Full wwPDB EM Validation Report ⓘ

May 12, 2025 – 07:31 PM EDT

PDB ID	:	9CM5 / pdb_00009cm5
EMDB ID	:	EMD-45739
Title	:	CryoEM Strucuture of TcdB in complex with De Novo Minibinder fzd48
Authors	:	Weidle, C.; Carr, K.D.; Borst, A.J.
Deposited on	:	2024-07-12
Resolution	:	4.61 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

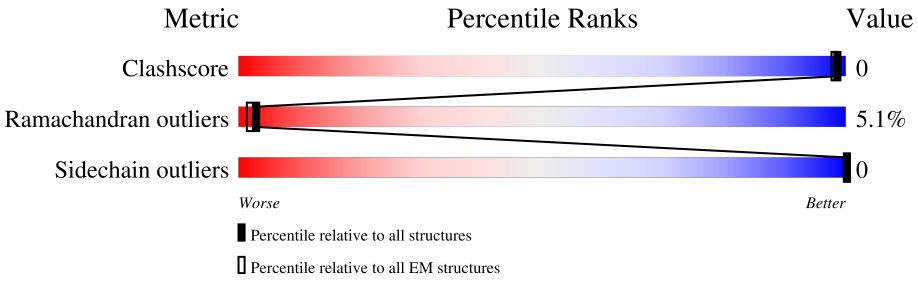
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 4.61 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.

Mol	Chain	Length	Quality of chain
1	B	76	17% 75% 25%
2	A	2119	21% 83% 5% 12%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14029 atoms, of which 4396 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 De Novo Minibinder fzd48.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	57	Total	C	H	N	O	0	0
			415	172	129	57	57		

- Molecule 2 is a protein called Toxin B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1870	Total	C	H	N	O	0	0
			13614	5607	4267	1870	1870		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P18177
A	0	TYR	-	expression tag	UNP P18177
A	102	ALA	TRP	conflict	UNP P18177
A	286	ASN	ASP	conflict	UNP P18177
A	288	ASN	ASP	conflict	UNP P18177
A	543	ALA	LEU	conflict	UNP P18177
A	2101	GLY	-	expression tag	UNP P18177
A	2102	TYR	-	expression tag	UNP P18177
A	2103	ARG	-	expression tag	UNP P18177
A	2104	PRO	-	expression tag	UNP P18177
A	2105	HIS	-	expression tag	UNP P18177
A	2106	ALA	-	expression tag	UNP P18177
A	2107	GLY	-	expression tag	UNP P18177
A	2108	LEU	-	expression tag	UNP P18177
A	2109	ARG	-	expression tag	UNP P18177
A	2110	GLY	-	expression tag	UNP P18177
A	2111	SER	-	expression tag	UNP P18177
A	2112	HIS	-	expression tag	UNP P18177
A	2113	HIS	-	expression tag	UNP P18177
A	2114	HIS	-	expression tag	UNP P18177
A	2115	HIS	-	expression tag	UNP P18177

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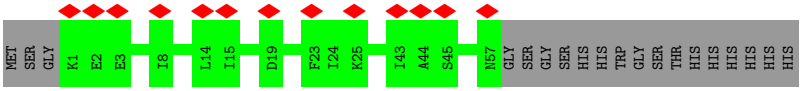
Chain	Residue	Modelled	Actual	Comment	Reference
A	2116	HIS	-	expression tag	UNP P18177
A	2117	HIS	-	expression tag	UNP P18177

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.

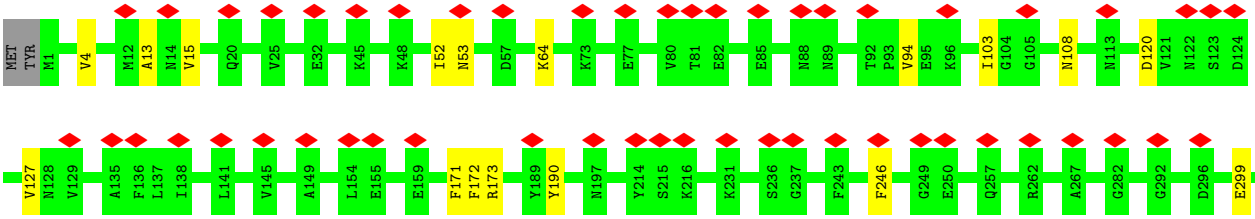
- Molecule 1: De Novo Minibinder fzd48

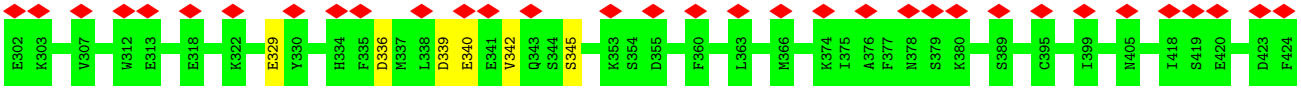
Chain B:

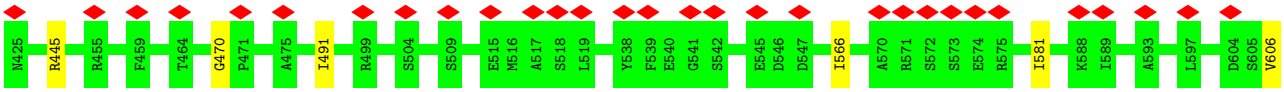


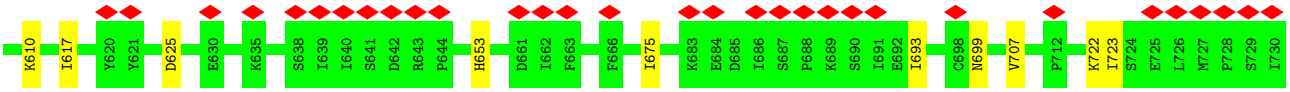
- Molecule 2: Toxin B

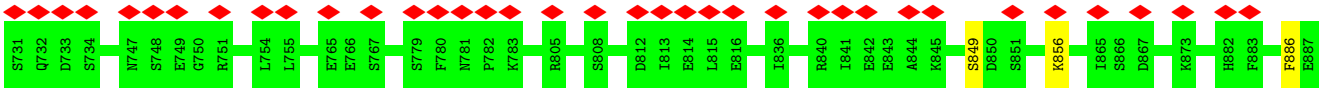
Chain A:

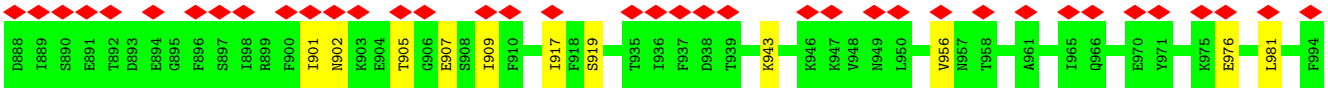


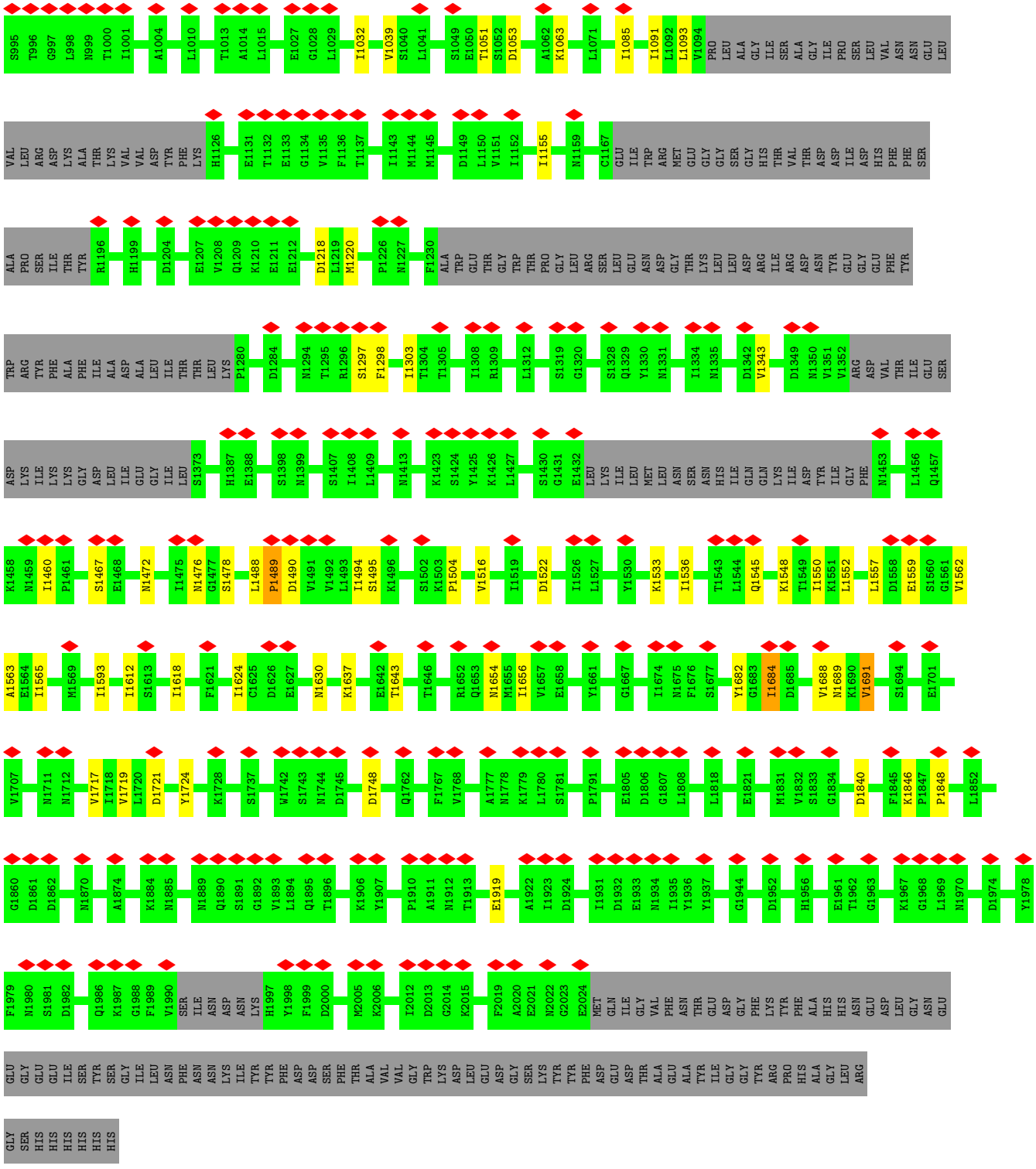











S995 T996 G997 L998 N999 T1000 I1001 A1004 L1010 T1013 A1014 L1015 E1027 G1028 L1029 I1032 V1039 S1040 L1041 S1049 E1050 T1051 S1052 D1053 A1062 K1063 L1071 I1085 I1091 L1092 L1093 V1094 PRO LEU ALA GLY ILE SER ALA GLY ILE PRO SER LEU VAL ASN ASN GLU LEU
VAL LEU ARG ASP LYS ALA THR LYS VAL VAL ASP TYR PHE LYS H1126 E1131 T1132 E1133 G1134 V1135 F1136 T1137 I1143 M1144 M1145 D1149 L1150 V1151 I1152 I1155 N1159 C1167 GLU ILE TRP ARG MET GLU GLY GLY SER GLY HIS THR VAL THR ASP ASP ILE ASP HIS PHE PHE SER
ALA PRO SER ILE THR TYR R1196 H1199 D1204 E1207 V1208 Q1209 K1210 E1211 E1212 D1218 L1219 M1220 P1226 N1227 F1230 ALA TRP GLU THR GLY TRP THR PRO GLY LEU ARG SER LEU GLU ASN ASP GLY THR LYS LEU LEU ASP ARG ILE ARG ASP ASN TYR GLU GLY GLU PHE TYR
TRP ARG TYR PHE ALA PHE ILE ALA ASP ALA LEU ILE THR THR LEU LYS P1280 D1284 N1294 T1295 R1296 S1297 F1298 I1303 T1304 T1305 I1308 R1309 L1312 S1319 G1320 S1328 Q1329 Y1330 N1331 I1334 N1335 D1342 V1343 D1349 N1350 V1351 V1352 ARG ASP VAL THR ILE GLU SER
ASP LYS ILE LYS LYS GLY ASP LEU ILE GLU GLY ILE LEU S1373 H1387 E1388 S1398 N1399 S1407 I1408 L1409 N1413 K1423 S1424 Y1425 K1426 L1427 S1430 G1431 E1432 LEU LYS ILE LEU MET LEU ASN SER ASN HIS ILE GLN GLN LYS ILE ASP TYR ILE GLY PHE N1453 L1456 Q1457
K1458 N1459 I1460 P1461 S1467 E1468 N1472 I1475 N1476 G1477 S1478 L1488 P1489 D1490 V1491 V1492 L1493 I1494 S1495 K1496 S1502 K1503 P1504 V1516 I1519 D1522 I1526 L1527 Y1530 K1533 I1536 T1543 L1544 Q1545 K1548 T1549 I1550 K1551 L1552 L1557 D1558 E1559 S1560 G1561 V1562
A1563 E1564 I1565 M1569 I1593 I1612 S1613 I1618 F1621 I1624 C1625 D1626 E1627 N1630 K1637 E1642 T1643 T1646 R1652 Q1653 N1654 M1655 I1656 V1657 E1658 Y1661 G1667 I1674 N1675 F1676 S1677 Y1682 G1683 I1684 D1685 V1688 N1689 K1690 V1691 S1694 E1701
V1707 N1711 N1712 V1717 I1718 V1719 L1720 D1721 Y1724 K1728 S1737 W1742 S1743 N1744 D1745 D1748 Q1762 F1767 V1768 A1777 N1778 K1779 L1780 S1781 P1791 E1805 D1806 G1807 L1808 L1818 E1821 M1831 V1832 S1833 G1834 D1840 F1845 K1846 P1847 P1848 L1852
G1860 D1861 D1862 N1870 A1874 K1884 N1885 N1889 Q1890 S1891 G1892 V1893 L1894 Q1895 T1896 K1906 Y1907 P1910 A1911 N1912 T1913 E1919 A1922 I1923 D1924 I1931 D1932 E1933 N1934 I1935 Y1936 Y1937 G1944 D1952 H1956 E1961 T1962 G1963 K1967 G1968 L1969 N1970 D1974 Y1978
F1979 N1980 S1981 D1982 Q1986 K1987 G1988 F1989 V1990 SER ILE ASN ASP ASN LYS H1997 Y1998 F1999 D2000 M2005 K2006 I2012 D2013 G2014 K2015 F2019 A2020 E2021 N2022 G2023 E2024 MET GLN ILE GLY VAL PHE ASN THR GLU ASP GLY PHE LYS TYR PHE ALA HIS HIS ASN GLU ASP LEU GLY ASN GLU
GLU GLY GLU GLU ILE SER TYR SER GLY ILE LEU ASN PHE ASN ASN LYS ILE TYR TYR PHE ASP ASP SER PHE THR ALA VAL VAL GLY TRP LYS ASP LEU GLU GLU ASP GLY SER LYS TYR TYR PHE ASP GLU ASP THR ALA GLU ALA TYR ILE GLY GLY TYR TYR ARG PRO HIS ALA GLY LEU ARG
GLY SER HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	108076	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.482	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.0803	Depositor
Map size (Å)	387.78, 387.78, 387.78	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.843, 0.843, 0.843	Depositor

