



wwPDB EM Validation Summary Report ⓘ

Oct 21, 2024 – 10:43 AM JST

PDB ID : 5X6O
EMDB ID : EMD-6708
Title : Intact ATR/Mec1-ATRIP/Ddc2 complex
Authors : Wang, X.; Ran, T.; Cai, G.
Deposited on : 2017-02-22
Resolution : 3.90 Å(reported)

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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.dev113
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) : 2.39

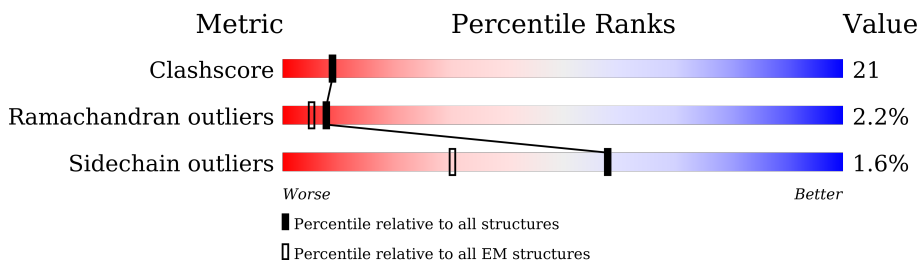
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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 $\leq 5\%$. 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	C	2368	
2	G	747	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19309 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.

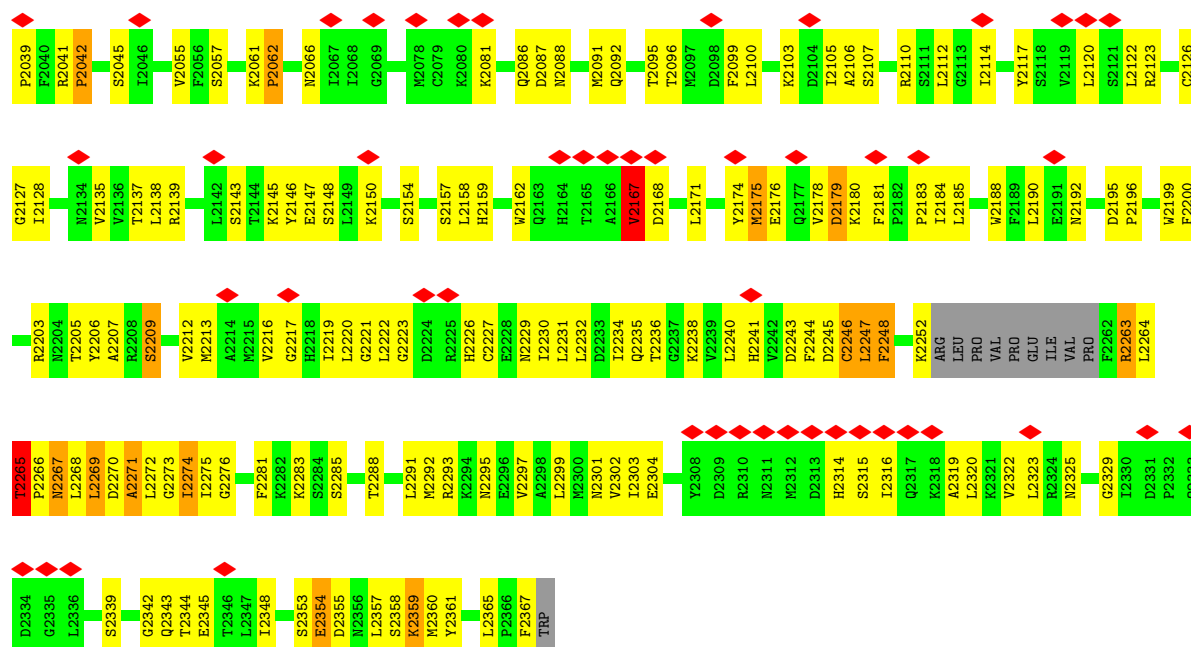
- Molecule 1 is a protein called Serine/threonine-protein kinase MEC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	1997	Total	C	N	O	S	0	0
			14240	8995	2502	2692	51		

- Molecule 2 is a protein called DNA damage checkpoint protein LCD1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	704	Total	C	N	O	S	0	0
			5069	3234	875	941	19		

