	TYR
C1774	ASN	C1908	Y1968	S2081	P2258	ASN	ASN	GLY
M1775	VAL	K1909	I1969	V2084	D2277	GLU	GLU	ALA
K1776	ASN	M1910	S1970	R2085	L2278	THR	THR	ALA
K1777	PRO	D1911	GLU	V2084	L2279	ALA	ALA	ALA
V1778	GLU	D1912	LEU	R2085	F2280	HIS	HIS	HIS
D1779	SER	D1913	ALA	F2094	V2281	GLY	GLY	ASN
T1780	GLN	E1914	ILE	R2099	K2288	TYR	TYR	ASN
V1781	LEU	E1915	THR	A2117	S2296	PHE	PHE	ASN
K1782	ILE	E1916	ARG	D2130	T2299	LEU	LEU	PRO
R1783	GLN	M1917	PRO	P2136	E2309	GLU	GLU	GLN
L1784	GLN	K1917	HIS	F2137	L2321	ARG	ARG	ARG
L1785	SER	M1918	ILE	ALA	L2339	GLU	GLU	ALA
L1786	GLU	Q1919	ILE	E1987	L2355	GLU	GLU	GLN
K1787	SER	C1920	MET	E1988	L2359	PRO	PRO	GLU
K1788	GLU	F1921	PRO	F1991	T2359	ASP	ASP	GLY
L1789	THR	G1922	SER	M1995	ALA	ASP	ASP	SER
I1795	ALA	G1923	ALA	R2002	TYR	ALA	ALA	ALA
K1798	G1859	E1924	I1987	M2007	E2008	GLU	GLU	ALA
R1799	S1860	Y1925	E1988	E2009	Y2010	GLU	GLU	GLN
F1800	T1861	M1926	V1991	F2010	Q2011	PRO	PRO	GLU
D1801	K1862	G1927	M1995	Q2011		TYR	TYR	ASP
Y1802	R1864	E1928	M1995			GLU	GLU	GLY
D1803	L1869	F1930	R2002			GLN	GLN	SER
W1804	V1870	D1931	M2007			ARG	ARG	ALA
E1805	H1871	H1932	E2008			ALA	ALA	ALA
R1806	S1872	M1933	Y2009			GLN	GLN	ALA
E1807	G1873	M1934	F2010			GLU	GLU	ALA
C1808	Q1874	K1935	Q2011			GLY	GLY	ALA
A1809	A1875	R1936				ASP	ASP	ALA
I1810	S1876	M1937				ASP	ASP	ALA
K1811		S1938						
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 (Å)	372.73602, 372.73602, 372.73602	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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.