5 Model quality

5.1 Standard geometry

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	0.57	0/286	0.95	0/399
2	A	0.75	0/9384	1.55	17/13106 (0.1%)
All	All	0.75	0/9670	1.53	17/13505 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1691	VAL	N-CA-C	8.23	120.98	112.83
2	A	1846	LYS	N-CA-C	7.62	114.85	108.07
2	A	905	THR	N-CA-C	7.37	121.67	112.24
2	A	1489	PRO	CA-N-CD	-6.32	103.16	112.00
2	A	723	ILE	N-CA-C	6.08	116.55	110.23
2	A	1155	ILE	N-CA-C	6.02	116.30	107.75
2	A	1467	SER	N-CA-C	5.82	118.57	111.82
2	A	902	ASN	N-CA-C	5.62	115.65	108.24
2	A	1476	ASN	N-CA-C	5.57	116.73	108.60
2	A	675	ILE	N-CA-C	5.43	115.63	110.53
2	A	1298	PHE	N-CA-C	5.40	117.05	108.79
2	A	470	GLY	CA-C-N	5.36	124.81	119.24
2	A	470	GLY	C-N-CA	5.36	124.81	119.24
2	A	329	GLU	N-CA-C	5.25	116.82	108.79
2	A	1684	ILE	N-CA-C	5.17	120.09	109.34
2	A	299	GLU	N-CA-C	5.12	116.53	110.19
2	A	1721	ASP	N-CA-C	5.02	115.93	108.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	286	129	131	0	0
2	A	9347	4267	4270	2	0
All	All	9633	4396	4401	2	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 0.

All (2) 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)
2:A:1691:VAL:H	2:A:1717:VAL:HA	1.83	0.44
2:A:171:PHE:C	2:A:173:ARG:H	2.27	0.43

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	55/76 (72%)	54 (98%)	1 (2%)	0	100 100
2	A	1856/2119 (88%)	1390 (75%)	368 (20%)	98 (5%)	1 16
All	All	1911/2195 (87%)	1444 (76%)	369 (19%)	98 (5%)	3 16

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	4	VAL
2	A	103	ILE
2	A	445	ARG
2	A	909	ILE
2	A	956	VAL
2	A	1032	ILE
2	A	1303	ILE
2	A	1460	ILE
2	A	1488	LEU
2	A	1489	PRO
2	A	1494	ILE
2	A	1536	ILE
2	A	1550	ILE
2	A	1565	ILE
2	A	1612	ILE
2	A	1618	ILE
2	A	1684	ILE
2	A	1688	VAL
2	A	1719	VAL
2	A	15	VAL
2	A	52	ILE
2	A	108	ASN
2	A	172	PHE
2	A	336	ASP
2	A	491	ILE
2	A	617	ILE
2	A	707	VAL
2	A	901	ILE
2	A	1091	ILE
2	A	1548	LYS
2	A	1682	TYR
2	A	53	ASN
2	A	64	LYS
2	A	246	PHE
2	A	345	SER
2	A	610	LYS
2	A	699	ASN
2	A	849	SER
2	A	886	PHE
2	A	919	SER
2	A	976	GLU
2	A	1478	SER
2	A	1495	SER

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Mol	Chain	Res	Type
2	A	1522	ASP
2	A	1545	GLN
2	A	1559	GLU
2	A	1748	ASP
2	A	339	ASP
2	A	653	HIS
2	A	693	ILE
2	A	943	LYS
2	A	1051	THR
2	A	1220	MET
2	A	1297	SER
2	A	1472	ASN
2	A	1490	ASP
2	A	1563	ALA
2	A	1643	THR
2	A	1848	PRO
2	A	13	ALA
2	A	120	ASP
2	A	340	GLU
2	A	625	ASP
2	A	722	LYS
2	A	856	LYS
2	A	907	GLU
2	A	981	LEU
2	A	1063	LYS
2	A	1085	ILE
2	A	1218	ASP
2	A	1516	VAL
2	A	1533	LYS
2	A	1552	LEU
2	A	1557	LEU
2	A	1624	ILE
2	A	1630	ASN
2	A	1637	LYS
2	A	1654	ASN
2	A	1689	ASN
2	A	1724	TYR
2	A	1840	ASP
2	A	190	TYR
2	A	1093	LEU
2	A	1919	GLU
2	A	94	VAL

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Mol	Chain	Res	Type
2	A	1039	VAL
2	A	1504	PRO
2	A	1562	VAL
2	A	127	VAL
2	A	1053	ASP
2	A	566	ILE
2	A	1593	ILE
2	A	1656	ILE
2	A	342	VAL
2	A	581	ILE
2	A	606	VAL
2	A	917	ILE
2	A	1343	VAL

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	1/68 (2%)	1 (100%)	0	100	100
2	A	44/1918 (2%)	44 (100%)	0	100	100
All	All	45/1986 (2%)	45 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

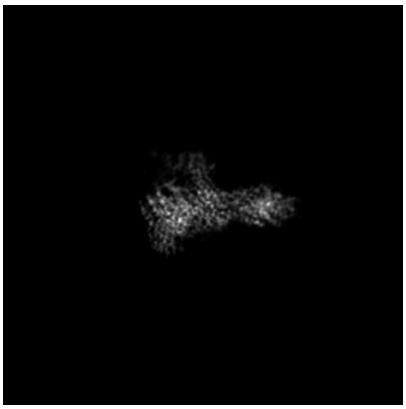
This section contains visualisations of the EMDB entry EMD-45739. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

