



## wwPDB EM Validation Summary Report ⓘ

Aug 16, 2025 – 12:44 PM EDT

PDB ID : 9BML / pdb\_00009bml  
EMDB ID : EMD-44702  
Title : State-2 of the motor domain from full-length human dynein-1 in 5mM AMPPNP  
Authors : Chai, P.; Zhang, K.  
Deposited on : 2024-05-02  
Resolution : 3.30 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](mailto: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.dev126  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
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) : 2.45.1

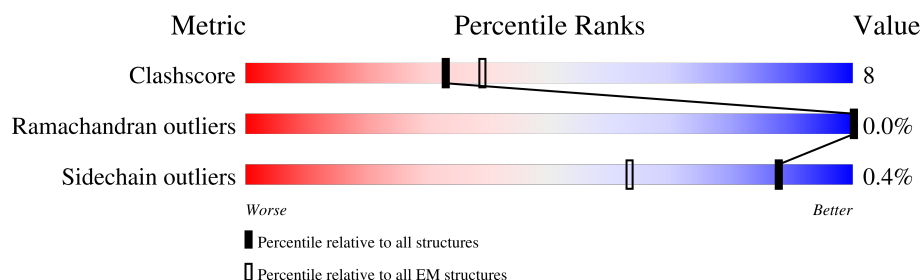
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 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	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  $\geq 3$ , 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 23706 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	2937	23593	15028	4070	4378	117	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
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

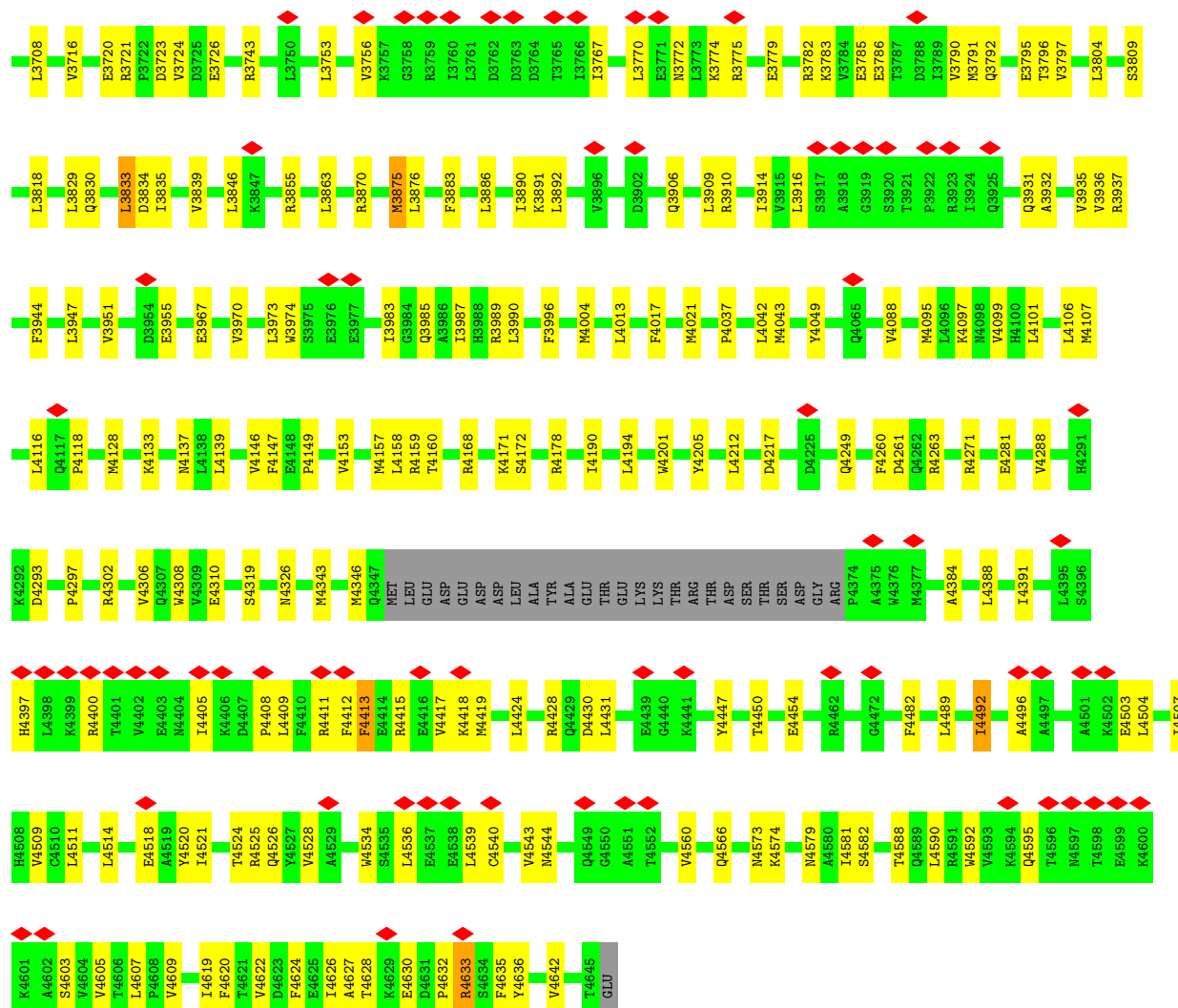
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	Mg 1	0



V1971	Q1818	L1638	Q1566	LYS	VAL	TRP	ARG	GLU	ALA	ASN	GLU	GLU	ASN	GLU	ASN	PHE
E1980	R1819	E1639	Q1567	ASN	ALA	GLU	PHE	GLN	ALA	ALA	LEU	LEU	LEU	LEU	LEU	PHE
H1984	D1820	I1640	F1568	ALA	GLU	GLU	THR	LYS	GLU	THR	ILE	ARG	ILE	ARG	ILE	PHE
H1985	D1831	K1645	Q1569	ILE	VAL	VAL	PRO	LYS	PRO	PRO	GLN	THR	GLY	GLY	GLY	LYS
S1986	L1839	N1646	S1570	VAL	GLN	GLN	SER	VAL	SER	ASP	ASN	VAL	ILE	ILE	ILE	VAL
N1987	R1843	K1652	I1571	LYS	ASP	ASP	TRP	THR	THR	THR	LYS	VAL	ARG	ARG	GLU	VAL
F1988	H1653	H1653	S1572	ASP	GLN	GLN	VAL	VAL	VAL	VAL	LYS	LEU	LEU	LEU	LEU	ASP
N1989	K1849	I1664	T1573	LEU	VAL	VAL	ARG	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	LEU
Y1990	Q1850	L1576	L1576	VAL	ALA	ALA	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	ILE
D1991	T1851	A1577	A1577	GLN	GLN	GLN	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	GLU
K1992	D1852	L1578	L1578	GLY	GLY	GLY	SER	SER	SER	SER	SER	SER	SER	SER	SER	GLU
T1993	V1853	K1579	K1579	ILE	ILE	ILE	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	LYS
S1994	L1854	K1580	M1578	ASN	ASN	ASN	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	ALA
A1995	Q1855	K1581	V1582	LEU	LEU	LEU	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	ASP
L2001	Q1856	V1582	S1583	LEU	LEU	LEU	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	LEU
L2002	N1867	R1679	K1584	VAL	VAL	VAL	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	GLU
Y1872	L1873	E1680	K1584	ILE	ILE	ILE	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL
L2016	L1873	G1681	S1585	GLU	GLU	GLU	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	THR
R2025	D1877	E1682	P1586	LYS	LYS	LYS	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	GLY
D2030	K1878	I1692	L1587	GLN	GLN	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL
N2031	L1879	T1693	V1588	GLU	GLU	GLU	MET	MET	MET	MET	MET	MET	MET	MET	MET	LEU
L2032	R1887	E1706	M1589	ALA	ALA	ALA	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	ARG
M2041	C1888	M1709	D1590	LYS	LYS	LYS	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	THR
D2045	S1903	L1713	V1591	ASP	ASP	ASP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	VAL
R2046	P1907	L1717	L1592	ARG	ARG	ARG	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	GLY
Q2047	T1910	K1729	G1596	HIS	HIS	HIS	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	THR
L2048	G1911	A1730	V1597	TRP	TRP	TRP	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	VAL
L2049	K1912	A1730	Q1598	LYS	LYS	LYS	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	LEU
E2063	T1913	T1731	Q1599	LEU	LEU	LEU	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	ILE
A2066	E1914	S1732	R1599	ARG	ARG	ARG	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	MET
N2067	H1921	L1749	L1601	HIS	HIS	HIS	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	CTR
K2068	R1925	M1769	E1602	VAL	VAL	VAL	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	GLN
L2069	F1930	G1770	R1603	VAL	VAL	VAL	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	VAL
V2070	D1934	G1771	D1606	VAL	VAL	VAL	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	SER
P2071	E1934	G1771	L1607	SER	SER	SER	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	ASP
L2075	D1933	G1772	L1608	GLU	GLU	GLU	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	LYS
L2080	T1935	G1773	G1609	LEU	LEU	LEU	THR	THR	THR	THR	THR	THR	THR	THR	THR	PRO </td
Q2083	M1941	A1775	K1610	LEU	LEU	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ASN
A2092	Q1950	P1777	I1611	THR	THR	THR	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
K2104	E1959	L1792	Q1612	GLY	GLY	GLY	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	HIS
E2117	F1960	A1793	I1611	LEU	LEU	LEU	SER	SER	SER	SER	SER	SER	SER	SER	SER	GLY
R2118	R1966	D1794	Y1618	GLN	GLN	GLN	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	THR
G2119	R1966	L1811	L1619	ILE	ILE	ILE	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	LYS
E2120	R1966	E1814	E1620	ASP	ASP	ASP	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ILE
A2121	R1966	L1815	E1622	VAL	VAL	VAL	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ASN
			P1627	THR	THR	THR	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL
			D1634	GLN	GLN	GLN	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	HIS
			E1635				VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	
			D1636				THR	THR	THR	THR	THR	THR	THR	THR	THR	
			L1637				ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40850	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	1.898	Depositor
Minimum map value	-1.110	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.3	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: ADP, ATP, MG

