wwPDB EM Validation Summary Report (i)

Nov 27, 2022 – 08:29 PM EST

PDB ID	:	7KVE
EMDB ID	:	EMD-23048
Title	:	Cryo-EM structure of human Factor V at 3.3 Angstrom resolution
Authors	:	Ruben, E.A.; Di Cera, E.
Deposited on	:	2020-11-27
Resolution	:	3.30 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 (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 (i)) were used in the production of this report:

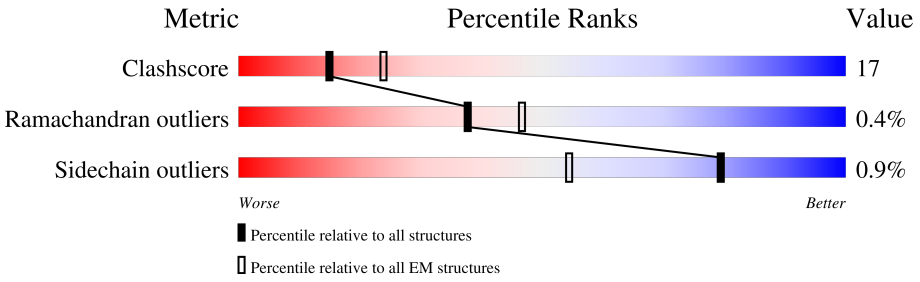
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

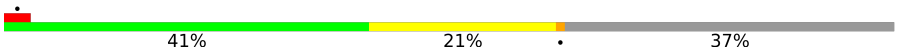
The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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 <=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	B	2196	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 11142 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 Coagulation factor V.

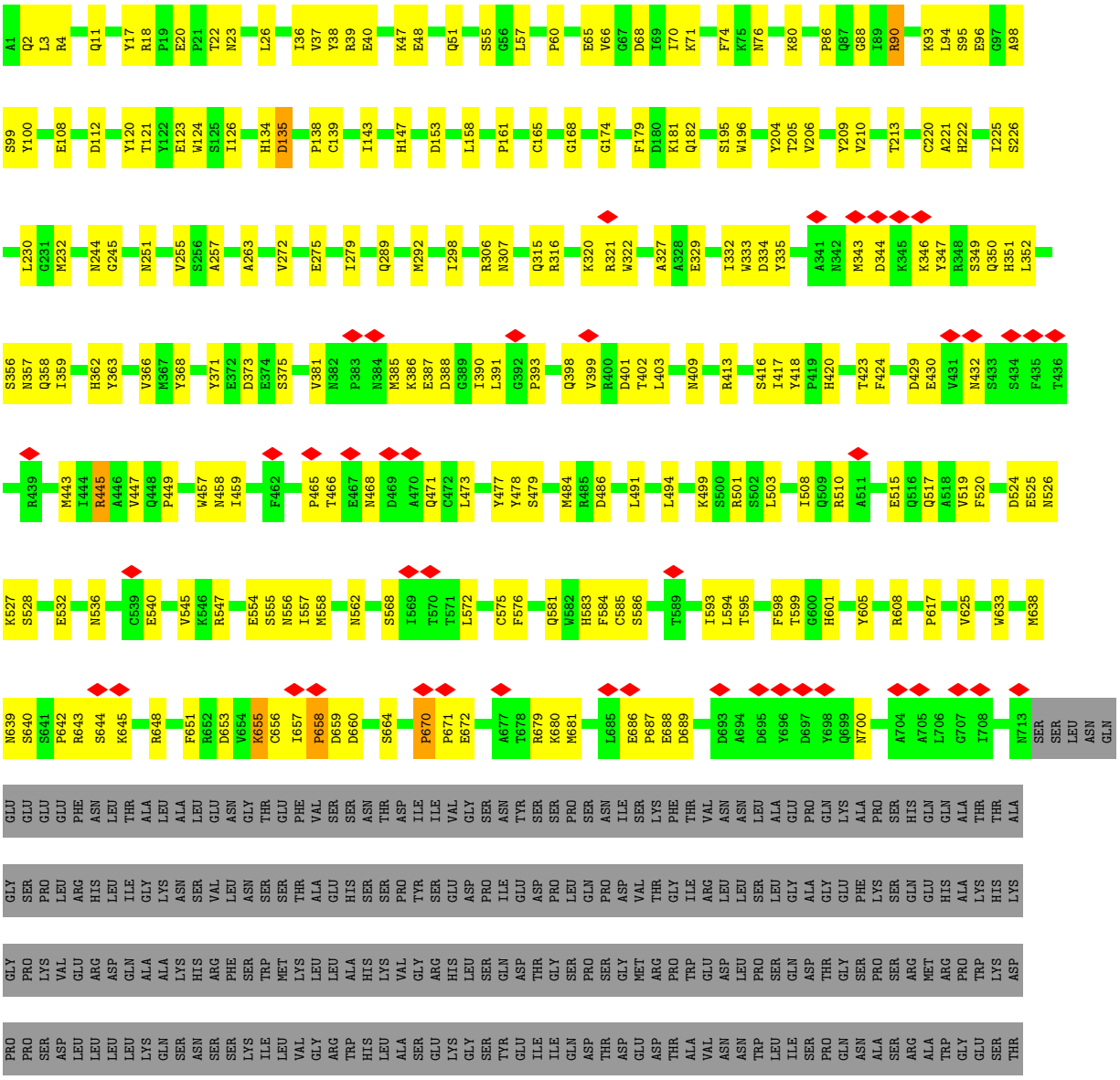
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	1374	11142	7074	1905	2108	55	0	0

