



wwPDB EM Validation Summary Report i

Sep 23, 2024 – 10:49 AM EDT

PDB ID : 8VDQ
EMDB ID : EMD-43155
Title : Cryogenic electron microscopy model of full-length talin
Authors : Izard, T.; Rangarajan, E.S.
Deposited on : 2023-12-17
Resolution : 5.50 Å(reported)
Based on initial model : 6r9t

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 i 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](#) ①) were used in the production of this report:

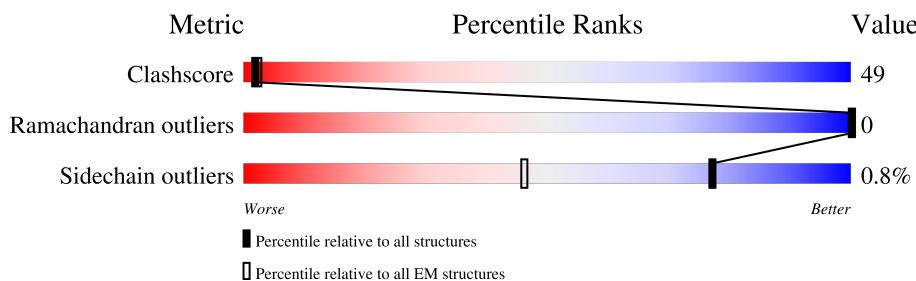
EMDB validation analysis : 0.0.1.dev112
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.3

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

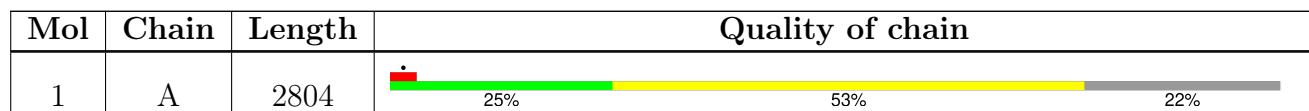
The reported resolution of this entry is 5.50 Å.

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	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 <=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.



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 16077 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 Green fluorescent protein, Talin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2192	16077	9904	2874	3221	78	0	0

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-262	MET	-	expression tag	UNP P42212
A	-261	HIS	-	expression tag	UNP P42212
A	-260	HIS	-	expression tag	UNP P42212
A	-259	HIS	-	expression tag	UNP P42212
A	-258	HIS	-	expression tag	UNP P42212
A	-257	HIS	-	expression tag	UNP P42212
A	-256	HIS	-	expression tag	UNP P42212
A	-255	HIS	-	expression tag	UNP P42212
A	-254	HIS	-	expression tag	UNP P42212
A	-253	HIS	-	expression tag	UNP P42212
A	-252	HIS	-	expression tag	UNP P42212
A	-251	MET	-	expression tag	UNP P42212
A	-250	VAL	-	expression tag	UNP P42212
A	-187	LEU	PHE	conflict	UNP P42212
A	-186	THR	SER	conflict	UNP P42212
A	-20	LEU	HIS	conflict	UNP P42212
A	-12	GLY	-	linker	UNP P42212
A	-11	SER	-	linker	UNP P42212
A	-10	LEU	-	linker	UNP P42212
A	-9	GLU	-	linker	UNP P42212
A	-8	VAL	-	linker	UNP P42212
A	-7	LEU	-	linker	UNP P42212
A	-6	PHE	-	linker	UNP P42212
A	-5	GLN	-	linker	UNP P42212
A	-4	GLY	-	linker	UNP P42212
A	-3	PRO	-	linker	UNP P42212
A	-2	ALA	-	linker	UNP P42212
A	-1	ALA	-	linker	UNP P42212

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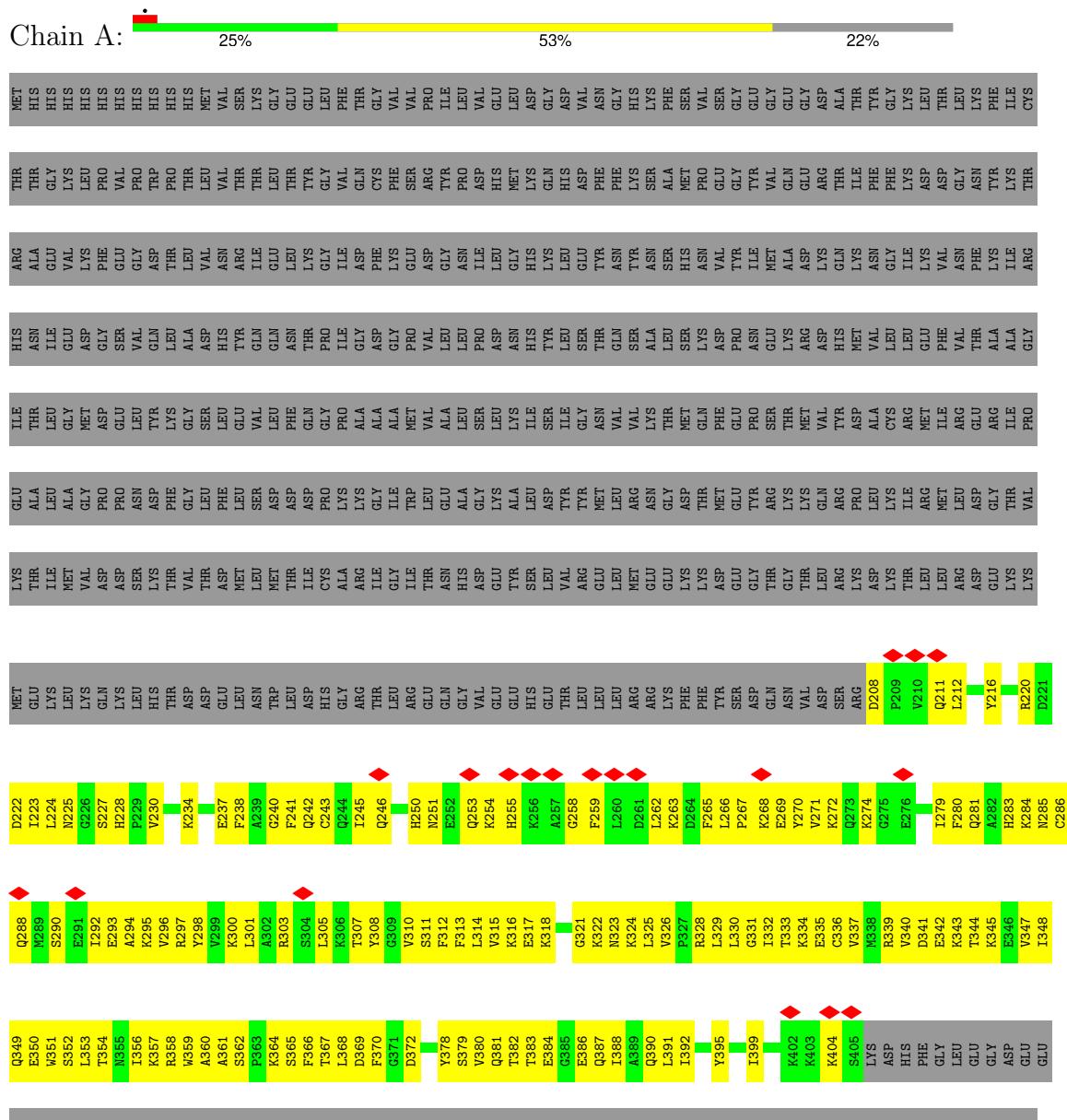
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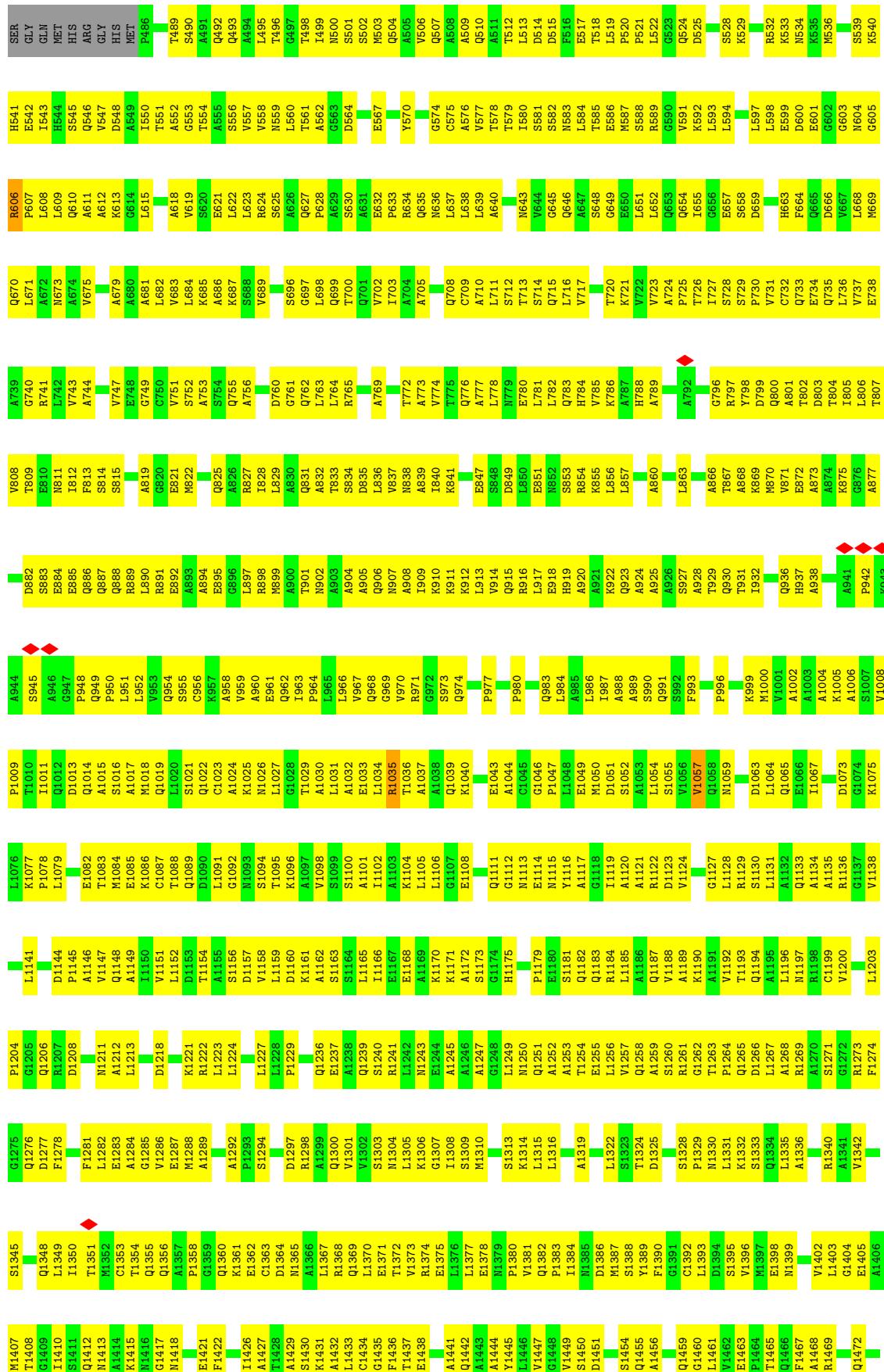
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	linker	UNP P42212
A	639	LEU	GLN	conflict	UNP P26039
A	673	ASN	LYS	conflict	UNP P26039
A	1227	LEU	SER	conflict	UNP P26039
A	2349	VAL	ALA	conflict	UNP P26039