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	0.15	0/24093	0.31	1/32651 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4628	THR	CB-CA-C	-5.07	110.71	116.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4633	ARG	Sidechain

### 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	23593	0	23658	387	0
2	A	81	0	36	3	0
3	A	31	0	12	0	0
4	A	1	0	0	0	0
All	All	23706	0	23706	387	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 8.

The worst 5 of 387 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:4574:LYS:HB3	1:A:4627:ALA:HB2	1.46	0.98
1:A:1480:TYR:HB2	1:A:1486:LEU:HD11	1.57	0.85
1:A:1526:LYS:HA	1:A:1529:ARG:HD3	1.62	0.82
1:A:2092:ALA:HB1	1:A:2145:MET:HE1	1.63	0.78
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.66	0.77

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	2929/4646 (63%)	2888 (99%)	40 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2530	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	A	2605/4125 (63%)	2595 (100%)	10 (0%)	<a href="#">89</a> <a href="#">93</a>

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

Mol	Chain	Res	Type
1	A	3875	MET
1	A	4413	PHE
1	A	4492	ILE
1	A	2247	VAL
1	A	2522	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3233	ASN
1	A	3744	GLN
1	A	4191	GLN
1	A	3526	GLN
1	A	3820	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

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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
2	ADP	A	4703	-	24,29,29	0.89	0	29,45,45	1.21	2 (6%)
2	ADP	A	4704	-	24,29,29	0.89	0	29,45,45	1.18	2 (6%)
3	ATP	A	4702	4	28,33,33	0.68	0	34,52,52	0.60	1 (2%)
2	ADP	A	4701	-	24,29,29	0.73	0	29,45,45	0.74	1 (3%)

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
2	ADP	A	4703	-	-	2/12/32/32	0/3/3/3
2	ADP	A	4704	-	-	1/12/32/32	0/3/3/3
3	ATP	A	4702	4	-	4/18/38/38	0/3/3/3
2	ADP	A	4701	-	-	2/12/32/32	0/3/3/3

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4703	ADP	N3-C2-N1	-3.70	123.65	128.67
2	A	4704	ADP	N3-C2-N1	-3.62	123.76	128.67
2	A	4704	ADP	C4-C5-N7	-2.50	106.69	109.34
2	A	4703	ADP	C4-C5-N7	-2.44	106.76	109.34
3	A	4702	ATP	C5-C6-N6	2.33	123.86	120.31

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

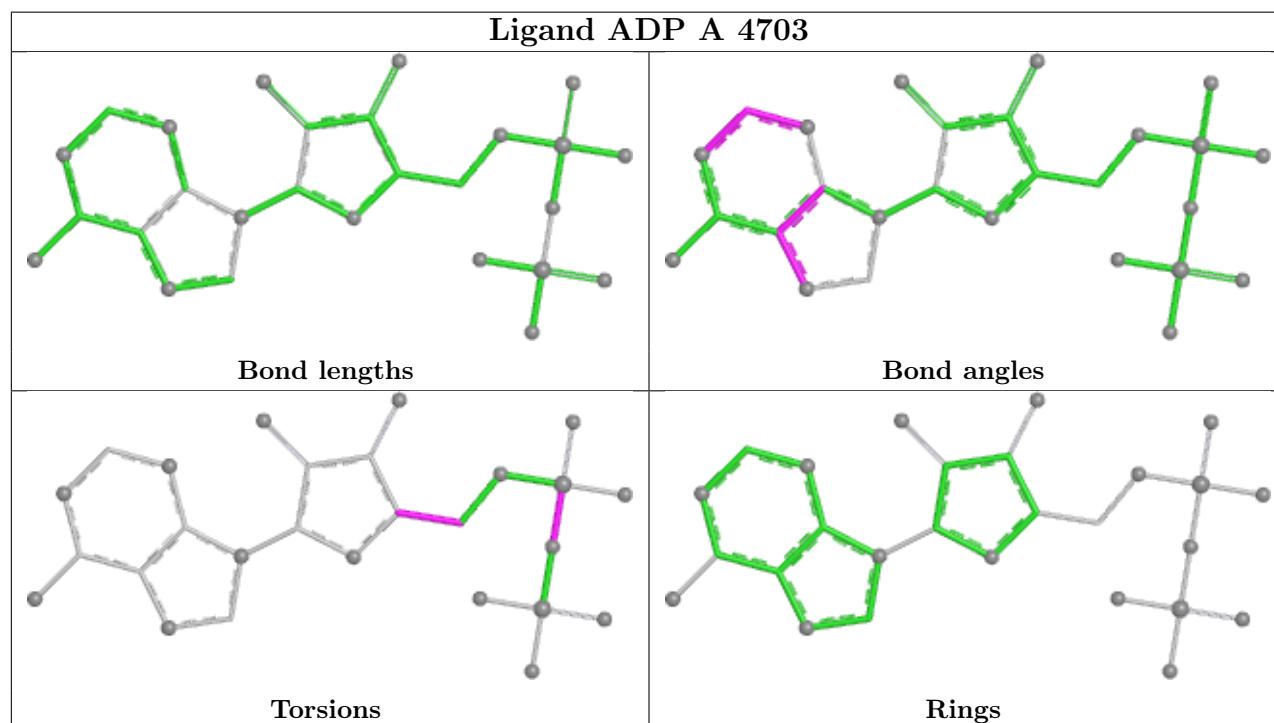
Mol	Chain	Res	Type	Atoms
3	A	4702	ATP	O4'-C4'-C5'-O5'
2	A	4701	ADP	O4'-C4'-C5'-O5'
3	A	4702	ATP	C3'-C4'-C5'-O5'
3	A	4702	ATP	PA-O3A-PB-O2B
2	A	4704	ADP	C5'-O5'-PA-O1A

