



wwPDB EM Validation Summary Report ⓘ

Mar 15, 2026 – 07:35 AM UTC

PDB ID : 9BMP / pdb_00009bmp
EMDB ID : EMD-44706
Title : State-7 of the motor domain from full-length human dynein-1 in 5mM AMPPNP
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.50 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 ⓘ 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

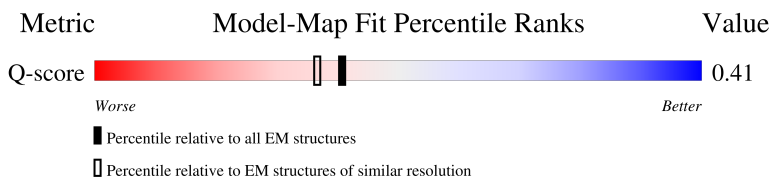
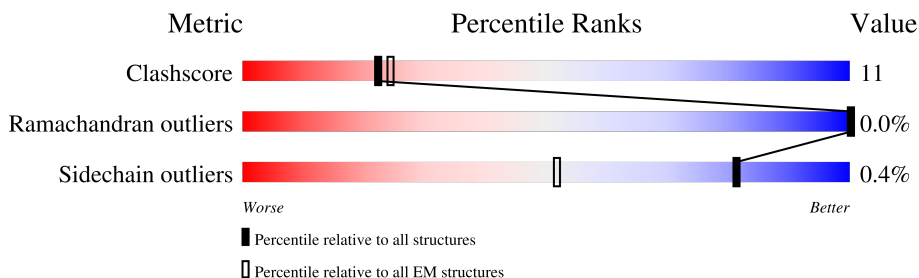
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

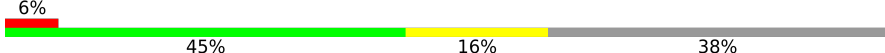
The reported resolution of this entry is 3.50 Å.

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	A	4646	

2 Entry composition [i](#)

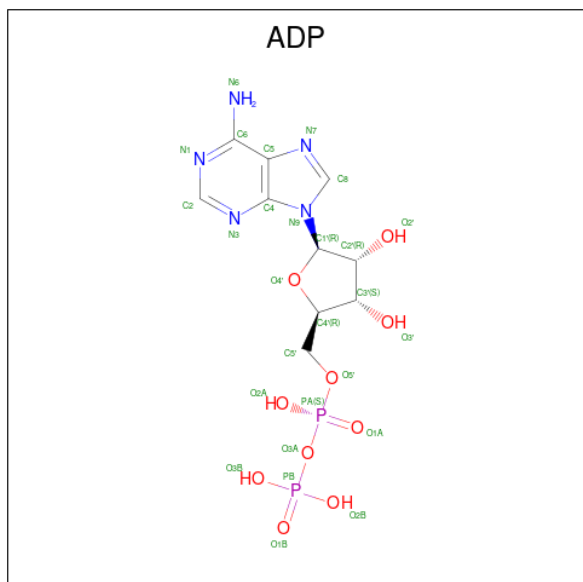
There are 4 unique types of molecules in this entry. The entry contains 23110 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cytoplasmic dynein 1 heavy chain 1.

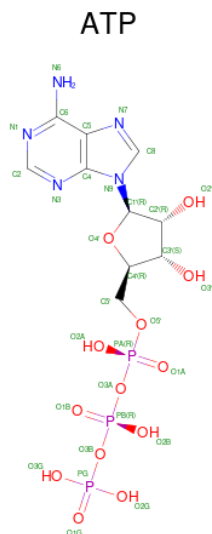
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2858	22994	14663	3967	4249	115	0	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



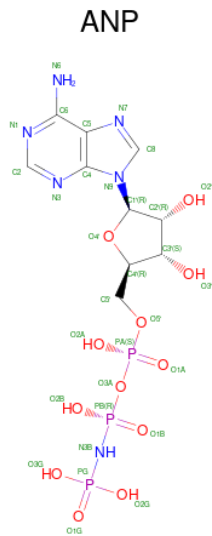
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	27	10	5	10	2	0
2	A	1	27	10	5	10	2	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 31	C 10	N 6	O 12	P 3	0

Q2139	ALA	E1871	K1687	M1579	S1505	LYS	ALA	VAL	TRP	ARG	GLU	ALA	ASN	PHE
Y2146	GLY	Y1872	K1580	K1581	A1506	ASN	SER	ALA	GLU	PHE	PHE	LEU	LEU	ASN
L2149	ARG	V1875	K1582	K1583	M1507	ALA	THR	GLU	LYS	THR	THR	GLN	GLN	GLN
G2200	SER	V1876	V1582	V1583	K1508	ILE	PHE	GLU	LYS	PRO	PRO	MET	GLY	LYS
G2201	N2027	R1887	L1701	K1584	S1509	VAL	VAL	LEU	VAL	THR	THR	ASN	GLY	GLY
M2202	P2029	C1888	L1702	S1585	L1510	LYS	GLN	GLN	ASP	SER	VAL	PRO	ILE	VAL
Q2203	R2037	Y1889	M1709	S1586	P1511	ASP	ARG	ASP	THR	TRP	GLY	GLY	GLY	ASP
Q2209	T2042	T1893	V1588	V1589	Y1512	VAL	LEU	LYS	GLY	TYR	LEU	LEU	LEU	ASP
I2213	T2043	K1715	D1590	D1591	Y1513	VAL	GLY	GLY	ARG	ASN	ASN	ASN	GLY	ILE
G2219	L2054	L1714	M1589	M1590	K1514	ALA	THR	TRP	ILE	ILE	LEU	PRO	VAL	ILE
G2221	R2060	S1720	M1593	M1594	V1515	GLN	VAL	SER	GLU	GLY	GLU	PRO	ARG	GLU
M2222	T2061	V1721	I1594	F1516	F1517	GLY	GLY	GLU	GLY	GLY	GLY	ILE	LEU	GLY
V2223	V2070	V1724	Q1595	E1517	E1518	MET	ASN	SER	LEU	SER	GLY	TYR	ALA	ILE
S2226	P2071	D1734	G1596	D1524	D1523	LYS	LEU	VAL	GLN	TRP	VAL	CYS	GLY	ASP
G2227	F2072	A1747	A1604	E1524	E1523	GLN	SER	GLN	GLY	MET	ASP	VAL	VAL	LEU
S2231	F2073	L1749	A1605	D1525	D1528	MET	GLY	TRP	LYS	ARG	ALA	ARG	LEU	GLY
V2234	F2074	S1753	D1606	M1528	M1531	ALA	ALA	LEU	ASP	LYS	LYS	VAL	ARG	GLY
E2245	N1931	G1772	L1607	M1532	A1532	LYS	ILE	GLU	GLY	THR	ALA	ALA	LEU	VAL
E2248	N1932	G1773	L1615	L1533	L1538	GLN	GLU	GLN	ARG	PHE	PHE	THR	ALA	GLY
D2255	N1933	D1774	L1619	L1538	I1538	ILE	GLY	ILE	ARG	THR	THR	THR	THR	THR
T2259	D1945	A1775	R1623	I1538	I1538	ASP	ASP	PRO	LYS	ILE	ILE	VAL	ALA	ALA
S2260	V1946	V1778	F1629	R1541	Q1541	LYS	THR	PRO	CYS	VAL	VAL	PRO	ASP	ASP
K2261	G1947	V1785	Y1630	R1542	R1543	ARG	LEU	ARG	LYS	GLN	GLN	LEU	ASP	ASP
Y2265	V1951	L1789	L1637	W1544	W1544	ASN	ASN	ASN	LYS	GLN	GLN	GLN	ASP	ASP
D2277	R1962	L1792	I1640	Y1545	Y1546	VAL	TRP	TRP	ALA	ILE	ILE	ILE	ILE	ILE
G2278	L1988	L1803	I1641	Y1546	L1547	VAL	VAL	VAL	GLY	GLY	GLY	GLY	GLY	GLY
L2279	H1985	K1807	K1645	E1548	E1548	VAL	VAL	VAL	GLY	GLY	GLY	GLY	GLY	GLY
T2288	N1989	L1815	K1649	G1549	G1549	VAL	VAL	VAL	GLY	GLY	GLY	GLY	GLY	GLY
D2289	Y1990	L1825	L1650	T1550	T1550	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
S2290	D1991	I1826	K1651	F1551	F1551	THR	THR	THR	THR	THR	THR	THR	THR	THR
V2291	K1992	L1835	K1652	G1553	G1553	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
R2292	T1993	K1827	M1657	S1554	S1554	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS
L2295	A1995	Q1850	M1667	A1555	A1555	THR	THR	THR	THR	THR	THR	THR	THR	THR
Q2296	T1998	Q1855	N1667	K1558	K1558	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
K2297	C1999	Q1855	E1668	L1561	L1561	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE
R2298	E2000	Q1860	D1669	E1564	E1564	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
Q2299	L2001	K1865	V1672	Q1566	Q1566	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
V2302	Q2005	Q1865	S1678	R1567	R1567	THR	THR	THR	THR	THR	THR	THR	THR	THR
E2310	T2017	Q1865	R1679	F1568	F1568	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
N2314	M2018	Q1865	E1680	T1571	T1571	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN
	N2019													
	PRO													
	GLY													
	TYR													