3 Residue-property plots [\(i\)](#)

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: Green fluorescent protein, Talin-1





M1476	L1747	V1684	A1618	R1685	P1686	S1480
V1683	E1805	S1684	A1806	V1807	E1808	A1619
A1617	V1872	T1873	S1940	R1885	P1886	R1656
A1744	A1873	T1874	P1941	K1874	V1746	A1656
R1656	A1745	V1746	V1888	V1887	D1809	G1747
S1480	A1656	V1747	L1810	K1843	D1810	T1877
N1554	V1688	A1688	K1751	T1811	P1689	P1624
R1555	R1688	V1688	P1878	T1812	R1690	R1559
S1483	C1556	A1689	P1879	T1812	D1625	E1560
P1484	R1556	V1689	E1807	E1813	E1691	A1561
						T1487
M1477	A1656	V1692	L1754	S1753	E1693	T1652
A1477	A1656	V1692	E1814	H1754	P1627	P1622
N1555	V1693	A1693	K1755	T1755	P1628	P1563
R1556	R1693	V1693	E1815	P1756	E1629	P1564
S1485	C1556	A1694	P1884	P1756	V1630	V1491
P1486	R1557	V1694	E1816	Q1757	W1630	A1494
M1478	A1656	V1695	A1817	V1757	P1631	V1656
A1478	A1656	V1695	E1818	Q1757	E1696	A1495
N1556	V1696	A1697	K1758	T1758	P1633	V1659
R1557	R1696	V1697	E1819	P1759	W1633	V1492
S1486	C1557	A1698	S1886	S1886	E1760	V1659
P1487	R1558	V1698	N1852	N1852	V1760	V1493
M1479	A1656	V1699	A1820	V1820	P1761	V1659
A1479	A1656	V1699	E1821	E1821	E1762	V1659
N1557	V1700	A1701	K1759	T1759	P1762	V1659
R1558	R1700	V1701	E1822	E1822	E1763	V1659
S1487	C1558	A1702	P1882	P1882	E1764	A1574
P1488	R1559	V1702	E1823	E1823	E1765	F1575
M1480	A1656	V1703	A1824	V1824	P1763	V1659
A1480	A1656	V1703	E1825	E1825	E1766	V1659
N1558	V1704	A1704	K1760	T1760	P1767	V1659
R1559	R1704	V1704	E1826	E1826	E1767	V1659
S1488	C1559	A1705	P1883	P1883	E1768	A1576
P1489	R1560	V1705	E1827	E1827	E1769	F1576
M1481	A1656	V1706	A1828	V1828	P1768	V1659
A1481	A1656	V1706	E1829	E1829	E1770	V1659
N1559	V1707	A1707	K1764	T1764	P1769	V1659
R1560	R1707	V1707	E1830	E1830	E1771	A1577
S1489	C1560	A1708	P1884	P1884	E1772	F1577
P1490	R1561	V1708	E1831	E1831	E1773	V1659
M1482	A1656	V1709	A1832	V1832	P1770	V1659
A1482	A1656	V1709	E1832	E1832	E1774	V1659
N1560	V1710	A1710	K1765	T1765	P1771	V1659
R1561	R1710	V1710	E1833	E1833	E1775	A1578
S1491	C1561	A1711	P1885	P1885	E1776	F1578
P1492	R1562	V1711	E1834	E1834	E1777	V1659
M1483	A1656	V1712	A1835	V1835	P1772	V1659
A1483	A1656	V1712	E1835	E1835	E1778	V1659
N1562	V1713	A1713	K1766	T1766	P1773	V1659
R1563	R1713	V1713	E1836	E1836	E1779	A1579
S1493	C1563	A1714	P1886	P1886	E1780	F1579
P1494	R1564	V1714	E1837	E1837	E1781	V1659
M1484	A1656	V1715	A1838	V1838	P1774	V1659
A1484	A1656	V1715	E1838	E1838	E1782	V1659
N1563	V1716	A1716	K1767	T1767	P1775	V1659
R1564	R1716	V1716	E1839	E1839	E1783	A1580
S1495	C1564	A1717	P1887	P1887	E1784	F1580
P1496	R1565	V1717	E1840	E1840	E1785	V1659
M1485	A1656	V1718	A1841	V1841	P1776	V1659
A1485	A1656	V1718	E1841	E1841	E1786	V1659
N1566	V1719	A1719	K1768	T1768	P1777	V1659
R1567	R1719	V1719	E1842	E1842	E1787	A1581
S1496	C1567	A1720	P1888	P1888	E1788	F1582
P1497	R1568	V1720	E1843	E1843	E1789	V1659
M1486	A1656	V1721	A1844	V1844	P1778	V1659
A1486	A1656	V1721	E1844	E1844	E1790	V1659
N1567	V1722	A1722	K1769	T1769	P1779	V1659
R1568	R1722	V1722	E1845	E1845	E1791	A1583
S1497	C1568	A1723	P1889	P1889	E1792	F1583
P1498	R1569	V1723	E1846	E1846	E1793	V1659
M1487	A1656	V1724	A1847	V1847	P1780	V1659
A1487	A1656	V1724	E1847	E1847	E1794	V1659
N1568	V1725	A1725	K1770	T1770	P1781	V1659
R1569	R1725	V1725	E1848	E1848	E1795	A1584
S1498	C1569	A1726	P1890	P1890	E1796	F1584
P1499	R1570	V1726	E1849	E1849	E1797	V1659
M1488	A1656	V1727	A1849	V1849	P1782	V1659
A1488	A1656	V1727	E1849	E1849	E1798	V1659
N1569	V1728	A1728	K1771	T1771	P1783	V1659
R1570	R1728	V1728	E1850	E1850	E1799	A1585
S1499	C1570	A1729	P1891	P1891	E1800	F1585
P1500	R1571	V1729	E1851	E1851	E1790	V1659
M1489	A1656	V1730	A1851	V1851	P1784	V1659
A1489	A1656	V1730	E1851	E1851	E1791	V1659
N1570	V1731	A1731	K1772	T1772	P1785	V1659
R1571	R1731	V1731	E1852	E1852	E1792	A1586
S1500	C1571	A1732	P1892	P1892	E1801	F1586
P1501	R1572	V1732	E1853	E1853	E1793	V1659
M1490	A1656	V1733	A1853	V1853	P1786	V1659
A1490	A1656	V1733	E1853	E1853	E1794	V1659
N1571	V1734	A1734	K1773	T1773	P1787	V1659
R1572	R1734	V1734	E1854	E1854	E1795	A1587
S1502	C1572	A1735	P1894	P1894	E1802	F1587
P1503	R1573	V1735	E1855	E1855	E1796	V1659
M1491	A1656	V1736	A1855	V1855	P1788	V1659
A1491	A1656	V1736	E1855	E1855	E1797	V1659
N1572	V1737	A1737	K1774	T1774	P1789	V1659
R1573	R1737	V1737	E1856	E1856	E1798	A1588
S1503	C1573	A1738	P1896	P1896	E1803	F1588
P1504	R1574	V1738	E1857	E1857	E1799	V1659
M1492	A1656	V1739	A1857	V1857	P1790	V1659
A1492	A1656	V1739	E1857	E1857	E1804	V1659
N1573	V1740	A1740	K1775	T1775	P1791	V1659
R1574	R1740	V1740	E1858	E1858	E1805	A1589
S1505	C1574	A1741	P1898	P1898	E1806	F1589
P1506	R1575	V1741	E1859	E1859	E1807	V1659
M1493	A1656	V1742	A1859	V1859	P1792	V1659
A1493	A1656	V1742	E1859	E1859	E1808	V1659
N1574	V1743	A1743	K1776	T1776	P1793	V1659
R1575	R1743	V1743	E1860	E1860	E1809	A1590
S1506	C1575	A1744	P1900	P1900	E1810	F1590
P1507	R1576	V1744	E1861	E1861	E1811	V1659
M1494	A1656	V1745	A1861	V1861	P1794	V1659
A1494	A1656	V1745	E1861	E1861	E1812	V1659
N1575	V1746	A1746	K1777	T1777	P1795	V1659
R1576	R1746	V1746	E1862	E1862	E1813	A1591
S1507	C1576	A1747	P1901	P1901	E1814	F1591
P1508	R1577	V1747	E1863	E1863	E1815	V1659
M1495	A1656	V1748	A1863	V1863	P1796	V1659
A1495	A1656	V1748	E1863	E1863	E1816	V1659
N1576	V1749	A1749	K1778	T1778	P1797	V1659
R1577	R1749	V1749	E1864	E1864	E1817	A1592
S1508	C1577	A1750	P1902	P1902	E1818	F1592
P1509	R1578	V1750	E1865	E1865	E1819	V1659
M1496	A1656	V1751	A1865	V1865	P1798	V1659
A1496	A1656	V1751	E1865	E1865	E1820	V1659
N1577	V1752	A1752	K1779	T1779	P1799	V1659
R1578	R1752	V1752	E1866	E1866	E1821	A1593
S1509	C1578	A1753	P1903	P1903	E1822	F1593
P1510	R1579	V1753	E1867	E1867	E1823	V1659
M1497	A1656	V1754	A1867	V1867	P1800	V1659
A1497	A1656	V1754	E1867	E1867	E1824	V1659
N1578	V1755	A1755	K1780	T1780	P1801	V1659
R1579	R1755	V1755	E1868	E1868	E1825	A1594
S1510	C1579	A1756	P1904	P1904	E1826	F1594
P1511	R1580	V1756	E1869	E1869	E1827	V1659
M1498	A1656	V1757	A1869	V1869	P1802	V1659
A1498	A1656	V1757	E1869	E1869	E1828	V1659
N1579	V1758	A1758	K1781	T1781	P1803	V1659
R1580	R1758	V1758	E1870	E1870	E1829	A1595
S1512	C1580	A1759	P1905	P1905	E1830	F1595
P1513	R1581	V1759	E1871	E1871	E1831	V1659
	</td					



