



## wwPDB EM Validation Summary Report ⓘ

Apr 24, 2025 – 11:20 AM EDT

PDB ID : 9DH5 / pdb\_00009dh5  
EMDB ID : EMD-46856  
Title : State-1 of the motor domain from full-length human dynein-1 in 5mM AMPPNP with 5mM Mg<sup>2+</sup>  
Authors : Chai, P.; Zhang, K.  
Deposited on : 2024-09-03  
Resolution : 2.60 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>.

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

EMDB validation analysis : 0.0.1.dev117  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
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) : 2.42

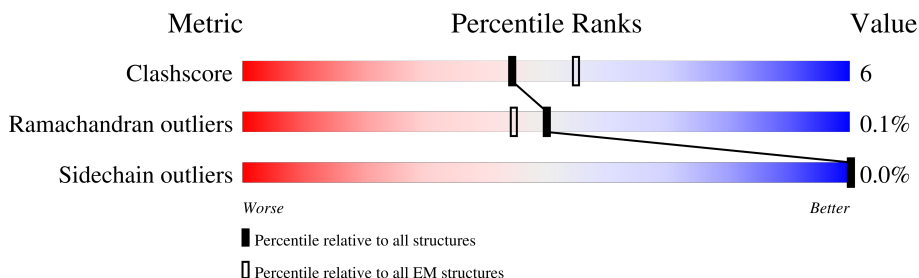
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.60 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 23689 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	2935	23575	15017	4067	4374	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	C	N	O	P	0
			31	10	5	13	3	

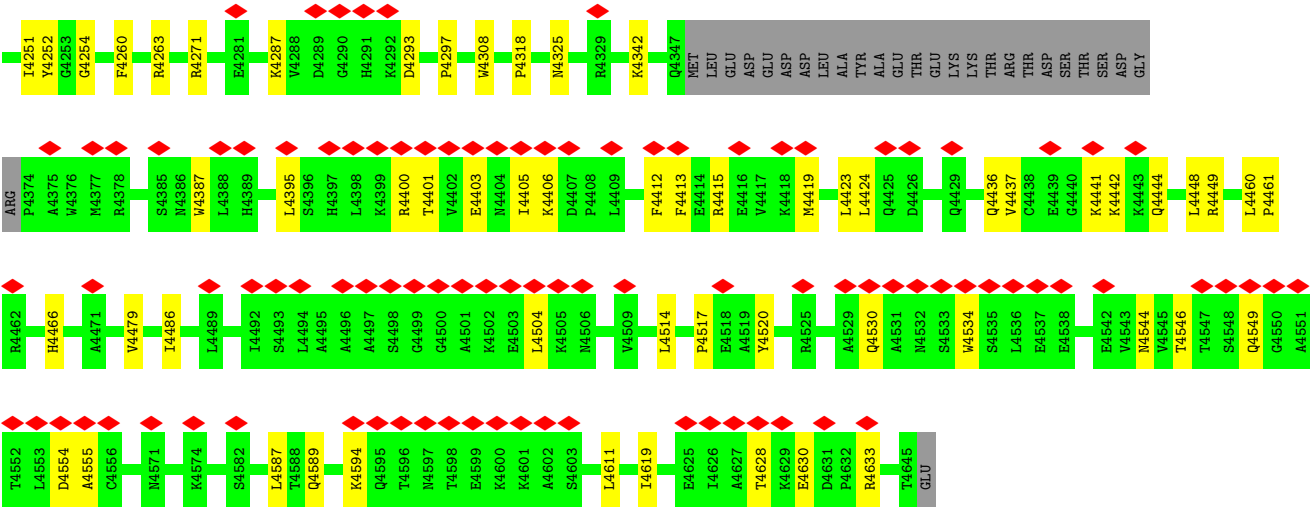
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
4	A	2	Total Mg 2 2	0