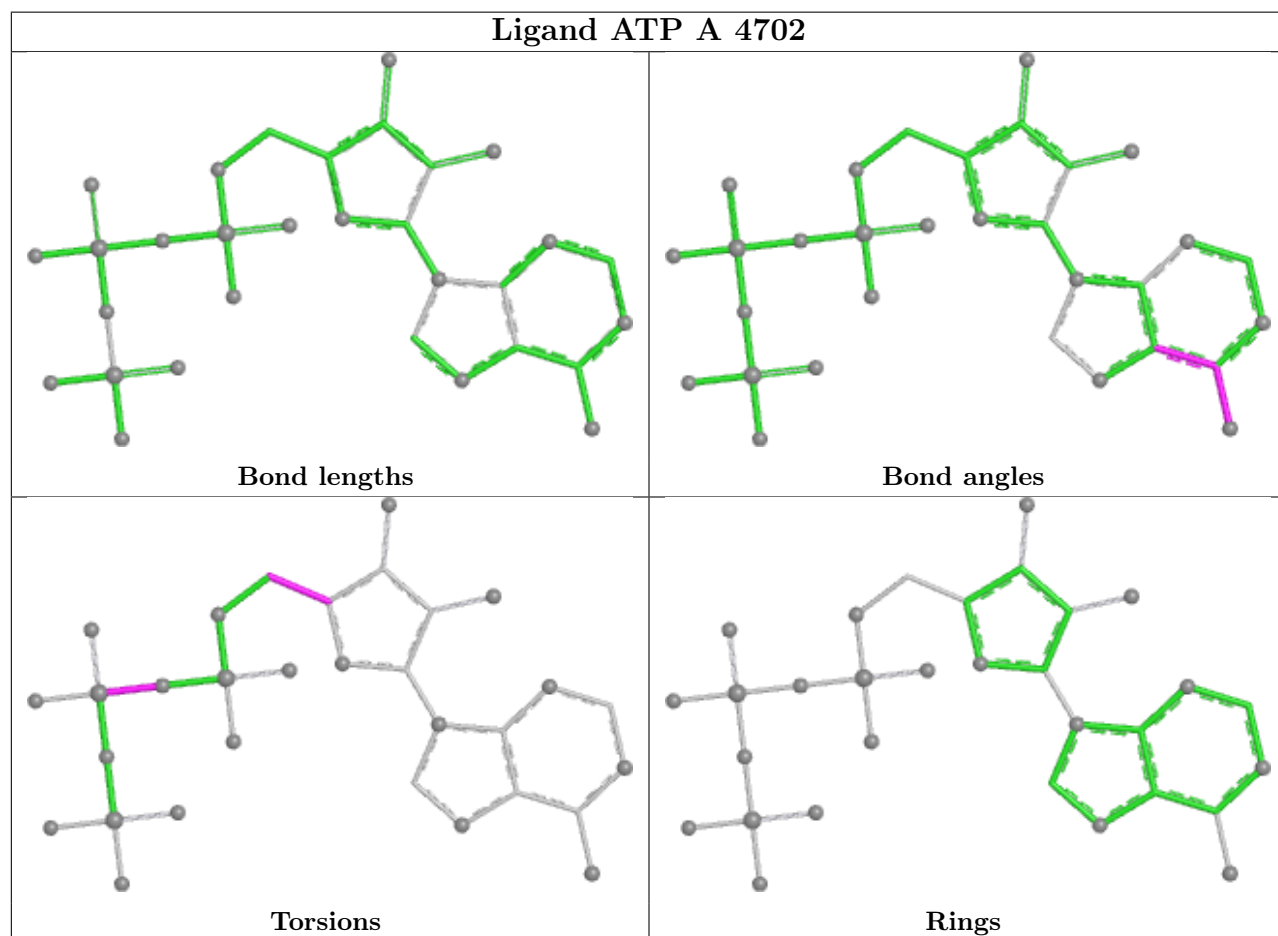
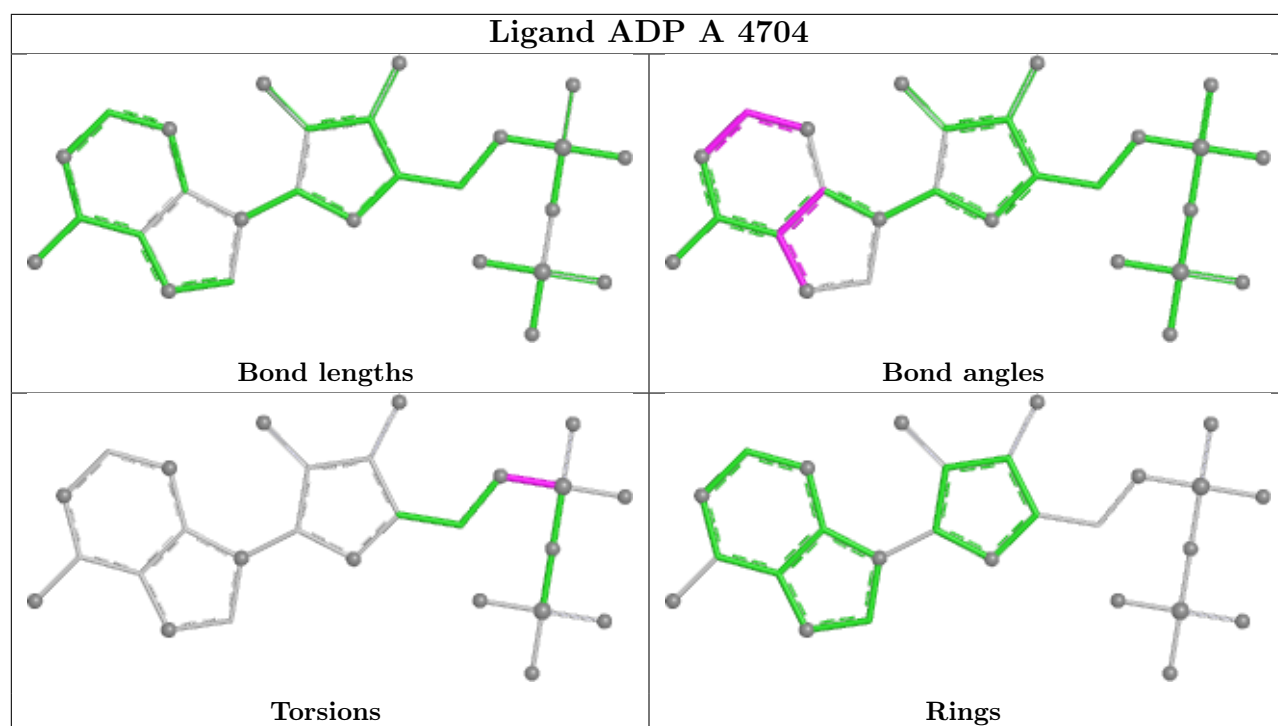
There are no ring outliers.

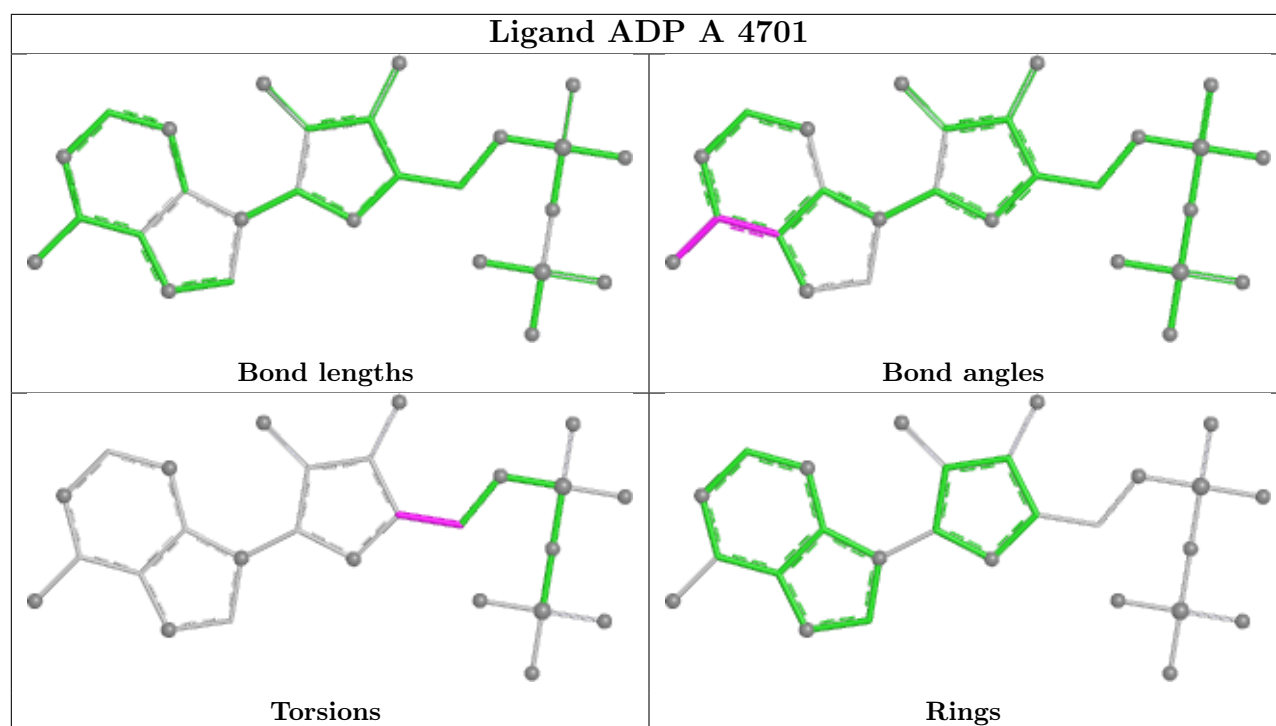
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4701	ADP	3	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.