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47831	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.499	Depositor
Minimum map value	-0.825	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	333.312, 333.312, 333.312	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.302, 1.302, 1.302	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ADP, ANP

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	0.14	0/23487	0.35	1/31835 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	2387	LEU	N-CA-C	-5.24	107.18	113.21

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	22994	0	23055	524	0
2	A	54	0	24	2	0
3	A	31	0	12	1	0
4	A	31	0	13	1	0
All	All	23110	0	23104	524	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 11.

The worst 5 of 524 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:3151:HIS:HD1	1:A:3516:TYR:HH	1.16	0.89
1:A:2836:ARG:HG3	1:A:3091:LEU:HB2	1.58	0.84
1:A:1698:ILE:HD12	1:A:1701:TRP:HE1	1.50	0.77
1:A:2762:LEU:HD13	1:A:2821:LEU:HD12	1.67	0.77
1:A:3727:LYS:HE2	1:A:3790:VAL:HG13	1.68	0.76

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	2844/4646 (61%)	2762 (97%)	81 (3%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4172	SER

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	2544/4125 (62%)	2534 (100%)	10 (0%)	84 81

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4431	LEU
1	A	4469	VAL
1	A	4617	ASP
1	A	3188	HIS
1	A	3952	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3202	ASN
1	A	3985	GLN
1	A	3772	ASN
1	A	4029	HIS
1	A	2414	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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ANP	A	4703	-	33,33,33	0.93	4 (12%)	45,52,52	0.59	0
3	ATP	A	4702	-	32,33,33	0.39	0	48,52,52	0.29	0
2	ADP	A	4701	-	28,29,29	1.40	4 (14%)	43,45,45	1.84	9 (20%)
2	ADP	A	4704	-	28,29,29	1.41	4 (14%)	43,45,45	1.85	10 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ANP	A	4703	-	-	4/18/38/38	0/3/3/3
3	ATP	A	4702	-	-	9/22/38/38	0/3/3/3
2	ADP	A	4701	-	-	3/16/32/32	0/3/3/3
2	ADP	A	4704	-	-	5/16/32/32	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4704	ADP	C5-C4	4.63	1.47	1.39
2	A	4701	ADP	C5-C4	4.63	1.47	1.39
2	A	4704	ADP	C5-C6	2.69	1.48	1.41
2	A	4701	ADP	C5-C6	2.62	1.48	1.41
4	A	4703	ANP	PG-O1G	2.53	1.50	1.46

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4701	ADP	C5-C4-N3	-5.79	118.75	126.72
2	A	4704	ADP	C5-C4-N3	-5.76	118.78	126.72
2	A	4701	ADP	N3-C4-N9	4.62	135.02	127.17
2	A	4704	ADP	N3-C4-N9	4.44	134.72	127.17
2	A	4701	ADP	C2-N3-C4	3.70	120.86	111.83

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4701	ADP	C5'-O5'-PA-O2A
2	A	4701	ADP	C5'-O5'-PA-O3A

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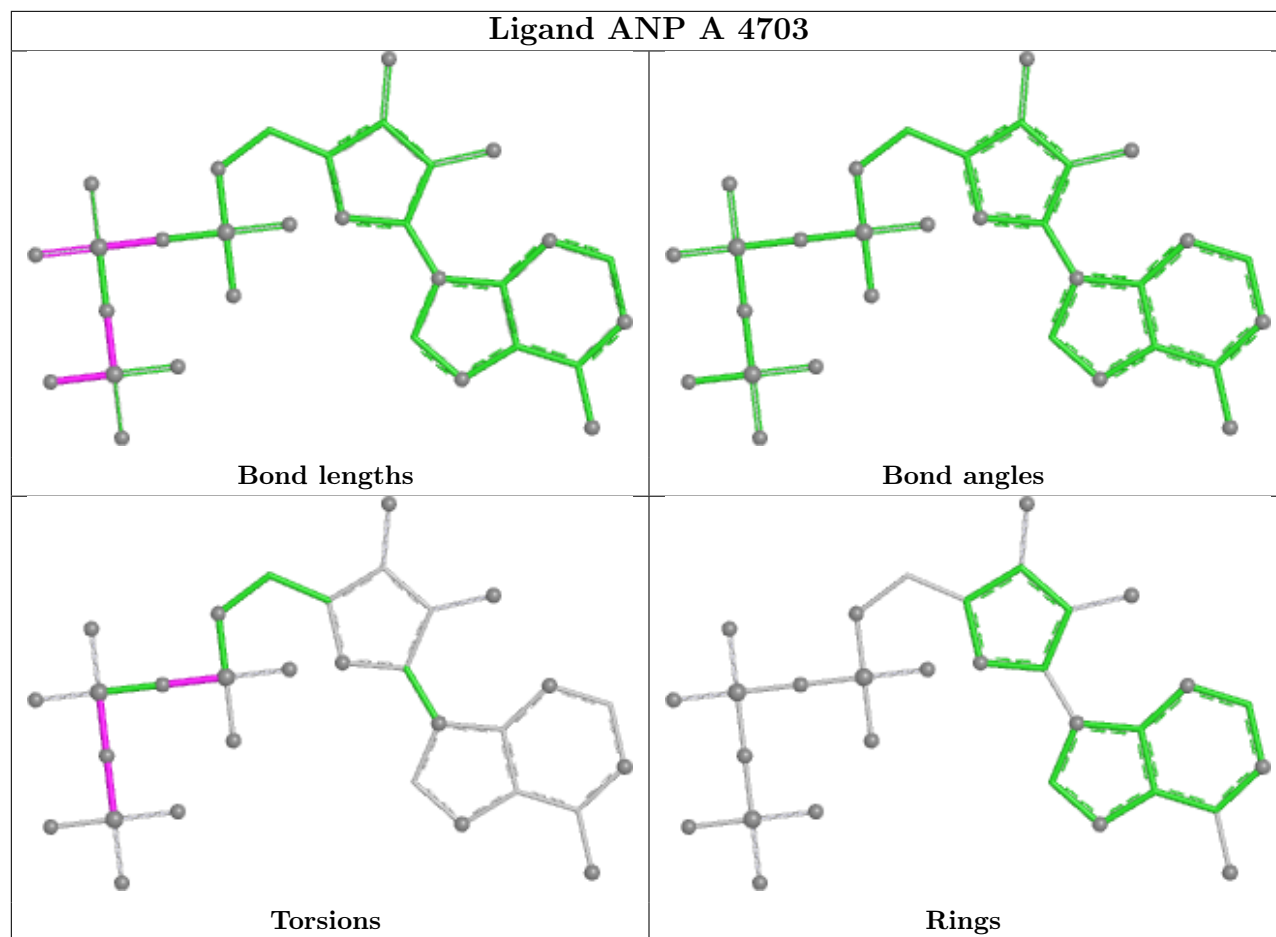
Mol	Chain	Res	Type	Atoms
2	A	4704	ADP	C5'-O5'-PA-O1A
2	A	4704	ADP	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O3A