All (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
1:A:1132:ARG:HH22	1:A:1134:ASN:HB2	1.56	0.70
1:A:1811:LYS:NZ	1:A:1945:TRP:O	2.24	0.70
1:A:508:LEU:HD11	1:A:544:ARG:HH12	1.58	0.69
1:A:1653:HIS:HD2	1:A:1991:VAL:HG22	1.57	0.69
1:A:702:SER:HA	1:A:742:ARG:HH12	1.58	0.68
1:A:1136:LEU:HB3	1:A:1144:ARG:HE	1.58	0.68
1:A:846:GLU:HA	1:A:849:ARG:HD3	1.77	0.67
1:A:1869:LEU:HD12	1:A:1950:ILE:HB	1.76	0.67
1:A:2045:ILE:HG21	1:A:2084:VAL:HG13	1.77	0.66
1:A:2067:ALA:HA	1:A:2070:TRP:HD1	1.61	0.66
1:A:1452:GLU:O	1:A:1457:ASN:ND2	2.23	0.65
1:A:1333:GLN:HB2	1:A:1378:LEU:HG	1.79	0.64
1:A:729:PRO:HB3	1:A:777:VAL:HG22	1.79	0.64
1:A:495:ALA:HB2	1:A:507:VAL:HG11	1.79	0.64
1:A:1380:ARG:HH21	1:A:1429:GLY:HA2	1.62	0.64
1:A:620:LEU:HD22	1:A:657:ARG:HD2	1.81	0.63
1:A:1664:PRO:HB2	1:A:1667:PHE:HB3	1.81	0.63
1:A:1863:TYR:HB3	1:A:1953:TYR:HB3	1.82	0.62
1:A:406:GLN:HE21	1:A:408:GLN:HE22	1.47	0.62
1:A:779:ILE:HG23	1:A:780:GLN:HG3	1.81	0.62
1:A:717:LYS:NZ	1:A:751:GLU:OE1	2.27	0.61
1:A:1041:ARG:HH22	1:A:1143:THR:HG22	1.66	0.61
1:A:337:LYS:O	1:A:341:ARG:HG2	2.01	0.61
1:A:805:GLN:O	1:A:808:GLN:NE2	2.33	0.61
1:A:2007:MET:O	1:A:2011:GLN:NE2	2.34	0.61
1:A:855:THR:HA	1:A:858:ARG:HG2	1.82	0.61
1:A:1435:LYS:HD2	1:A:1503:GLU:HB3	1.83	0.61
1:A:2209:SER:O	1:A:2288:LYS:NZ	2.32	0.61
1:A:1820:ARG:NH2	1:A:1911:ASP:O	2.34	0.60
1:A:755:VAL:HG23	1:A:762:MET:HB3	1.84	0.59
1:A:1707:PRO:HB3	1:A:1969:ILE:HD12	1.83	0.59
1:A:1267:ILE:HG22	1:A:1275:ASN:HD22	1.67	0.59
1:A:1084:SER:HB3	1:A:1087:GLN:HG2	1.84	0.59
1:A:1149:LEU:HG	1:A:1153:LYS:NZ	2.18	0.58
1:A:735:ASN:OD1	1:A:738:LYS:NZ	2.36	0.58
1:A:2046:GLN:HB3	1:A:2050:ARG:HH12	1.68	0.58
1:A:2117:ALA:HB1	1:A:2181:LEU:HB2	1.84	0.58
1:A:1461:GLU:O	1:A:1465:ASP:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:TRP:HE1	1:A:475:SER:HG	1.49	0.58
1:A:1475:LEU:HD11	1:A:1526:MET:HA	1.84	0.58
1:A:1520:VAL:HG13	1:A:2047:LEU:HD12	1.86	0.58
1:A:457:ALA:HA	1:A:460:PHE:HD2	1.68	0.58
1:A:754:LEU:HD22	1:A:763:MET:HA	1.85	0.58
1:A:509:ASN:O	1:A:513:ASN:ND2	2.37	0.57
1:A:1083:PRO:HD2	1:A:1084:SER:H	1.69	0.57
1:A:672:LEU:HB3	1:A:711:LEU:HG	1.86	0.57
1:A:1446:LYS:O	1:A:1515:ASN:ND2	2.37	0.57
1:A:536:LEU:O	1:A:548:LYS:NZ	2.38	0.57
1:A:705:MET:HE1	1:A:719:PHE:HZ	1.70	0.57
1:A:1653:HIS:CD2	1:A:1991:VAL:HG22	2.38	0.57
1:A:2387:CYS:O	1:A:2391:MET:HG3	2.03	0.57
1:A:557:GLU:HA	1:A:560:ARG:HD3	1.86	0.57
1:A:1159:LEU:HA	1:A:1162:ILE:HG22	1.86	0.57
1:A:552:ILE:HD11	1:A:573:ILE:HG23	1.87	0.57
1:A:1687:LEU:HD11	1:A:1739:THR:HG21	1.88	0.56
1:A:1140:ASP:OD1	1:A:1141:MET:N	2.38	0.56
1:A:1441:GLN:HB3	1:A:1445:LYS:HB2	1.87	0.56
1:A:454:ALA:HA	1:A:494:LEU:HD23	1.87	0.56
1:A:1144:ARG:HH12	1:A:1258:PHE:HE2	1.53	0.56
1:A:409:TYR:HD1	1:A:412:LYS:HZ1	1.54	0.56
1:A:779:ILE:O	1:A:849:ARG:NH1	2.39	0.55
1:A:1344:CYS:HB2	1:A:1349:PRO:HG2	1.88	0.55
1:A:1569:ASN:OD1	1:A:1570:SER:N	2.39	0.55
1:A:716:ASN:HA	1:A:719:PHE:CE1	2.42	0.55
1:A:1931:ASP:OD2	1:A:1936:ARG:NH2	2.40	0.55
1:A:1577:MET:HG3	1:A:1884:ILE:HG21	1.88	0.54
1:A:2172:GLY:O	1:A:2173:ARG:HG2	2.06	0.54
1:A:1987:ILE:O	1:A:1988:GLU:HG3	2.06	0.54
1:A:345:ILE:HG22	1:A:347:SER:H	1.72	0.54
1:A:700:TRP:HE1	1:A:704:LEU:HD12	1.73	0.54
1:A:704:LEU:HD21	1:A:710:ASP:HB2	1.90	0.54
1:A:1456:ALA:O	1:A:1458:LEU:N	2.41	0.54
1:A:1588:ILE:O	1:A:1648:GLN:NE2	2.30	0.54
1:A:1917:LYS:HA	1:A:1921:PHE:HB2	1.90	0.54
1:A:2236:ILE:HD13	1:A:2279:LEU:HD11	1.89	0.54
1:A:505:HIS:O	1:A:509:ASN:ND2	2.37	0.53
1:A:662:ARG:O	1:A:666:LYS:HG2	2.07	0.53
1:A:1581:ILE:HG22	1:A:1651:PHE:HE2	1.73	0.53
1:A:741:GLU:HG2	1:A:792:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1251:CYS:HB2	1:A:1268:TYR:HE1	1.73	0.53
1:A:492:ARG:NH1	1:A:496:GLU:OE2	2.42	0.53
1:A:1873:GLY:HA3	1:A:1878:GLY:HA2	1.89	0.53
1:A:496:GLU:OE2	1:A:538:TYR:OH	2.26	0.53
1:A:489:GLU:OE2	1:A:493:ARG:NH1	2.38	0.53
1:A:790:ILE:HG12	1:A:856:VAL:HG22	1.90	0.53
1:A:1061:CYS:HB3	1:A:1116:HIS:HB3	1.91	0.53
1:A:2355:ILE:HD13	1:A:2401:ALA:HB2	1.91	0.53
1:A:1520:VAL:HG22	1:A:2047:LEU:HD13	1.91	0.53
1:A:567:ILE:HG22	1:A:571:LYS:HZ3	1.74	0.53
1:A:563:ASP:HB3	1:A:565:TRP:NE1	2.24	0.52
1:A:1643:VAL:HG22	1:A:1671:PHE:CE1	2.44	0.52
1:A:2160:VAL:O	1:A:2178:TYR:OH	2.23	0.52
1:A:729:PRO:HG3	1:A:776:ARG:HG3	1.91	0.52
1:A:1333:GLN:HG2	1:A:1374:ASP:HB3	1.90	0.52
1:A:2117:ALA:HA	1:A:2181:LEU:HD12	1.91	0.52
1:A:1468:PHE:HB3	1:A:1471:SER:HB2	1.92	0.52
1:A:781:SER:H	1:A:852:ARG:HH12	1.58	0.52
1:A:780:GLN:HG2	1:A:849:ARG:NH2	2.25	0.51
1:A:1656:ALA:HB3	1:A:1991:VAL:HG11	1.91	0.51
1:A:1239:ILE:HG21	1:A:1306:LEU:HD11	1.92	0.51
1:A:1467:ILE:HG21	1:A:1502:PHE:HE1	1.74	0.51
1:A:2007:MET:HG2	1:A:2011:GLN:NE2	2.21	0.51
1:A:865:ASP:OD1	1:A:866:SER:N	2.43	0.51
1:A:724:VAL:HG21	1:A:743:PHE:HE1	1.74	0.51
1:A:451:ASP:OD1	1:A:452:LEU:N	2.44	0.51
1:A:567:ILE:HG22	1:A:571:LYS:NZ	2.25	0.51
1:A:1550:PRO:HB3	1:A:2002:ARG:HH12	1.74	0.51
1:A:1330:GLN:O	1:A:1333:GLN:HG3	2.10	0.51
1:A:1525:GLU:HA	1:A:1529:ILE:HB	1.93	0.50
1:A:340:LEU:HD23	1:A:341:ARG:HH12	1.76	0.50
1:A:553:ASP:HA	1:A:556:ILE:HD12	1.93	0.50
1:A:1040:ALA:O	1:A:1044:MET:HG3	2.12	0.50
1:A:2168:VAL:HG13	1:A:2175:LEU:HD21	1.93	0.50
1:A:2321:LEU:HD21	1:A:2339:LEU:HD22	1.94	0.50
1:A:544:ARG:HA	1:A:547:GLN:HE21	1.77	0.49
1:A:744:PHE:CE1	1:A:770:GLY:HA3	2.48	0.49
1:A:1520:VAL:HG21	1:A:2043:ILE:HG22	1.94	0.49
1:A:748:ASN:HB3	1:A:754:LEU:HG	1.94	0.49
1:A:1247:TRP:O	1:A:1268:TYR:OH	2.27	0.49
1:A:1307:SER:O	1:A:1313:GLN:NE2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ILE:HG23	1:A:395:ILE:HB	1.95	0.49
1:A:1263:GLU:O	1:A:1267:ILE:HD12	2.12	0.49
1:A:1579:PRO:HA	1:A:1582:ARG:HG2	1.93	0.49
1:A:1333:GLN:O	1:A:1378:LEU:HD21	2.12	0.49
1:A:1642:GLY:O	1:A:1646:HIS:ND1	2.34	0.49
1:A:662:ARG:HA	1:A:662:ARG:NE	2.27	0.49
1:A:1240:ARG:O	1:A:1243:GLN:HG3	2.12	0.49
1:A:1248:ALA:HB1	1:A:1254:LEU:HA	1.94	0.49
1:A:1262:GLU:O	1:A:1265:THR:OG1	2.27	0.49
1:A:1731:TYR:HH	1:A:1771:CYS:HG	1.49	0.49
1:A:1896:ARG:HH21	1:A:1907:GLU:HG2	1.77	0.49
1:A:381:LEU:HD11	1:A:386:MET:HE2	1.96	0.48
1:A:1243:GLN:O	1:A:1247:TRP:HD1	1.95	0.48
1:A:1536:CYS:HB2	1:A:2099:ARG:HH22	1.78	0.48
1:A:2359:LEU:HD22	1:A:2391:MET:HE2	1.94	0.48
1:A:678:LYS:O	1:A:682:LYS:HG2	2.12	0.48
1:A:2176:GLN:O	1:A:2180:ASN:HB2	2.14	0.48
1:A:1567:TYR:CZ	1:A:1684:HIS:HB2	2.48	0.48
1:A:1650:ILE:HD11	1:A:1667:PHE:HB2	1.95	0.48
1:A:2062:VAL:HG23	1:A:2063:VAL:HG23	1.95	0.48
1:A:400:LEU:HD23	1:A:404:LEU:HD21	1.95	0.48