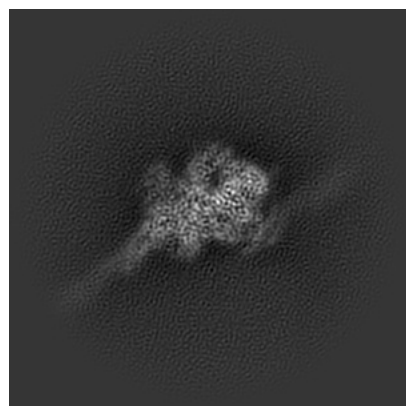
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44702. These allow visual inspection of the internal detail of the map and identification of artifacts.

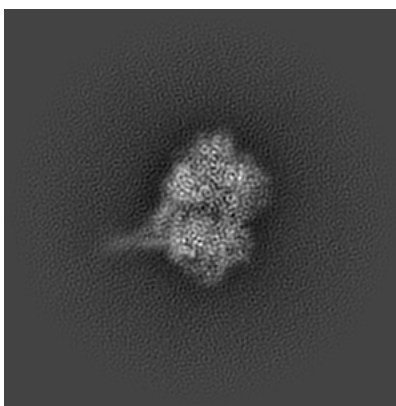
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

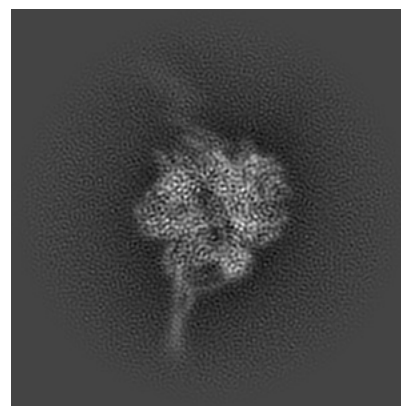
#### 6.1.1 Primary map



X

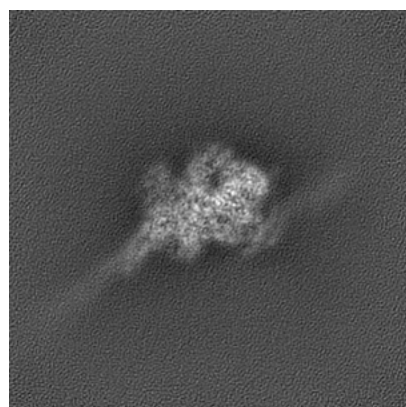


Y

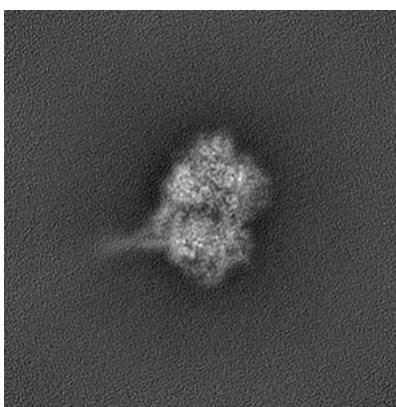


Z

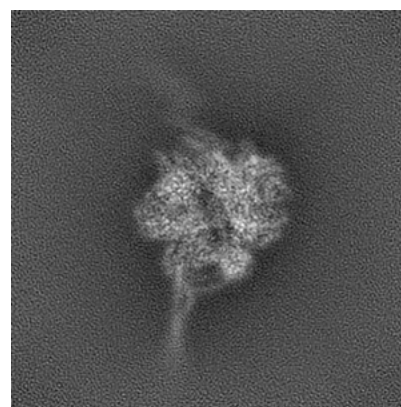
#### 6.1.2 Raw map



X



Y

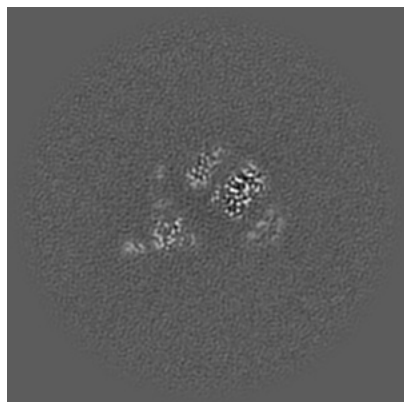


Z

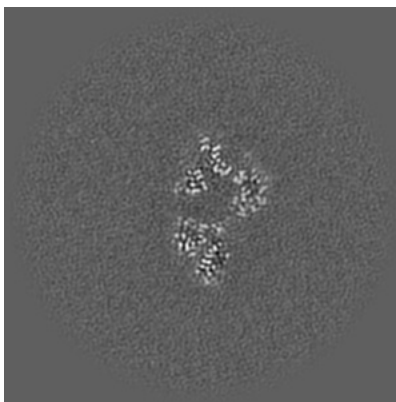
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

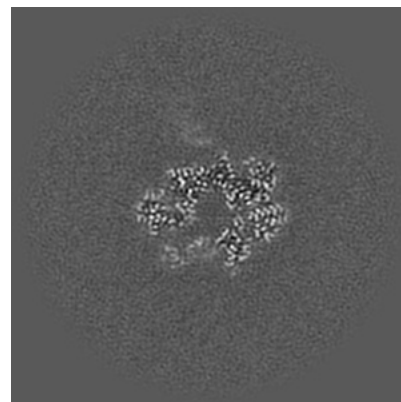
### 6.2.1 Primary map



X Index: 128

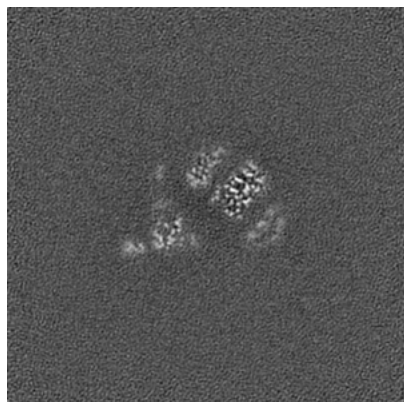


Y Index: 128

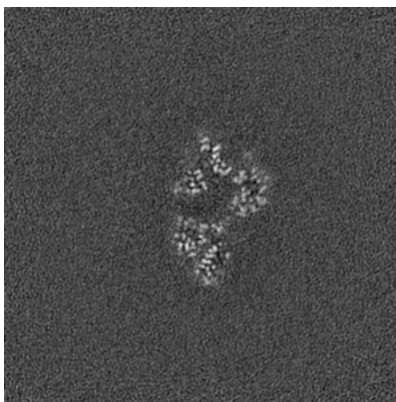


Z Index: 128

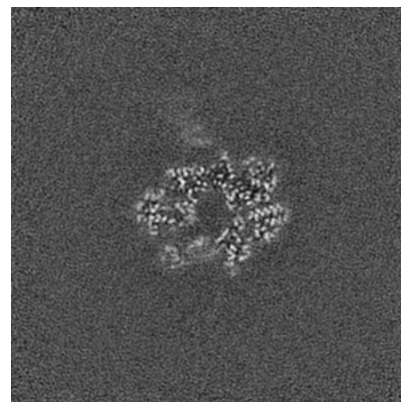
### 6.2.2 Raw map



X Index: 128



Y Index: 128

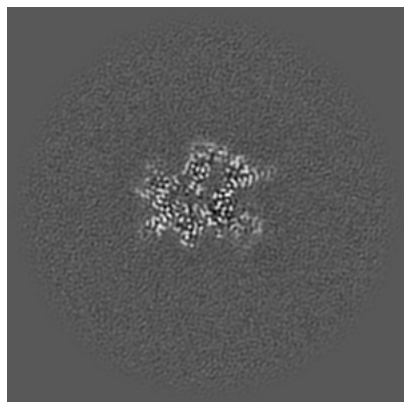


Z Index: 128

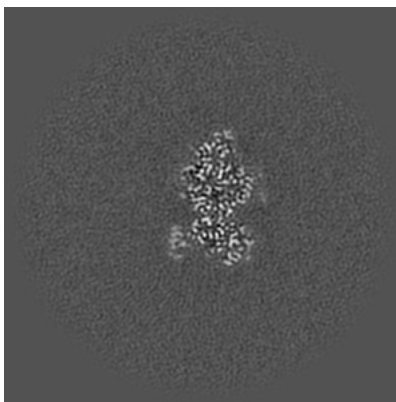
The images above show central slices of the map in three orthogonal directions.