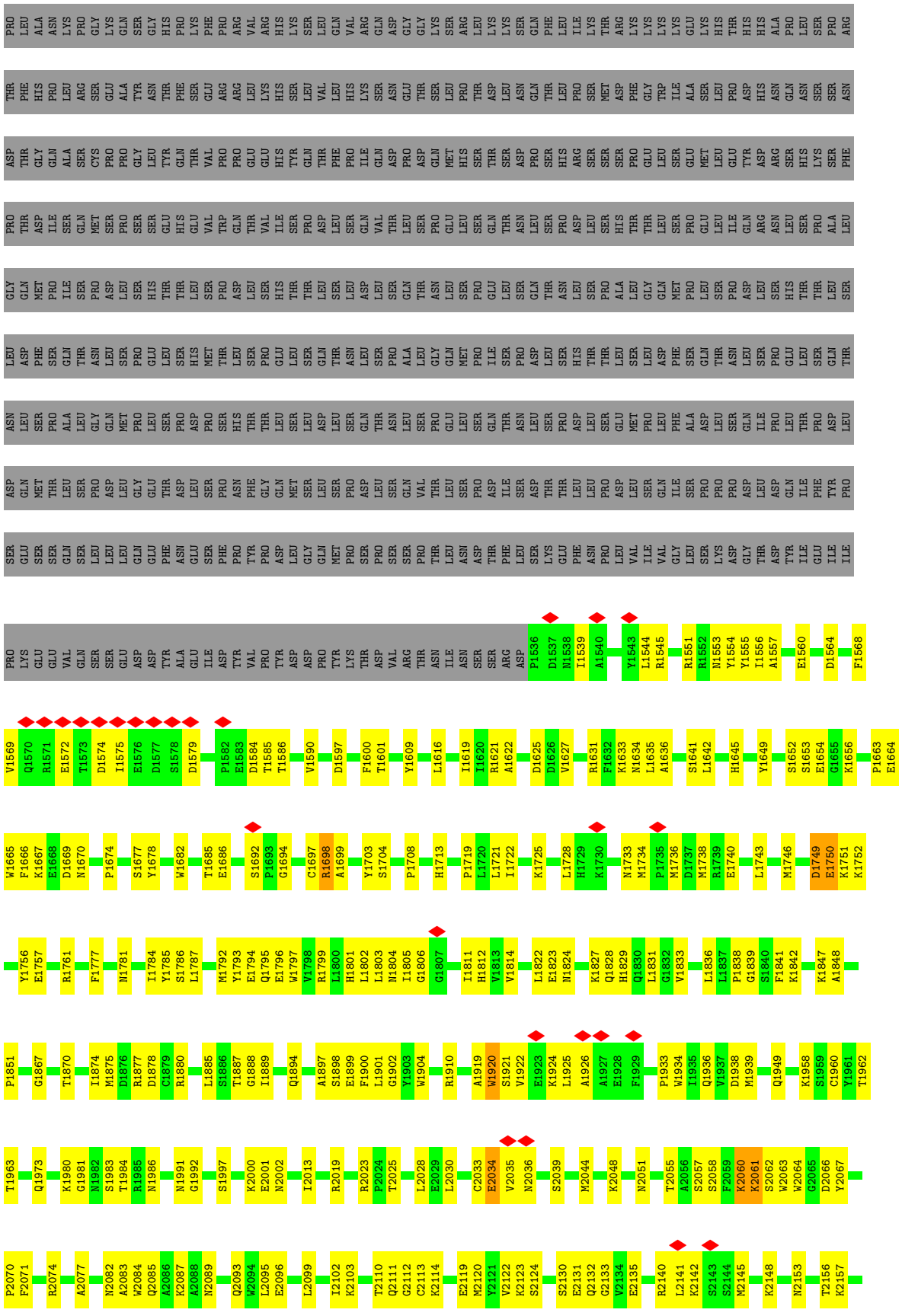
3 Residue-property plots (i)

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: Coagulation factor V

Chain B: 41% 21% 37%




PRO LEU ALA ASN LYS PRO GLY LYS GLN SER GLY HIS PRO LYS PHE PRO ARG VAL ARG HIS LYS SER LEU LEU GLN VAL ARG GLN ASP GLY GLY LYS SER ARG LEU LYS LYS SER GLN PHE LEU ILE LYS THR ARG LYS LYS LYS GLU LYS HIS THR HIS HIS ALA PRO LEU SER PRO ARG
THR PHE HIS PRO LEU ARG SER GLU ALA TYR ASN THR PHE SER GLU LYS HIS SER LEU VAL LEU HIS LYS SER ASN GLU THR SER LEU PRO THR ASP LEU ASN GLN THR LEU PRO SER MET ASP PHE GLY TRP ILE ALA SER LEU PRO ASP HIS ASN GLN ASN SER SER ASN
ASP THR GLY GLN ALA SER CYS PRO PRO GLY LEU TYR GLN THR VAL PRO PRO GLU GLU HIS TYR GLN THR PHE PRO ILE GLN ASP PRO ASP GLN MET HIS SER THR SER ASP PRO SER HIS ARG SER SER SER PRO GLU LEU SER GLU MET LEU GLU TYR ASP ARG SER HIS LYS SER PHE
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GLY GLN MET PRO ILE SER PRO ASP LEU SER SER HIS THR THR LEU SER PRO ASP LEU SER HIS THR THR LEU SER GLN THR ASN LEU SER PRO ALA LEU GLY GLN MET PRO GLU LEU SER PRO GLN THR THR LEU SER
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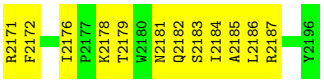
ASN LEU SER PRO ALA LEU GLY GLN MET PRO LEU LEU SER PRO ASP PRO SER HIS THR THR LEU SER LEU ASP LEU SER GLN THR ASN LEU SER PRO GLU LEU SER GLN THR ASN LEU SER PRO ASP LEU SER GLN ILE PRO LEU THR PRO ASP LEU
ASP GLN MET THR LEU SER PRO ASP LEU GLY GLU THR ASP LEU SER PRO ASN PHE GLY GLN MET SER LEU SER PRO ASP LEU SER GLN VAL THR LEU SER PRO GLU ASP THR THR LEU LEU PRO ASP LEU SER GLN ILE SER PRO PRO ASP LEU ASP GLN ILE PHE TYR PRO
SER GLU SER SER GLN SER LEU LEU LEU LEU GLN GLU PHE ASN GLU SER PHE PRO TYR PRO ASP LEU GLY GLN MET PRO SER PRO SER SER PRO THR LEU ASN ASP THR PHE LEU SER LYS GLU PHE ASN PRO LEU VAL ILE ASN GLY THR LEU SER LYS ASP GLY THR ASP TYR ILE GLU ILE ILE
PRO LYS GLU GLU VAL GLN SER SER GLU ASP ASP TYR ALA GLU ILE ASP TYR VAL PRO TYR ASP ASP PRO TYR LYS THR ASP VAL ARG THR ASN ILE ASN SER SER ARG ASP P1536 D1537 N1538 I1539 A1540 Y1543 L1544 R1545 R1551 R1552 N1553 Y1554 Y1555 I1556 A1557 E1560 D1564 F1568
V1569 Q1570 R1571 E1572 T1573 D1574 I1575 E1576 D1577 S1578 D1579 P1582 E1583 D1584 T1585 T1586 V1590 D1597 F1600 T1601 Y1609 L1616 I1619 I1620 R1621 A1622 D1625 D1626 V1627 R1631 F1632 K1633 N1634 L1635 A1636 S1641 L1642 H1645 Y1649 S1652 S1653 E1654 G1655 K1656 P1663 E1664
W1665 F1666 K1667 E1668 D1669 N1670 P1674 S1677 Y1678 W1682 T1685 E1686 S1692 P1693 G1694 C1697 R1698 A1699 Y1703 S1704 P1708 H1713 P1719 L1720 L1721 I1722 K1725 L1728 H1729 K1730 N1733 M1734 P1735 M1736 D1737 M1738 R1739 E1740 L1743 M1746 D1749 E1750 K1751 K1752
Y1756 E1757 R1761 F1777 N1781 I1784 Y1785 S1786 L1787 M1792 Y1793 E1794 Q1795 E1796 W1797 V1798 R1799 L1800 H1801 L1802 L1803 N1804 I1805 G1806 G1807 I1811 H1812 V1813 V1814 L1822 E1823 N1824 K1827 Q1828 H1829 Q1830 L1831 G1832 V1833 L1836 L1837 P1838 G1839 S1840 F1841 K1842 K1847 A1848
P1851 G1867 T1870 I1874 M1875 D1876 R1877 D1878 C1879 R1880 L1885 S1886 T1887 G1888 I1889 Q1894 A1897 S1898 E1899 F1900 L1901 G1902 Y1903 W1904 R1910 A1919 W1920 S1921 V1922 E1923 K1924 L1925 A1926 A1927 E1928 F1929 P1933 W1934 I1935 Q1936 V1937 D1938 M1939 Q1949 K1958 S1959 C1960 Y1961 T1962
T1963 Q1973 K1980 G1981 N1982 S1983 T1984 R1985 N1986 N1991 G1992 S1997 K2000 E2001 N2002 I2013 R2019 R2023 P2024 T2025 L2028 E2029 L2030 C2033 E2034 V2035 N2036 S2039 M2044 K2048 N2051 T2055 A2056 S2057 S2058 F2059 K2060 K2061 S2062 W2063 W2064 G2065 D2066 Y2067
P2070 F2071 R2074 A2077 N2082 A2083 W2084 Q2085 A2086 K2087 A2088 N2089 Q2093 W2094 L2095 E2096 L2099 I2102 K2103 T2110 Q2111 G2112 C2113 K2114 E2119 M2120 Y2121 V2122 K2123 S2124 S2130 E2131 Q2132 G2133 V2134 E2135 R2140 L2141 K2142 S2143 S2144 M2145 K2148 N2153 T2156 K2157