1:A:1152:LEU:HB3	1:A:1287:GLU:HG3	1.96	0.48
1:A:1290:GLU:CD	1:A:1335:GLN:HE22	2.17	0.48
1:A:1639:TYR:O	1:A:1643:VAL:HG23	2.14	0.48
1:A:516:HIS:HB3	1:A:565:TRP:CZ3	2.49	0.48
1:A:1560:LYS:HB2	1:A:1663:VAL:HG22	1.95	0.48
1:A:741:GLU:HG2	1:A:792:LEU:HD21	1.96	0.48
1:A:1139:ALA:HB1	1:A:1144:ARG:HG2	1.96	0.47
1:A:1366:ARG:HD2	1:A:1426:ILE:HD13	1.96	0.47
1:A:658:LEU:O	1:A:662:ARG:HG2	2.14	0.47
1:A:1021:LEU:HG	1:A:1044:MET:HE3	1.95	0.47
1:A:2046:GLN:HB3	1:A:2050:ARG:NH1	2.29	0.47
1:A:791:ASP:O	1:A:794:LYS:HG3	2.14	0.47
1:A:1080:PHE:HE1	1:A:1091:LEU:HD22	1.78	0.47
1:A:1309:GLU:O	1:A:1313:GLN:NE2	2.47	0.47
1:A:1012:SER:OG	1:A:1013:LEU:N	2.47	0.47
1:A:336:LEU:HD11	1:A:386:MET:HE1	1.95	0.47
1:A:396:LEU:HD11	1:A:430:ASP:HB3	1.95	0.47
1:A:1049:PRO:HB3	1:A:1094:VAL:HG23	1.97	0.47
1:A:1323:CYS:SG	1:A:1324:HIS:N	2.88	0.47
1:A:800:LEU:HD11	1:A:808:GLN:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1448:HIS:HA	1:A:1452:GLU:HB2	1.97	0.47
1:A:390:ILE:HG12	1:A:395:ILE:HD12	1.97	0.47
1:A:842:CYS:HA	1:A:845:GLN:HE22	1.80	0.47
1:A:1502:PHE:CD2	1:A:2012:PHE:HB2	2.50	0.47
1:A:1885:ILE:O	1:A:1887:ARG:NH1	2.48	0.47
1:A:1467:ILE:HG21	1:A:1502:PHE:CE1	2.50	0.46
1:A:1815:TYR:HD1	1:A:1923:GLY:HA3	1.81	0.46
1:A:1083:PRO:HD2	1:A:1084:SER:N	2.29	0.46
1:A:755:VAL:O	1:A:762:MET:N	2.42	0.46
1:A:450:HIS:ND1	1:A:490:LEU:HD22	2.30	0.46
1:A:776:ARG:HH11	1:A:776:ARG:HG2	1.80	0.46
1:A:402:ASP:O	1:A:405:HIS:ND1	2.39	0.46
1:A:606:LEU:HD13	1:A:612:LEU:HG	1.98	0.46
1:A:775:TRP:HA	1:A:778:VAL:HG12	1.98	0.46
1:A:1458:LEU:HD22	1:A:1508:LEU:HD11	1.98	0.46
1:A:2085:ARG:NH1	1:A:2130:ASP:OD2	2.48	0.46
1:A:328:VAL:O	1:A:331:LEU:HG	2.16	0.45
1:A:702:SER:O	1:A:742:ARG:NH1	2.49	0.45
1:A:1445:LYS:C	1:A:1447:PHE:H	2.19	0.45
1:A:1664:PRO:HG2	1:A:1668:TRP:CE2	2.51	0.45
1:A:1658:ARG:N	1:A:1995:ASN:OD1	2.42	0.45
1:A:1591:THR:O	1:A:1645:ARG:NH1	2.49	0.45
1:A:711:LEU:O	1:A:715:ILE:HB	2.16	0.45
1:A:1383:LEU:HD22	1:A:1440:PHE:HE2	1.81	0.45
1:A:1568:MET:O	1:A:1572:ILE:HG12	2.16	0.45
1:A:2165:ARG:O	1:A:2215:GLY:HA3	2.16	0.45
1:A:1694:VAL:HG12	1:A:1710:LEU:HD23	1.99	0.45
1:A:2035:PRO:O	1:A:2039:GLU:HG3	2.16	0.45
1:A:1924:GLU:HG2	1:A:1943:LYS:HG2	1.99	0.45
1:A:355:LEU:HD23	1:A:412:LYS:HE2	1.99	0.44
1:A:1091:LEU:HA	1:A:1094:VAL:HG12	1.99	0.44
1:A:1740:LEU:HD23	1:A:1795:ILE:HG12	1.98	0.44
1:A:1742:VAL:HB	1:A:1753:SER:HB2	1.99	0.44
1:A:1149:LEU:HB2	1:A:1284:VAL:HG22	1.98	0.44
1:A:1145:ARG:NE	1:A:1281:ASP:OD1	2.49	0.44
1:A:2094:PHE:HB3	1:A:2136:PRO:HB2	1.99	0.44
1:A:508:LEU:HD23	1:A:511:LEU:HD12	2.00	0.44
1:A:744:PHE:HE2	1:A:774:LEU:HD22	1.82	0.44
1:A:2034:LEU:HD12	1:A:2037:ALA:H	1.82	0.44
1:A:720:PHE:CD1	1:A:743:PHE:HD1	2.35	0.44
1:A:2052:LEU:HA	1:A:2056:GLY:HA3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2154:ASP:OD1	1:A:2195:GLN:NE2	2.33	0.44
1:A:625:GLU:O	1:A:629:LEU:HG	2.18	0.44
1:A:1554:LYS:NZ	1:A:1898:TYR:OH	2.40	0.44
1:A:1741:ASN:O	1:A:1757:TYR:OH	2.25	0.44
1:A:1251:CYS:HB2	1:A:1268:TYR:CE1	2.53	0.44
1:A:1531:THR:HG21	1:A:1537:GLU:HG2	2.00	0.43
1:A:1673:LEU:HG	1:A:1674:TRP:CD1	2.53	0.43
1:A:482:LYS:O	1:A:485:GLU:HG3	2.18	0.43
1:A:1140:ASP:HB3	1:A:1143:THR:HG23	1.99	0.43
1:A:1149:LEU:HG	1:A:1153:LYS:HZ2	1.82	0.43
1:A:1447:PHE:HB2	1:A:1512:CYS:SG	2.58	0.43
1:A:2376:SER:HB2	1:A:2384:ALA:HB2	2.00	0.43
1:A:444:ALA:O	1:A:447:LYS:HG3	2.18	0.43
1:A:749:CYS:SG	1:A:761:TYR:HD2	2.40	0.43
1:A:1502:PHE:CG	1:A:2012:PHE:HB2	2.53	0.43
1:A:2209:SER:HB2	1:A:2288:LYS:HZ3	1.83	0.43
1:A:737:MET:HE1	1:A:785:ILE:HG23	1.99	0.43
1:A:1641:ILE:HG22	1:A:1645:ARG:HH12	1.83	0.43
1:A:2296:SER:HB3	1:A:2299:THR:HG22	1.99	0.43
1:A:1080:PHE:CE1	1:A:1091:LEU:HD22	2.53	0.43
1:A:798:THR:HG21	1:A:863:GLU:HB2	2.00	0.43
1:A:2009:TYR:O	1:A:2013:MET:HG2	2.19	0.43
1:A:570:LEU:HD21	1:A:657:ARG:HA	2.00	0.43
1:A:2247:SER:HA	1:A:2309:GLU:OE1	2.18	0.43
1:A:1820:ARG:NH2	1:A:1916:MET:SD	2.92	0.43
1:A:2081:SER:OG	1:A:2084:VAL:HB	2.18	0.43
1:A:1126:VAL:O	1:A:1129:MET:HB3	2.19	0.43
1:A:1899:LYS:HE3	1:A:1901:ASP:HB3	2.01	0.42
1:A:2277:ASP:HA	1:A:2281:VAL:HB	2.00	0.42
1:A:1427:LEU:HD21	1:A:1491:VAL:HG12	2.00	0.42
1:A:516:HIS:HB3	1:A:565:TRP:HZ3	1.84	0.42
1:A:556:ILE:HA	1:A:559:LEU:HD23	2.00	0.42
1:A:622:THR:HA	1:A:625:GLU:HG2	2.01	0.42
1:A:851:VAL:HG21	1:A:1035:PRO:HB2	2.01	0.42
1:A:1314:THR:HG22	1:A:1318:ASP:OD2	2.18	0.42
1:A:483:GLN:O	1:A:486:LYS:HG3	2.20	0.42
1:A:745:LYS:HD3	1:A:761:TYR:CE1	2.55	0.42
1:A:1333:GLN:HA	1:A:1378:LEU:HD11	2.01	0.42
1:A:493:ARG:NH2	1:A:496:GLU:OE1	2.41	0.42
1:A:1247:TRP:HE1	1:A:1315:PHE:HB2	1.84	0.42
1:A:1286:CYS:O	1:A:1290:GLU:OE1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:LEU:HD22	1:A:532:HIS:ND1	2.35	0.42
1:A:574:ARG:HB2	1:A:660:PHE:HD1	1.85	0.42
1:A:1094:VAL:O	1:A:1098:LEU:HG	2.19	0.42
1:A:1027:LEU:HA	1:A:1030:SER:HB2	2.00	0.41
1:A:1127:LEU:O	1:A:1131:THR:HG23	2.20	0.41
1:A:1667:PHE:HD1	1:A:1668:TRP:HD1	1.68	0.41
1:A:1757:TYR:HD1	1:A:1784:LEU:HB2	1.85	0.41
1:A:1267:ILE:O	1:A:1275:ASN:ND2	2.52	0.41
1:A:1296:PHE:CE1	1:A:1303:LEU:HB3	2.55	0.41
1:A:1319:LEU:O	1:A:1329:ARG:HG2	2.19	0.41
1:A:1640:ASN:HB3	1:A:1700:ALA:HB2	2.02	0.41
1:A:2164:LEU:HD11	1:A:2208:VAL:HG21	2.03	0.41
1:A:1376:PHE:CG	1:A:1429:GLY:HA3	2.55	0.41
1:A:852:ARG:O	1:A:856:VAL:HG23	2.21	0.41
1:A:1442:THR:OG1	1:A:1443:SER:N	2.54	0.41
1:A:650:HIS:HD2	1:A:692:CYS:SG	2.44	0.41
1:A:1451:CYS:SG	1:A:1515:ASN:HA	2.61	0.41
1:A:2256:PRO:O	1:A:2258:PRO:HD3	2.21	0.41
1:A:398:ILE:O	1:A:401:ARG:HG2	2.20	0.41
1:A:858:ARG:HH21	1:A:1039:GLY:HA2	1.86	0.41
1:A:1495:PRO:N	1:A:1496:PRO:HD2	2.36	0.41
1:A:545:ASP:O	1:A:546:THR:OG1	2.27	0.41
1:A:603:ILE:HA	1:A:606:LEU:HG	2.03	0.41
1:A:620:LEU:HG	1:A:680:ILE:HD11	2.03	0.41
1:A:662:ARG:CZ	1:A:700:TRP:NE1	2.84	0.41
1:A:1326:LYS:HG3	1:A:1329:ARG:HH12	1.86	0.41
1:A:1789:LEU:HD11	1:A:1828:THR:HG21	2.03	0.41
1:A:1871:HIS:HE2	1:A:1878:GLY:HA3	1.85	0.41
1:A:559:LEU:HB2	1:A:566:VAL:HG12	2.03	0.41
1:A:1286:CYS:O	1:A:1289:LEU:HB2	2.21	0.41
1:A:1356:LEU:O	1:A:1359:THR:HG22	2.21	0.41
1:A:1357:LEU:O	1:A:1375:TYR:OH	2.30	0.41
1:A:2011:GLN:O	1:A:2015:LYS:HG2	2.20	0.41
1:A:1568:MET:HG2	1:A:1667:PHE:HE1	1.86	0.40
1:A:524:ILE:H	1:A:524:ILE:HD12	1.87	0.40
1:A:599:ARG:HA	1:A:602:LEU:HB2	2.03	0.40
1:A:2041:THR:HG22	1:A:2084:VAL:HG21	2.04	0.40
1:A:1763:LEU:HB3	1:A:1767:ASN:O	2.21	0.40
1:A:1887:ARG:H	1:A:1887:ARG:HG2	1.72	0.40
1:A:404:LEU:HD13	1:A:449:VAL:HG22	2.03	0.40