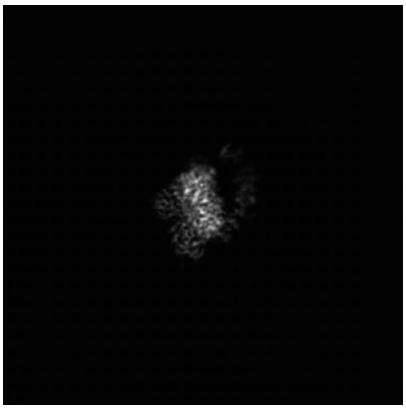
6.1 Orthogonal projections

6.1.1 Primary map

X

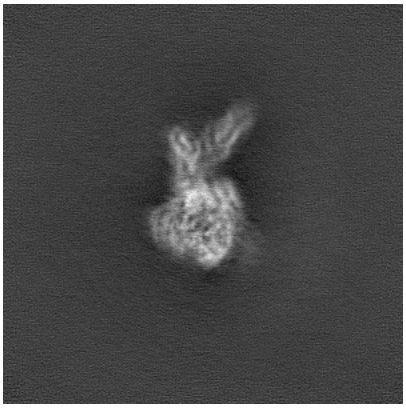


Y

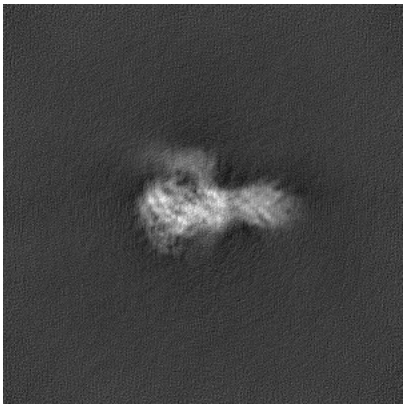


Z

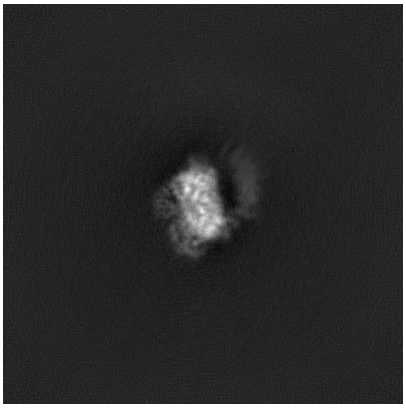
6.1.2 Raw map



X



Y



Z

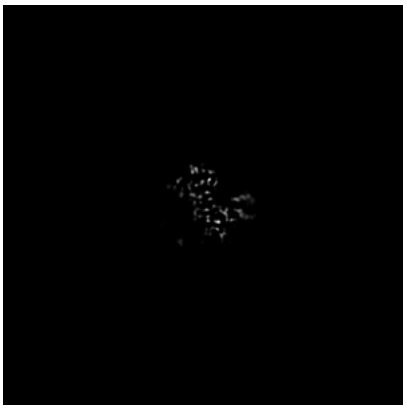
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

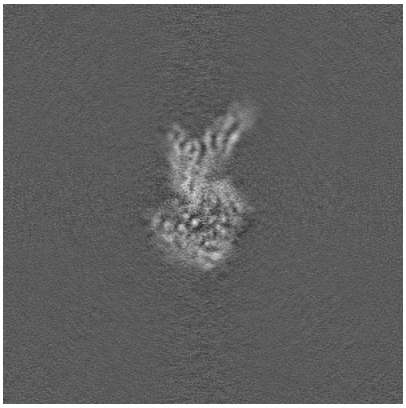
X Index: 230

Y Index: 230

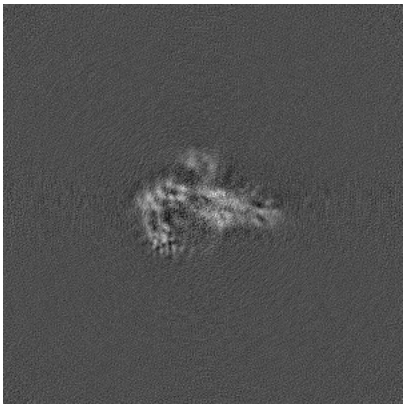


Z Index: 230

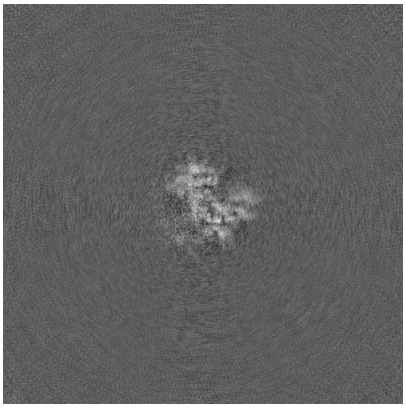
6.2.2 Raw map



X Index: 230



Y Index: 230



Z Index: 230

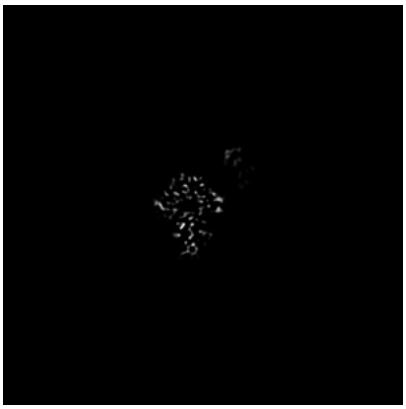
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

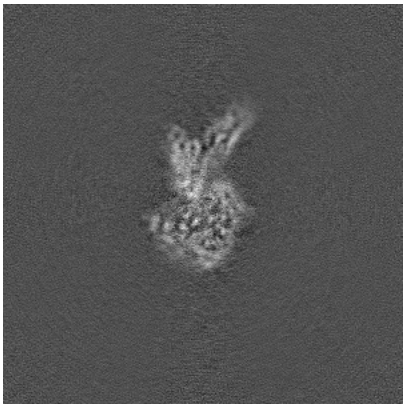
X Index: 232

Y Index: 234

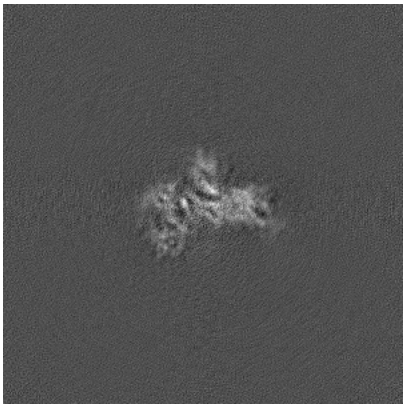


Z Index: 196

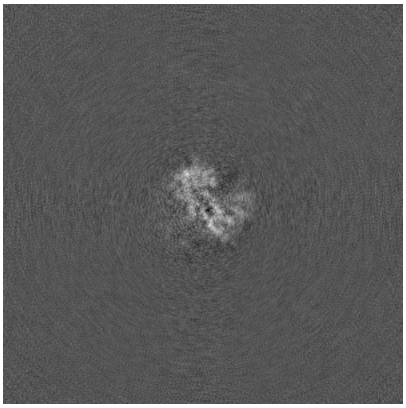
6.3.2 Raw map



X Index: 228



Y Index: 220

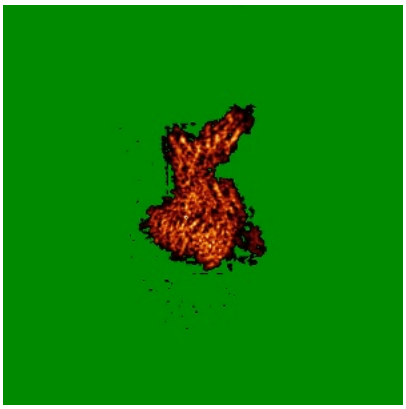


Z Index: 235

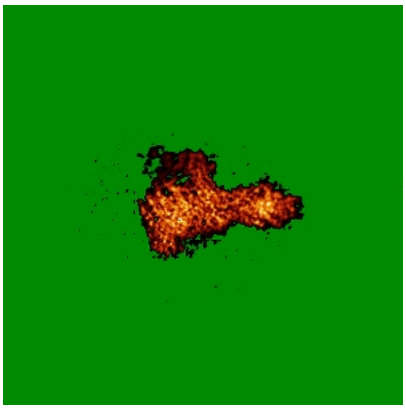
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