L2413	G2224	R2091	F1930	T1712	A1555	LYS	ALA	VAL	TRP	ARG	GLU	ALA	ASN	GLU	ASN	GLU	ASN	PHE
I2422	P2225	K2104	M1931	V1721	D1556	ASN	SER	ALA	GLU	PHE	PHE	GLN	LEU	LEU	LEU	LEU	LEU	ASN
N2430	S2226	R2107	D1937	V1724	R1567	ILE	PHE	GLU	GLU	THR	THR	THR	THR	THR	THR	THR	THR	LEU
Y2433	K2230	R2113	D1958	K1729	I1571	VAL	GLN	GLN	VAL	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	GLY
L2437	L2279	E2114	E1959	Y1738	F1575	ASP	ARG	ASP	THR	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	ASP
L2443	S2290	K2115	R1962	K1744	M1579	VAL	LEU	LEU	GLY	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	ASP
E2444	E2294	E2116	E1965	Y1745	V1591	LEU	GLY	VAL	VAL	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	GLY
H2445	L2295	E2117	R1966	V1751	V1591	VAL	THR	THR	THR	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	THR
L2449	D2308	G2118	M1967	L1601	L1607	GLN	MET	SER	GLU	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	LEU
T2450	N2316	E2120	E1980	S1753	L1611	GLY	LEU	GLU	GLU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLU
R2451	S2317	A2121	R1983	N1761	Q1612	GLU	VAL	VAL	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ARG
L2452	V2318	V2122	E1984	V1762	E1617	ILE	LEU	TRP	LEU	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	LEU
R2453	L2319	H1985	H1985	E1763	L1463	LEU	GLU	GLN	ILE	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	THR
C2454	D2123	S1986	S1986	G1771	R1621	SER	SER	GLN	GLY	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	GLY
S2457	E2124	M1987	P1988	G1772	E1622	GLU	GLU	MET	LYS	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	GLU
N2461	G2125	N1989	P1988	G1773	R1623	ALA	ALA	LYS	PRO	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	THR
Q2471	X1992	D1991	D1991	D1774	S1624	LEU	LEU	GLU	GLN	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	GLN
D2478	T1993	X1992	X1992	A1775	S1625	LYS	LYS	GLN	TRP	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ALA
F2479	S1994	K1834	K1834	V1781	Y1630	ASP	ASP	TRP	LYS	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	LYS
Q2482	A1995	L1792	L1792	E1635	F1631	TRP	TRP	VAL	ASP	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	VAL
E2487	P1996	L1832	L1832	E1635	G1633	SER	SER	GLN	GLU	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	THR
R2488	T1997	N1832	N1832	E1635	G1633	GLN	GLN	VAL	ARG	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	PHE
Q2491	I1997	K1834	K1834	E1635	G1633	LEU	LEU	PRO	ARG	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	ALA
R2492	Q2005	L1834	L1834	E1635	G1633	LYS	LYS	GLN	VAL	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	THR
I2498	A2023	V1838	V1838	E1635	G1633	ARG	ARG	LEU	ALA	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	VAL
D2505	S2026	V1853	V1853	E1635	G1633	HIS	HIS	GLN	ALA	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	ARG
E2513	L2028	Q1856	Q1856	E1635	G1633	ASN	ASN	ASN	GLU	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	GLN
E2516	L2032	Q1860	Q1860	E1635	G1633	TRP	TRP	VAL	ASP	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	VAL
T2528	R2037	K1865	K1865	E1635	G1633	VAL	VAL	LEU	ALA	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL
A2529	S2038	K1878	K1878	E1635	G1633	GLU	GLU	ASN	ASP	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	SER
P2530	L2039	L1879	L1879	E1635	G1633	THR	THR	LEU	GLY	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	GLY
N2531	Q2047	R1887	R1887	E1635	G1633	LYS	LYS	LEU	GLY	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	ASN
D2536	F2059	A1895	A1895	E1635	G1633	LEU	LEU	THR	GLY	THR	THR	THR	THR	THR	THR	THR	THR	PRO
Y2537	R2061	K1897	K1897	E1635	G1633	GLY	GLY	LEU	GLY	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLY
E2538	T2061	V1672	V1672	E1635	G1633	THR	THR	LEU	GLY	THR	THR	THR	THR	THR	THR	THR	THR	ASN
Y2544	I2069	K1697	K1697	E1635	G1633	LEU	LEU	VAL	GLY	THR	THR	THR	THR	THR	THR	THR	THR	LEU
W2548	V2070	N1698	N1698	E1635	G1633	ASP	ASP	VAL	GLY	THR	THR	THR	THR	THR	THR	THR	THR	LEU
V2557	P2071	E1914	E1914	E1635	G1633	GLN	GLN	THR	GLY	THR	THR	THR	THR	THR	THR	THR	THR	ASN







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	301002	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	4.272	Depositor
Minimum map value	-2.173	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.068	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	444.4032, 444.4032, 444.4032	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1573, 1.1573, 1.1573	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: MG, ADP, ATP

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	0.27	0/24075	0.48	2/32628 (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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1669	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	2308	ASP	CB-CG-OD1	5.17	122.95	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4195	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	23575	0	23638	290	0
2	A	81	0	36	3	0
3	A	31	0	12	3	0
4	A	2	0	0	0	0
All	All	23689	0	23686	292	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 6.