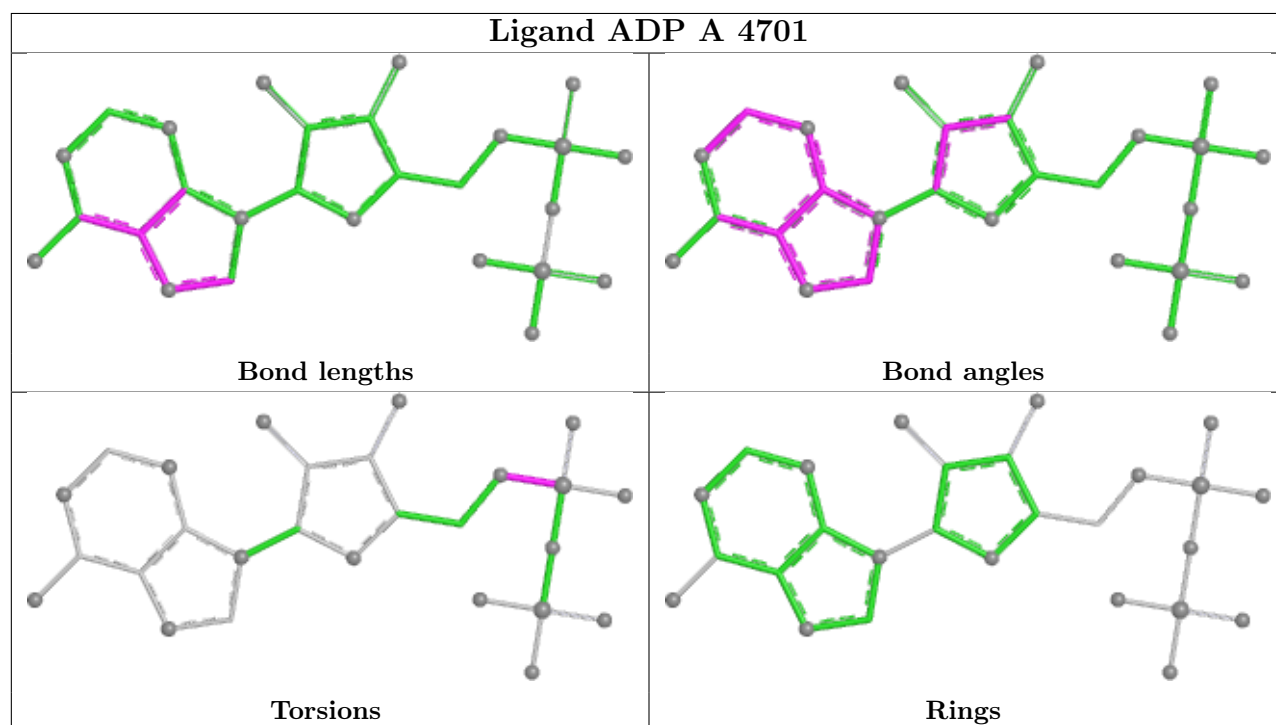
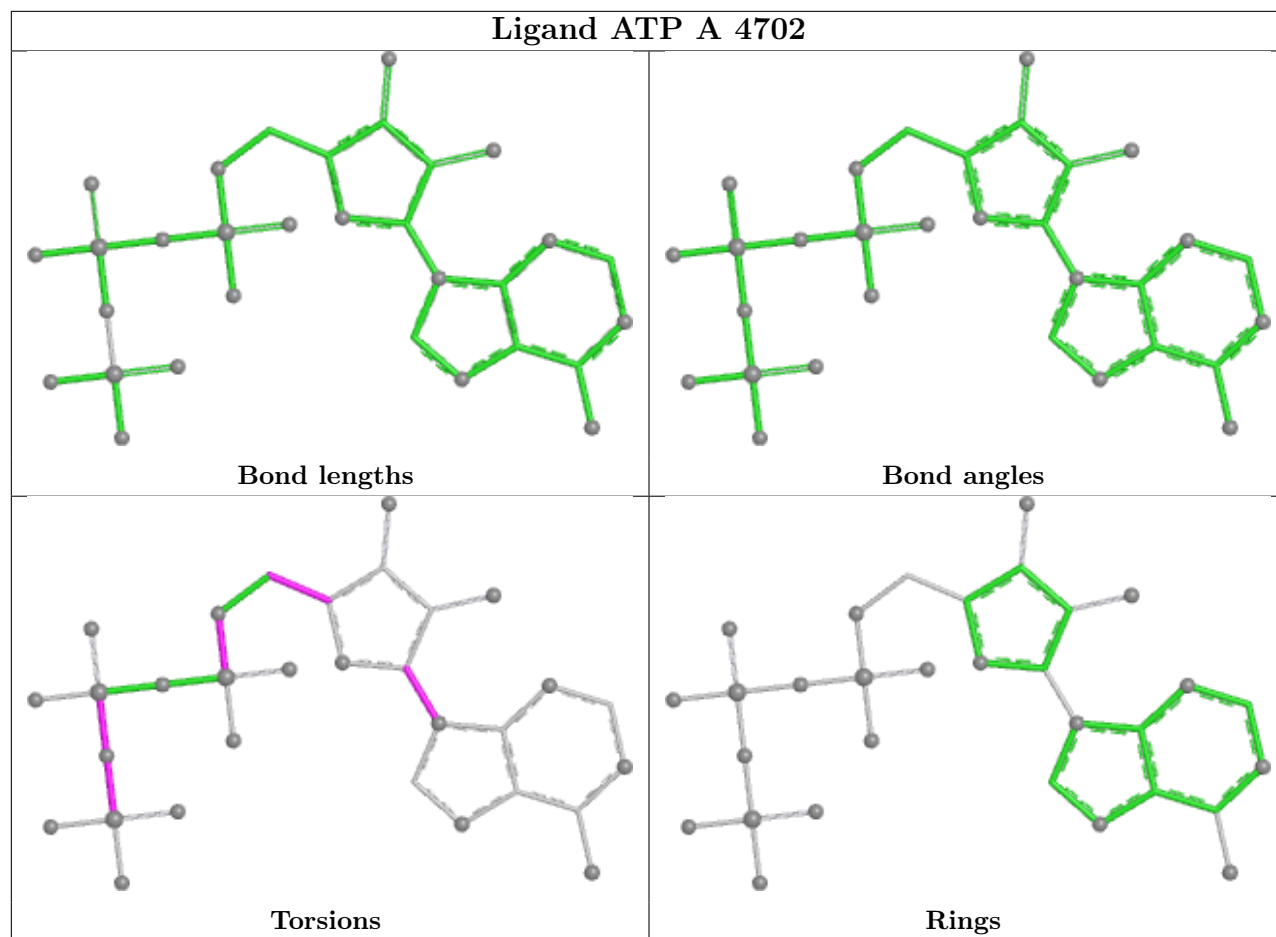
There are no ring outliers.

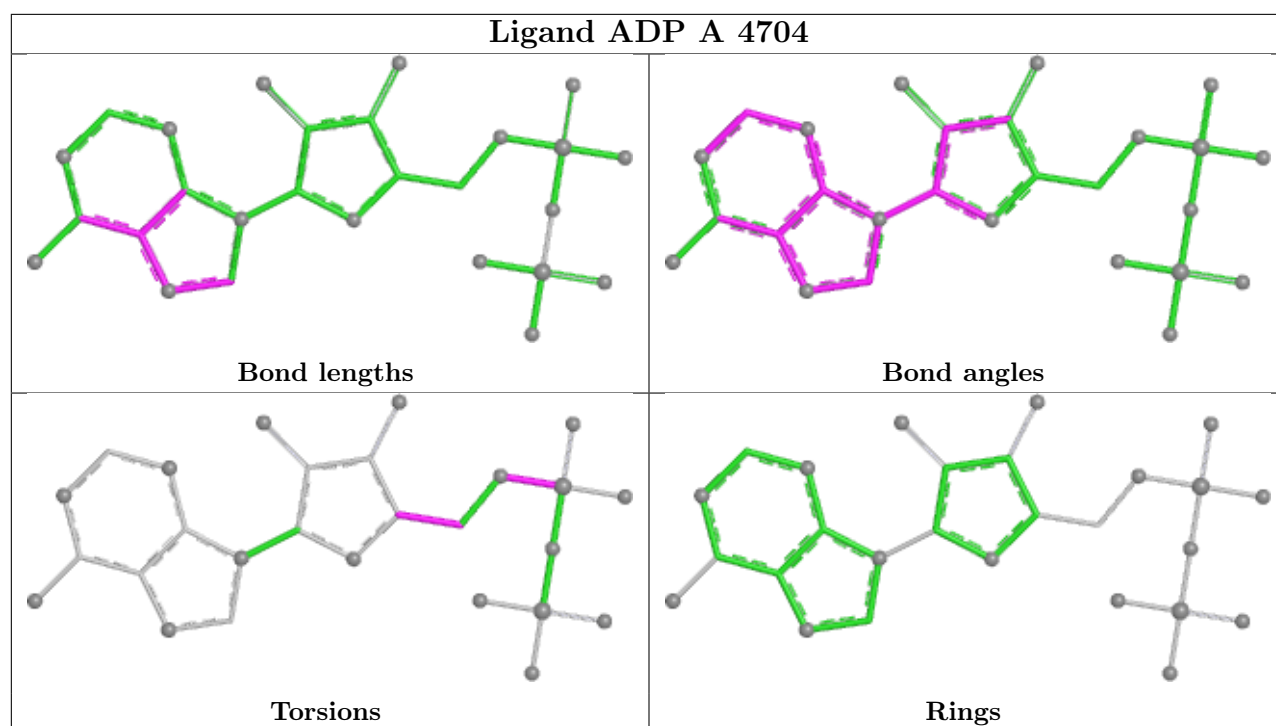
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4703	ANP	1	0
3	A	4702	ATP	1	0
2	A	4701	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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.