D1969	S1875	L1782	S1672	D1566	T1460	Y1355	N1249	I1157	R1071	G982	D893	L819
S1972	K1876	Q1785	R1567	R1567	L1463	K1357	F1250	W1158	K1072	K983	V894	S823
S1973	L1877	Y1786	V1568	V1568	K1466	K1357	LYS	V1159	Q1073	N986	E895	THR
A1974	E1878	Q1787	L1570	L1570	L1470	K1358	E1252	T1074	R1076	I987	G896	VAL
L1975	D1880	D1788	L1573	Y1573	Y1573	W1359	K1255	E1075	S1077	S890	T898	LYS
ASP	E1887	D1789	M1574	M1574	E1474	A1360	K1259	R1076	D1078	S991	T899	ASP
LEU	L1888	L1792	A1576	A1576	A1479	E1362	G1269	F1080	D1079	T994	R905	ALA
LYS	Q1890	S1794	P1587	P1587	A1479	F1363	G1269	L995	F1080	T996	N908	THR
Q1891	F1795	Q1795	Q1589	Q1589	F1489	K1364	E1272	W1169	THR	K997	N908	S831
L1891	CYS	W1796	Q1591	Q1591	ASP	Q1365	N1273	Q1170	LYS	E998	S911	D830
L1982	P1893	D1797	K1592	K1592	ASP	H1371	H1273	W1173	LYS	K999	S911	S831
L1983	T1894	P1799	Y1593	Y1593	T1496	G1372	P1275	N1173	VAL	D1001	F912	E832
L1986	I1895	R1717	I1594	I1594	T1496	T1382	P1275	F1179	GLY	L1002	L913	A834
Q1987	L1896	E1722	H1595	H1595	T1496	L1386	ASP	W1180	GLN	L1006	I914	M836
V1988	W1897	L1723	N1596	N1596	T1496	L1386	ASP	A1181	THR	L1006	I915	I837
L1990	L1901	E1724	S1597	S1597	T1496	L1386	ASP	W1180	THR	L1006	I916	L838
S1991	S1802	F1725	F1598	F1598	I1512	T1394	S1289	Q1185	THR	L1006	I916	L838
L1992	G1804	F1725	L1600	L1600	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
T1993	L1805	E1728	L1601	L1601	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
S1994	Y1806	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
R1907	S1807	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1908	L1808	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1909	L1809	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
S1906	S1810	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
R1907	L1811	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1908	L1812	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1909	L1813	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
S1906	L1814	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
R1907	L1815	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1908	L1816	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1909	L1817	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
S1906	L1818	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
R1907	L1819	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1908	L1820	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1909	L1821	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
S1906	L1822	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
R1907	L1823	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1908	L1824	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1909	L1825	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
S1906	L1826	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
R1907	L1827	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1908	L1828	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1909	L1829	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
S1906	L1830	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
R1907	L1831	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1908	L1832	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1909	L1833	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
S1906	L1834	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
R1907	L1835	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1908	L1836	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1909	L1837	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
S1906	L1838	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
R1907	L1839	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1908	L1840	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1909	L1841	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
S1906	L1842	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
R1907	L1843	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1908	L1844	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1909	L1845	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
S1906	L1846	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
R1907	L1847	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1908	L1848	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1909	L1849	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
S1906	L1850	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
R1907	L1851	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1908	L1852	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1909	L1853	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
S1906	L1854	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
R1907	L1855	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
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L1909	L1857	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
S1906	L1858	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
R1907	L1859	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1908	L1860	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1909	L1861	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
S1906	L1862	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
R1907	L1863	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1908	L1864	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1909	L1865	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
S1906	L1866	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
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L1908	L1868	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
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S1906	L1870	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
R1907	L1871	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1908	L1872	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1909	L1873	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
S1906	L1874	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
R1907	L1875	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1908	L1876	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1909	L1877	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
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S1906	L1882	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
R1907	L1883	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
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R1907	L1887	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
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L1909	L1889	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
S1906	L1890	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
R1907	L1891	E1734	G1602	G1602	S1514	T1394	S1289	L1188	THR	L1006	I916	L838
L1908	L1892	E1734	G1602	G1602	S1514	T1394</						





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63132	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.244	Depositor
Minimum map value	-0.151	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0518	Depositor
Map size (Å)	345.6, 345.6, 345.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	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	C	0.36	0/14428	0.55	20/19608 (0.1%)
2	G	0.41	0/5140	0.58	6/6985 (0.1%)
All	All	0.37	0/19568	0.56	26/26593 (0.1%)

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2018	PRO	N-CA-CB	6.85	111.52	103.30
2	G	160	PRO	N-CA-CB	6.70	111.34	103.30
1	C	356	PRO	N-CA-CB	6.57	111.18	103.30
2	G	171	PRO	N-CA-CB	6.24	110.79	103.30
1	C	1849	PRO	N-CA-CB	6.14	110.67	103.30

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	C	14240	0	12588	563	0
2	G	5069	0	4486	194	0
All	All	19309	0	17074	747	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 21.