The worst 5 of 292 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:2221:MET:HG2	1:A:2343:PHE:HB2	1.55	0.89
1:A:4271:ARG:HD3	1:A:4633:ARG:HH12	1.43	0.83
1:A:2629:GLU:OE2	1:A:2633:LYS:NZ	2.12	0.82
1:A:1490:TRP:HH2	1:A:1537:TRP:HD1	1.29	0.79
1:A:4088:VAL:HG11	1:A:4116:LEU:HD21	1.67	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	2927/4646 (63%)	2880 (98%)	45 (2%)	2 (0%)	48 71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4197	ALA
1	A	4198	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	2603/4125 (63%)	2602 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2471	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3735	GLN
1	A	3754	ASN
1	A	4335	GLN
1	A	2713	ASN
1	A	3092	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are 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	4701	4	24,29,29	0.73	0	29,45,45	0.75	1 (3%)
2	ADP	A	4704	-	24,29,29	0.73	0	29,45,45	0.74	1 (3%)
3	ATP	A	4702	4	28,33,33	0.76	0	34,52,52	0.79	1 (2%)
2	ADP	A	4703	-	24,29,29	0.75	0	29,45,45	0.73	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	4701	4	-	0/12/32/32	0/3/3/3
2	ADP	A	4704	-	-	2/12/32/32	0/3/3/3
3	ATP	A	4702	4	-	2/18/38/38	0/3/3/3
2	ADP	A	4703	-	-	1/12/32/32	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4704	ADP	C5-C6-N6	2.34	123.87	120.31
2	A	4701	ADP	C5-C6-N6	2.31	123.83	120.31
2	A	4703	ADP	C5-C6-N6	2.29	123.79	120.31
3	A	4702	ATP	C5-C6-N6	2.23	123.71	120.31

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4704	ADP	PA-O3A-PB-O2B
3	A	4702	ATP	O4'-C4'-C5'-O5'
2	A	4704	ADP	PA-O3A-PB-O1B

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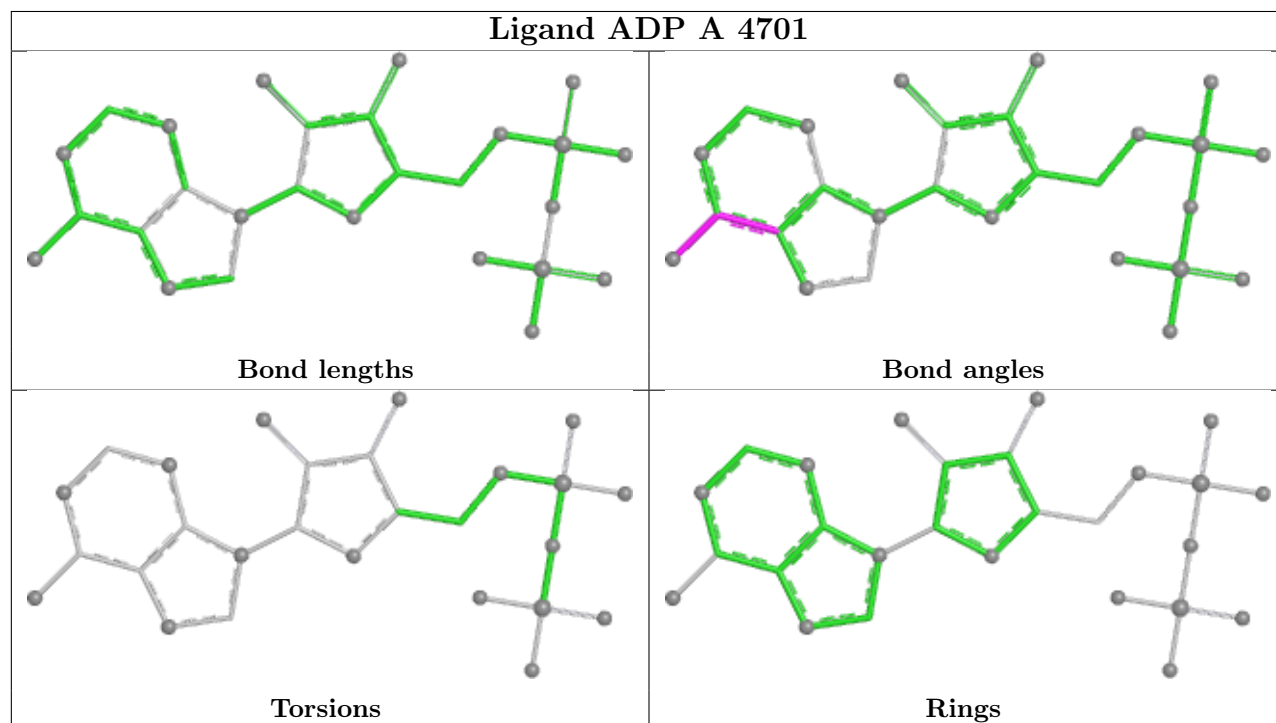
Mol	Chain	Res	Type	Atoms
3	A	4702	ATP	C3'-C4'-C5'-O5'
2	A	4703	ADP	PA-O3A-PB-O3B