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. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	547	GLN

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Mol	Chain	Res	Type
1	A	716	ASN
1	A	845	GLN
1	A	1653	HIS
1	A	1994	GLN
1	A	2011	GLN
1	A	2408	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 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.

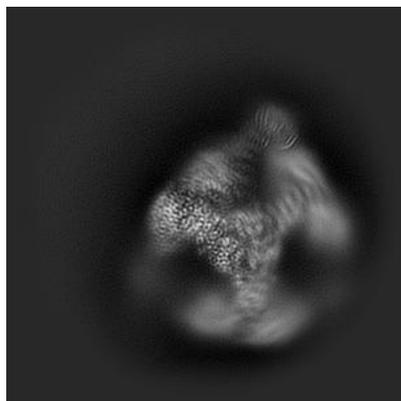
## 6 Map visualisation [i](#)

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.

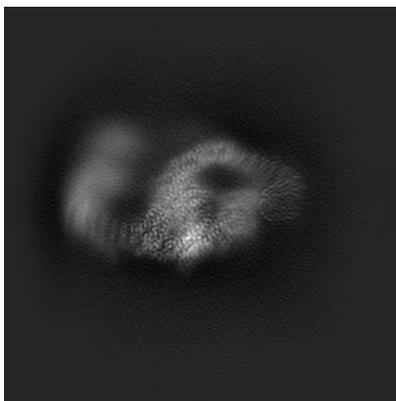
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

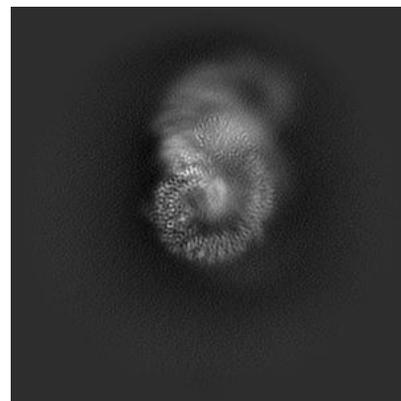
#### 6.1.1 Primary map



X

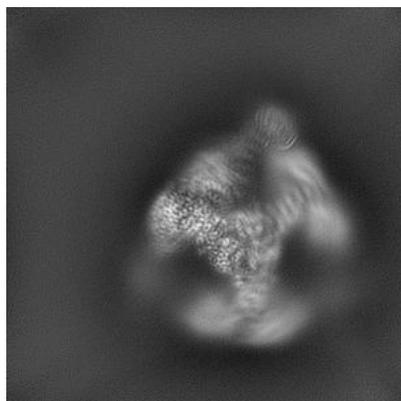


Y

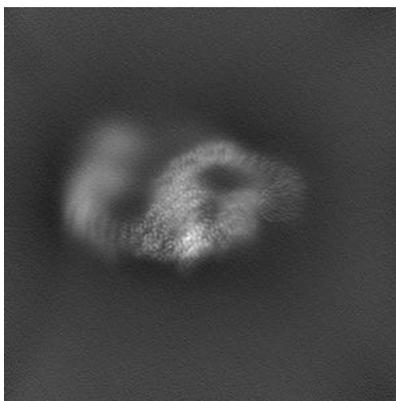


Z

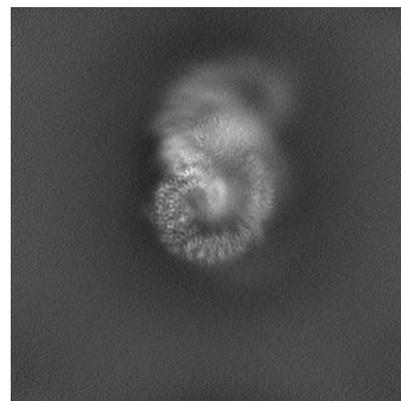
#### 6.1.2 Raw map



X



Y

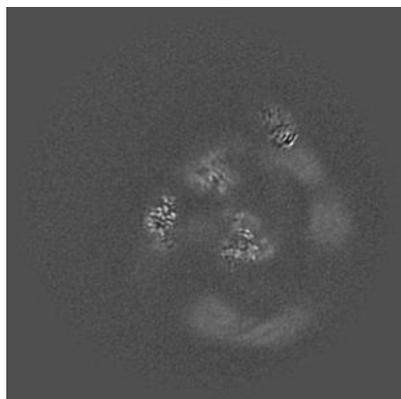


Z

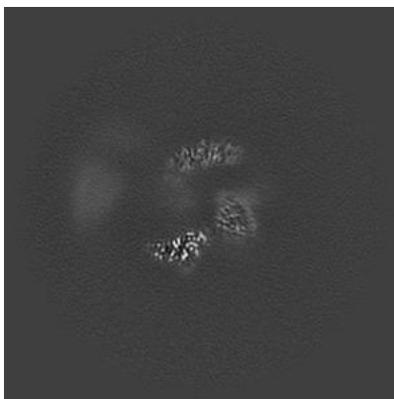
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