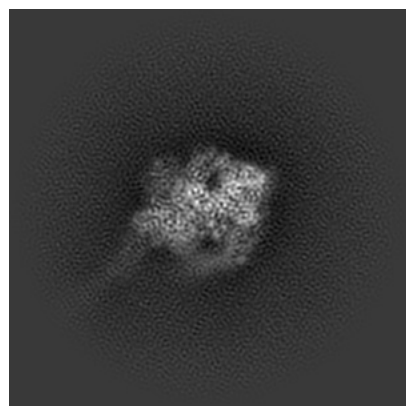
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44706. These allow visual inspection of the internal detail of the map and identification of artifacts.

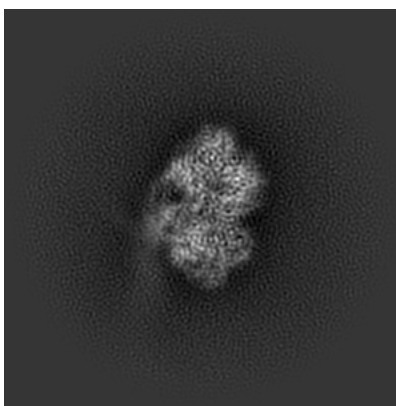
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

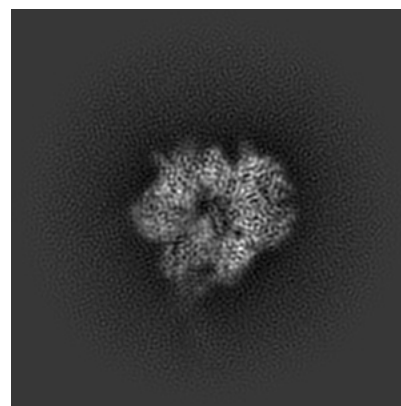
6.1.1 Primary map



X

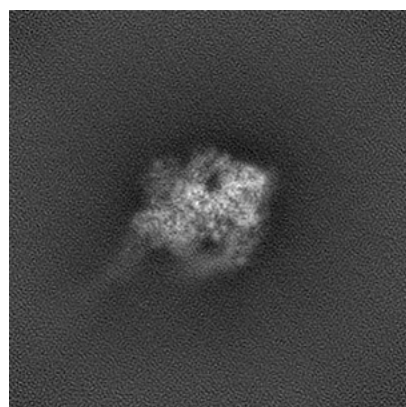


Y

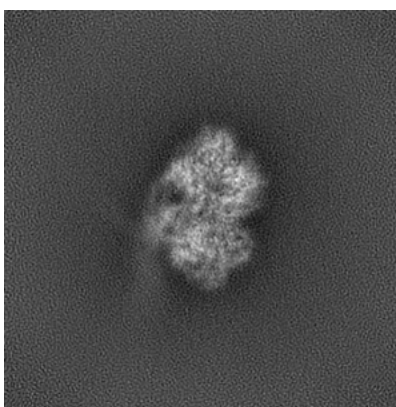


Z

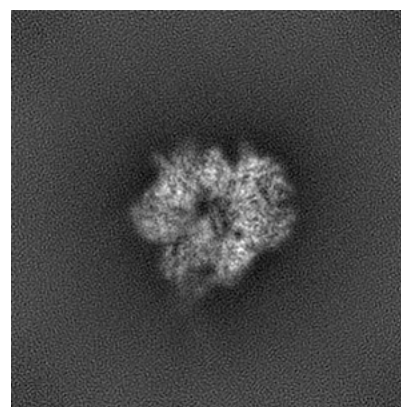
6.1.2 Raw map



X



Y

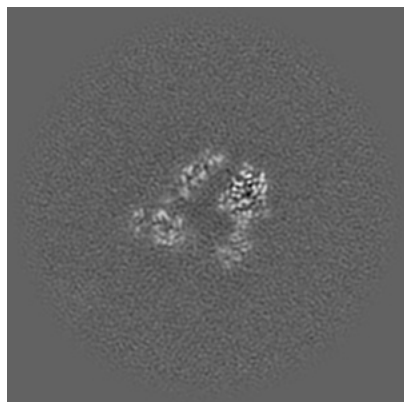


Z

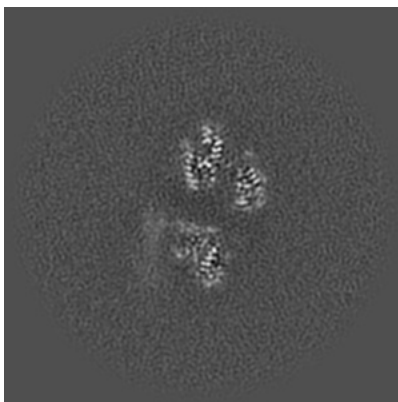
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

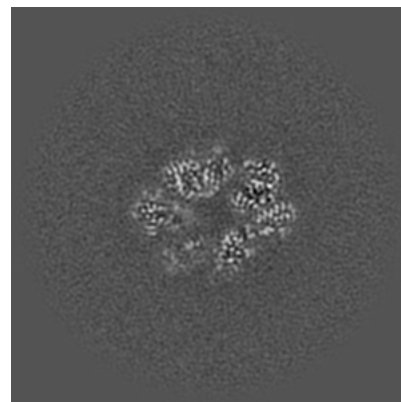
6.2.1 Primary map



X Index: 128

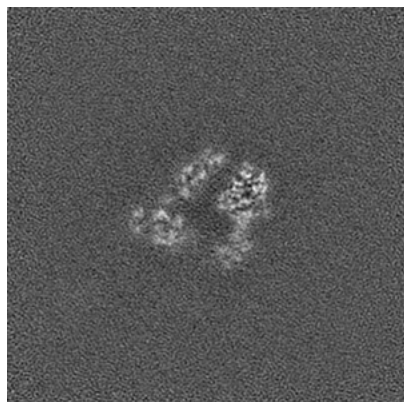


Y Index: 128

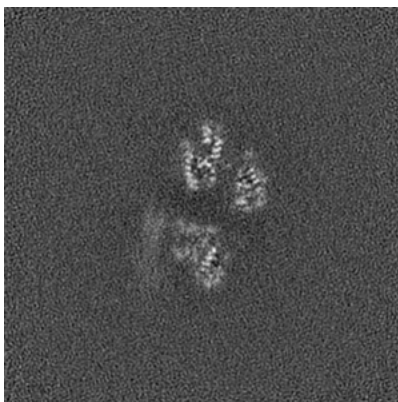


Z Index: 128

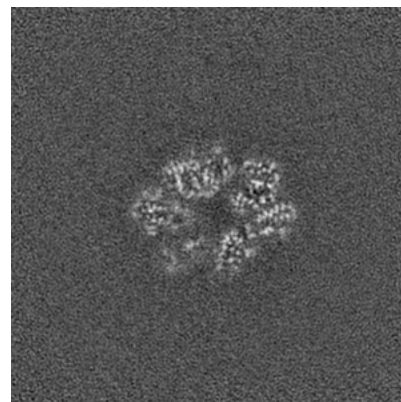
6.2.2 Raw map



X Index: 128



Y Index: 128

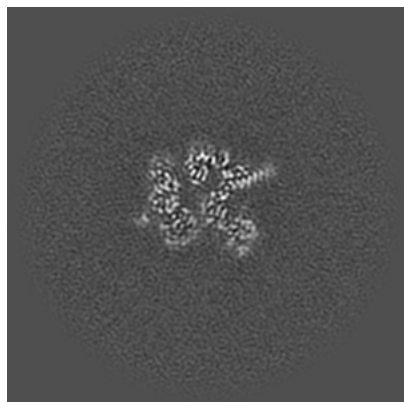


Z Index: 128

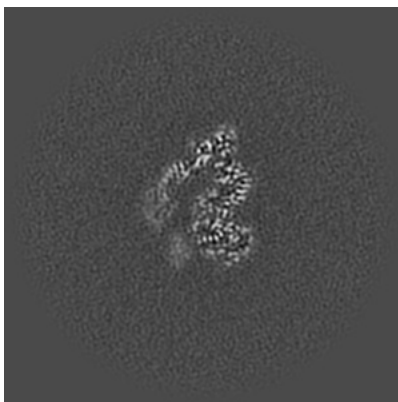
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