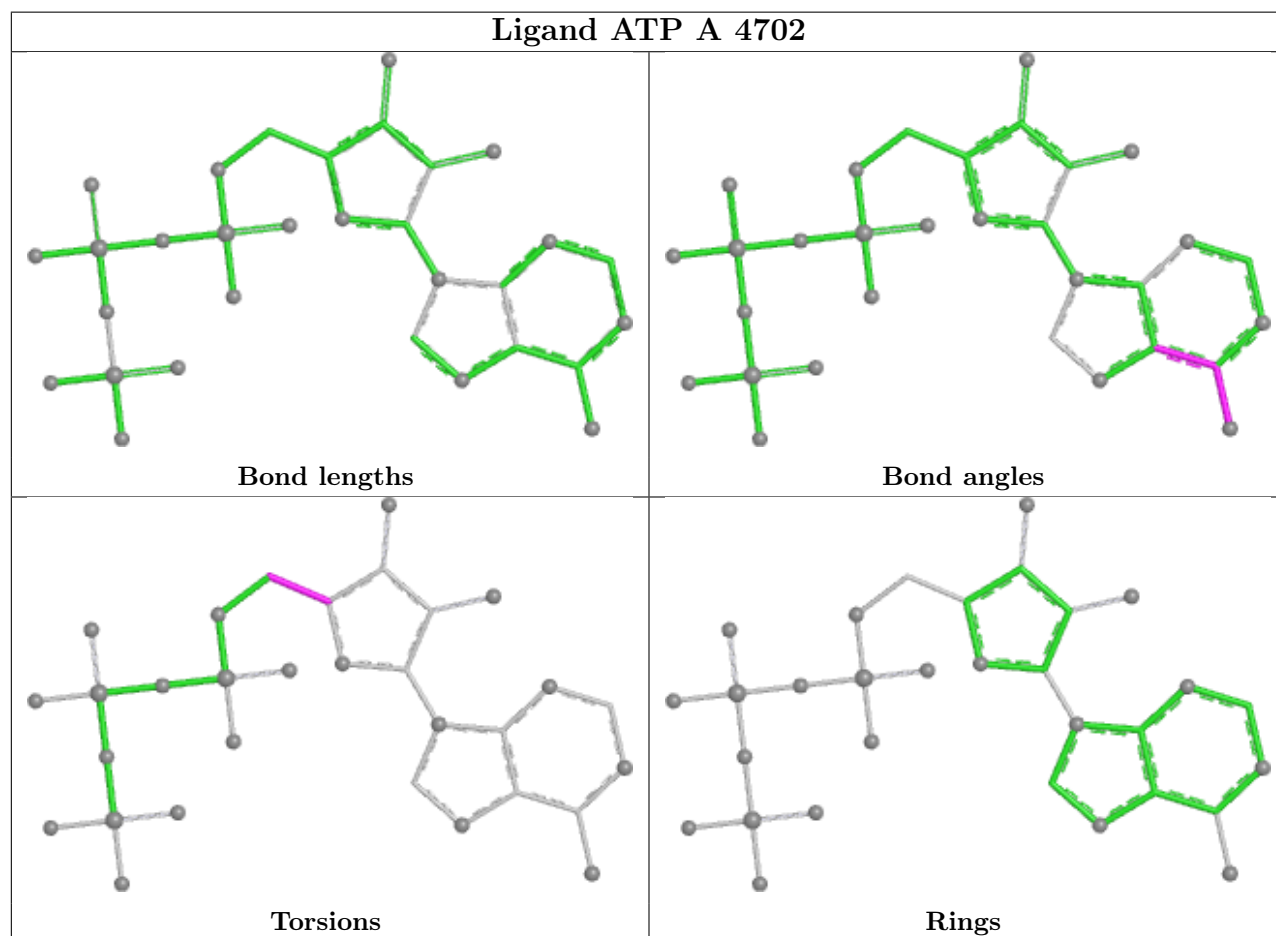