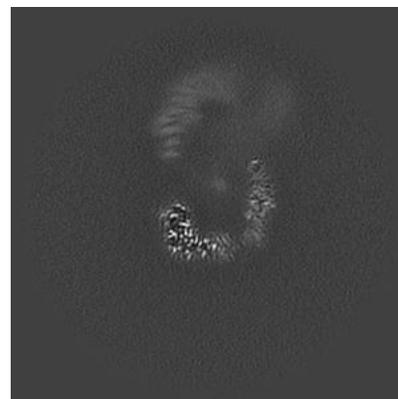
### 6.2.1 Primary map



X Index: 224

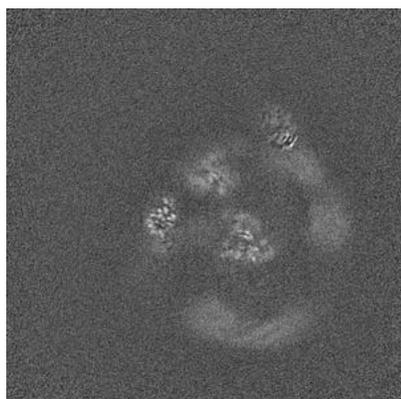


Y Index: 224

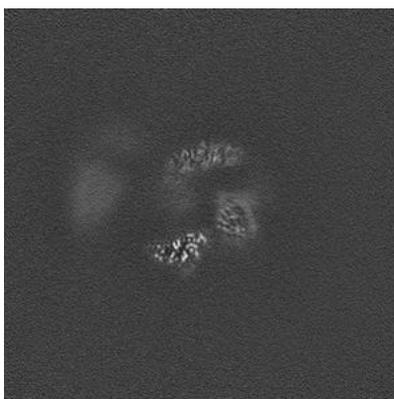


Z Index: 224

### 6.2.2 Raw map



X Index: 224



Y Index: 224

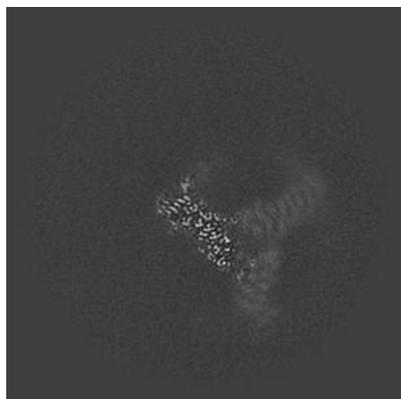


Z Index: 224

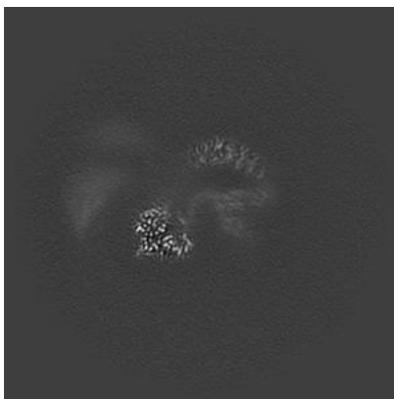
The images above show central slices of the map in three orthogonal directions.

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

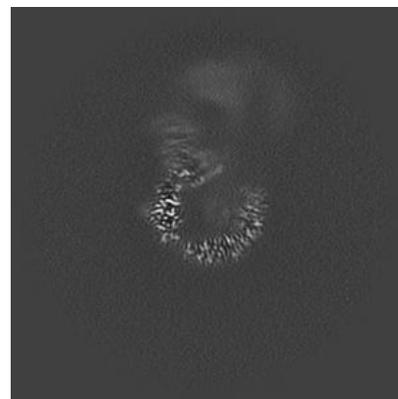
### 6.3.1 Primary map



X Index: 182

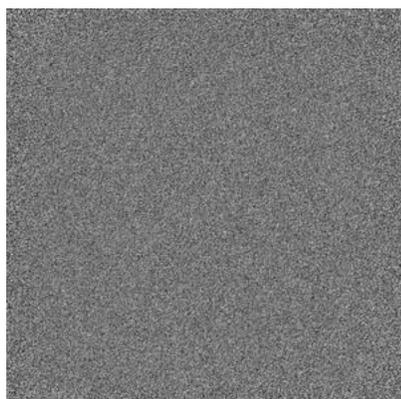


Y Index: 246

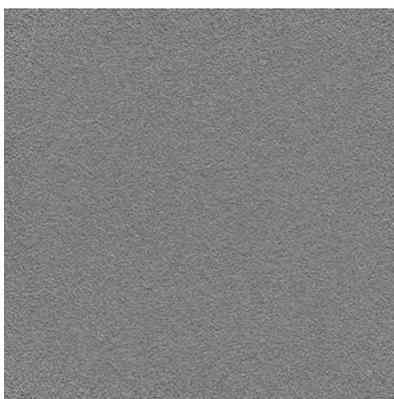


Z Index: 202

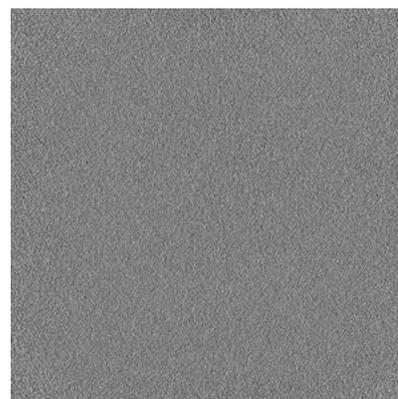
### 6.3.2 Raw map



X Index: 0



Y Index: 0

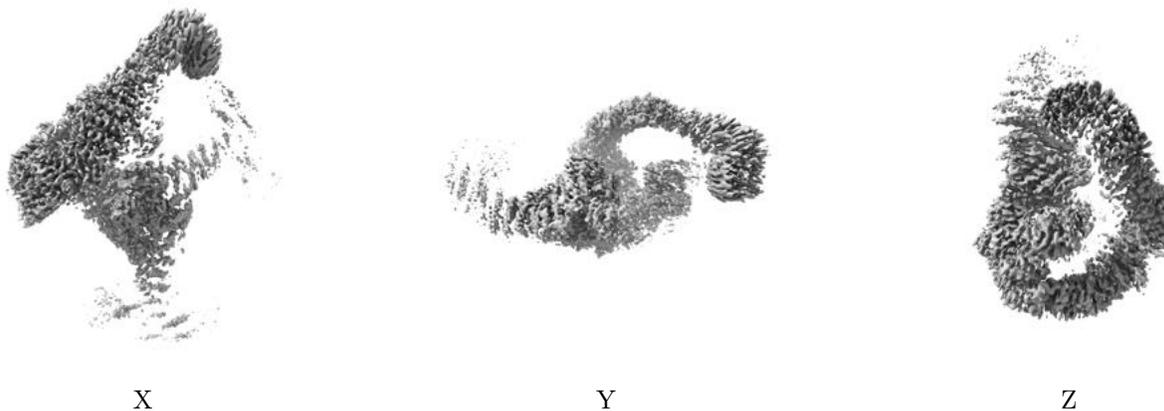


Z Index: 0

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

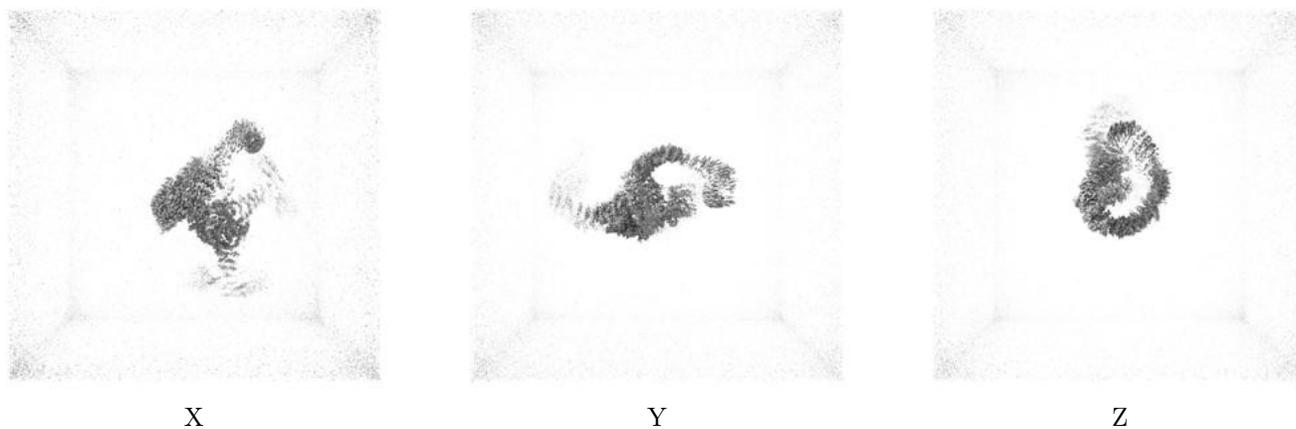
## 6.4 Orthogonal surface views [i](#)