R2171
F2172
I2176
P2177
K2178
T2179
W2180
N2181
Q2182
S2183
I2184
A2185
L2186
R2187
Y2196

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	299182	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.65	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	2.803	Depositor
Minimum map value	-1.629	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.067	Depositor
Recommended contour level	0.43	Depositor
Map size (Å)	325.6, 325.6, 325.6	wwPDB
Map dimensions	296, 296, 296	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	B	0.31	0/11436	0.51	0/15488

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	B	11142	0	10800	369	0
All	All	11142	0	10800	369	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 17.

The worst 5 of 369 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:B:656:CYS:H	1:B:660:ASP:HB2	1.16	1.10
1:B:2060:LYS:CG	1:B:2087:LYS:HA	1.84	1.08
1:B:2061:LYS:HD2	1:B:2067:TYR:HB3	1.10	1.08
1:B:2060:LYS:HG3	1:B:2087:LYS:HA	1.39	1.03
1:B:2061:LYS:CD	1:B:2067:TYR:HB3	1.91	0.99

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	B	1370/2196 (62%)	1115 (81%)	250 (18%)	5 (0%)	34 66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2060	LYS
1	B	135	ASP
1	B	700	ASN
1	B	658	PRO
1	B	670	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	1225/1989 (62%)	1214 (99%)	11 (1%)	78 87

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2033	CYS
1	B	2034	GLU
1	B	2061	LYS
1	B	2036	ASN

Continued on next page...

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Mol	Chain	Res	Type
1	B	1749	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1713	HIS
1	B	1819	GLN
1	B	1781	ASN
1	B	1936	GLN
1	B	562	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.

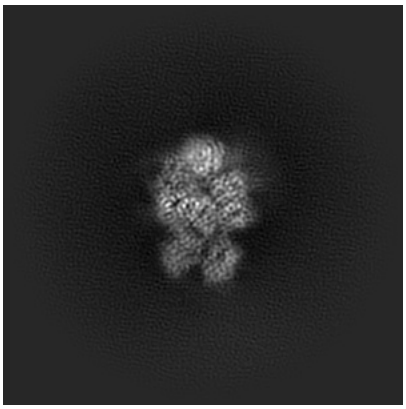
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-23048. These allow visual inspection of the internal detail of the map and identification of artifacts.

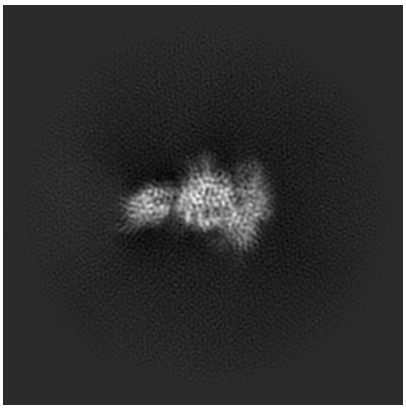
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