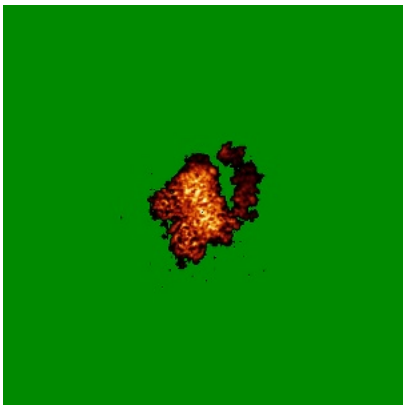
6.4.1 Primary map



X

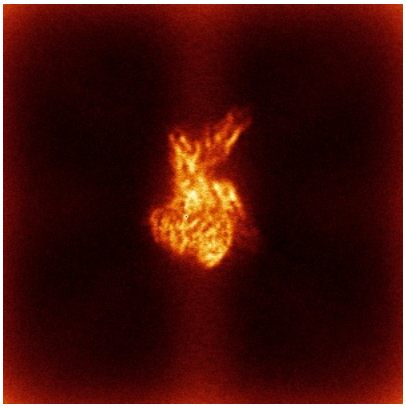


Y

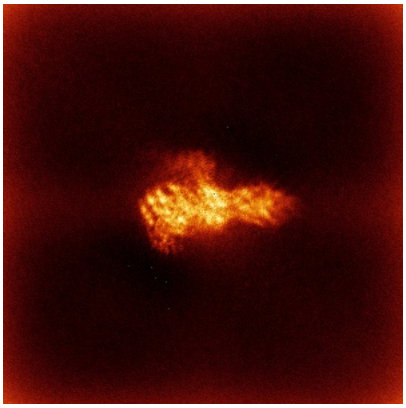


Z

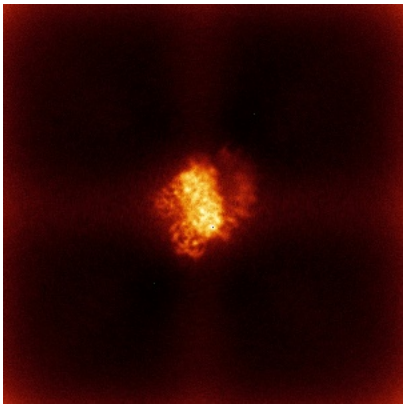
6.4.2 Raw map



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.

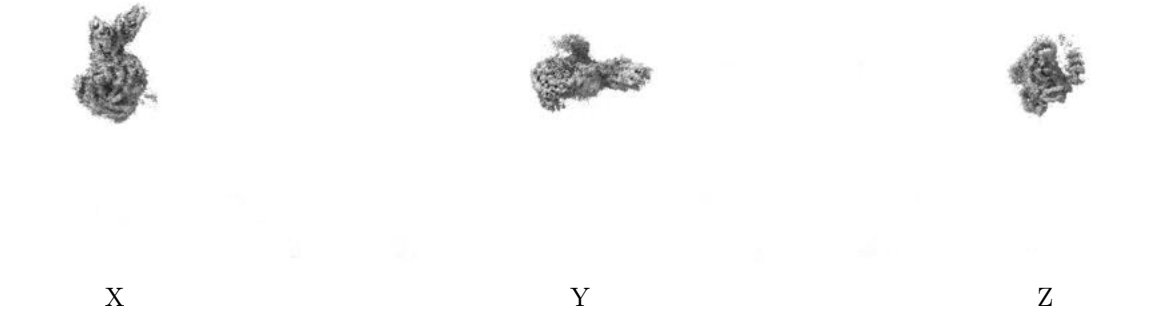
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0803. 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



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.

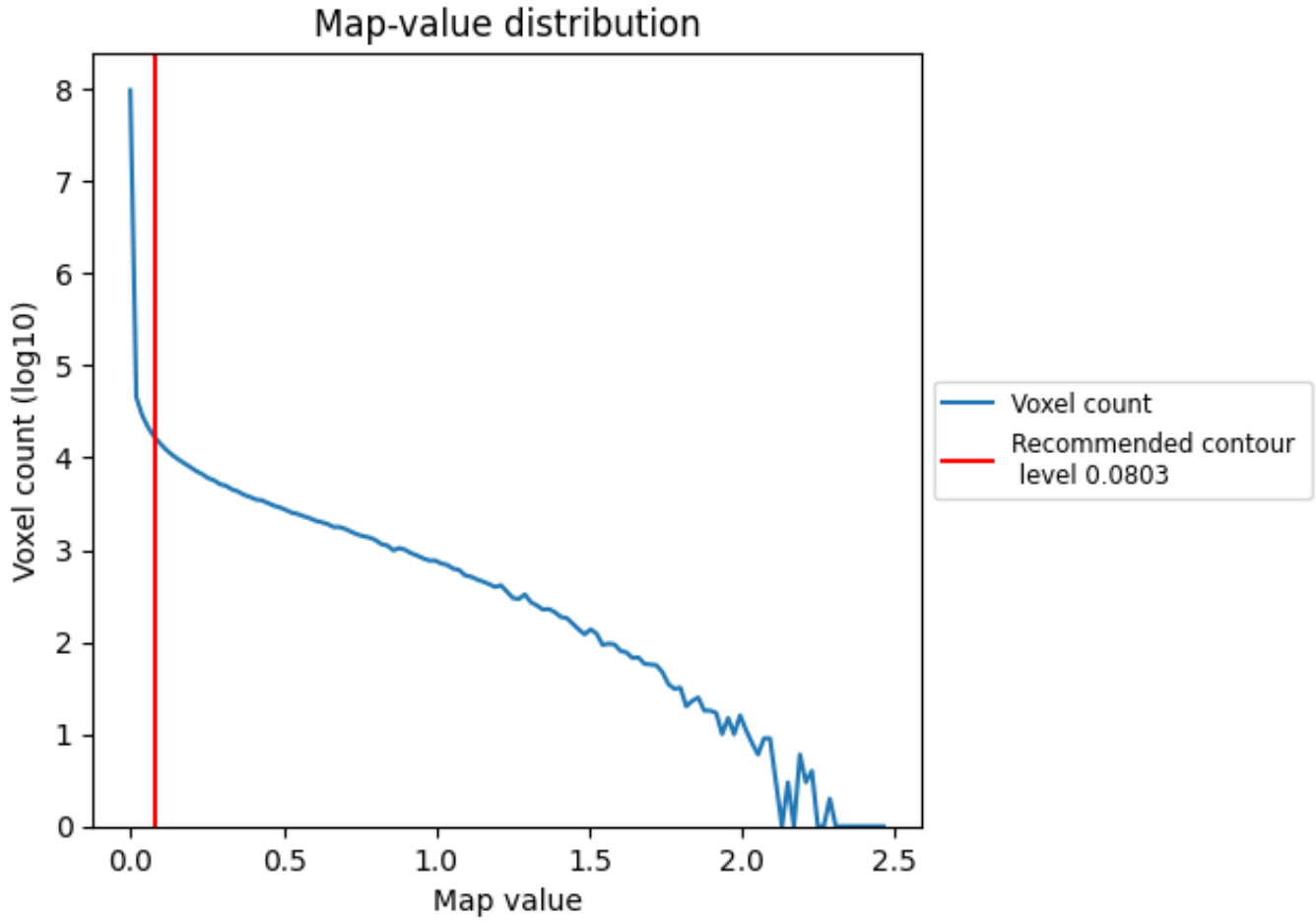
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