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

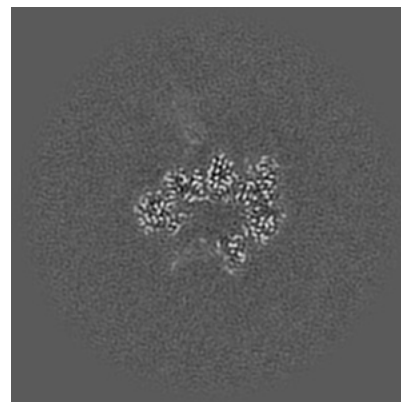
### 6.3.1 Primary map



X Index: 146

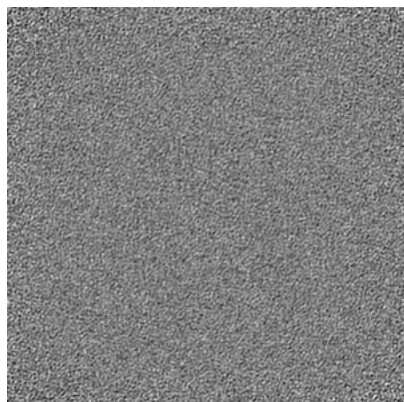


Y Index: 143

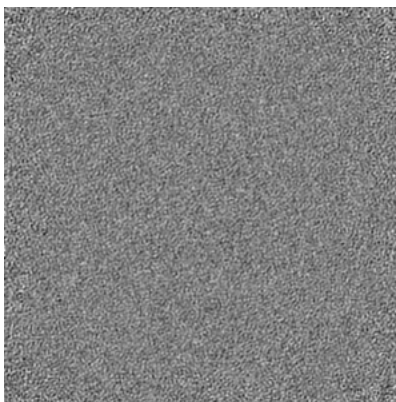


Z Index: 131

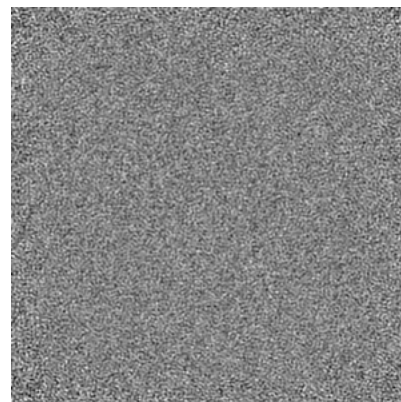
### 6.3.2 Raw map



X Index: 0



Y Index: 0



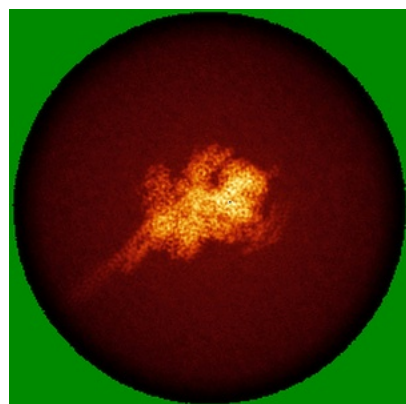
Z Index: 0

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

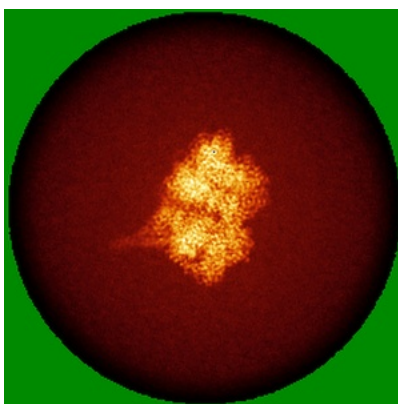


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

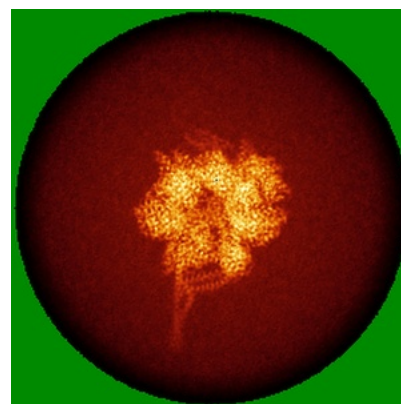
### 6.4.1 Primary map



X

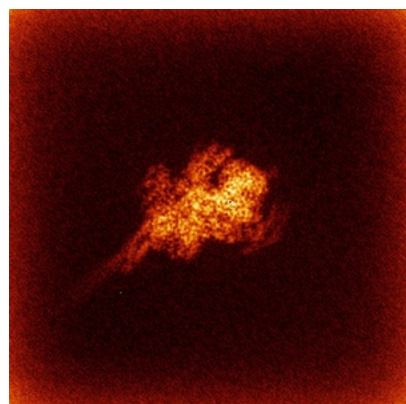


Y

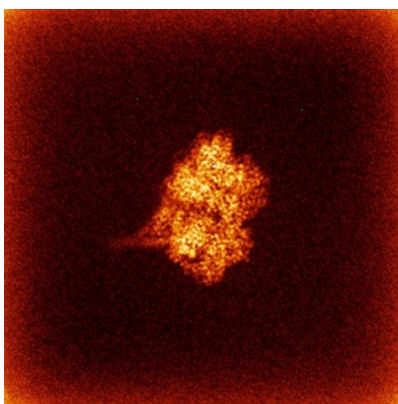


Z

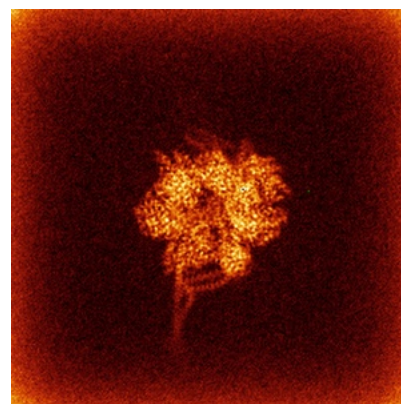
### 6.4.2 Raw map



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.

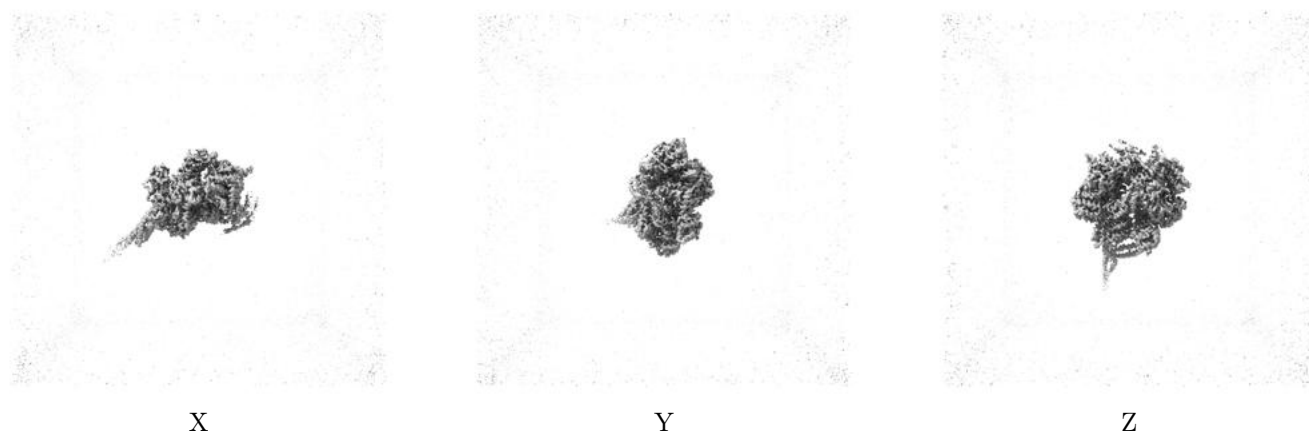
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

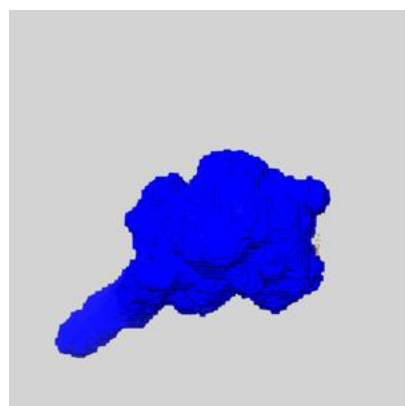
## 6.6 Mask visualisation [i](#)

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

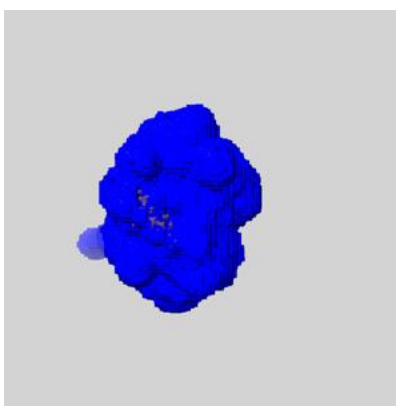
A mask typically either:

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

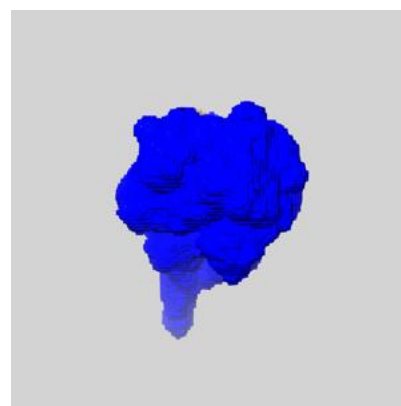
### 6.6.1 emd\_44702\_msk\_1.map [i](#)



X



Y

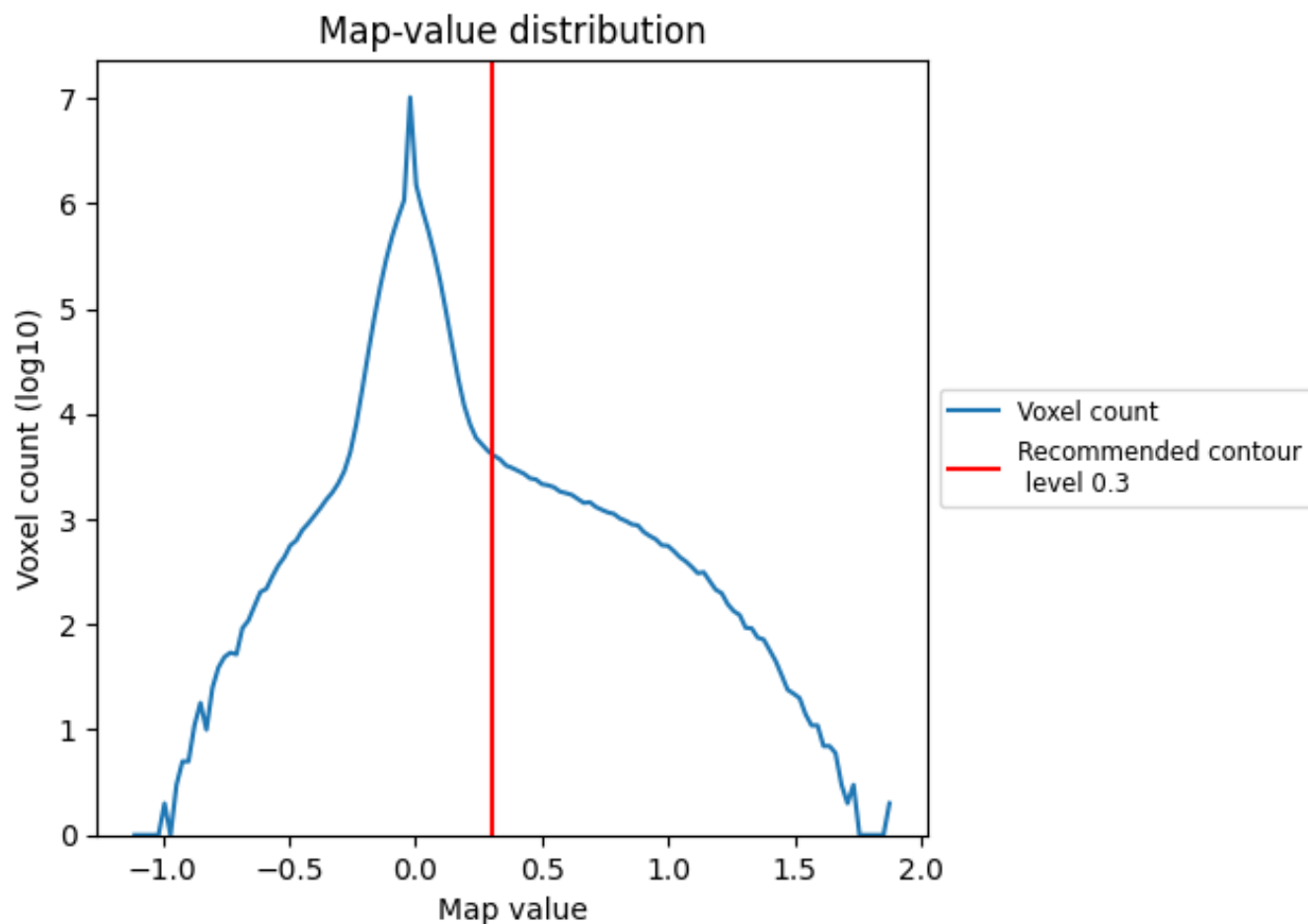


Z

## 7 Map analysis [i](#)

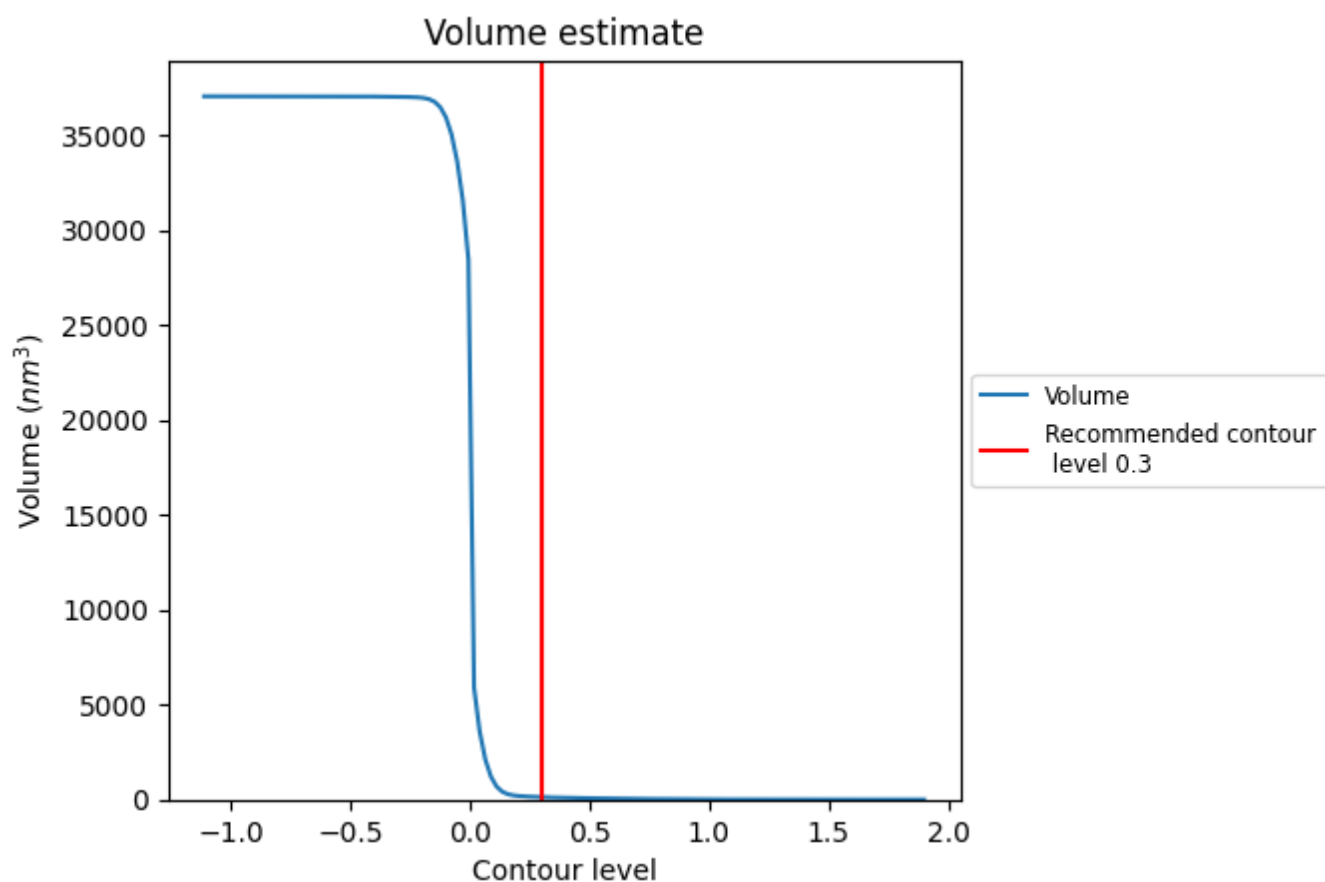
This section contains the results of statistical analysis of the map.