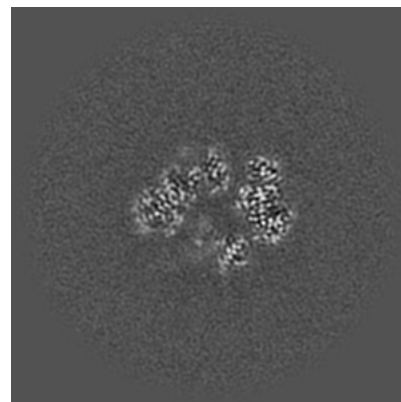
6.3.1 Primary map



X Index: 147

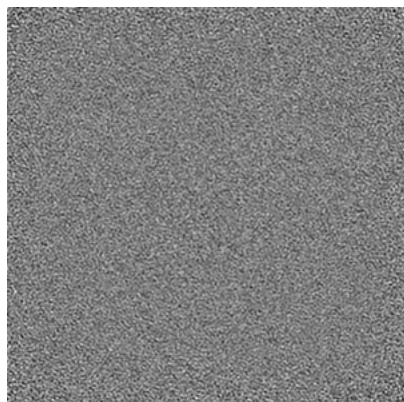


Y Index: 143

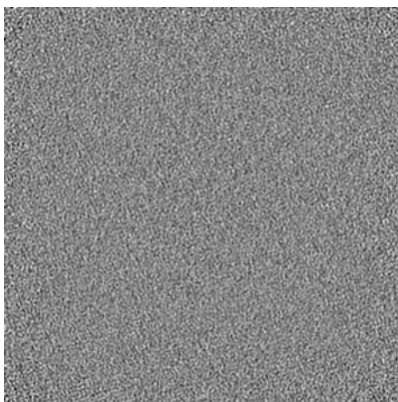


Z Index: 133

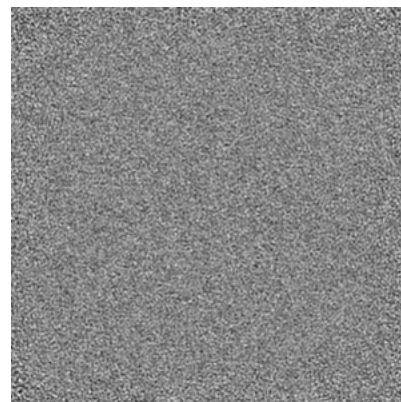
6.3.2 Raw map



X Index: 0



Y Index: 0

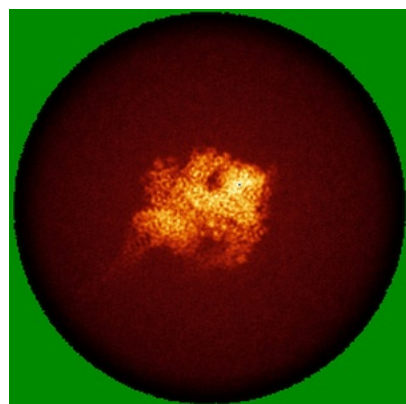


Z Index: 0

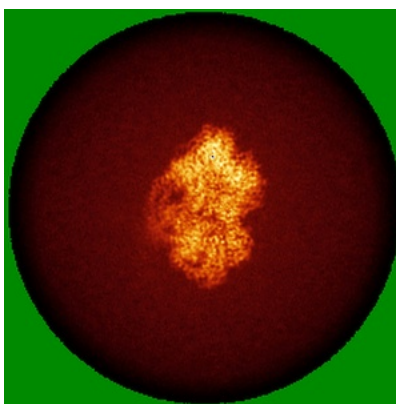
The images above show the largest variance slices of the map in three orthogonal directions.

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

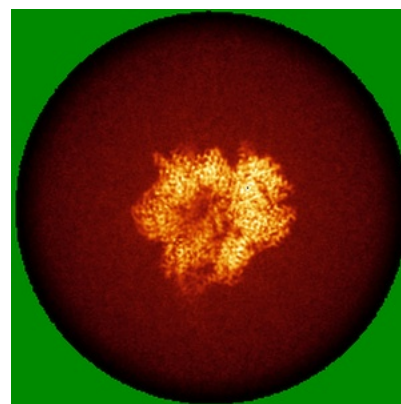
6.4.1 Primary map



X

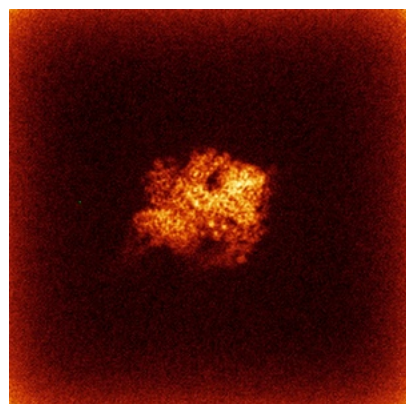


Y

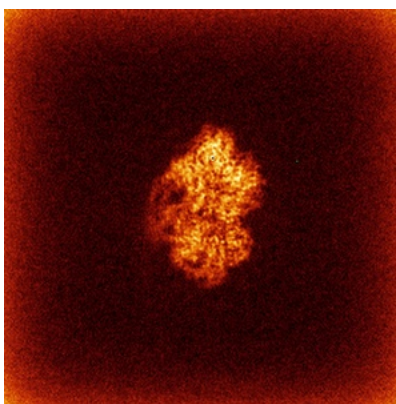


Z

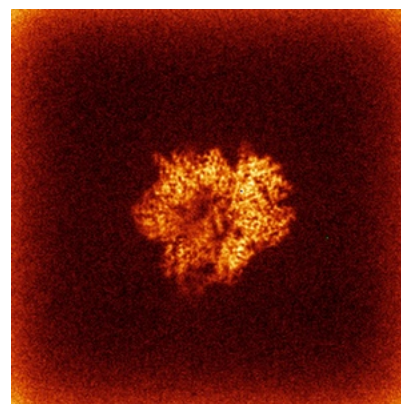
6.4.2 Raw map



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](#)

This section was not generated.

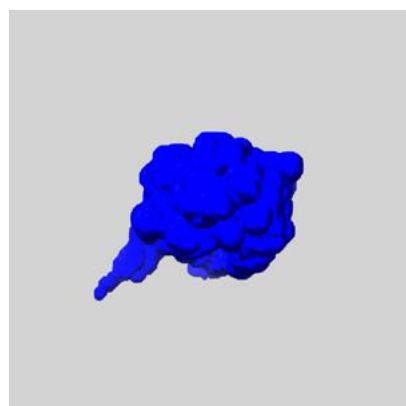
6.6 Mask visualisation [i](#)

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

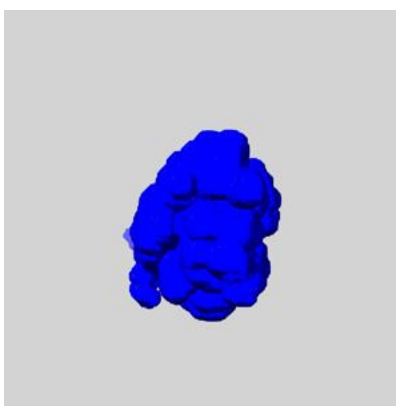
A mask typically either:

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

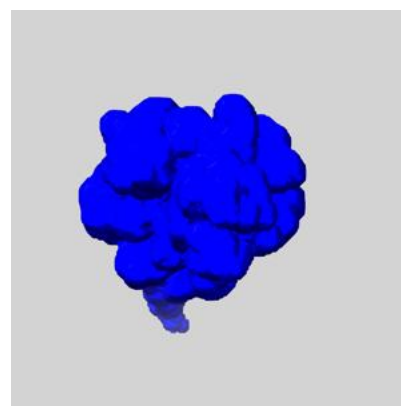
6.6.1 emd_44706_msk_1.map [i](#)