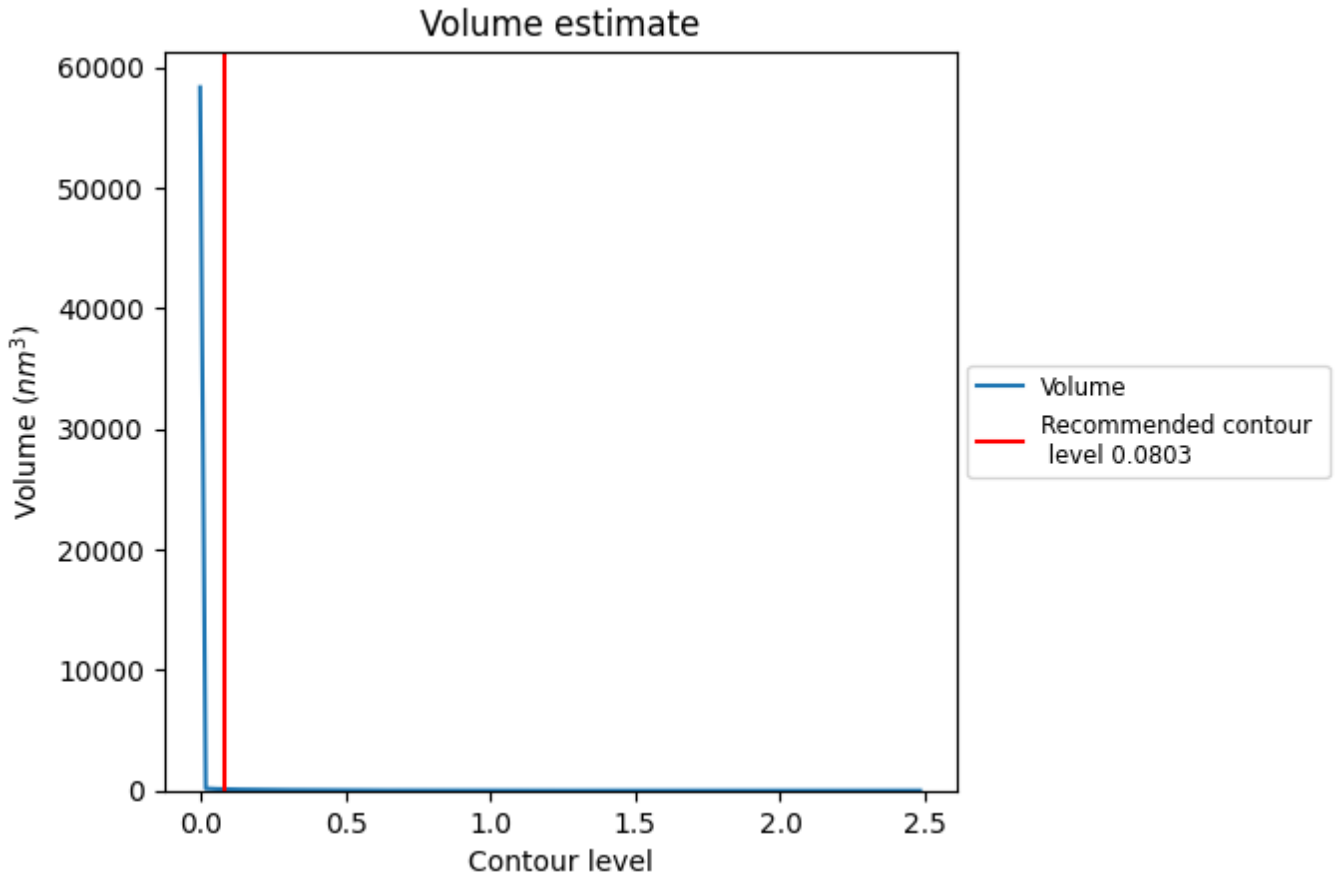
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