The worst 5 of 747 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:C:685:SER:HB3	1:C:686:PRO:CD	1.30	1.44
1:C:2167:VAL:CG1	1:C:2168:ASP:H	1.32	1.38
2:G:191:VAL:CB	2:G:195:PRO:HD2	1.54	1.37
1:C:2265:THR:HB	1:C:2266:PRO:CD	1.57	1.29
1:C:1124:GLY:O	1:C:1125:VAL:HG22	1.35	1.24

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	C	1943/2368 (82%)	1595 (82%)	311 (16%)	37 (2%)	6	34
2	G	678/747 (91%)	556 (82%)	102 (15%)	20 (3%)	3	27
All	All	2621/3115 (84%)	2151 (82%)	413 (16%)	57 (2%)	8	32

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	356	PRO
1	C	685	SER
1	C	845	ILE
1	C	1241	VAL
1	C	1395	THR

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	C	1257/2174 (58%)	1233 (98%)	24 (2%)	52	70
2	G	447/698 (64%)	443 (99%)	4 (1%)	75	83
All	All	1704/2872 (59%)	1676 (98%)	28 (2%)	58	73

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2246	CYS
2	G	435	MET
1	C	2265	THR
2	G	194	ASN
1	C	2263	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1756	ASN
1	C	2314	HIS
1	C	2229	ASN
2	G	196	ASN
1	C	877	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

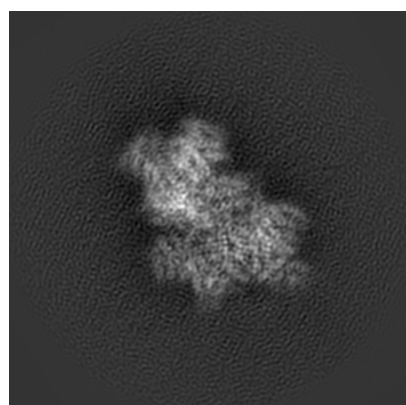
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6708. These allow visual inspection of the internal detail of the map and identification of artifacts.

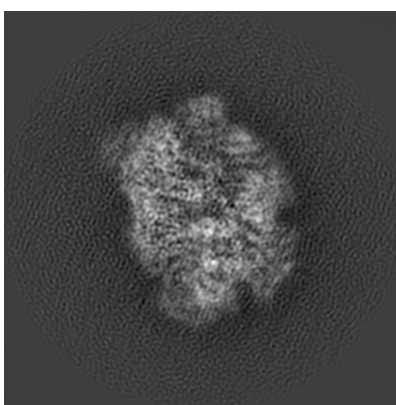
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

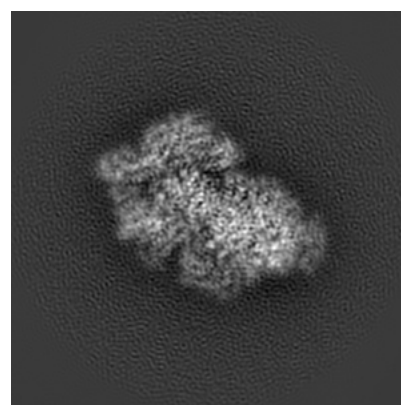
6.1.1 Primary map



X



Y

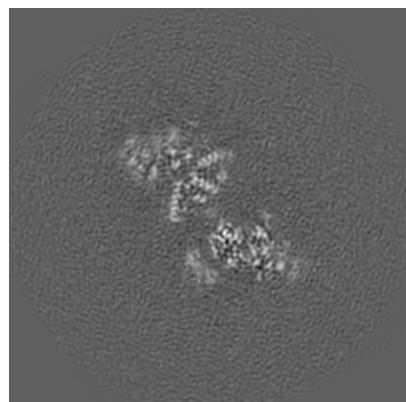


Z

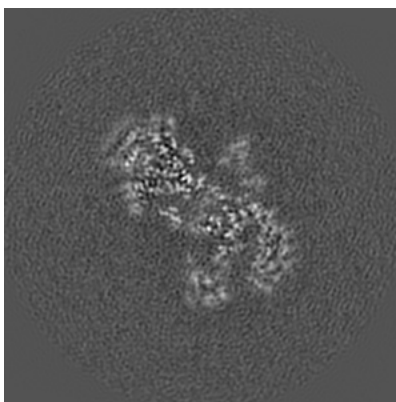
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

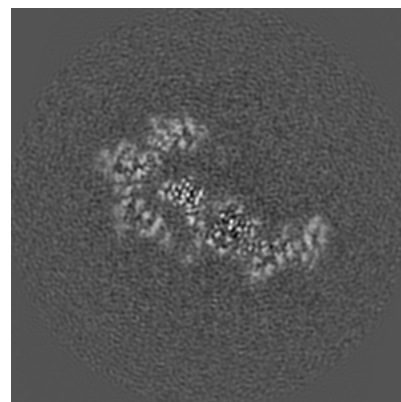
6.2.1 Primary map



X Index: 128



Y Index: 128

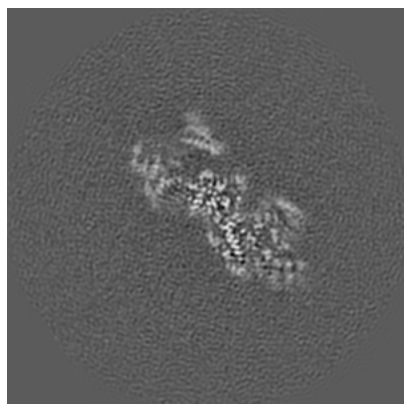


Z Index: 128

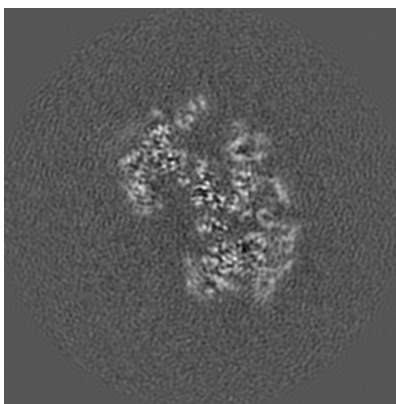
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