4 Experimental information i

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8318	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.816	Depositor
Minimum map value	-0.325	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.138	Depositor
Map size (Å)	368.64, 368.64, 368.64	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.44, 1.44, 1.44	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	0.37	0/16258	0.54	0/22030

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	16077	0	16278	1581	0
All	All	16077	0	16278	1581	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 49.

The worst 5 of 1581 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:1067:ILE:HG22	1:A:1152:LEU:HD21	1.25	1.15
1:A:1213:LEU:HB2	1:A:1316:LEU:HD23	1.45	0.94
1:A:1392:CYS:HB3	1:A:1442:GLN:HE21	1.32	0.93
1:A:1695:GLN:HB3	1:A:1699:HIS:HE1	1.33	0.93
1:A:1850:PHE:HB3	1:A:1973:ARG:HD3	1.51	0.92

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	2188/2804 (78%)	2040 (93%)	148 (7%)	0	100 100

There are no Ramachandran outliers to report.

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	1677/2215 (76%)	1664 (99%)	13 (1%)	79 85

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1064	LEU
1	A	1065	GLN
1	A	2177	ARG
1	A	1211	ASN
1	A	1955	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1472	GLN

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Mol	Chain	Res	Type
1	A	1869	GLN
1	A	1527	GLN
1	A	1736	GLN
1	A	1969	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 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.

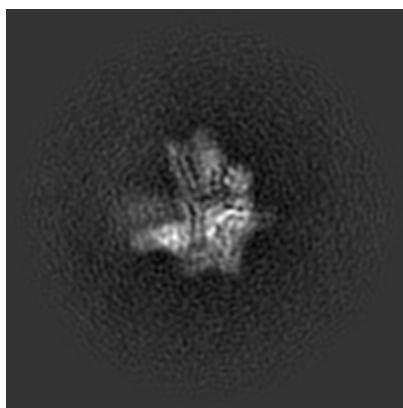
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-43155. These allow visual inspection of the internal detail of the map and identification of artifacts.

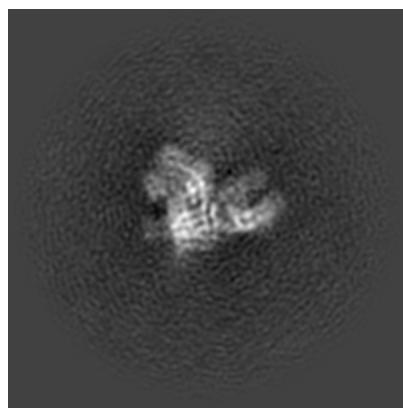
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