### 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](#)

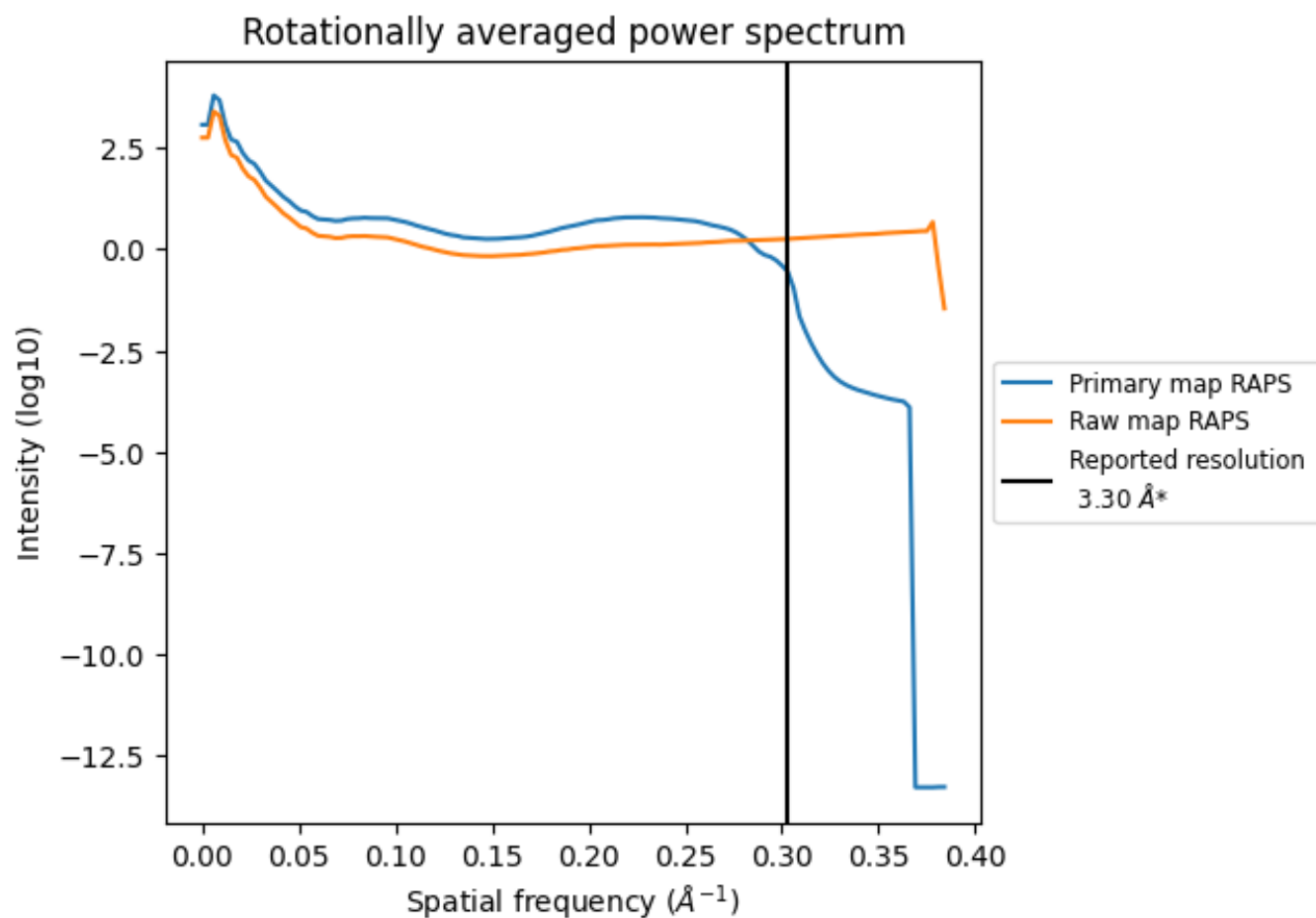


The volume at the recommended contour level is 128  $\text{nm}^3$ ; this corresponds to an approximate mass of 116 kDa.

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 ⓘ

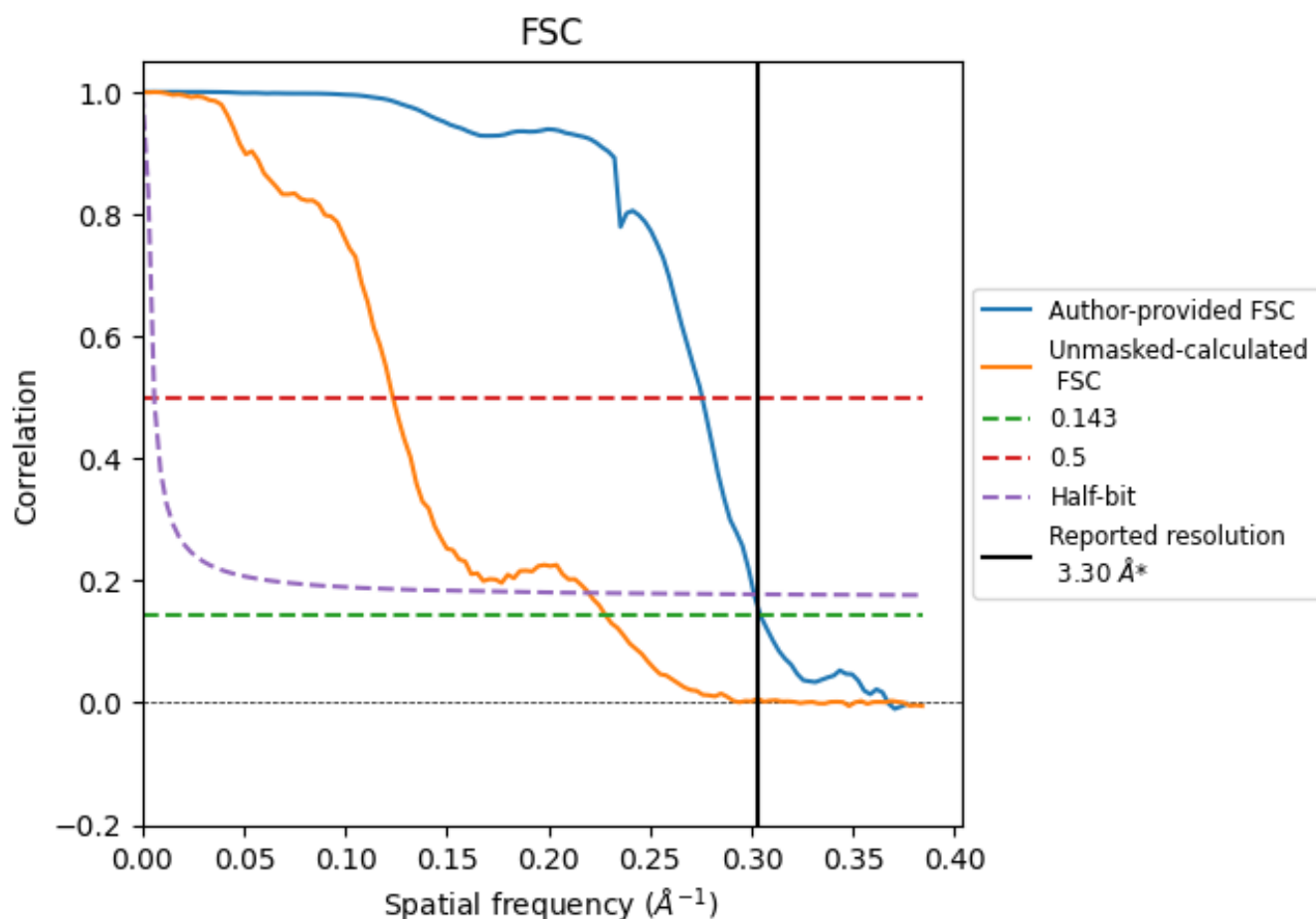


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

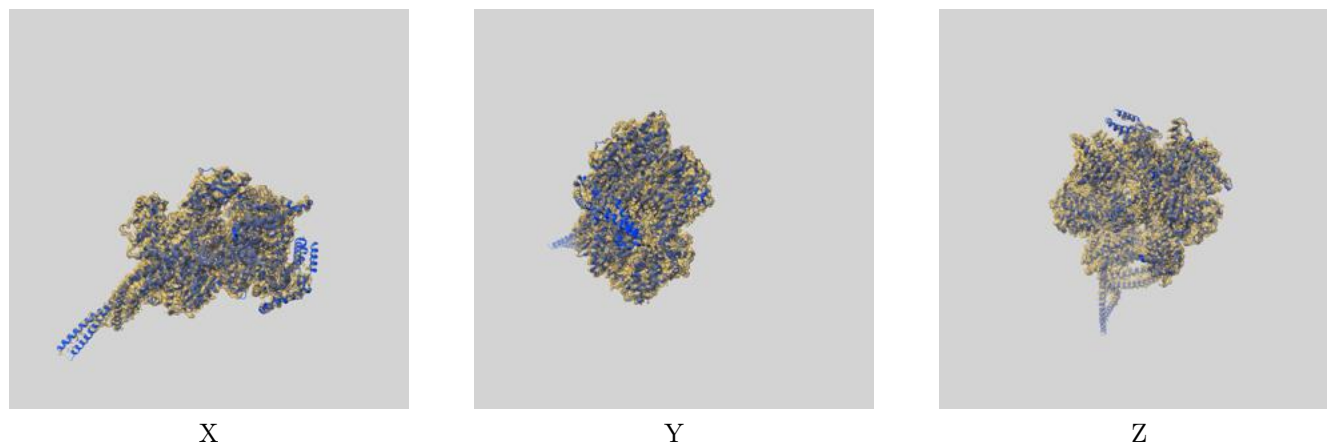
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.29	3.63	3.32
Unmasked-calculated*	4.38	8.10	4.55