X



Y

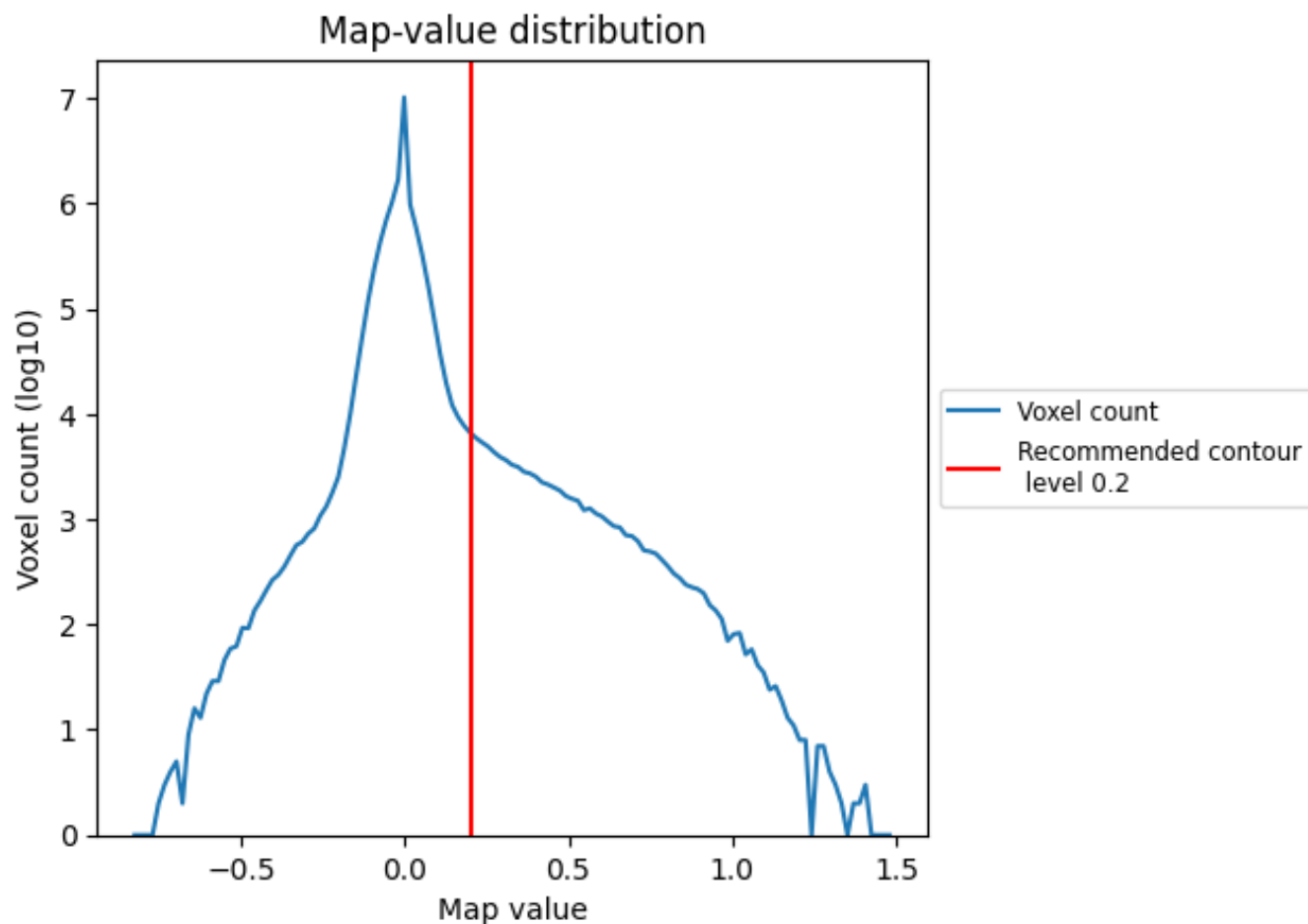


Z

7 Map analysis [i](#)

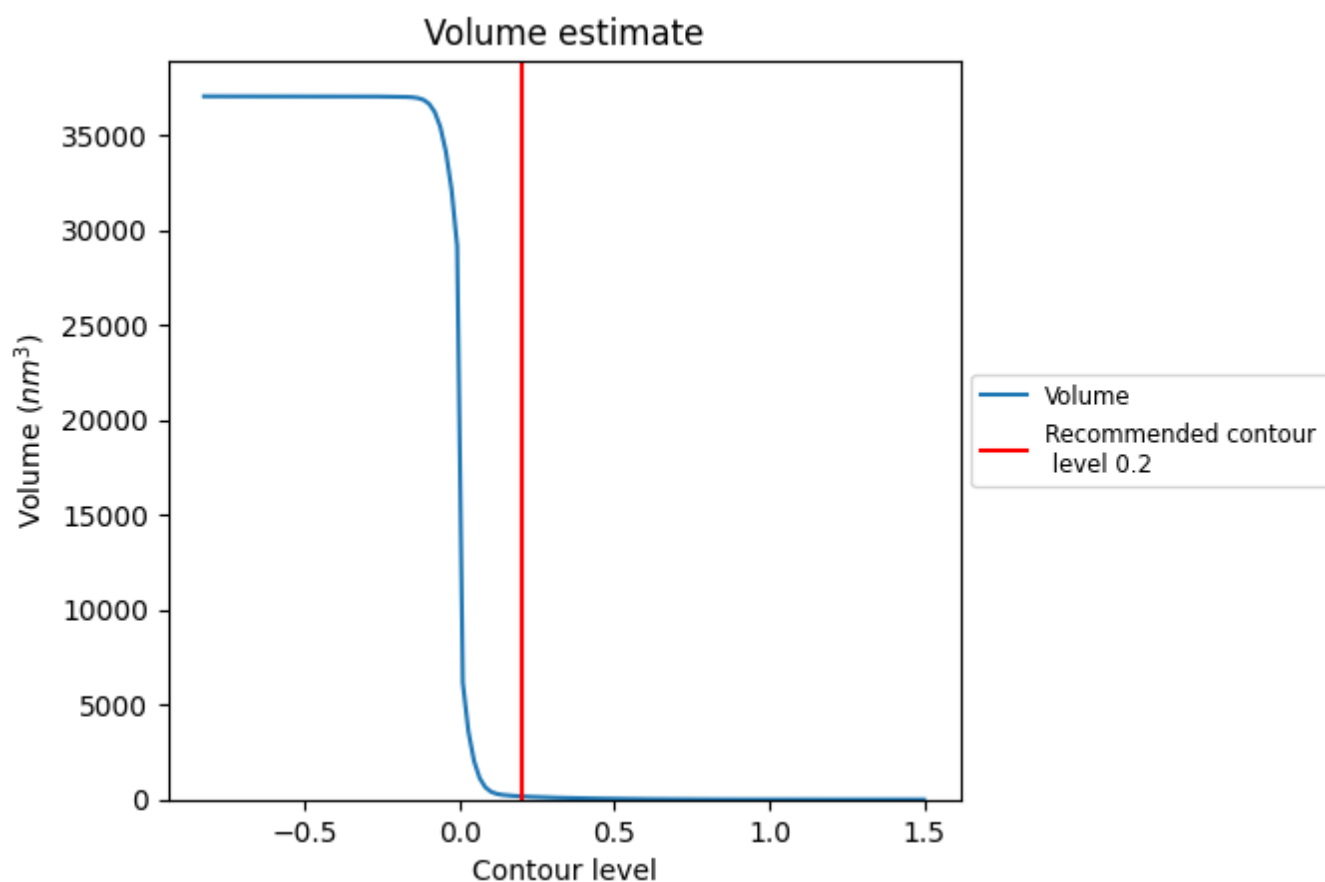
This section contains the results of statistical analysis of the map.

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.