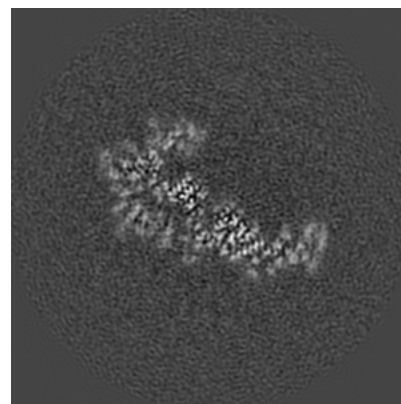
6.3.1 Primary map



X Index: 115



Y Index: 119

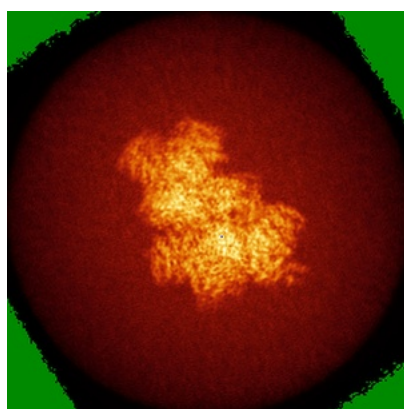


Z Index: 130

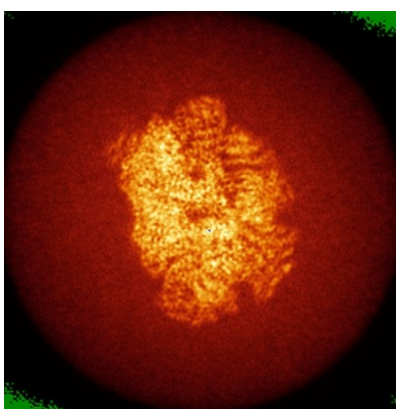
The images above show the largest variance slices of the map in three orthogonal directions.

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

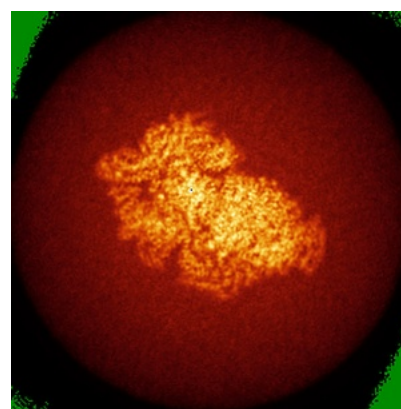
6.4.1 Primary map



X



Y



Z

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 0.0518. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