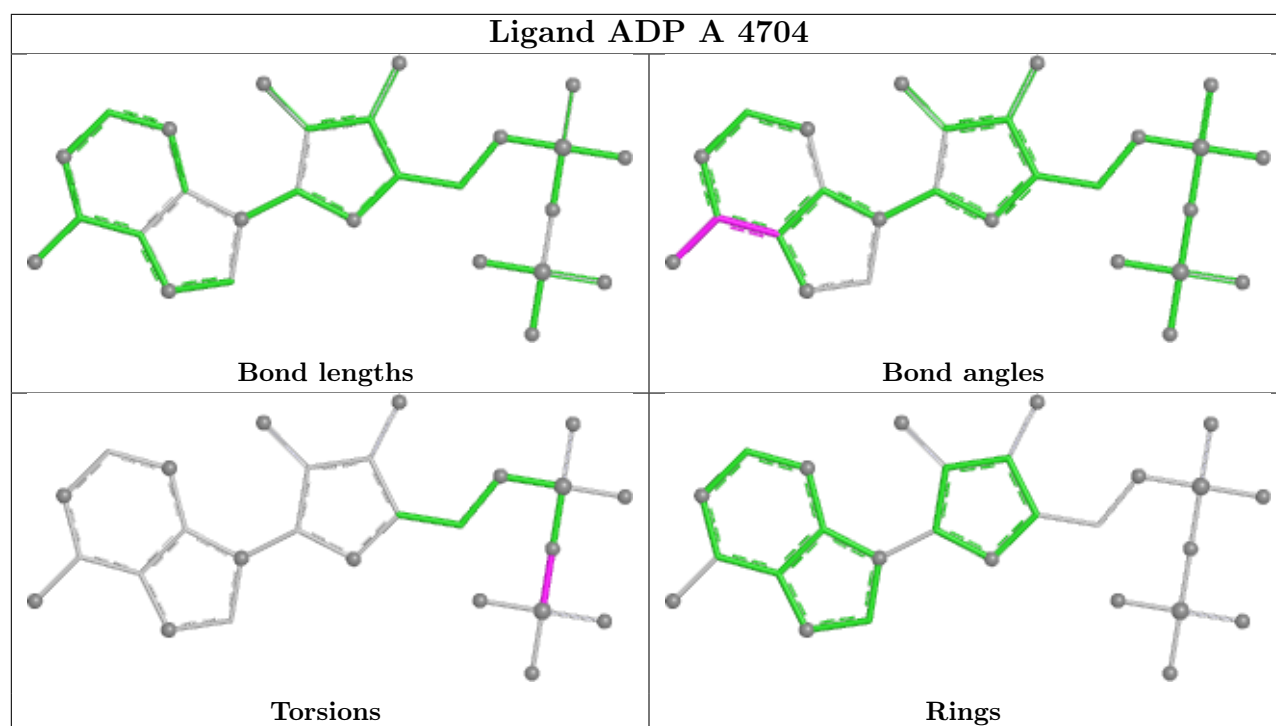
There are no ring outliers.