### 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.

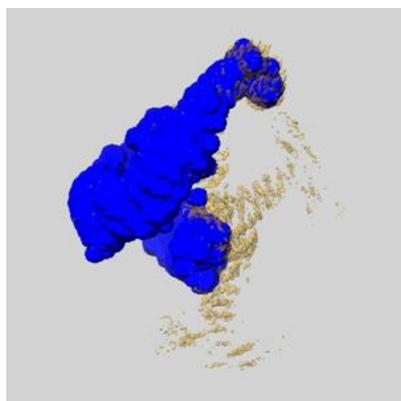
## 6.5 Mask visualisation [i](#)

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

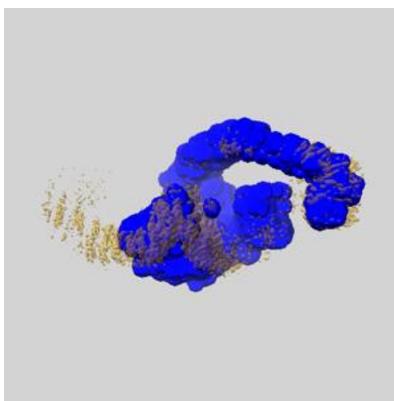
A mask typically either:

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

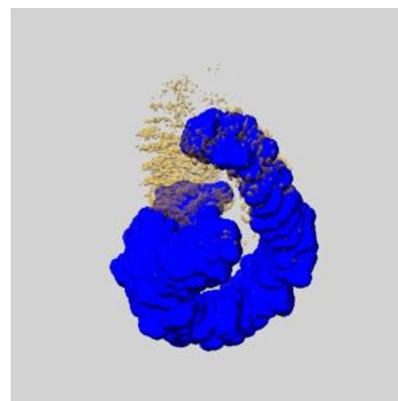
### 6.5.1 emd\_14369\_msk\_1.map [i](#)