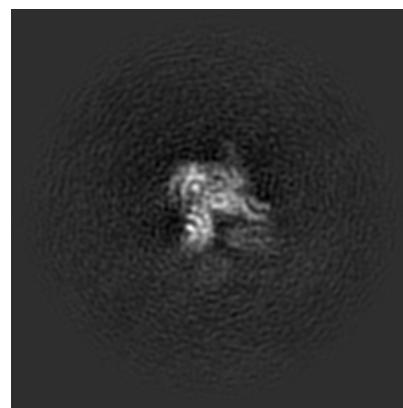
6.1.1 Primary map



X

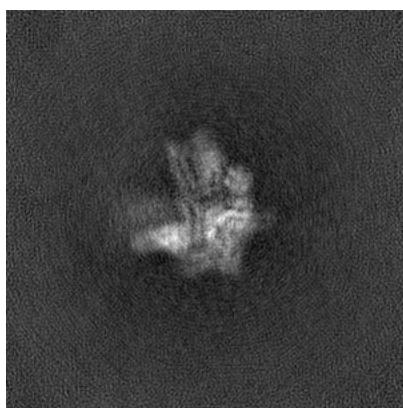


Y

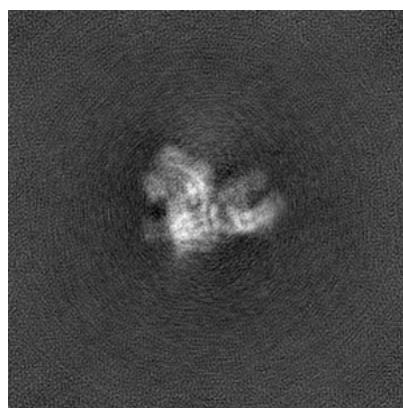


Z

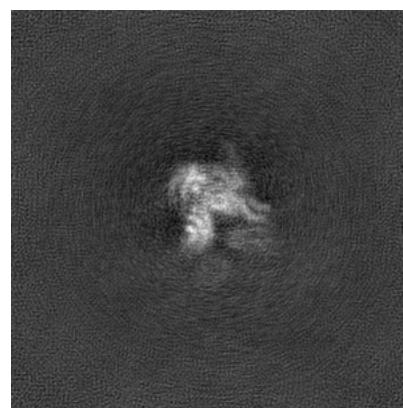
6.1.2 Raw map



X



Y

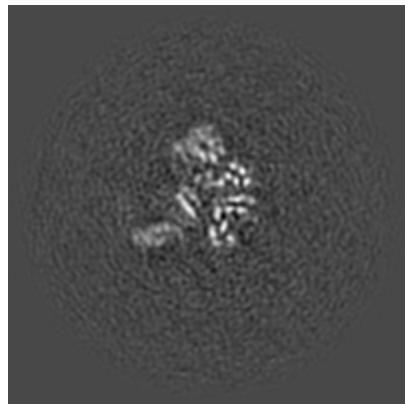


Z

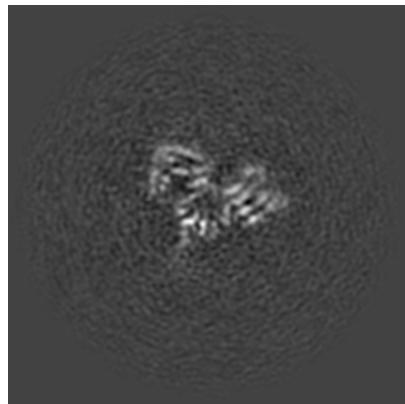
The images above show the map projected in three orthogonal directions.

6.2 Central slices [\(i\)](#)

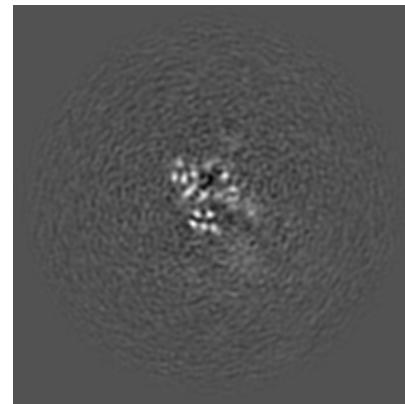
6.2.1 Primary map



X Index: 128

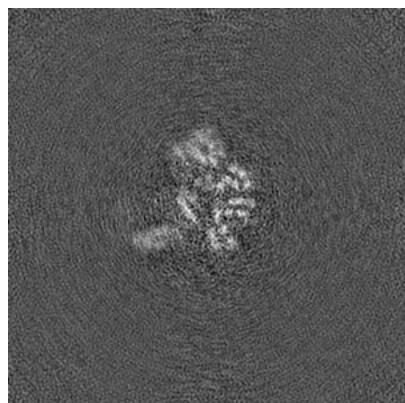


Y Index: 128

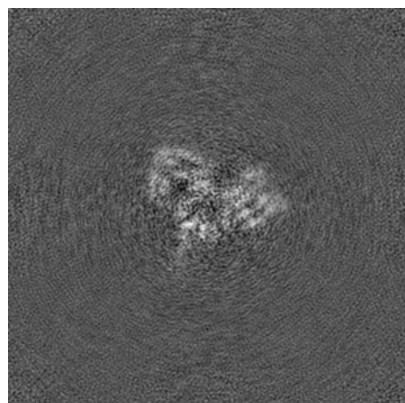


Z Index: 128

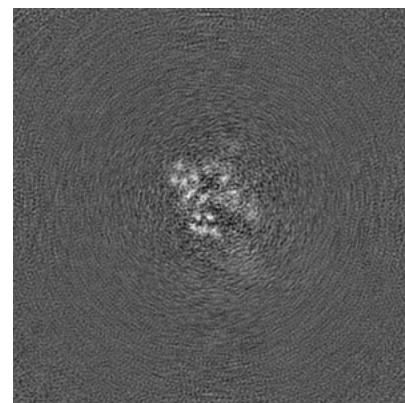
6.2.2 Raw map



X Index: 128



Y Index: 128

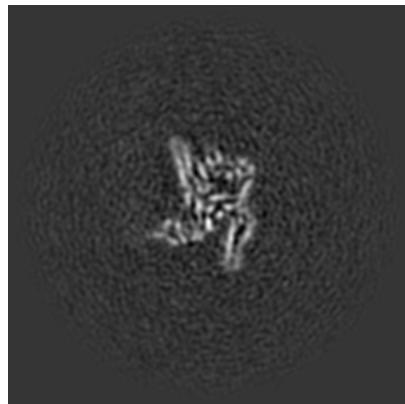


Z Index: 128

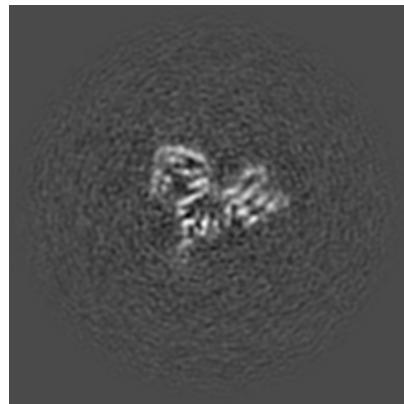
The images above show central slices of the map in three orthogonal directions.

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

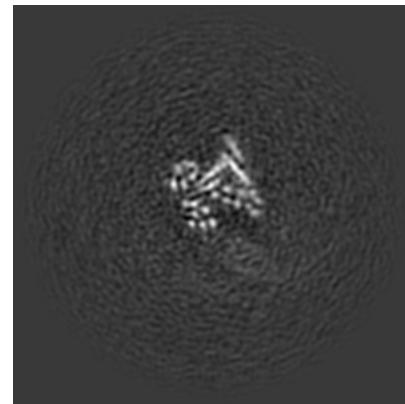
6.3.1 Primary map



X Index: 117

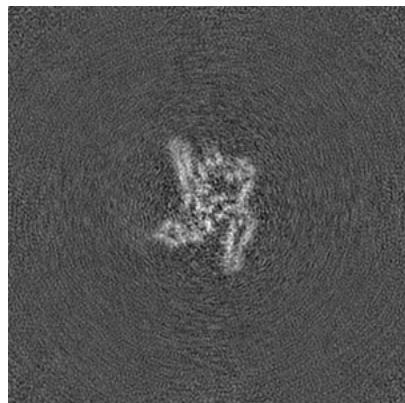


Y Index: 129

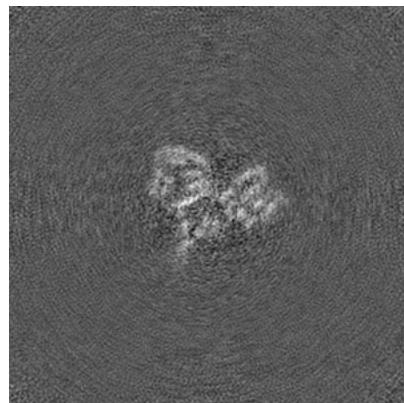


Z Index: 124

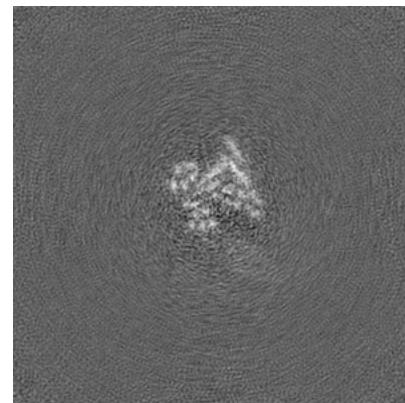
6.3.2 Raw map



X Index: 117



Y Index: 130

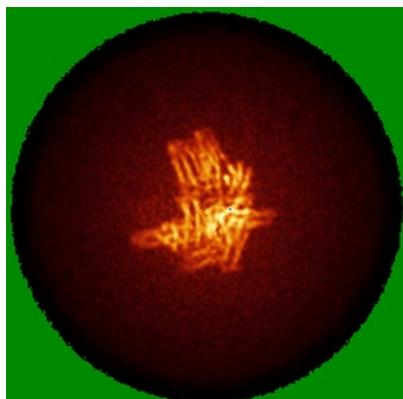


Z Index: 124

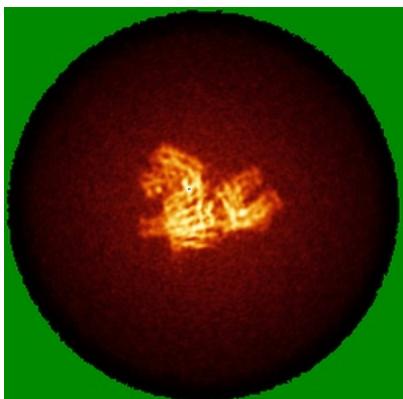
The images above show the largest variance slices of the map in three orthogonal directions.