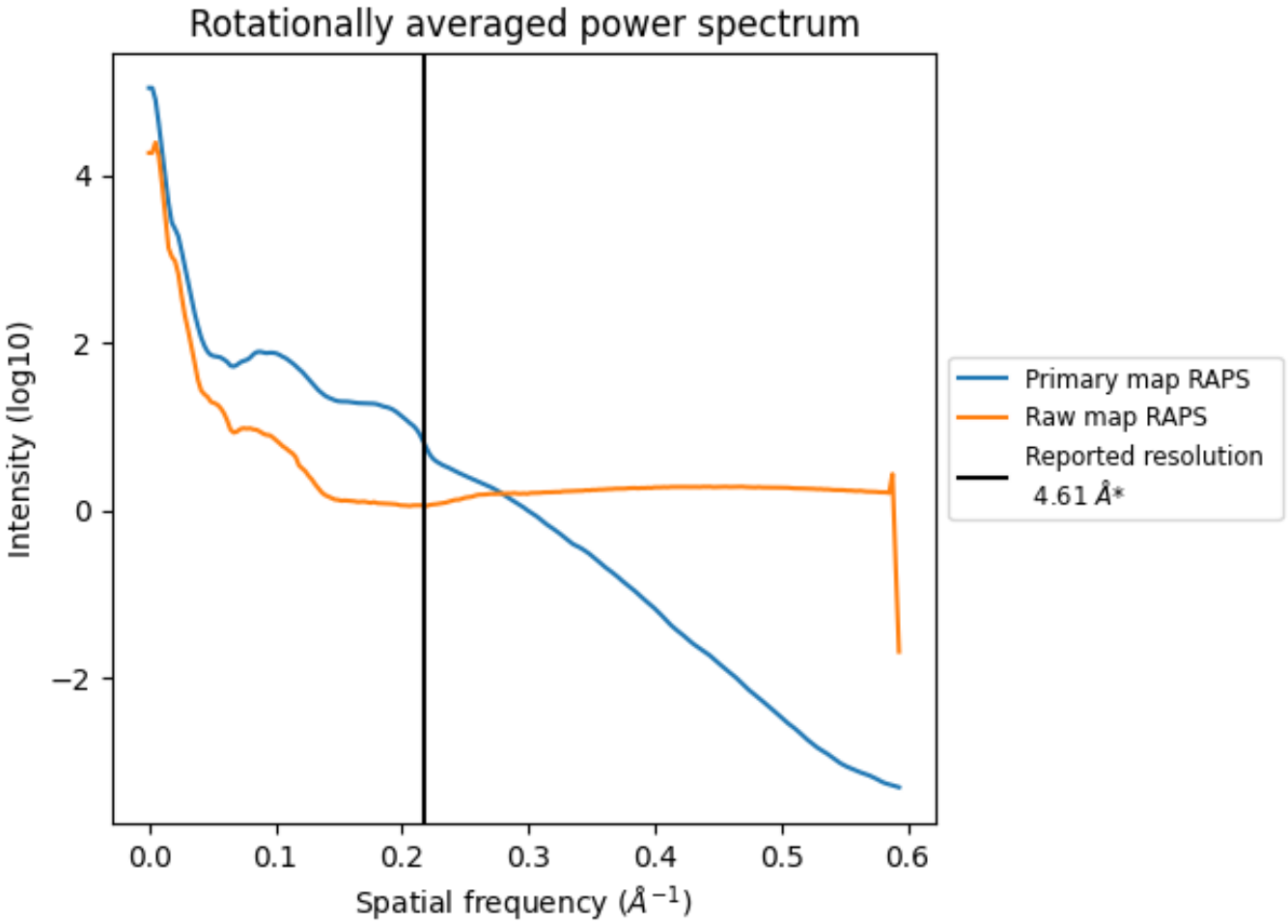
7.2 Volume estimate



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)

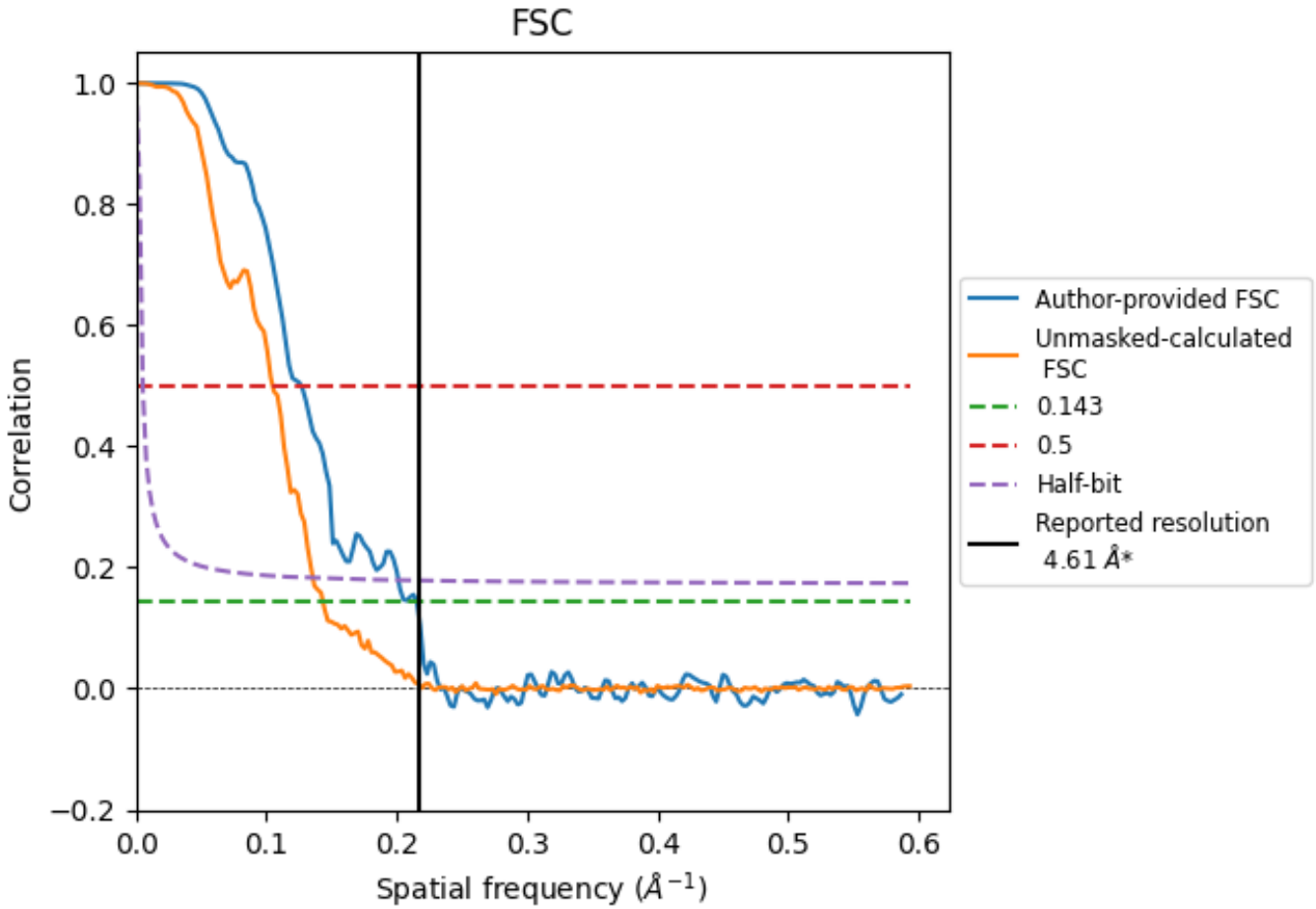


*Reported resolution corresponds to spatial frequency of 0.217 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

8.2 Resolution estimates (i)

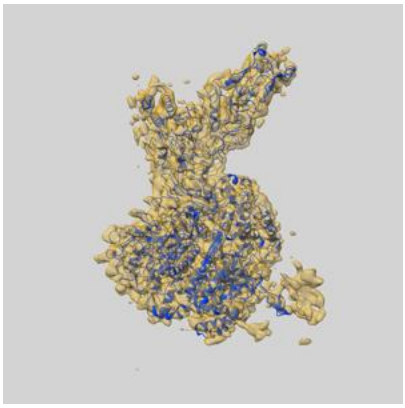
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.61	-	-
Author-provided FSC curve	4.64	7.91	4.97
Unmasked-calculated*	6.98	9.55	7.37

*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 6.98 differs from the reported value 4.61 by more than 10 %

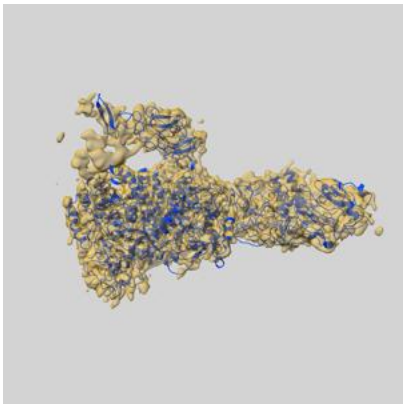
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-45739 and PDB model 9CM5. Per-residue inclusion information can be found in section 3 on page 5.