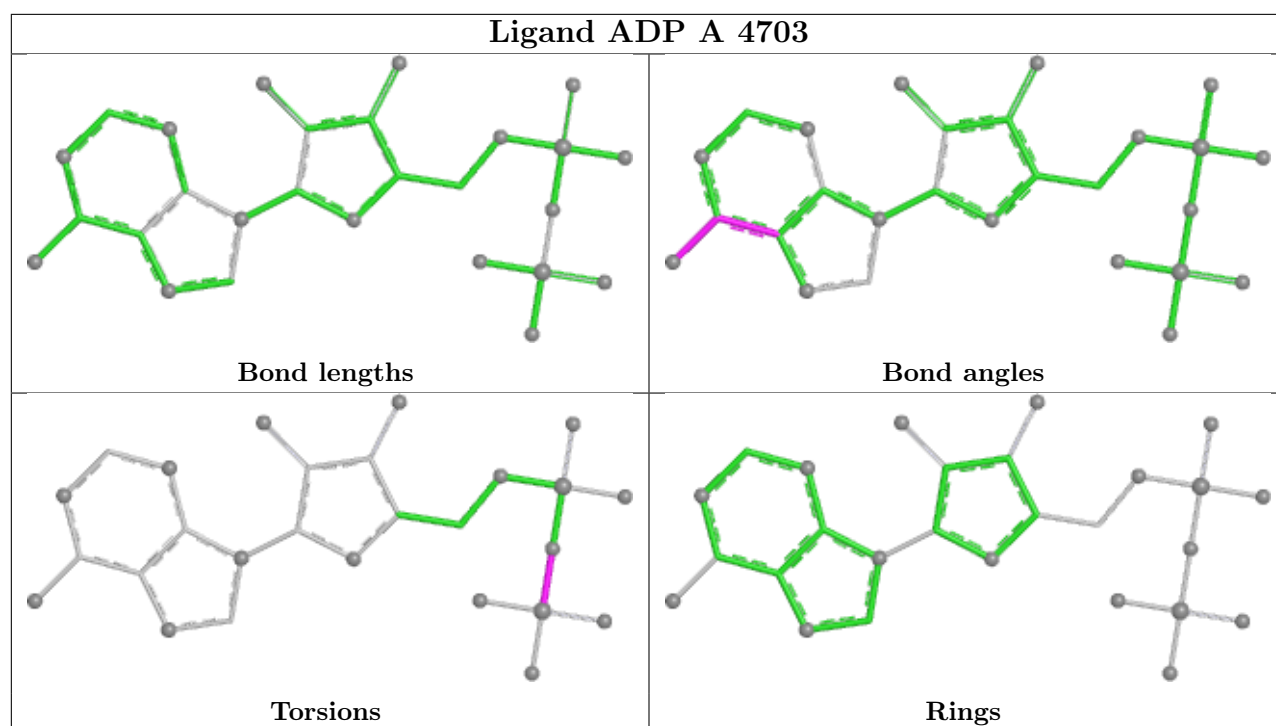
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4701	ADP	3	0
3	A	4702	ATP	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.