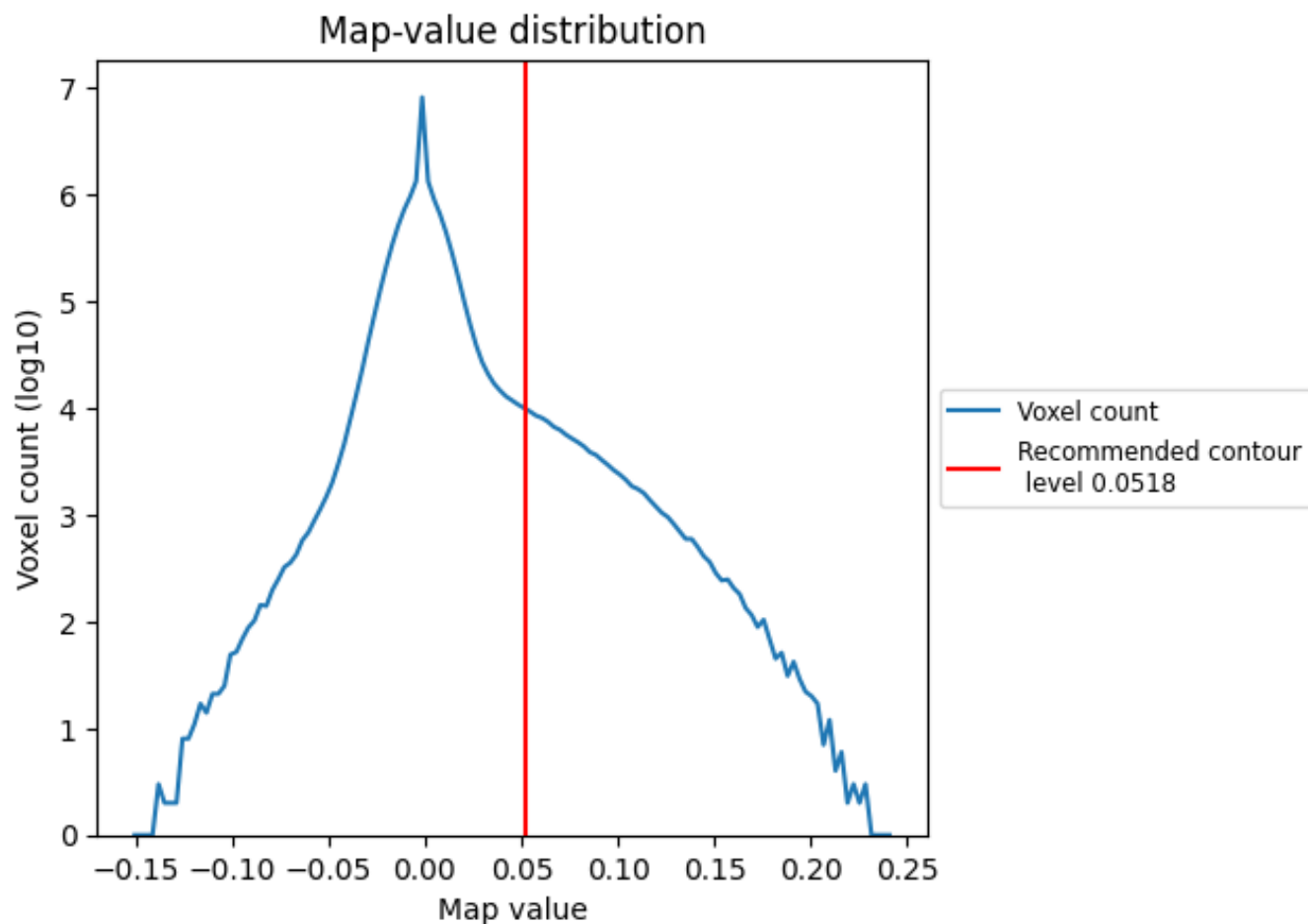
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

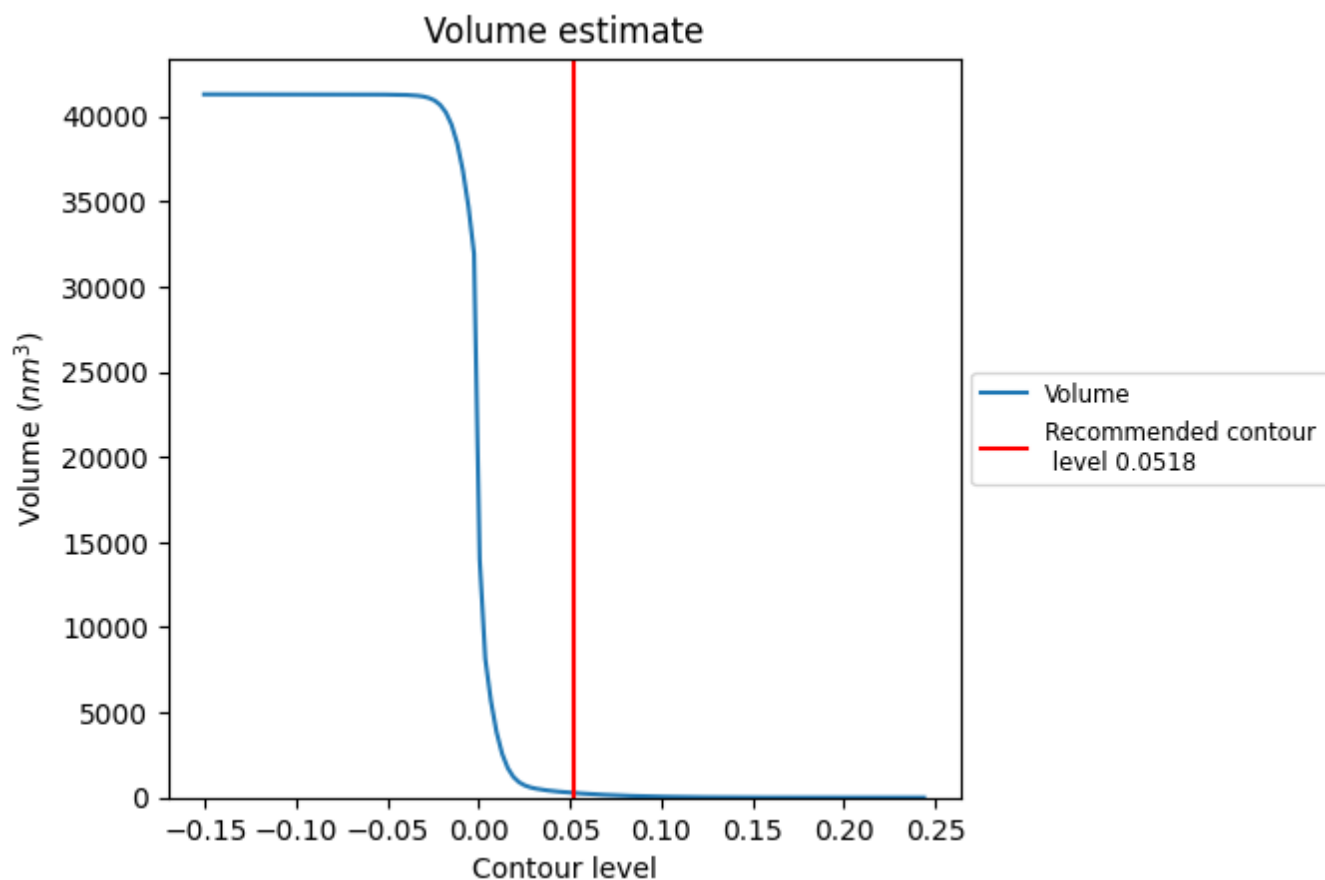
This section contains the results of statistical analysis of the map.