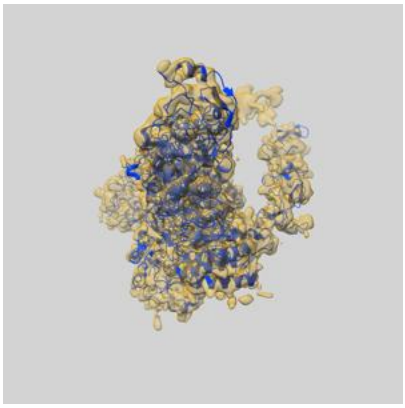
9.1 Map-model overlay



X



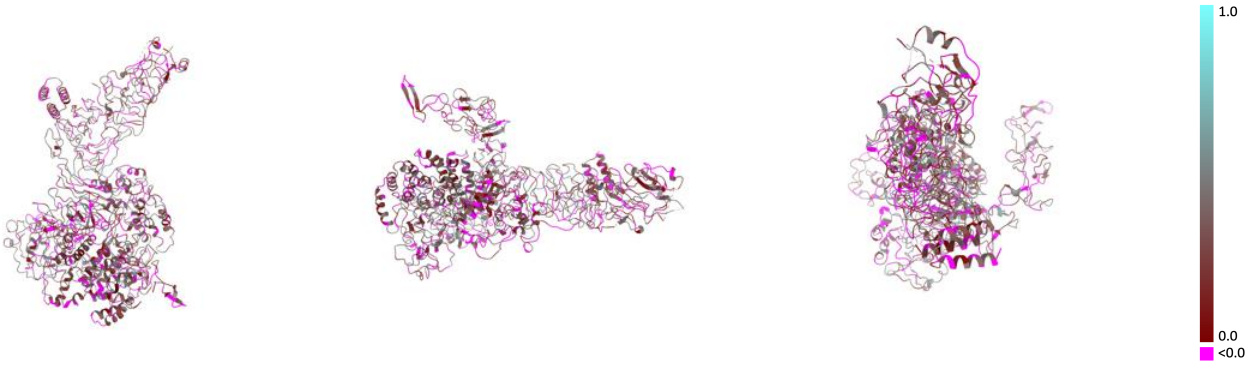
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0803 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.

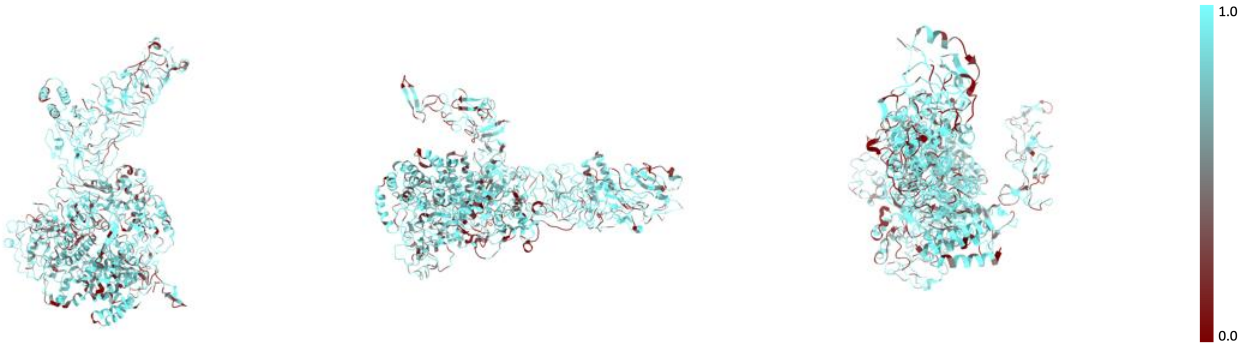
9.2 Q-score mapped to coordinate model (i)



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.

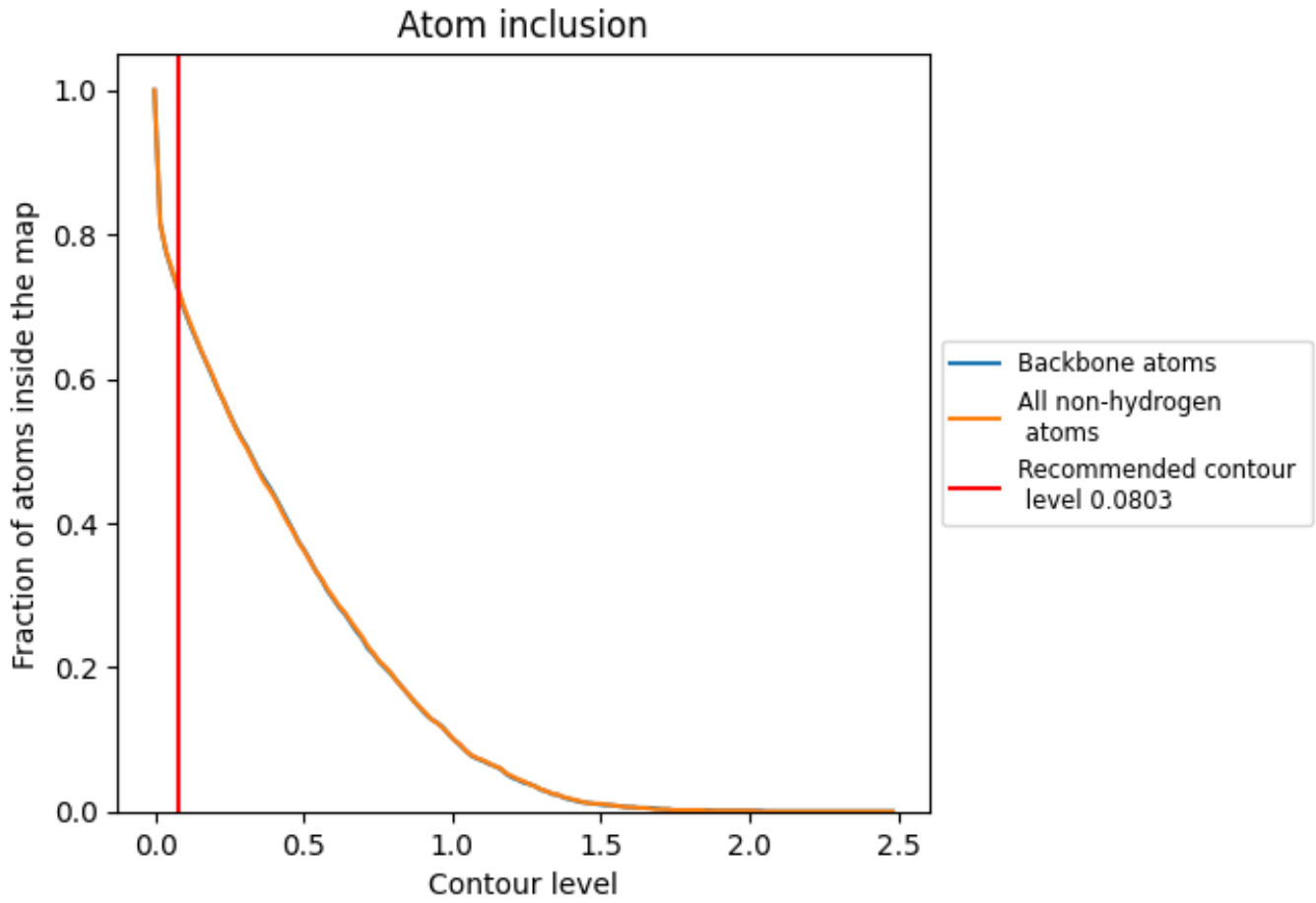
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0803).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 72% 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 (0.0803) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7210	0.2350
A	0.7200	0.2380
B	0.7450	0.1530