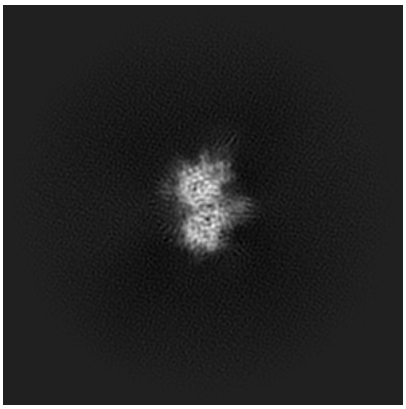
6.1.1 Primary map



X

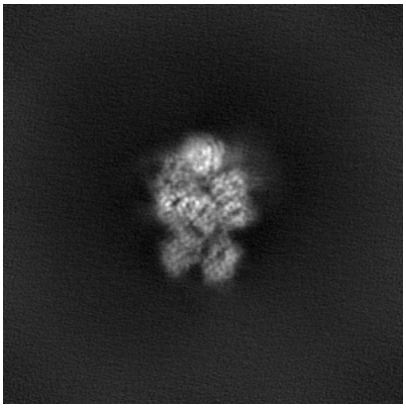


Y

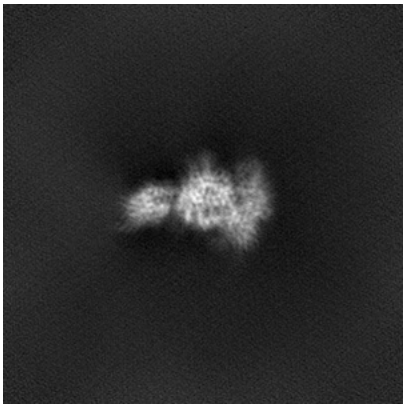


Z

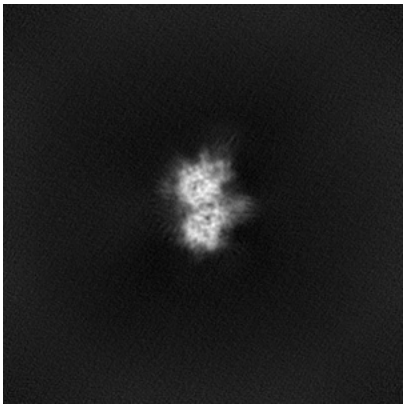
6.1.2 Raw map



X



Y

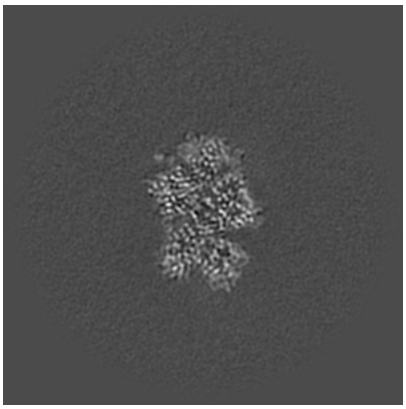


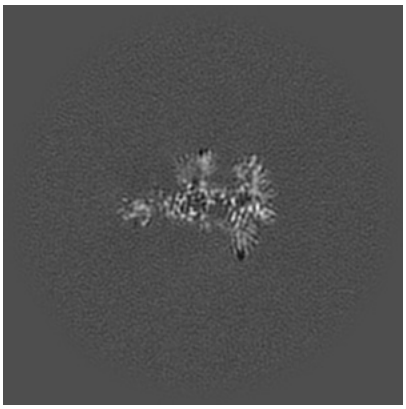
Z

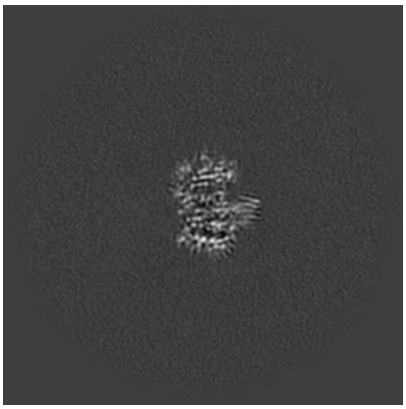
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

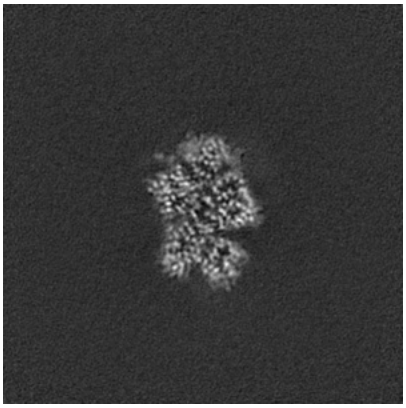
6.2.1 Primary map

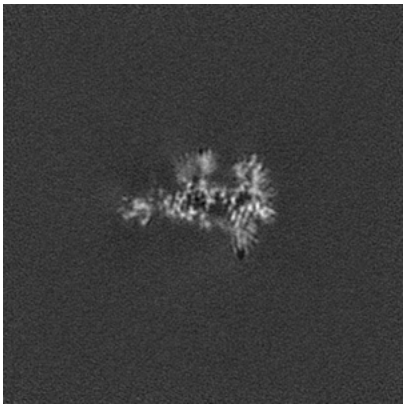

X Index: 148

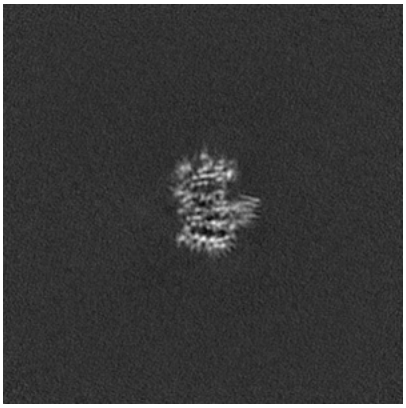

Y Index: 148


Z Index: 148

6.2.2 Raw map


X Index: 148

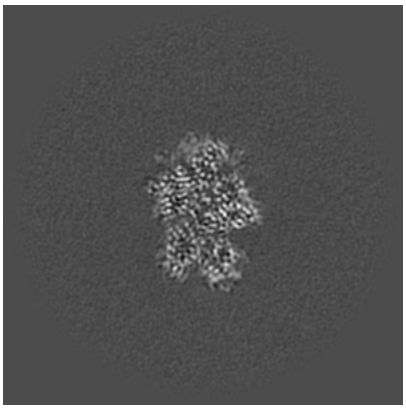

Y Index: 148

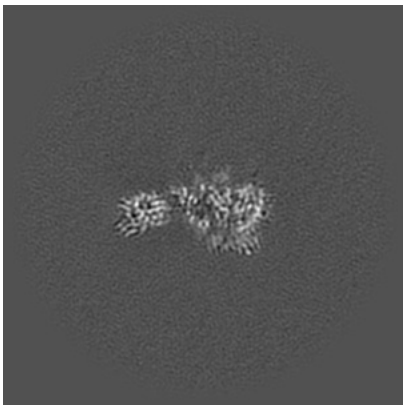

Z Index: 148

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: 149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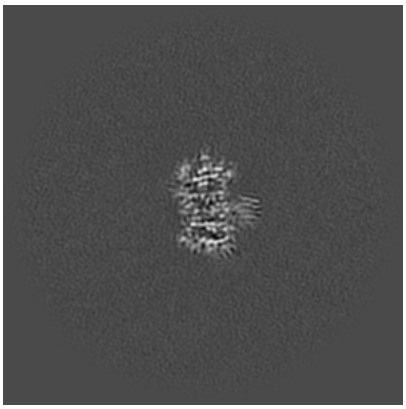
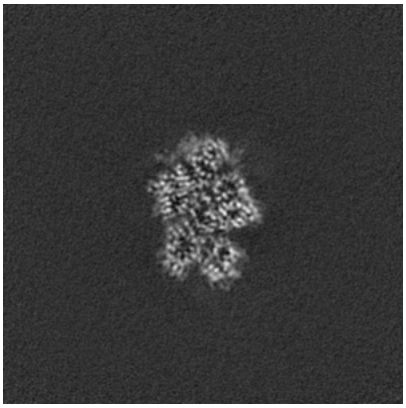
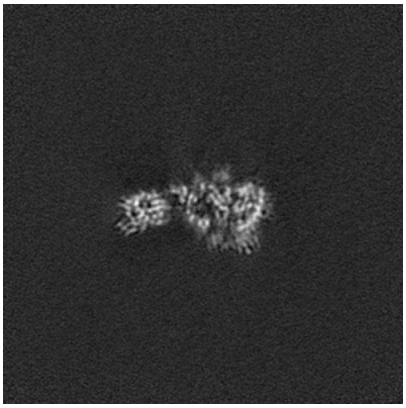
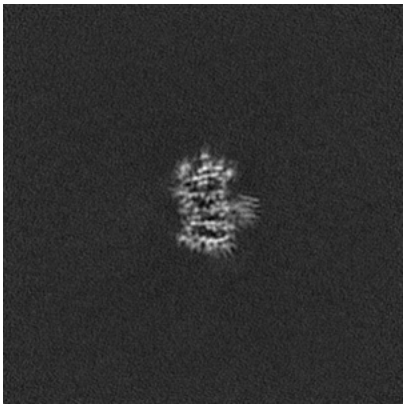