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.

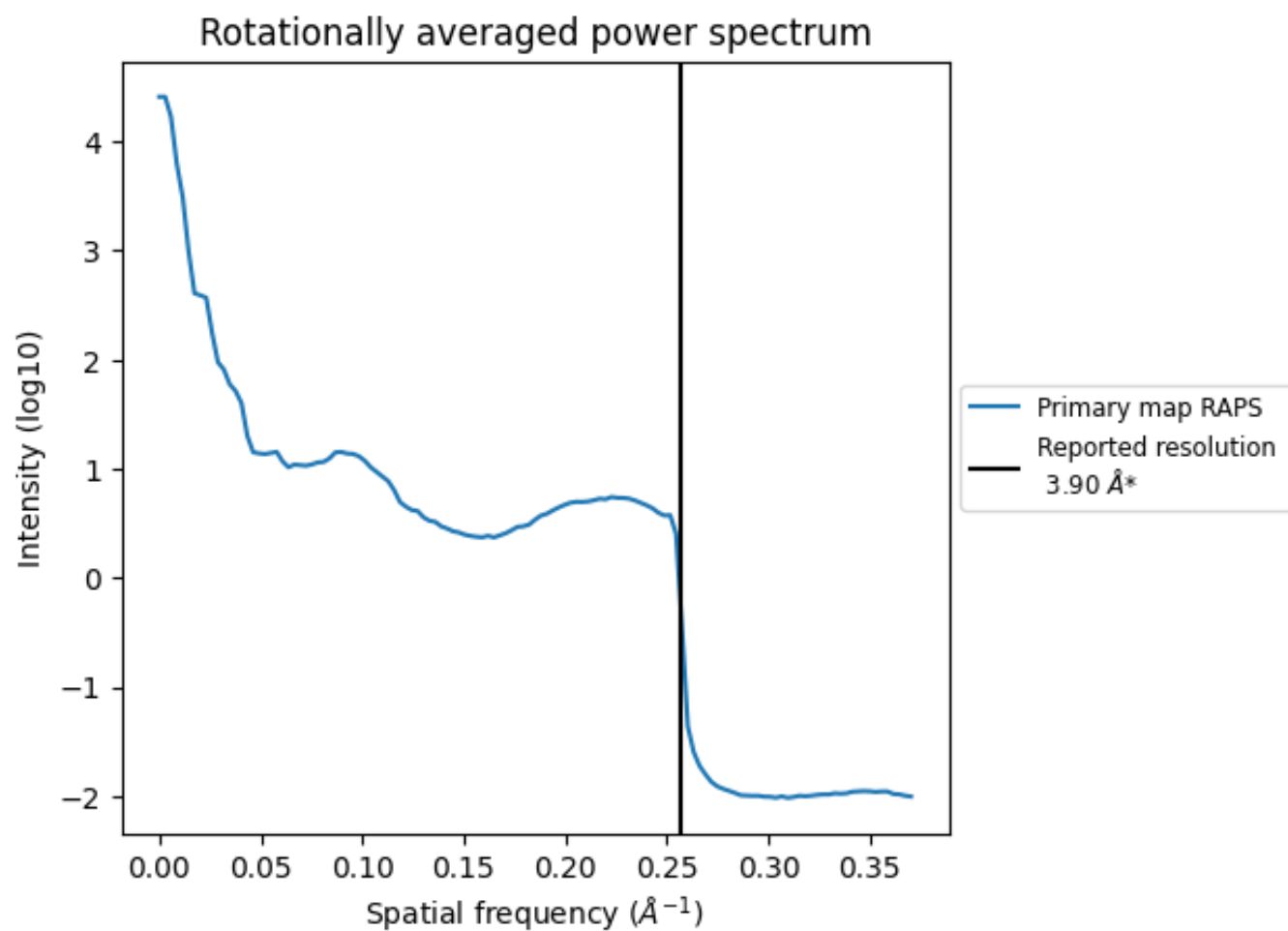
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 274 nm³; this corresponds to an approximate mass of 248 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