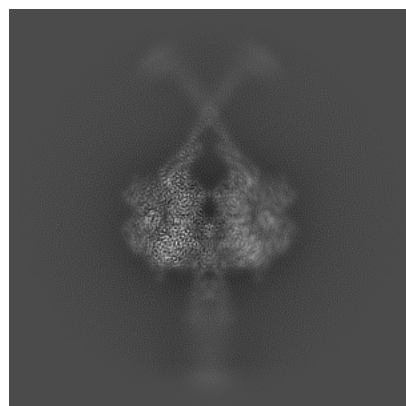
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46856. These allow visual inspection of the internal detail of the map and identification of artifacts.

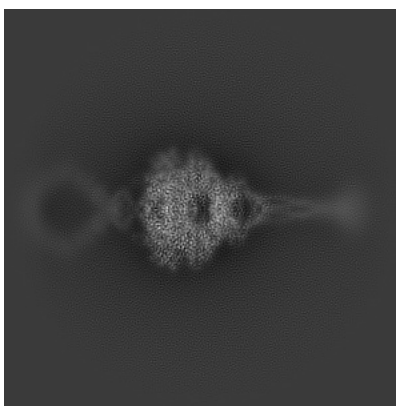
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

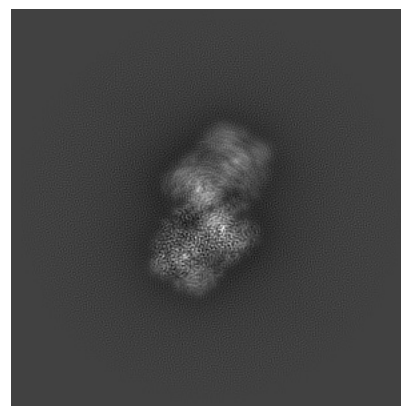
#### 6.1.1 Primary map



X

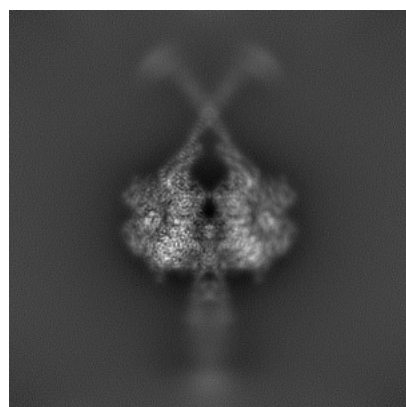


Y

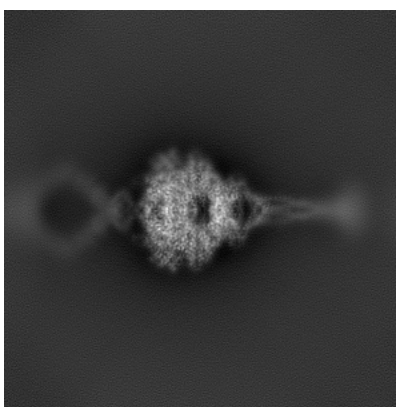


Z

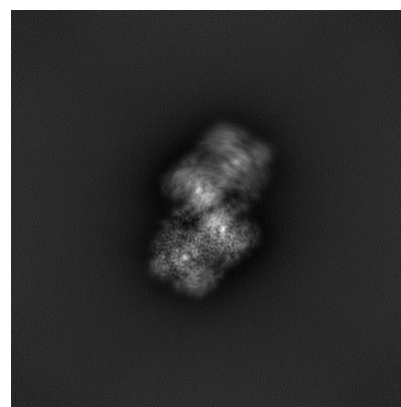
#### 6.1.2 Raw map



X



Y

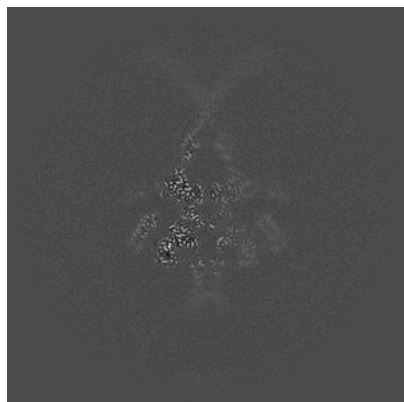


Z

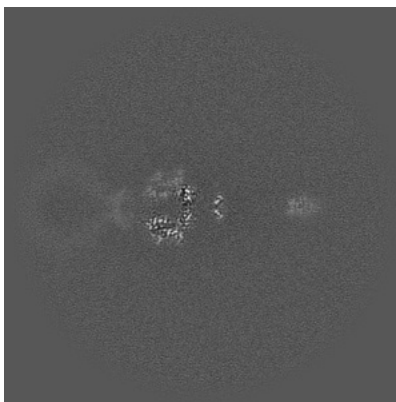
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