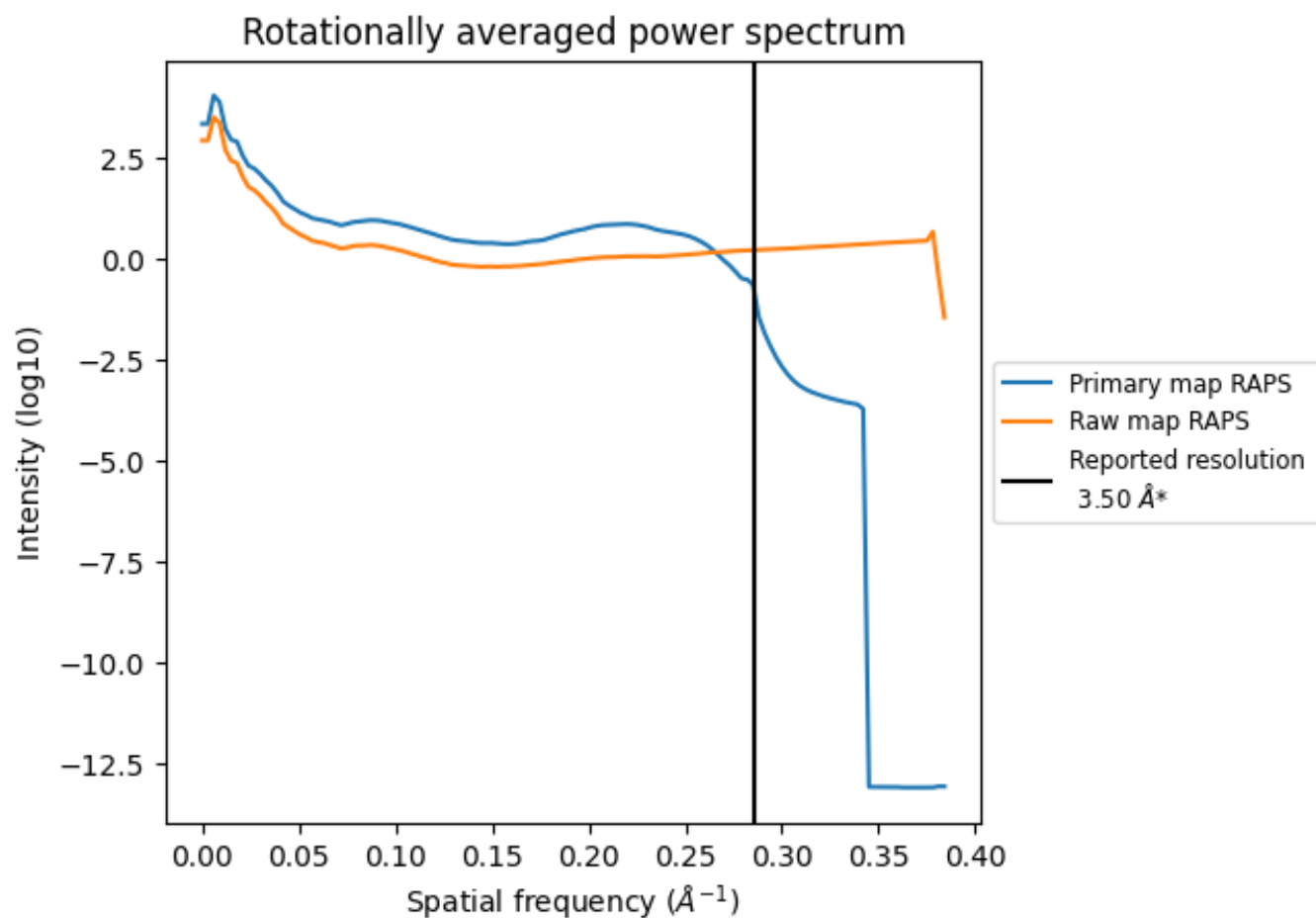
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 168 nm³; this corresponds to an approximate mass of 152 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 ⓘ

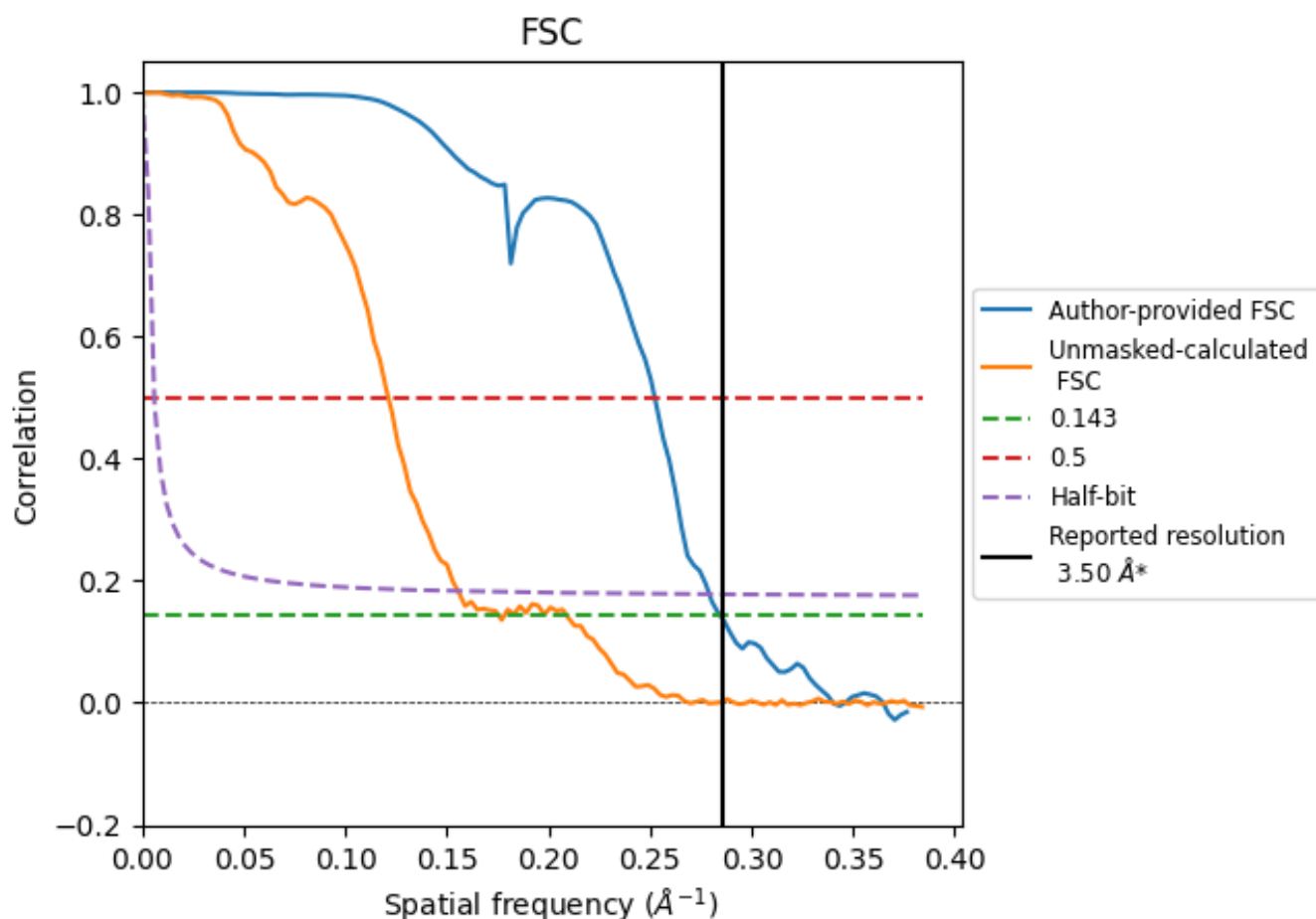


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 $0.286 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

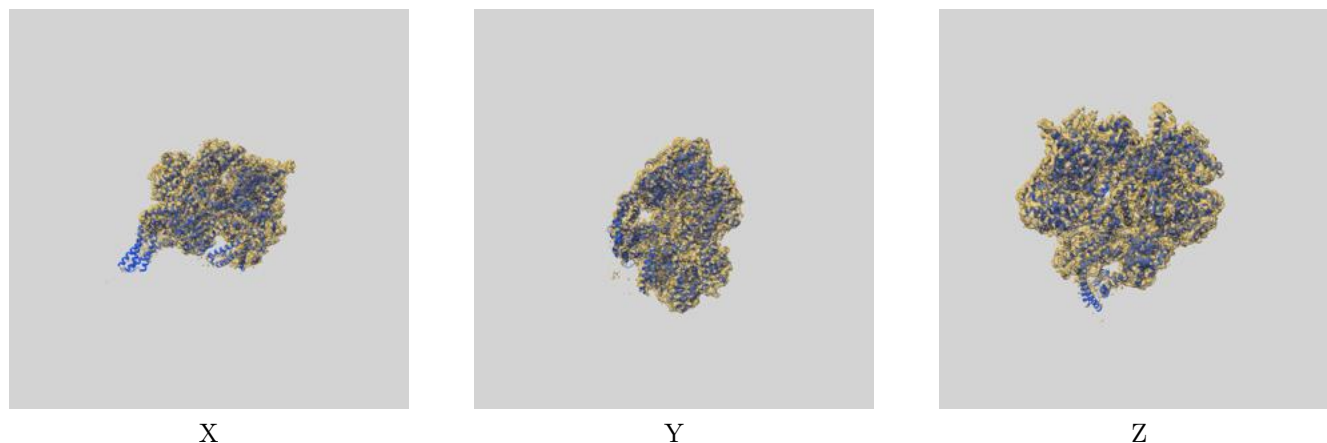
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.51	3.96	3.58
Unmasked-calculated*	5.70	8.25	6.43