X



Y

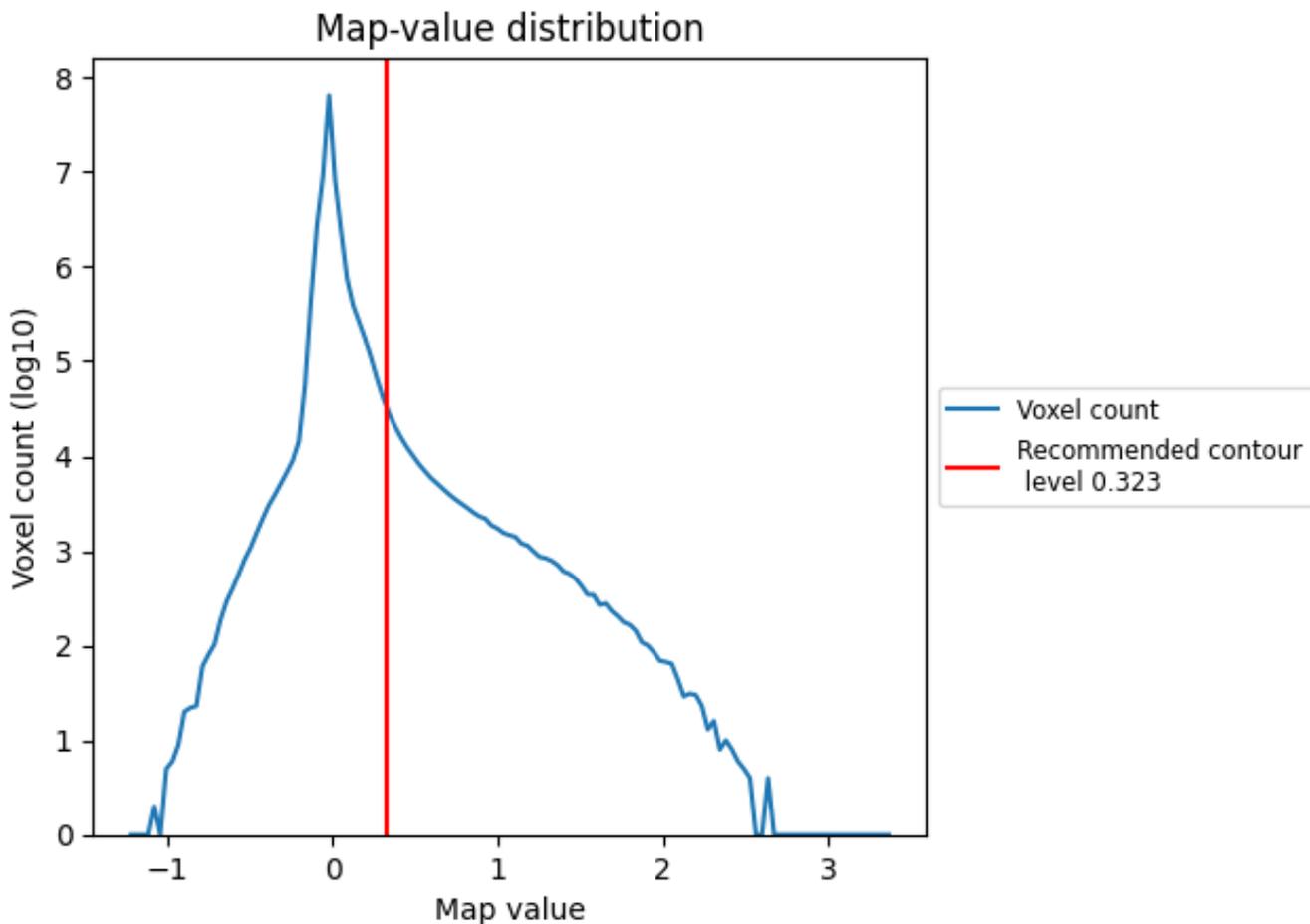


Z

## 7 Map analysis [i](#)

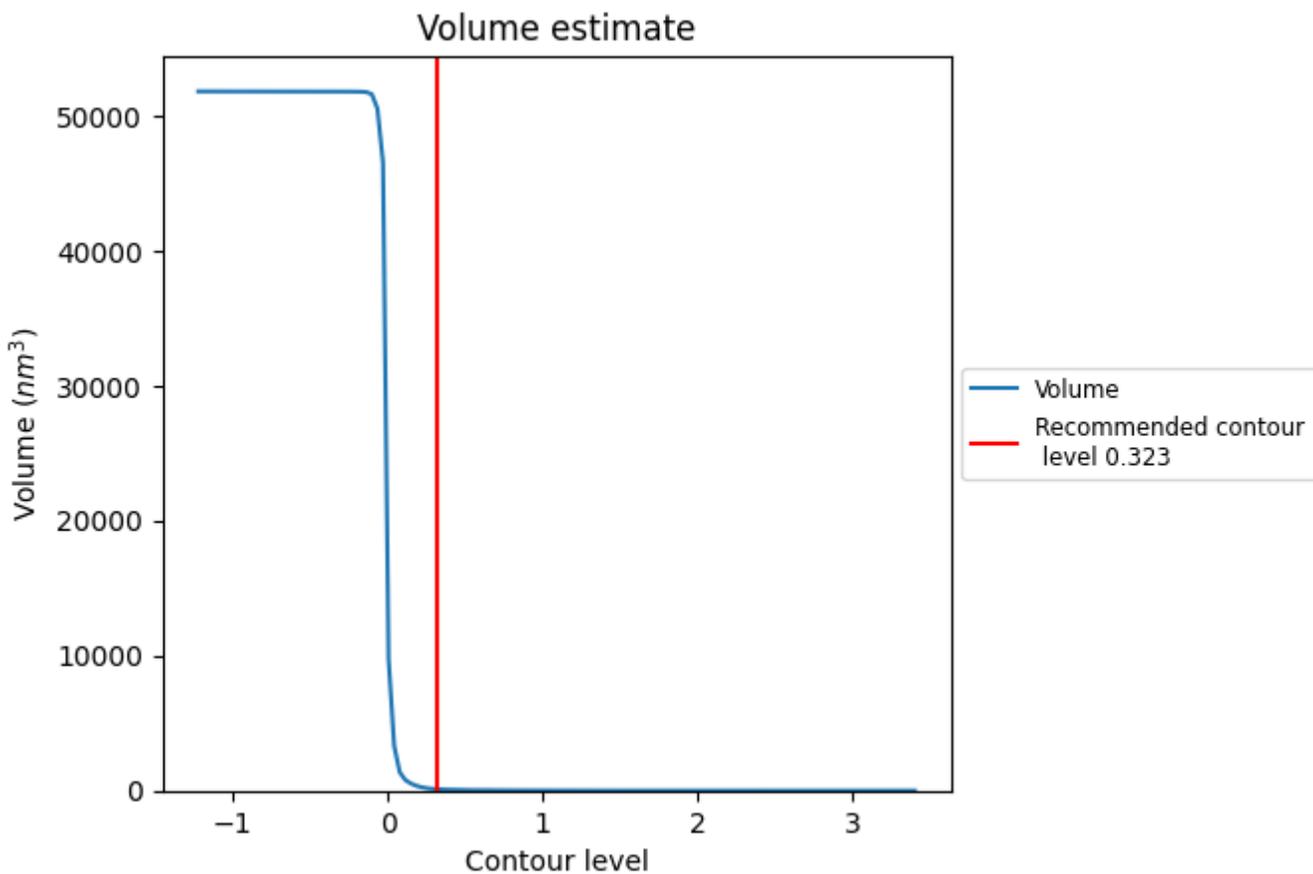
This section contains the results of statistical analysis of the map.

### 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.

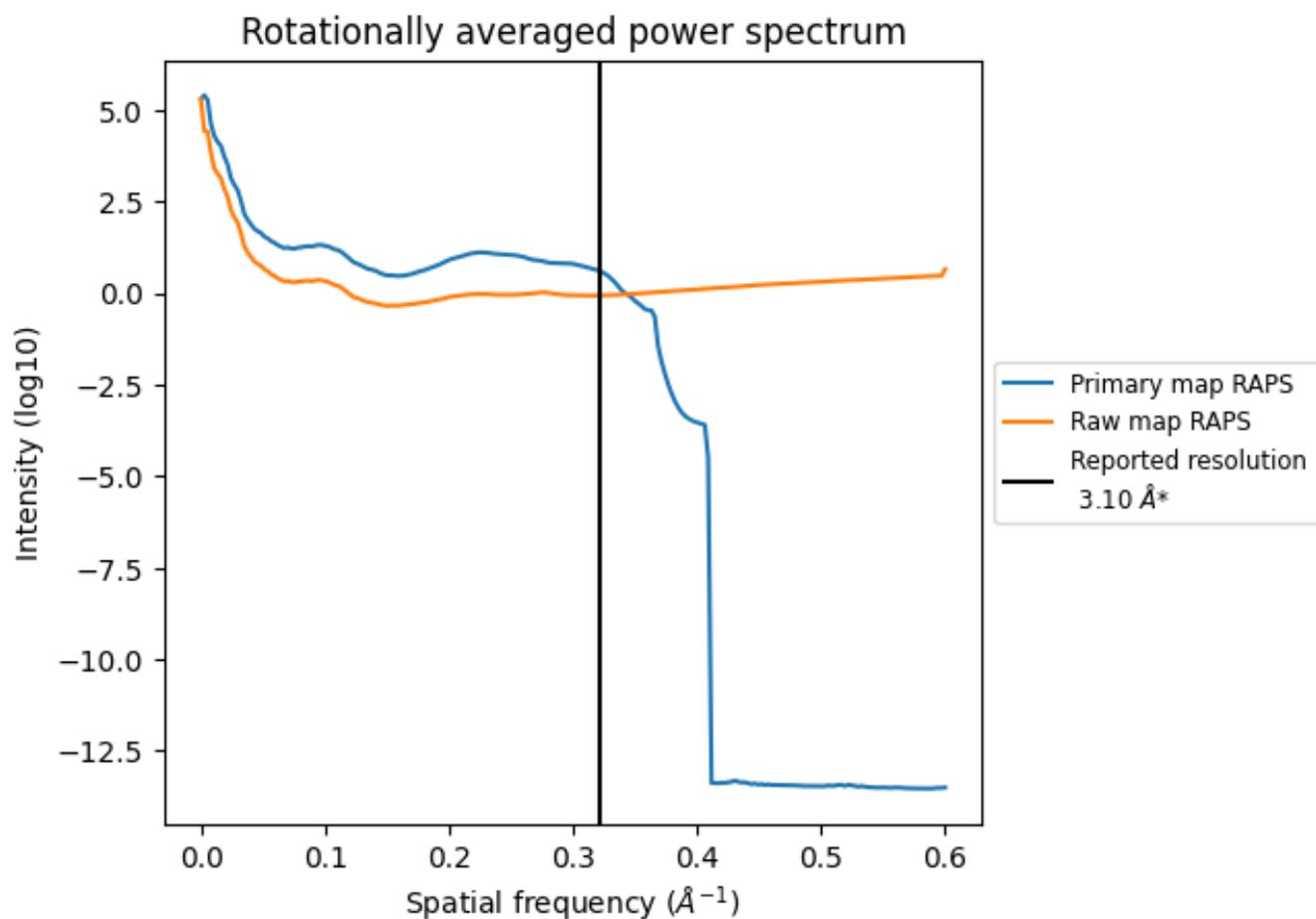
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 104 nm<sup>3</sup>; 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](#)