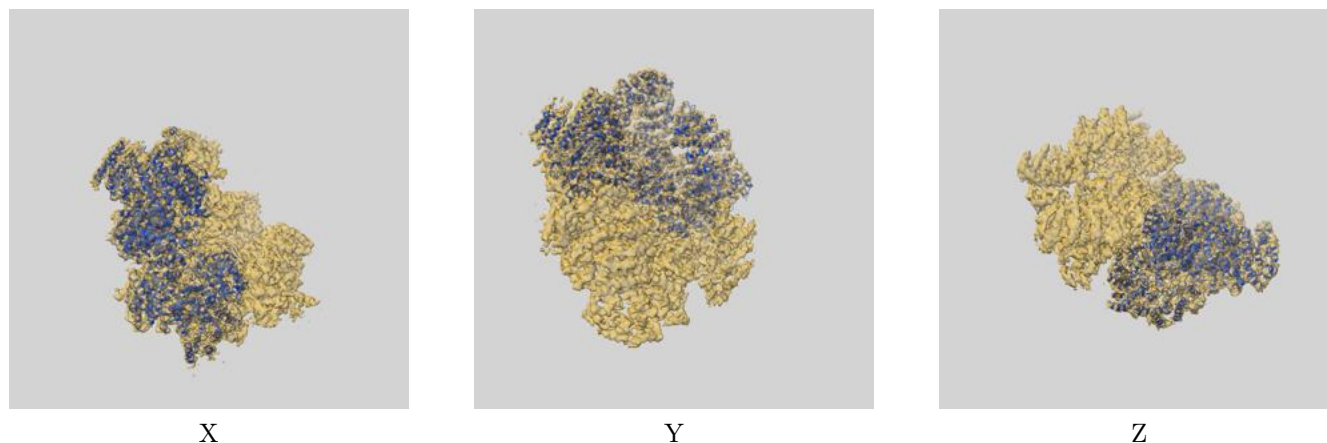
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

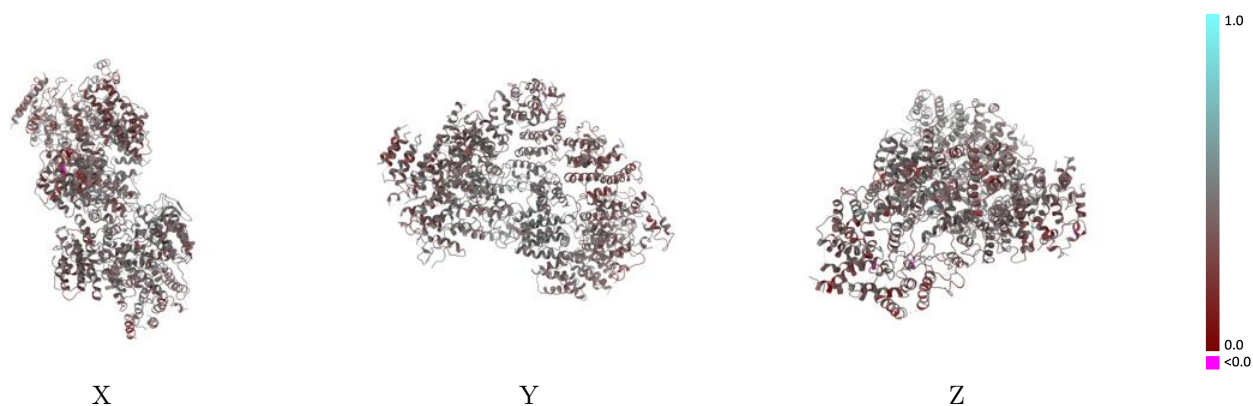
This section contains information regarding the fit between EMDB map EMD-6708 and PDB model 5X6O. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



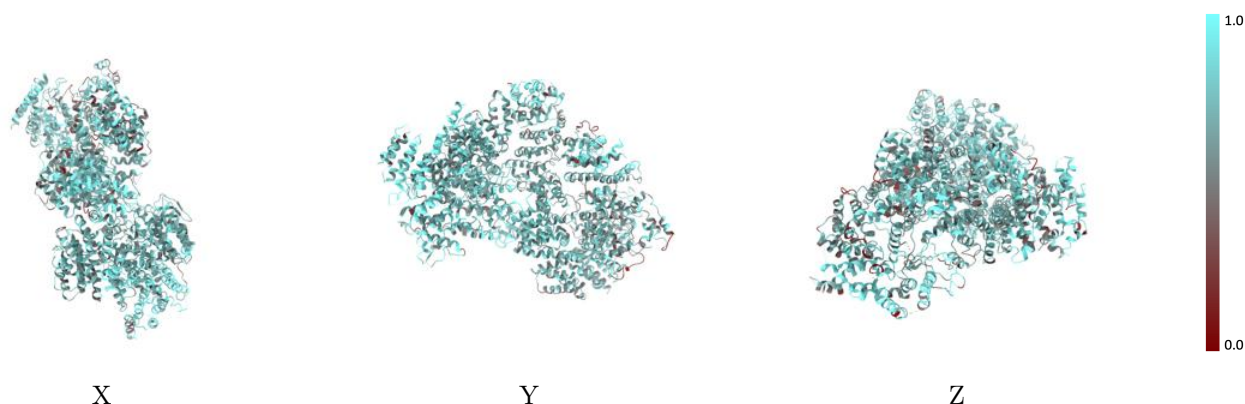
The images above show the 3D surface view of the map at the recommended contour level 0.0518 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