Z Index: 147

6.3.2 Raw map


X Index: 149


Y Index: 157


Z Index: 147

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

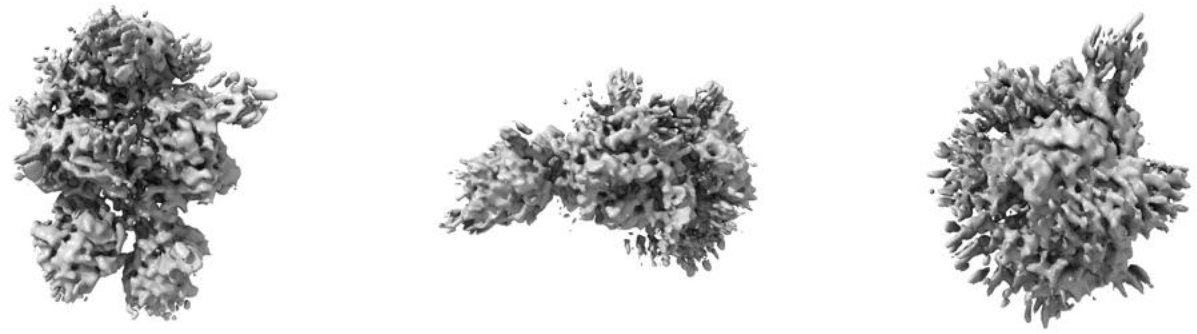
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.43. 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



X Y Z

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.

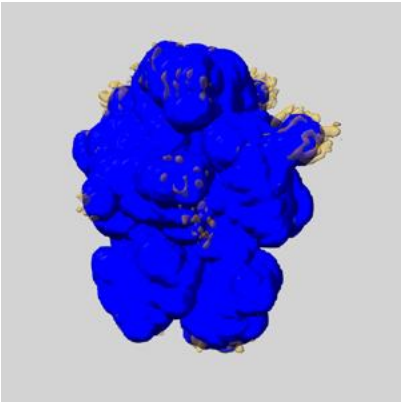
6.5 Mask visualisation (i)

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

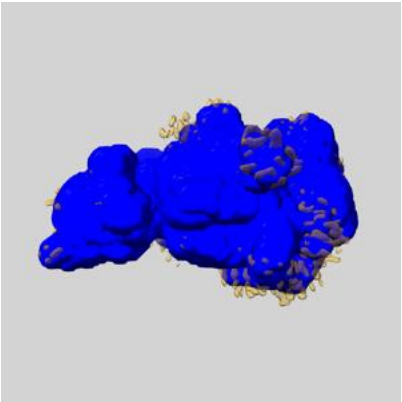
A mask typically either:

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

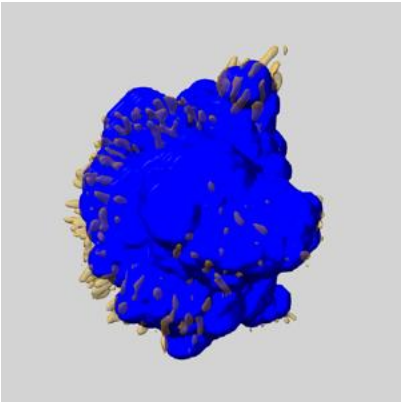
6.5.1 emd_23048_msk_1.map (i)