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

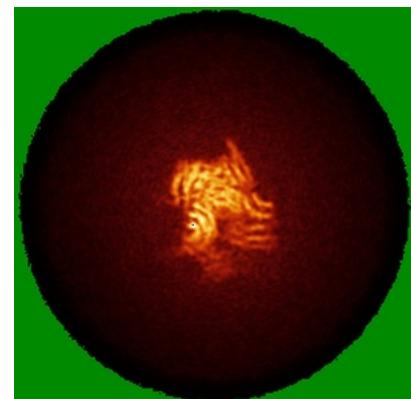
6.4.1 Primary map



X

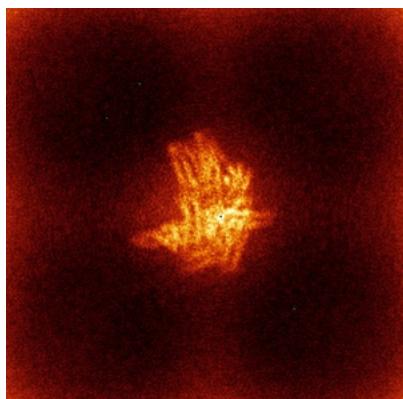


Y

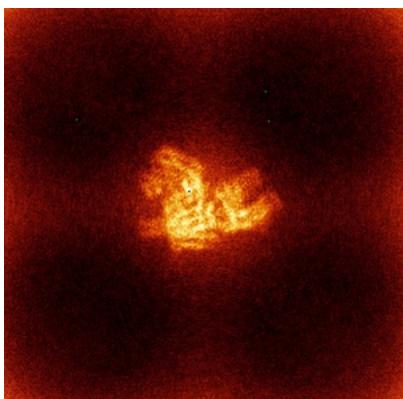


Z

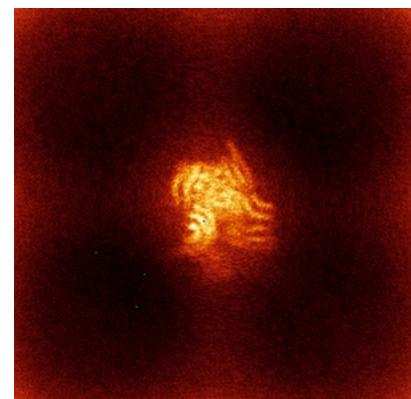
6.4.2 Raw map



X



Y

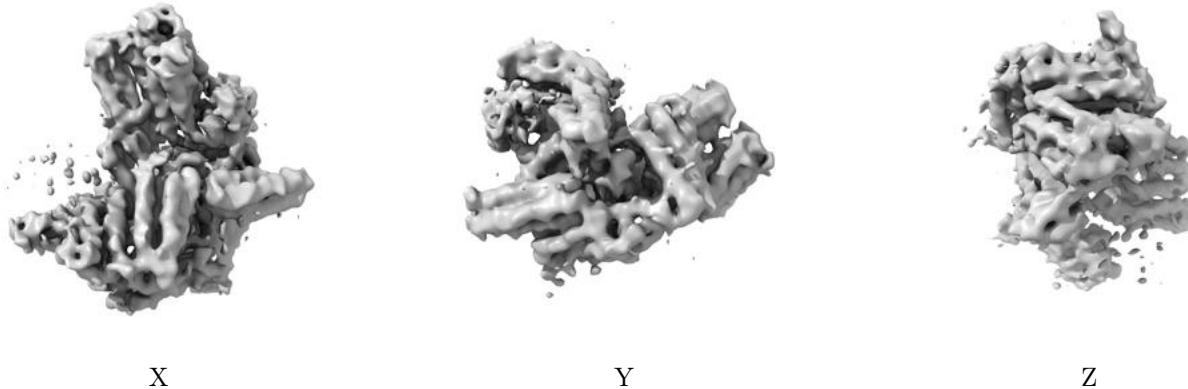


Z

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.

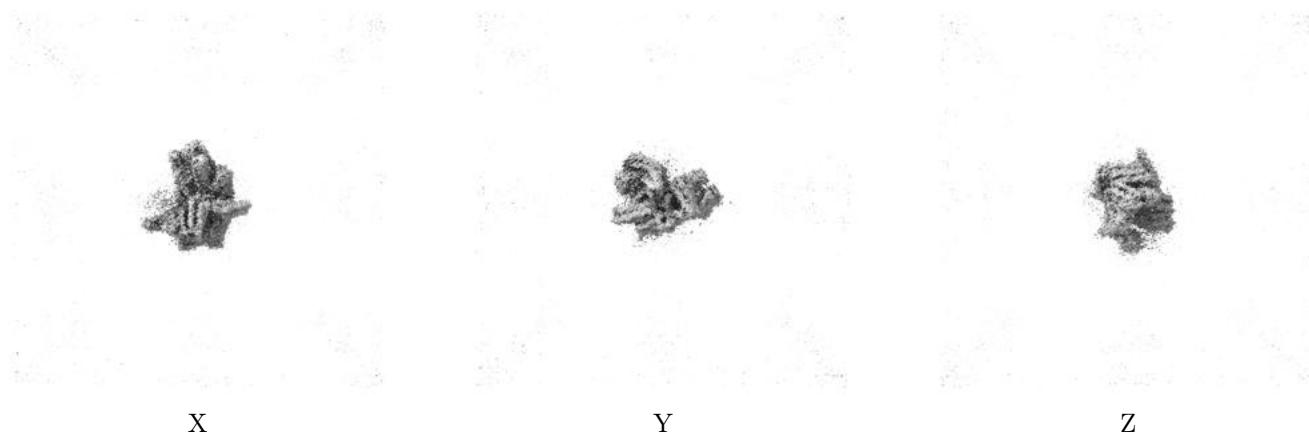
6.5 Orthogonal surface views [\(i\)](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.138. 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.

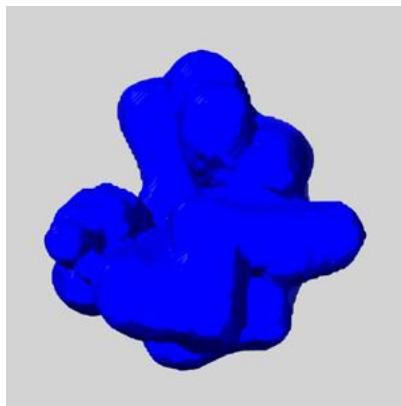
6.6 Mask visualisation [\(i\)](#)

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

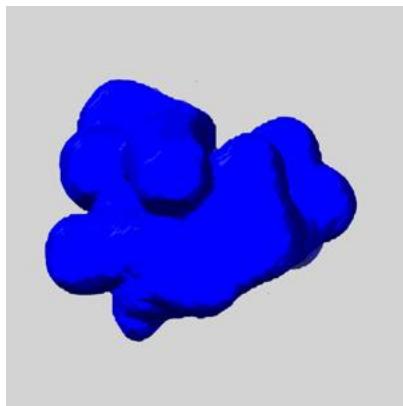
A mask typically either:

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

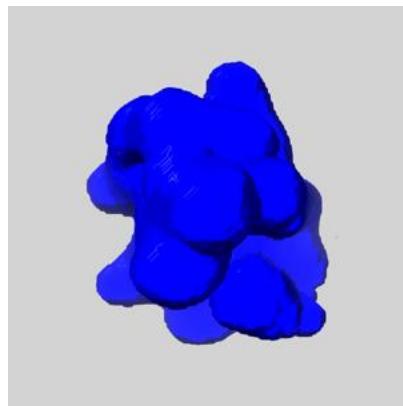
6.6.1 emd_43155_msk_1.map [\(i\)](#)