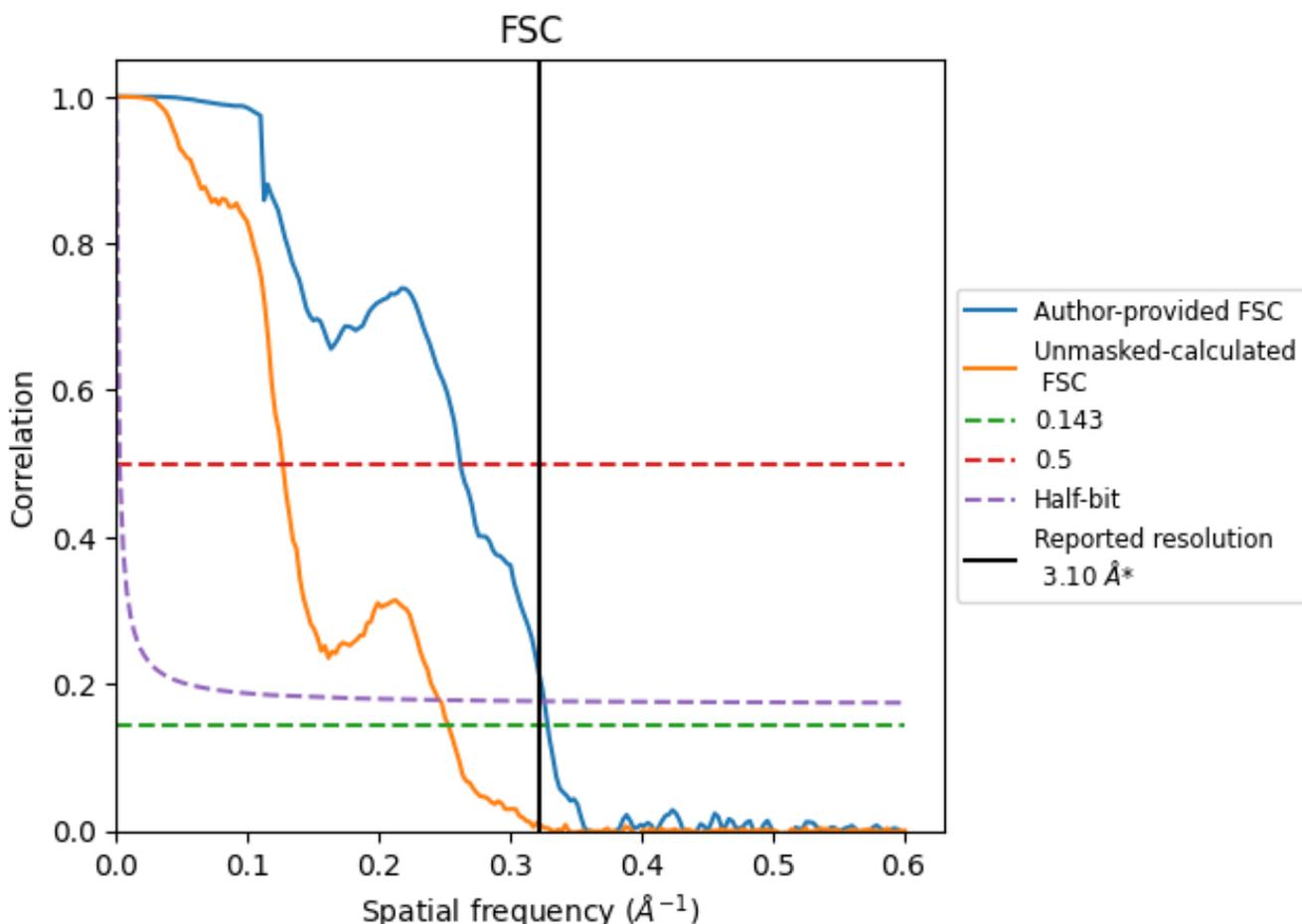


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 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<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

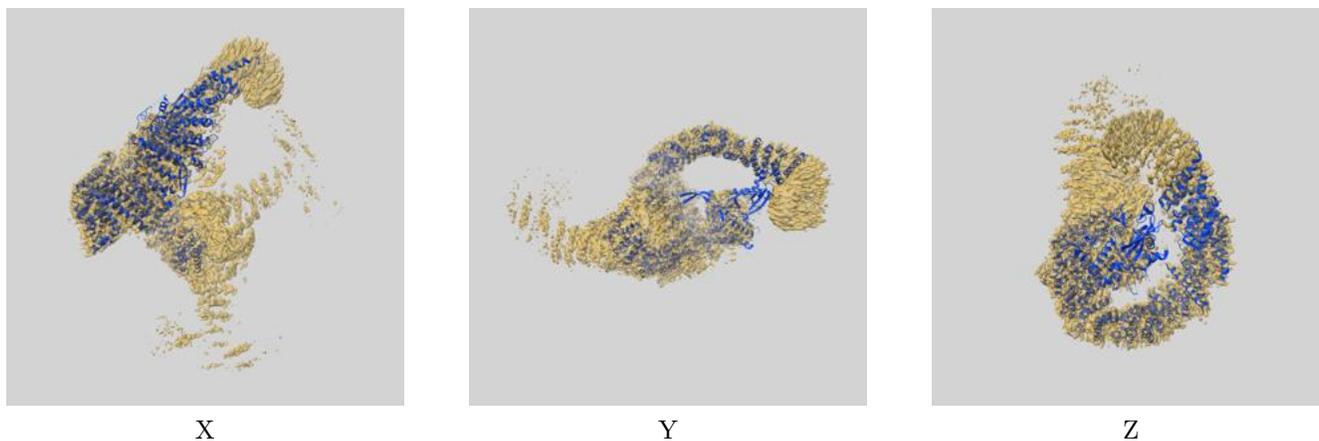
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.04	3.81	3.07
Unmasked-calculated*	3.95	7.88	4.06

\*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](#)

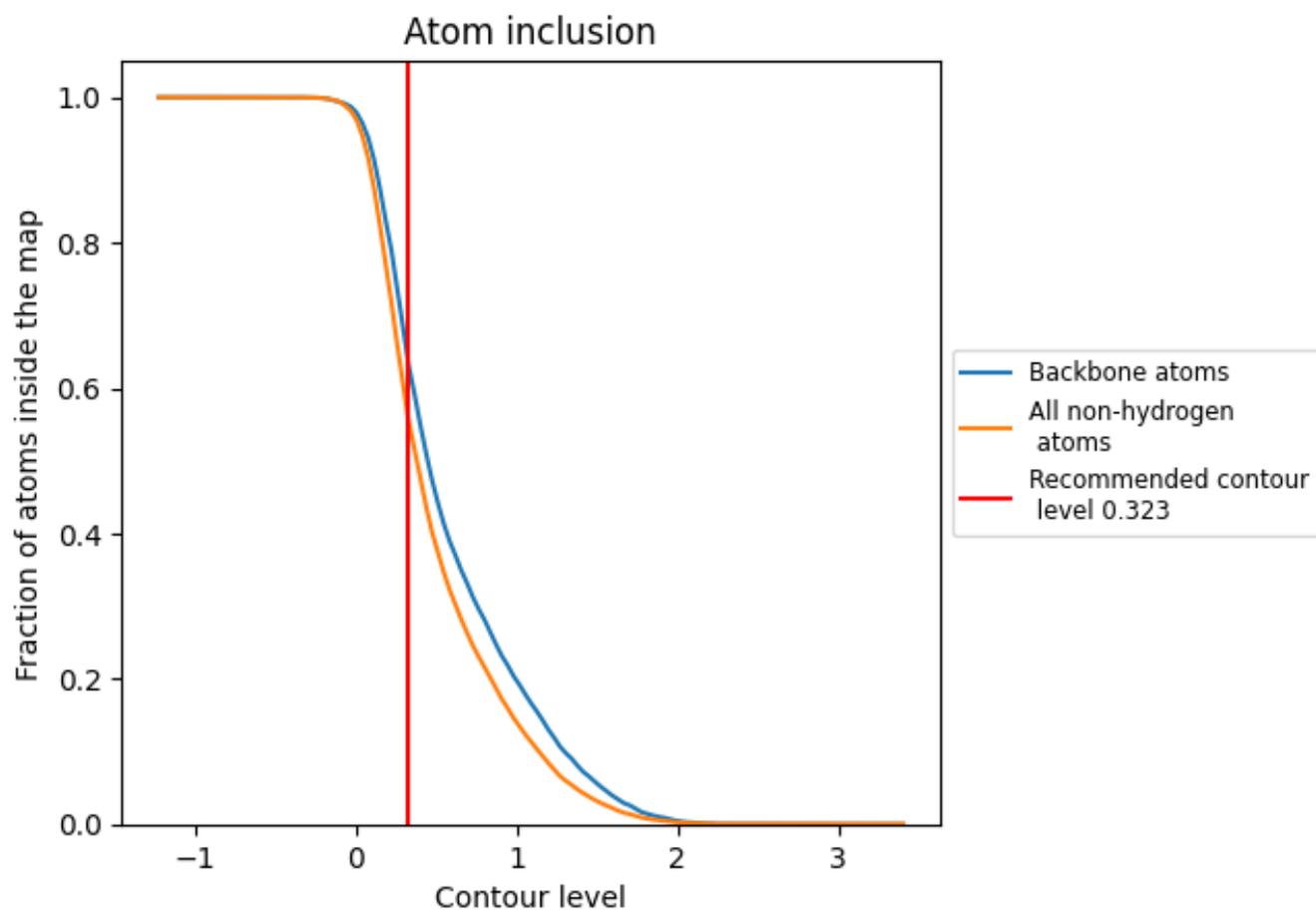
This section contains information regarding the fit between EMDB map EMD-14369 and PDB model 7YXY. Per-residue inclusion information can be found in section [3](#) on page [4](#).

### 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.