X



Y

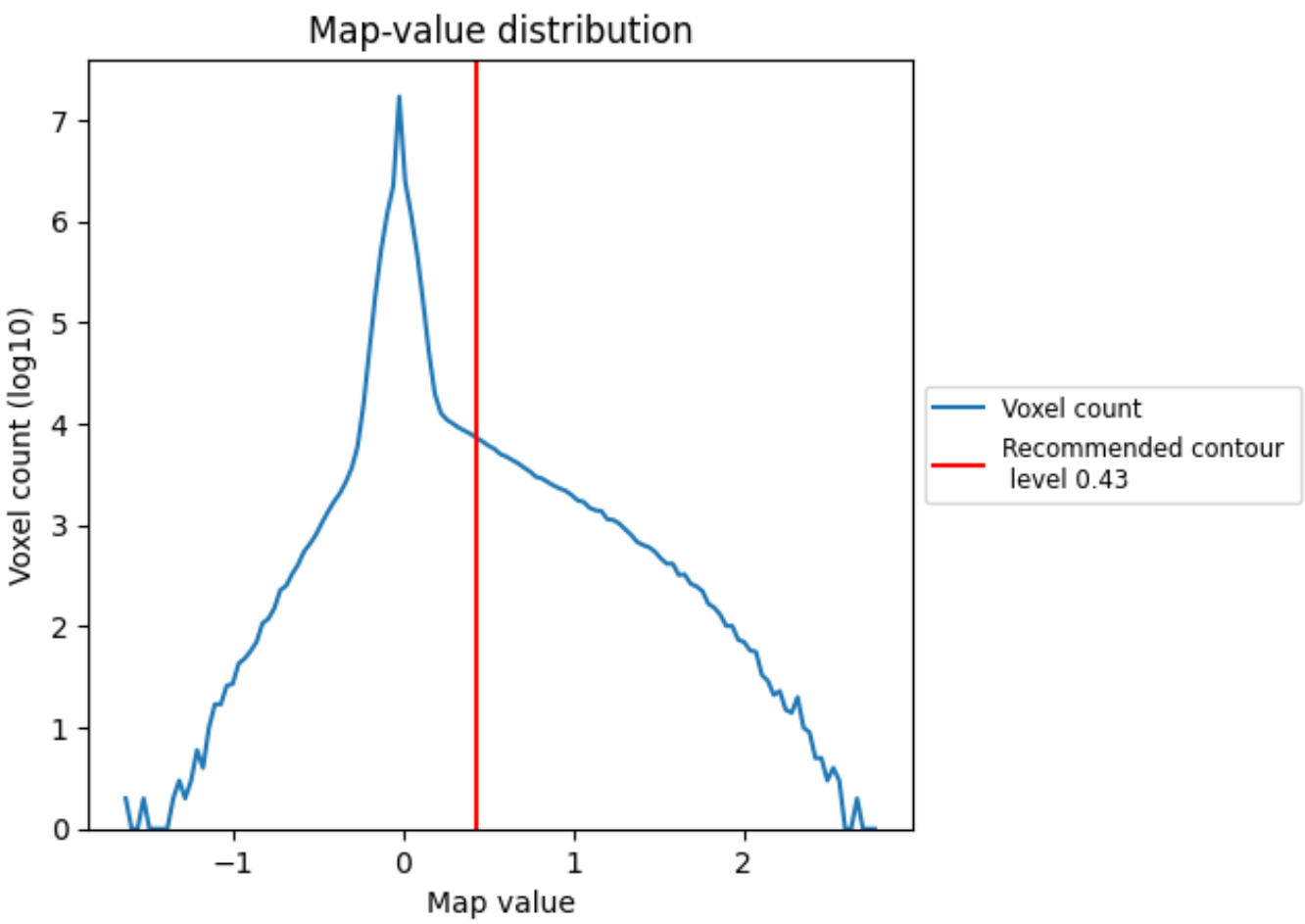


Z

7 Map analysis (i)

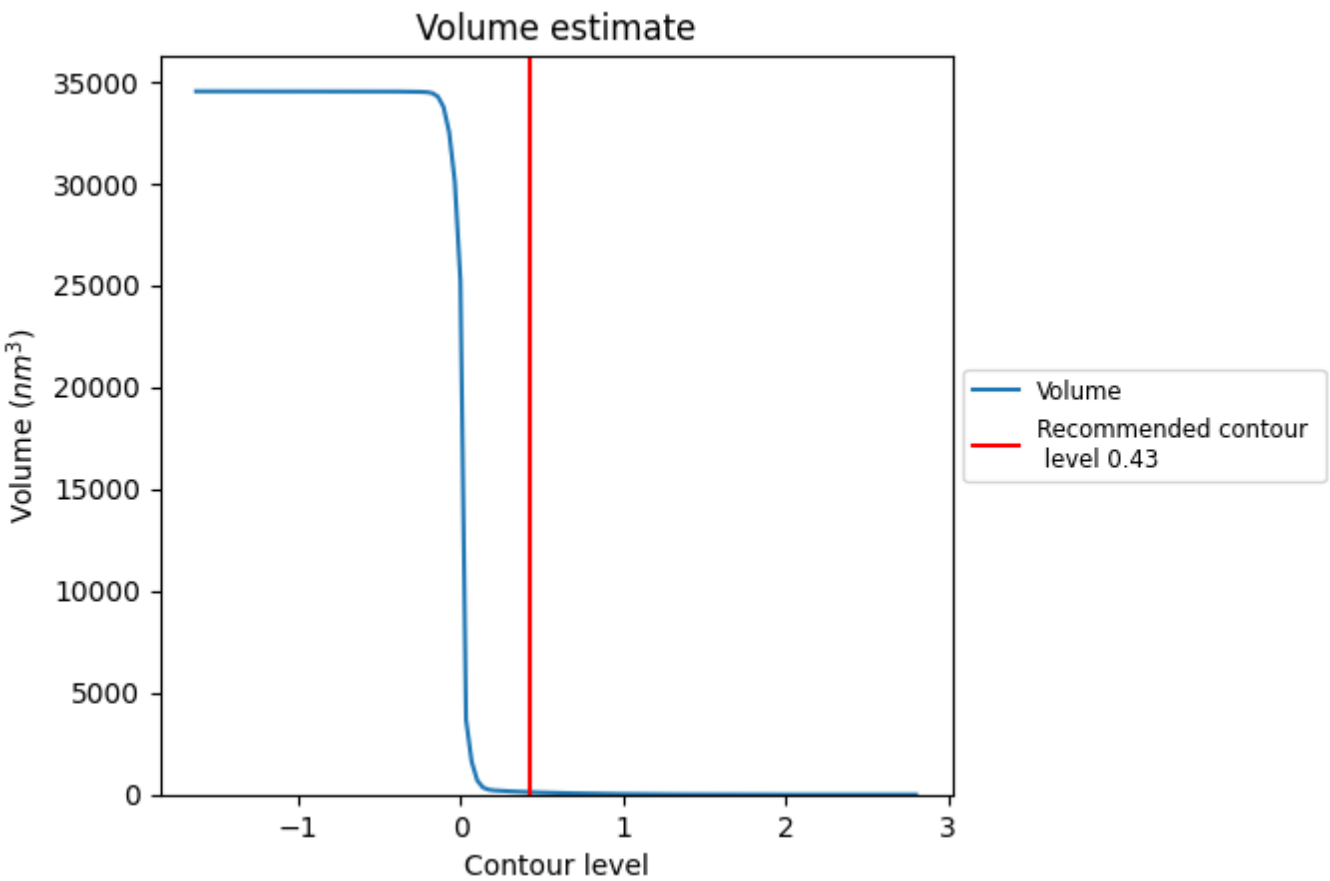
This section contains the results of statistical analysis of the map.

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.

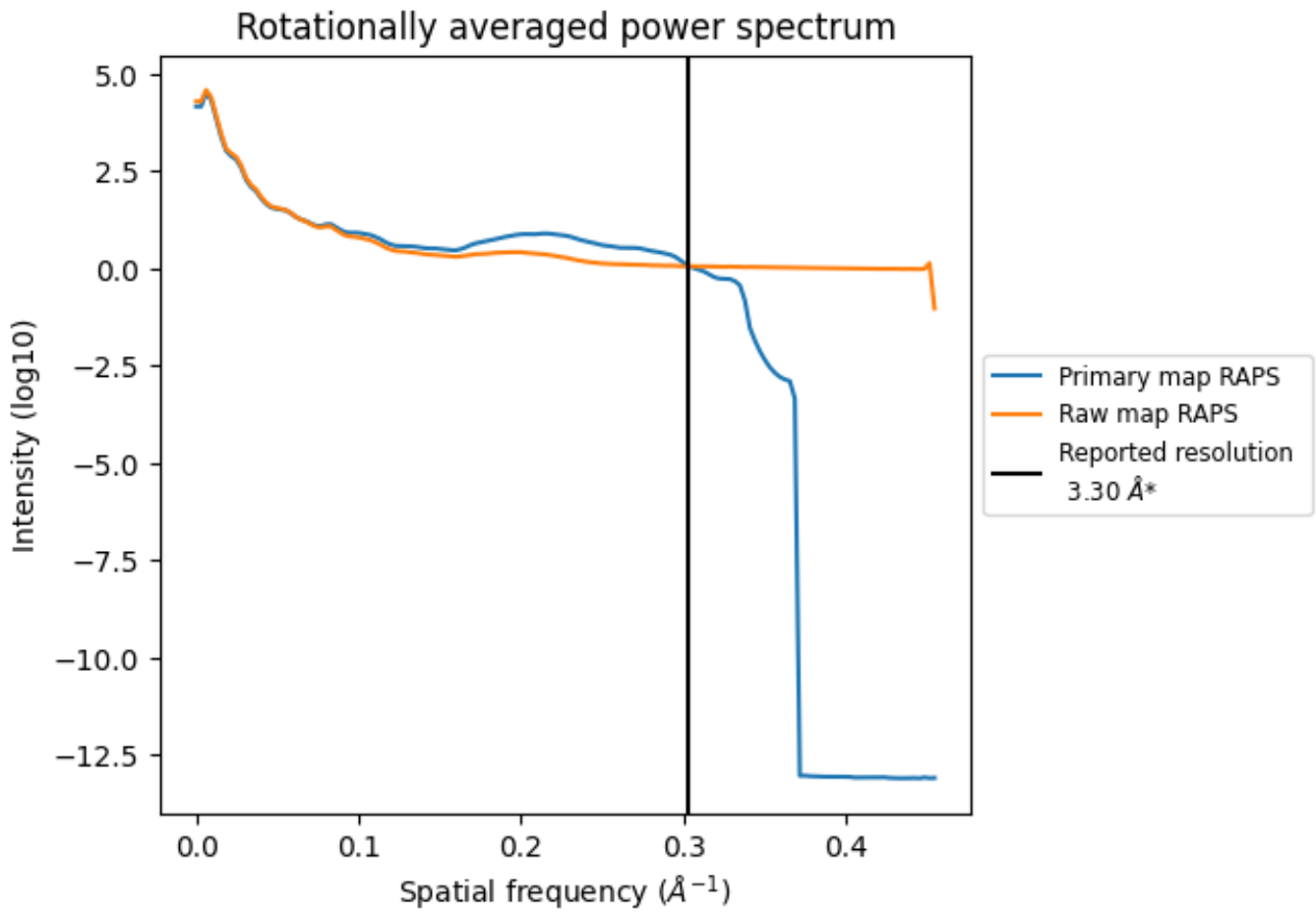
7.2 Volume estimate (i)