X



Y

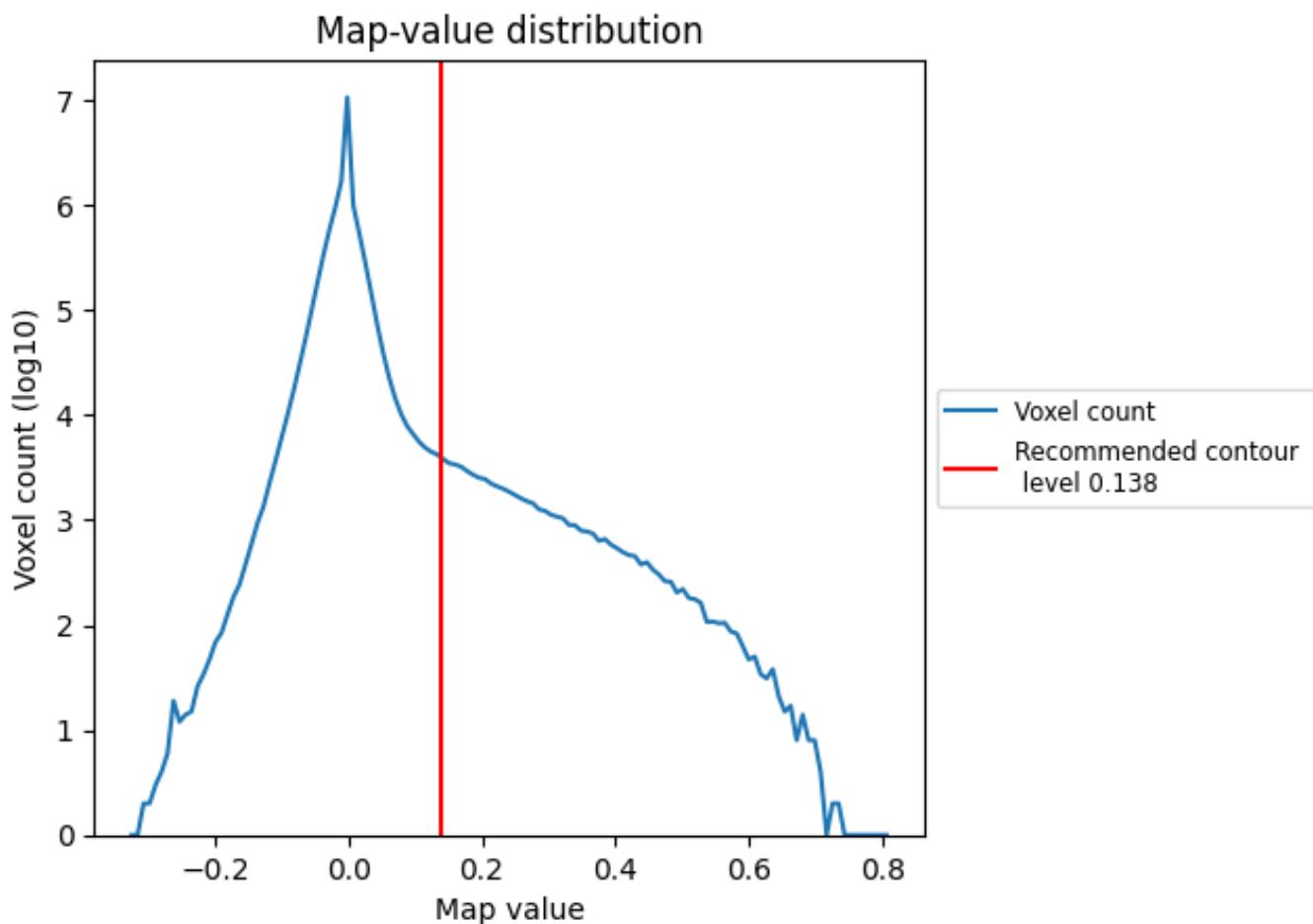


Z

7 Map analysis (i)

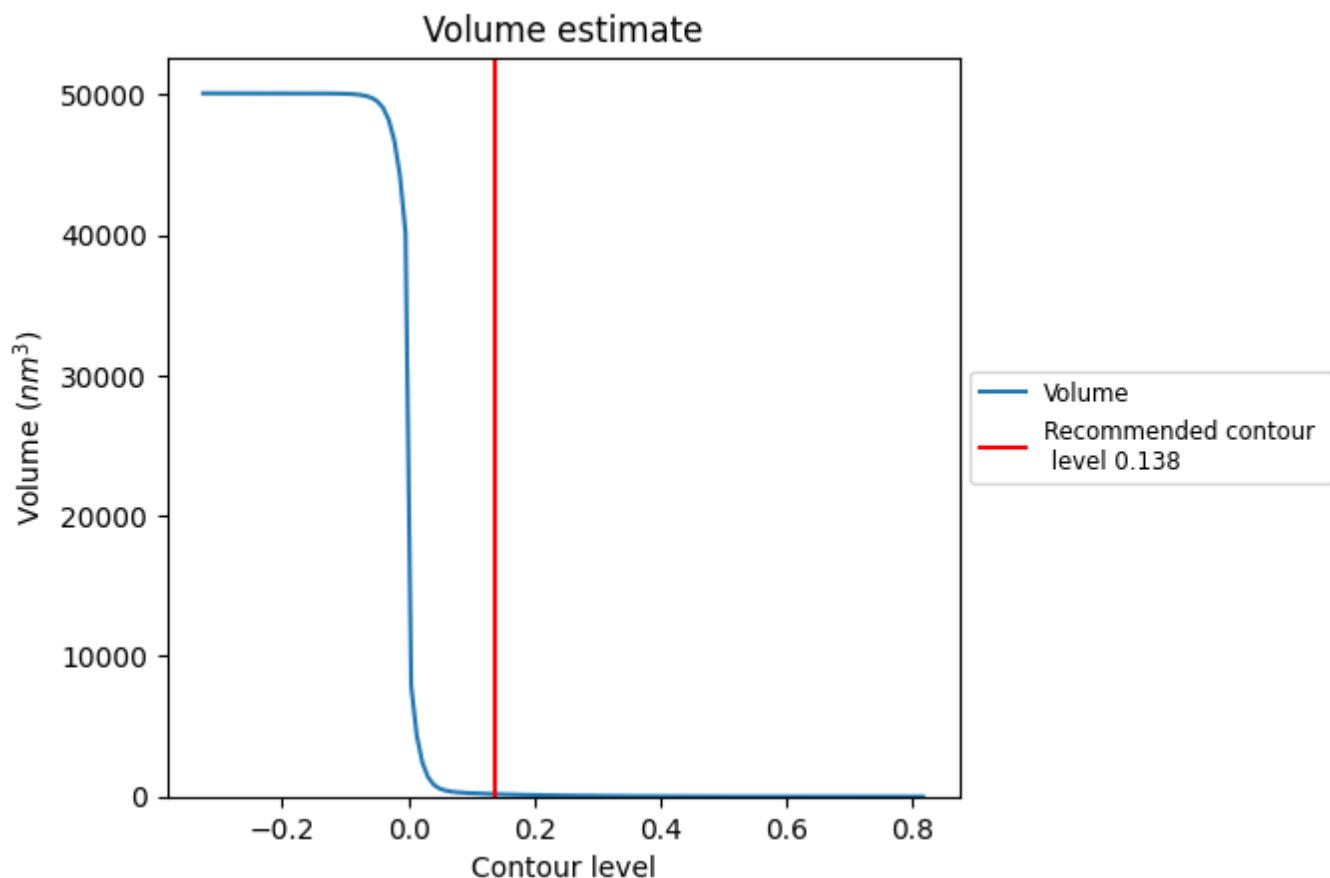
This section contains the results of statistical analysis of the map.

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.