\*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 4.38 differs from the reported value 3.3 by more than 10 %

## 9 Map-model fit [i](#)

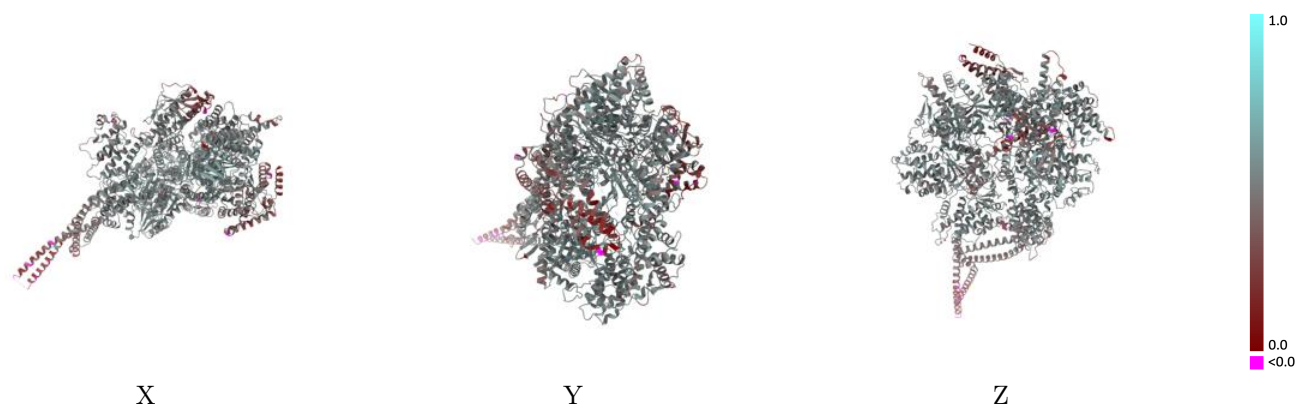
This section contains information regarding the fit between EMDB map EMD-44702 and PDB model 9BML. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

### 9.1 Map-model overlay [i](#)



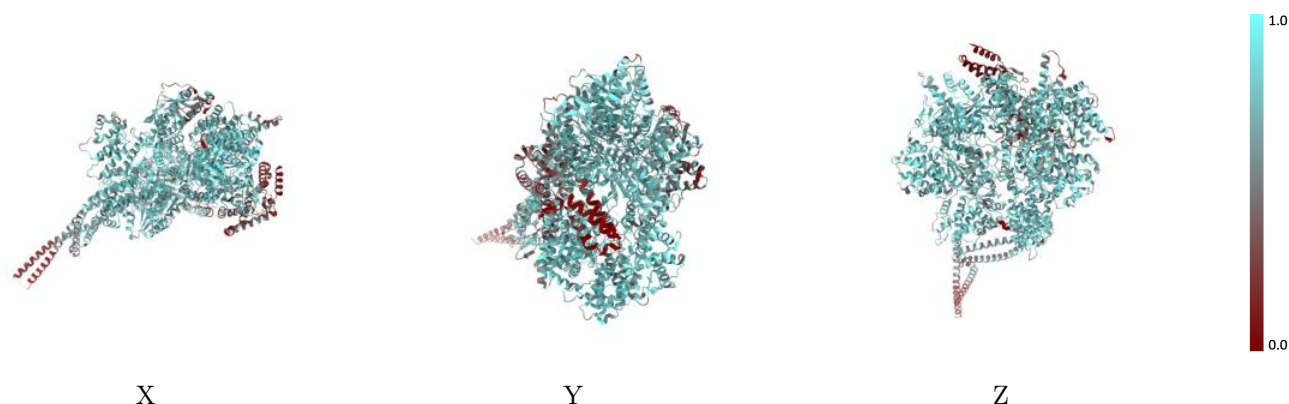
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



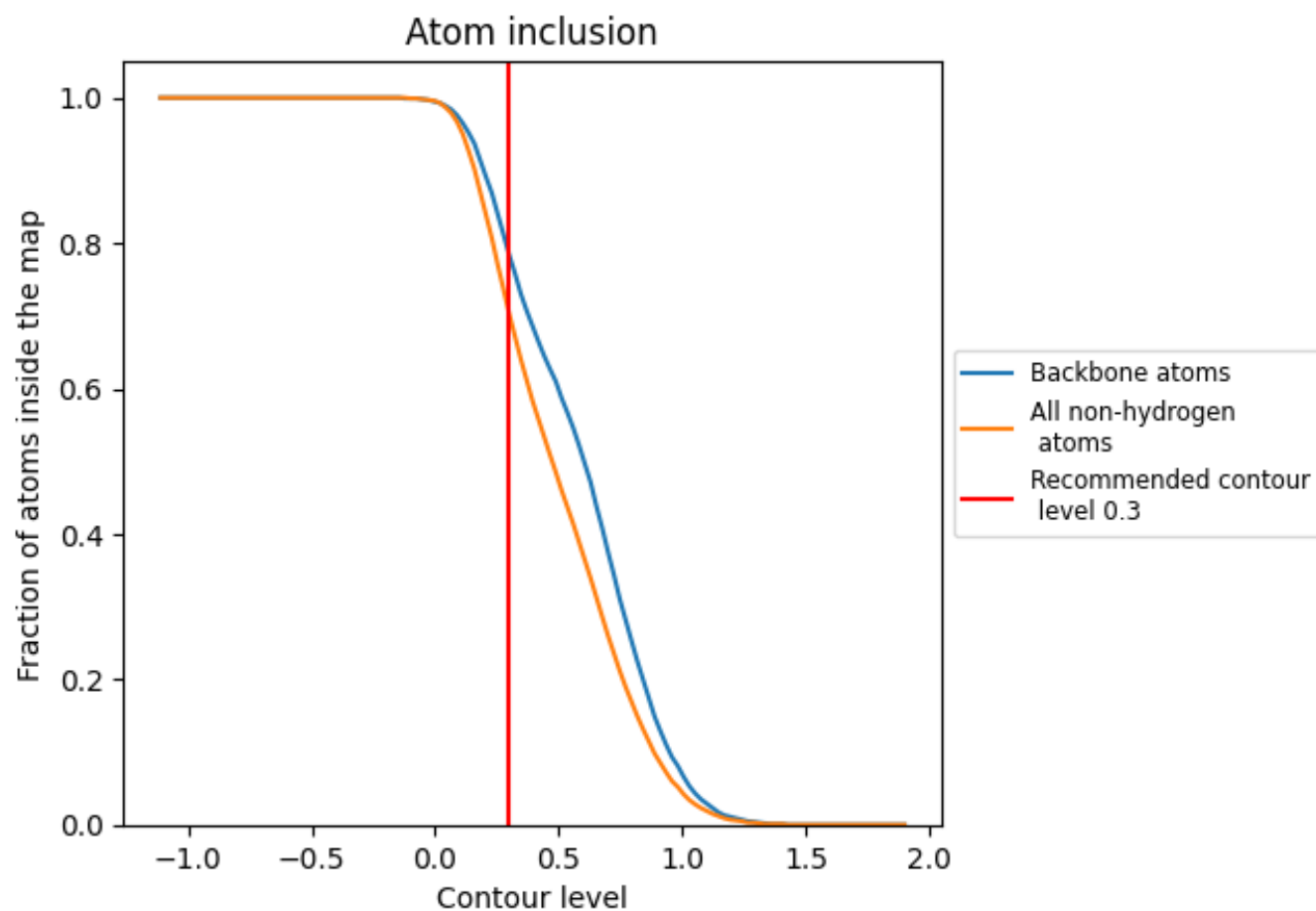
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 70% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7020	<div></div> 0.4800
A	<div></div> 0.7020	<div></div> 0.4800