The volume at the recommended contour level is 117 nm^3; this corresponds to an approximate mass of 106 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)

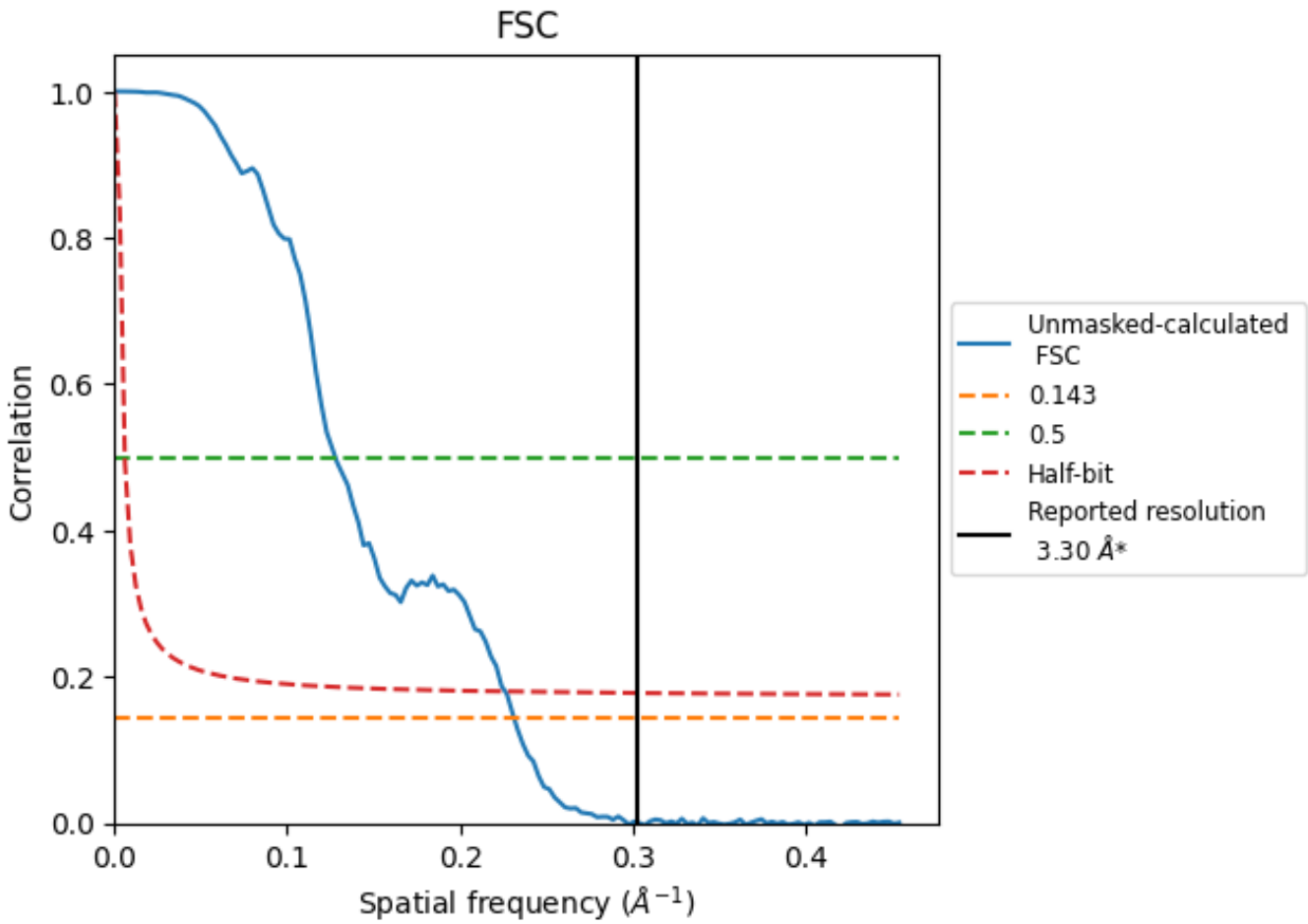


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8.2 Resolution estimates (i)

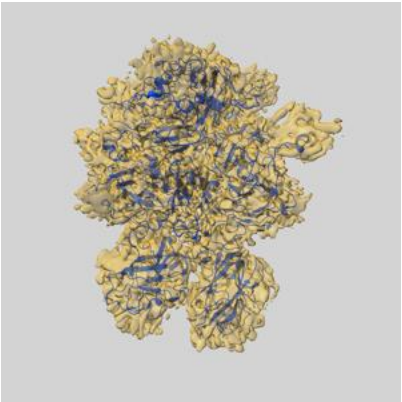
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.32	7.82	4.42

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

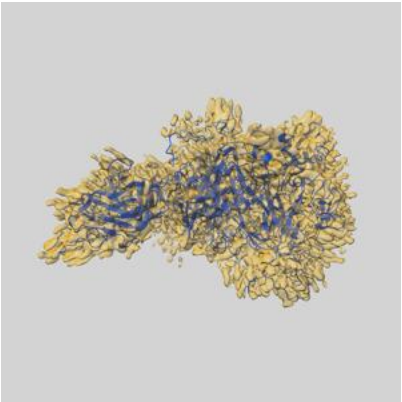
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-23048 and PDB model 7KVE. Per-residue inclusion information can be found in section 3 on page 4.