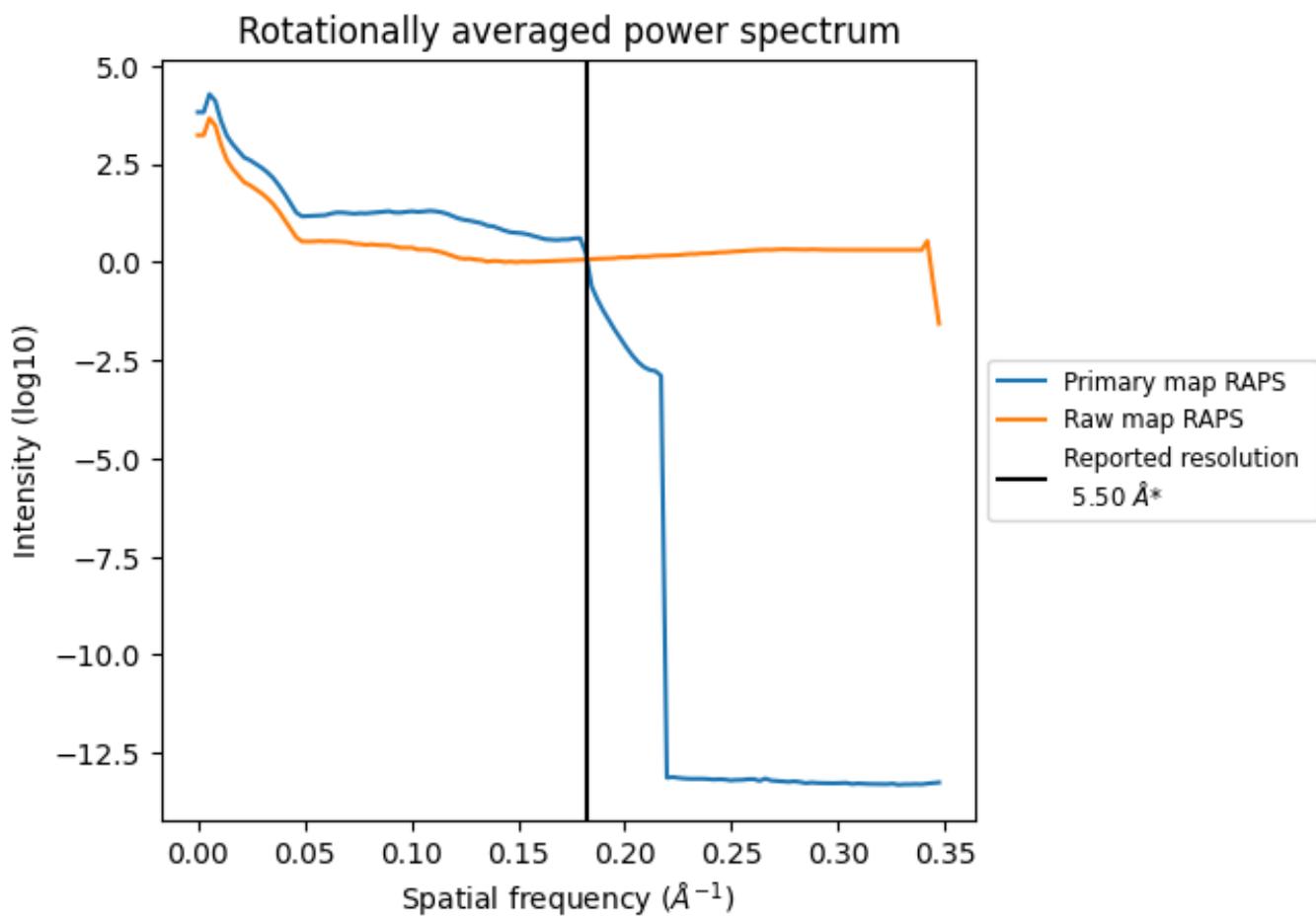
7.2 Volume estimate (i)



The volume at the recommended contour level is 174 nm^3 ; this corresponds to an approximate mass of 157 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 [\(i\)](#)

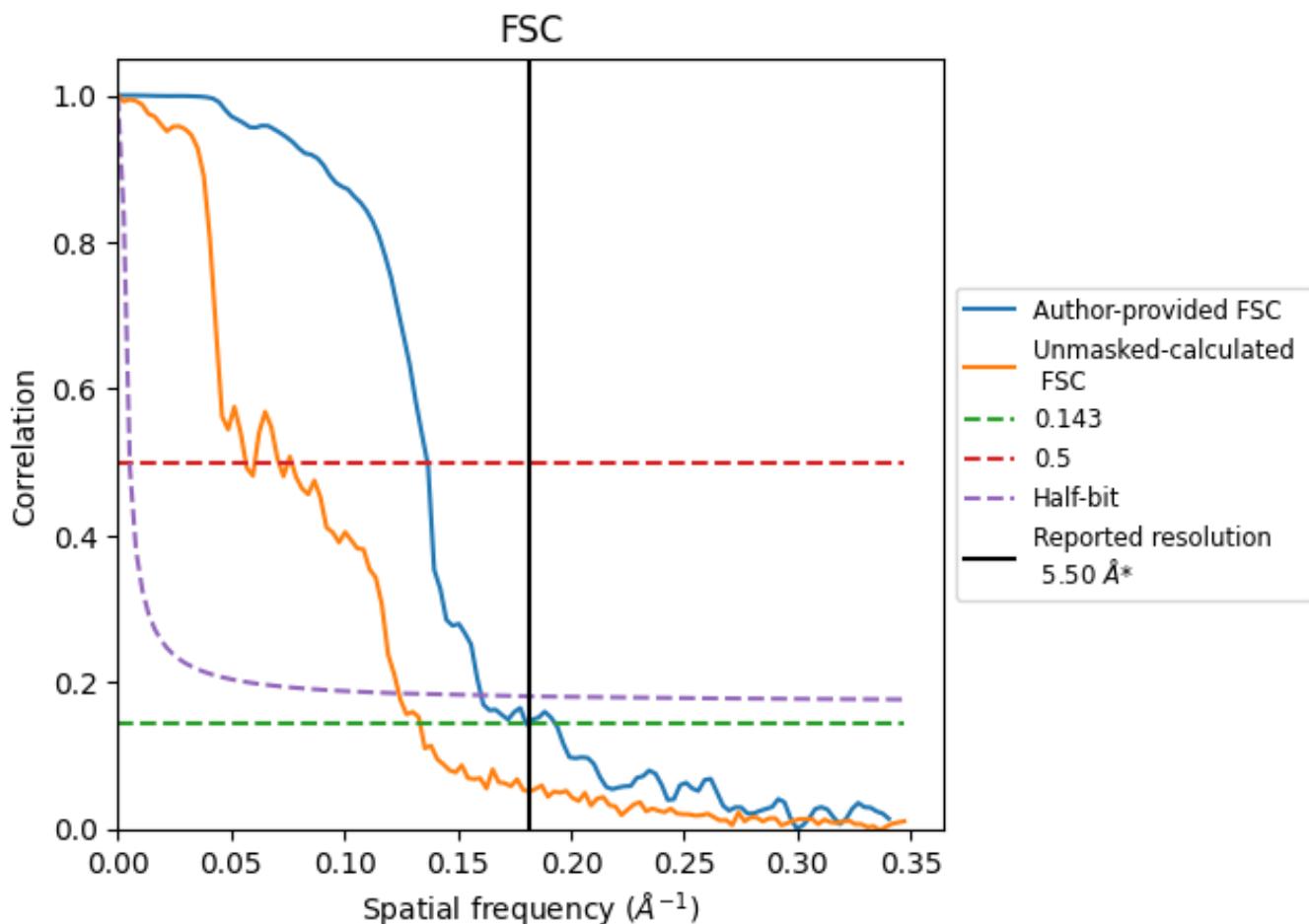


*Reported resolution corresponds to spatial frequency of 0.182 \AA^{-1}

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 0.182 \AA^{-1}

8.2 Resolution estimates [\(i\)](#)

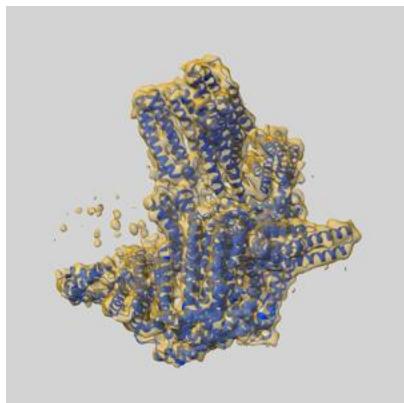
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.50	-	-
Author-provided FSC curve	5.55	7.32	6.23
Unmasked-calculated*	7.49	17.70	8.06

*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 7.49 differs from the reported value 5.5 by more than 10 %

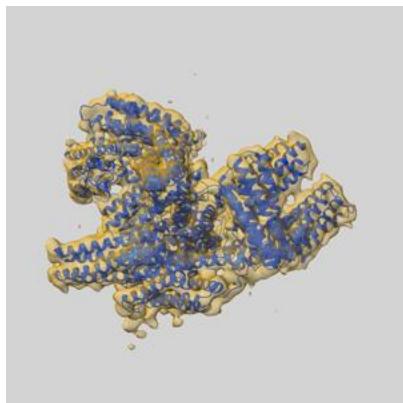
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-43155 and PDB model 8VDQ. Per-residue inclusion information can be found in section 3 on page 5.