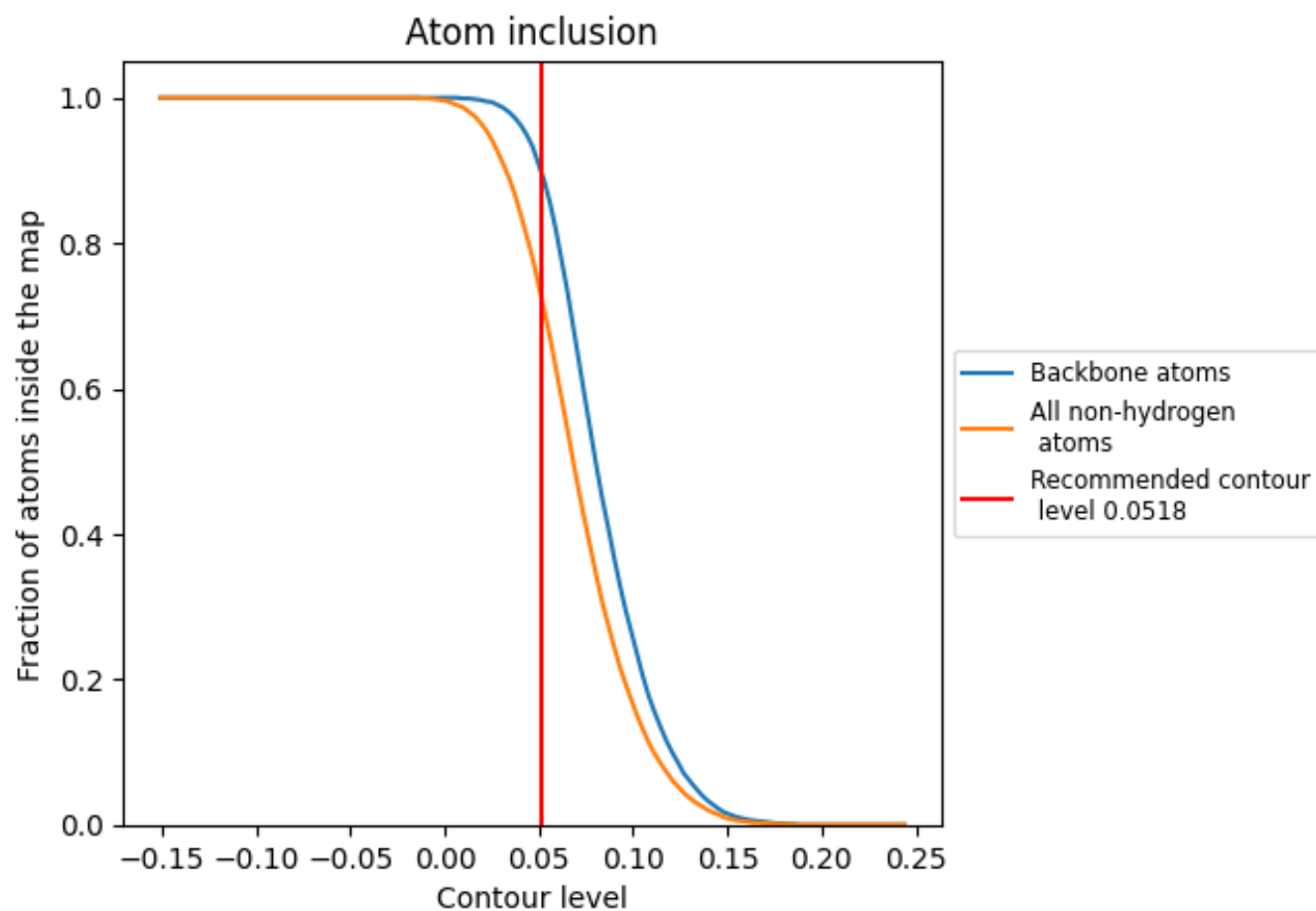
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0518).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0518) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7210	<div></div> 0.4100
C	<div></div> 0.7060	<div></div> 0.4020
G	<div></div> 0.7640	<div></div> 0.4310