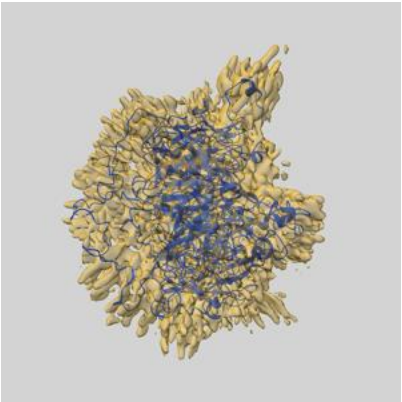
9.1 Map-model overlay (i)



X



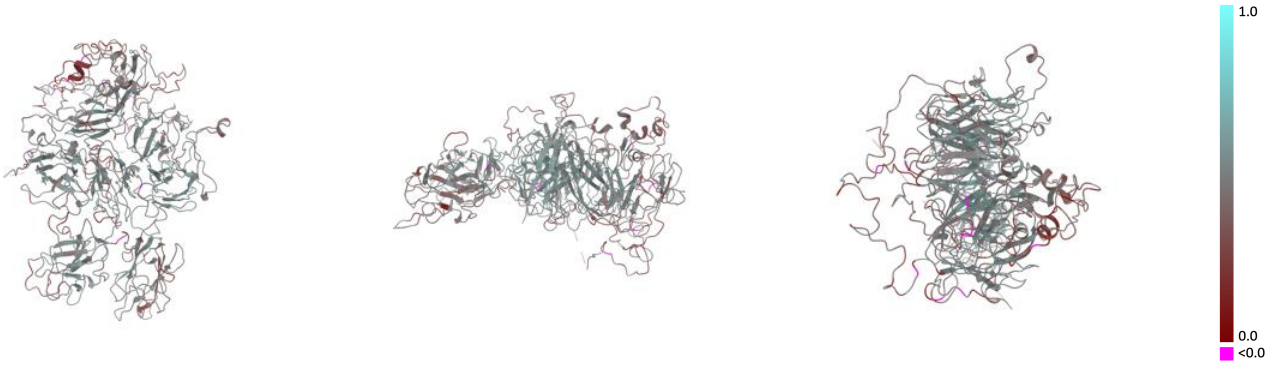
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.43 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.

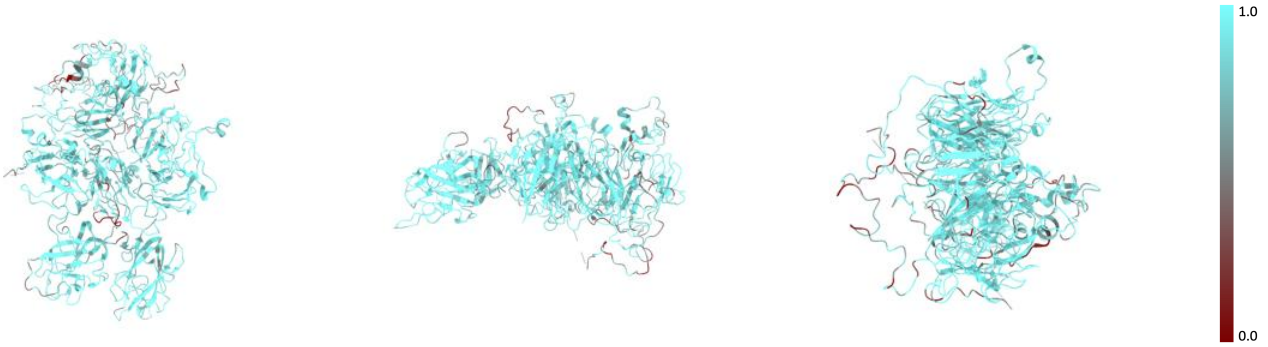
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

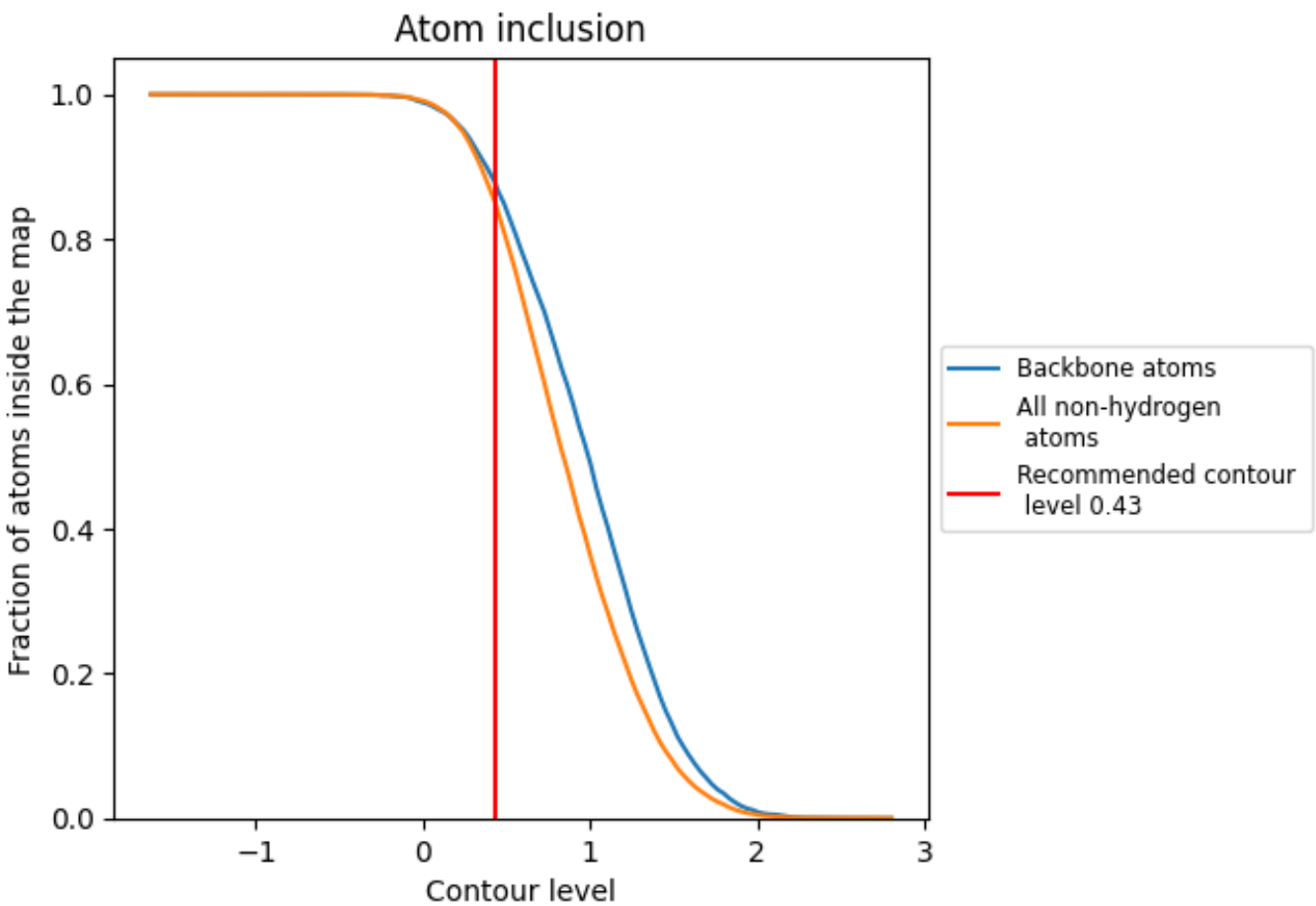
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.43).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 85% 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 (0.43) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8512	0.4510
B	0.8512	0.4510