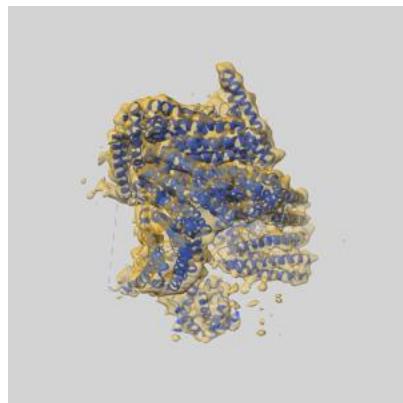
9.1 Map-model overlay (i)



X



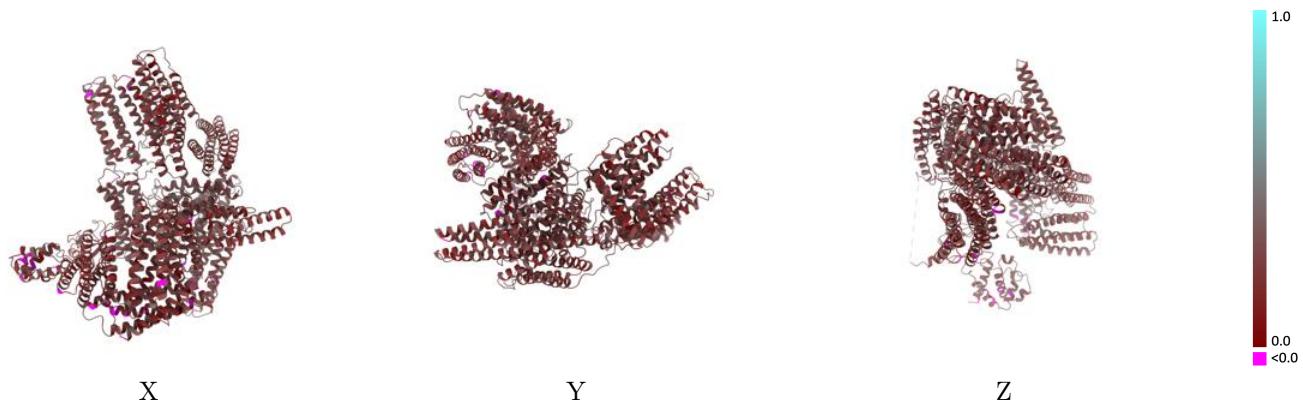
Y



Z

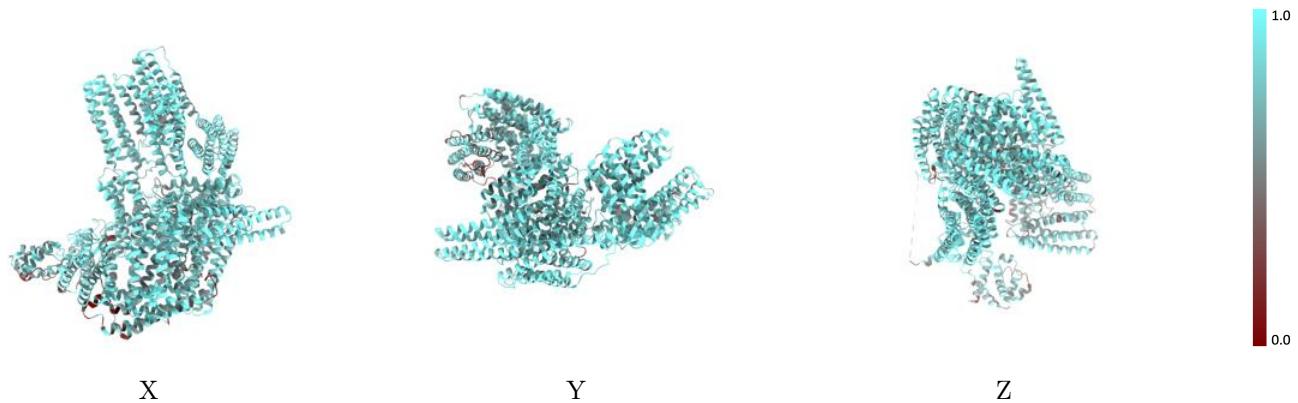
The images above show the 3D surface view of the map at the recommended contour level 0.138 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



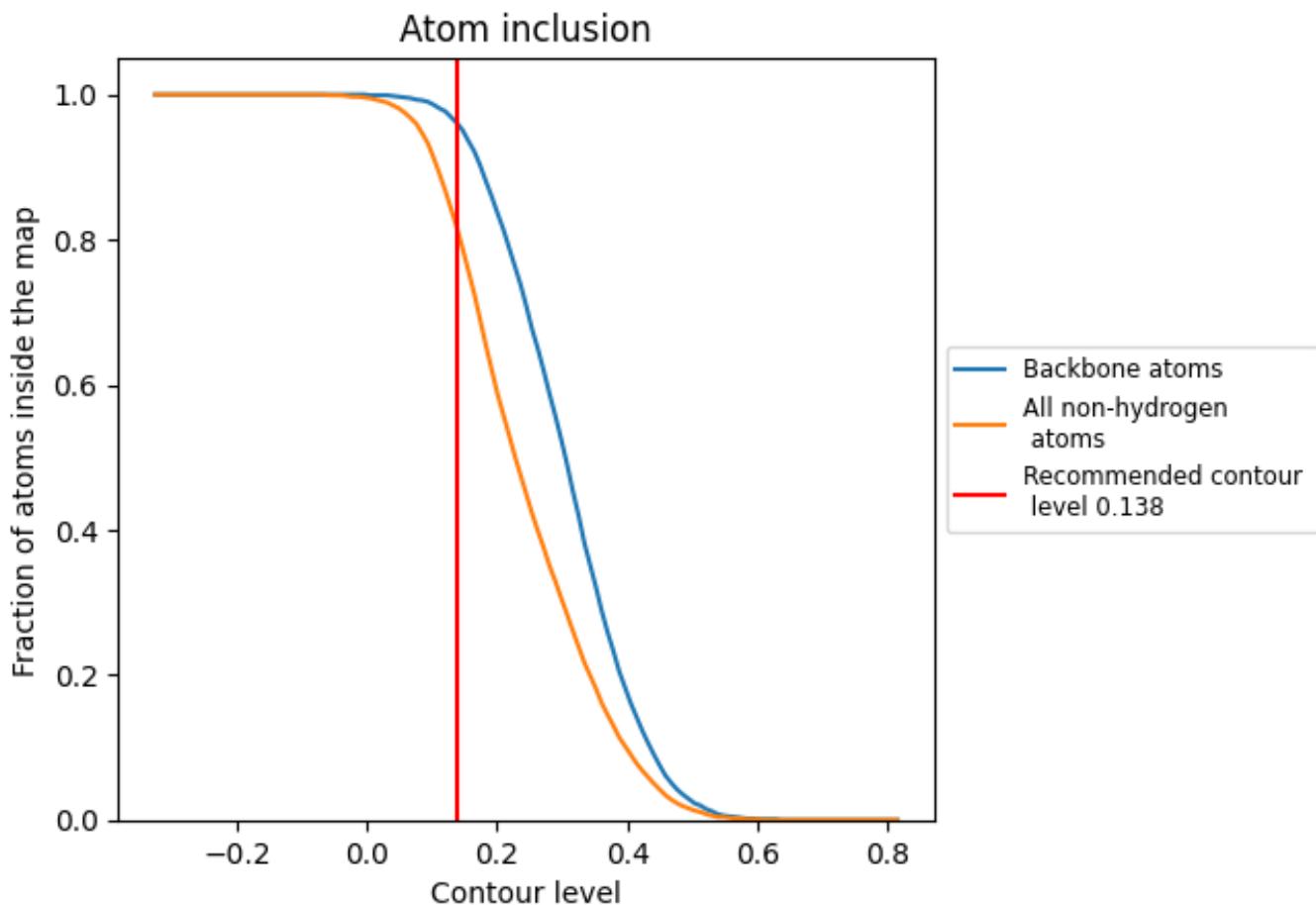
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.138).

9.4 Atom inclusion [\(i\)](#)



At the recommended contour level, 96% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [\(i\)](#)

The table lists the average atom inclusion at the recommended contour level (0.138) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8170	0.2390
A	0.8170	0.2390