*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 5.70 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

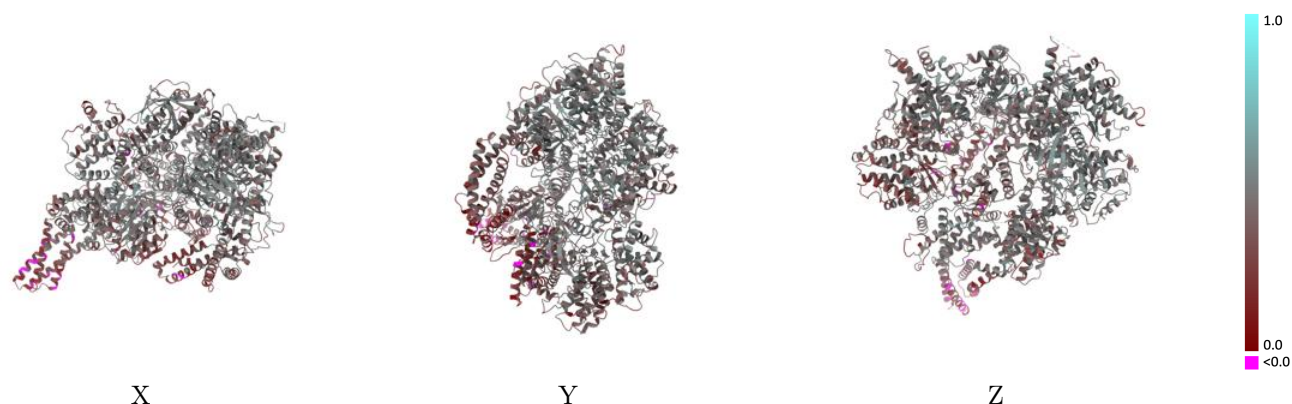
This section contains information regarding the fit between EMDB map EMD-44706 and PDB model 9BMP. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



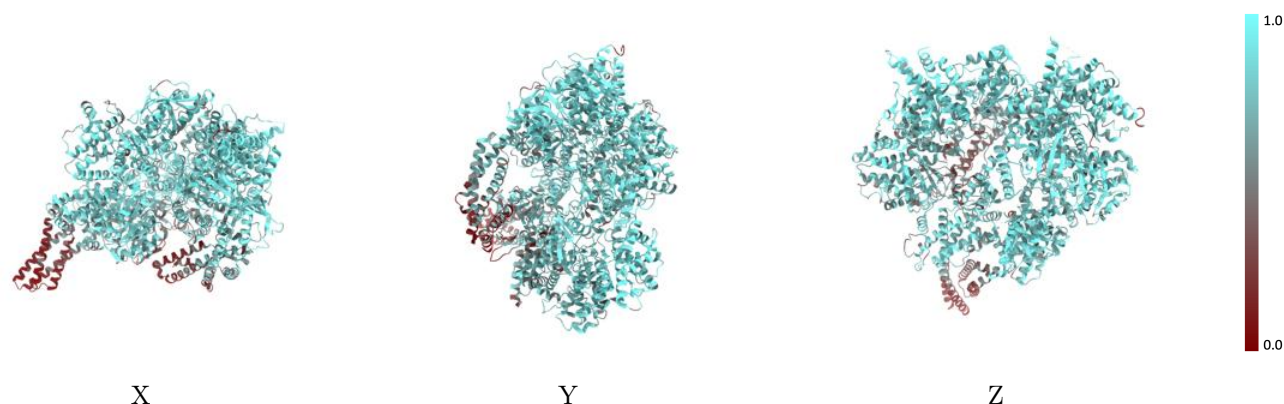
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



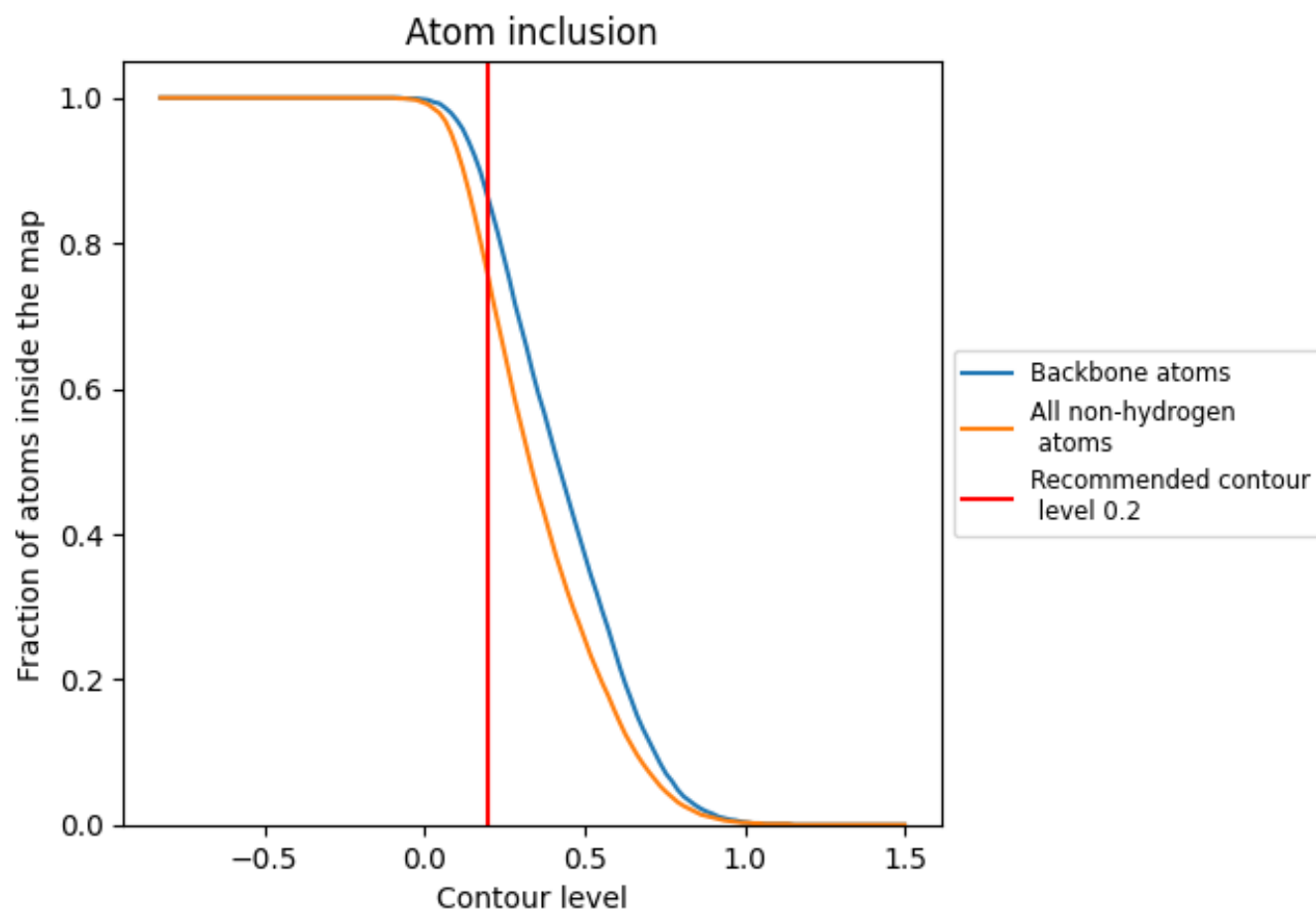
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 75% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7510	0.4100
A	0.7510	0.4100