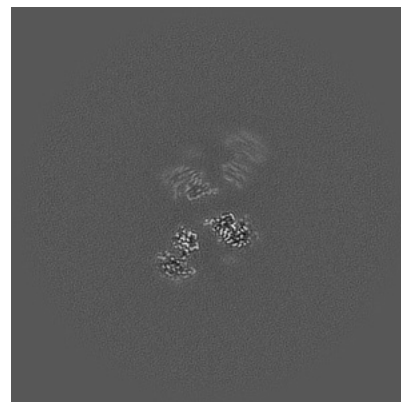
### 6.2.1 Primary map



X Index: 192

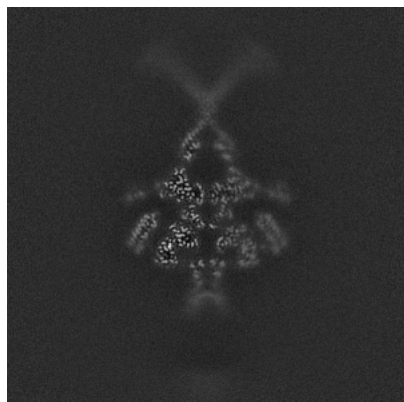


Y Index: 192

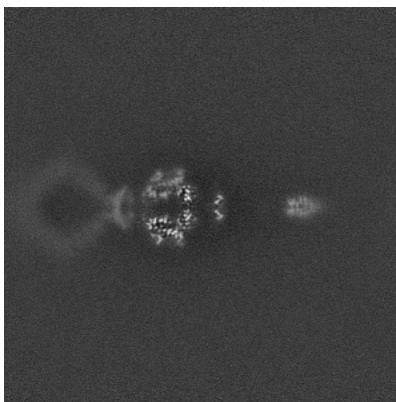


Z Index: 192

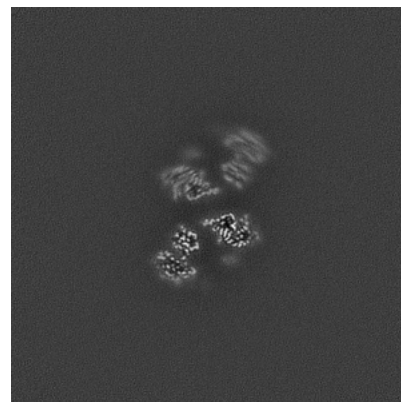
### 6.2.2 Raw map



X Index: 192



Y Index: 192



Z Index: 192

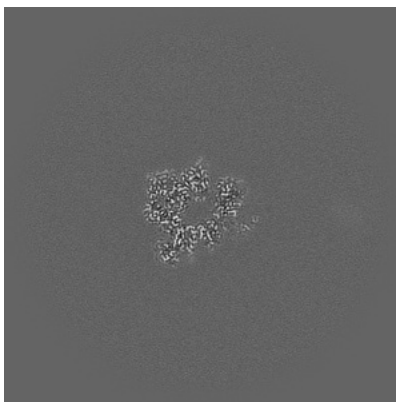
The images above show central slices of the map in three orthogonal directions.

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

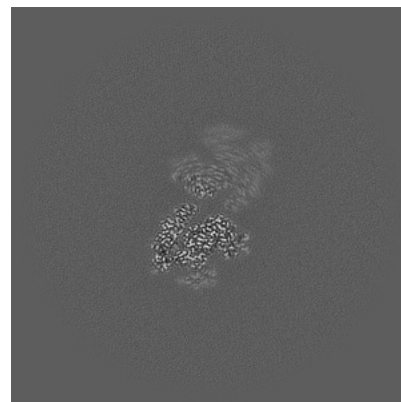
### 6.3.1 Primary map



X Index: 204



Y Index: 159

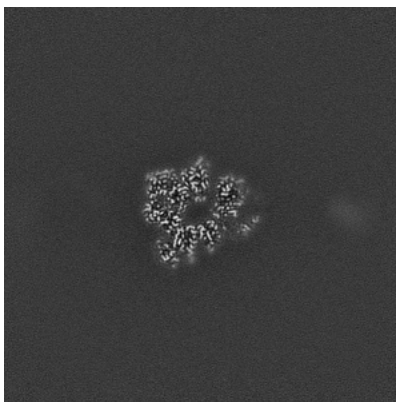


Z Index: 159

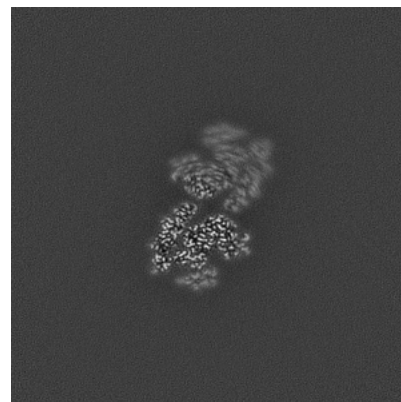
### 6.3.2 Raw map



X Index: 204



Y Index: 159

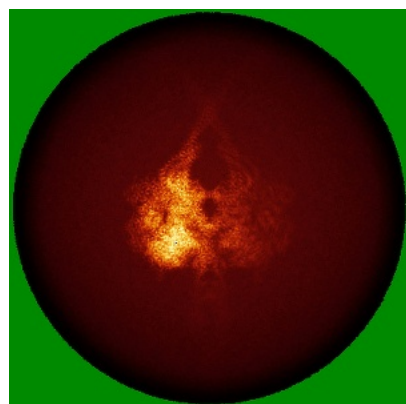


Z Index: 159

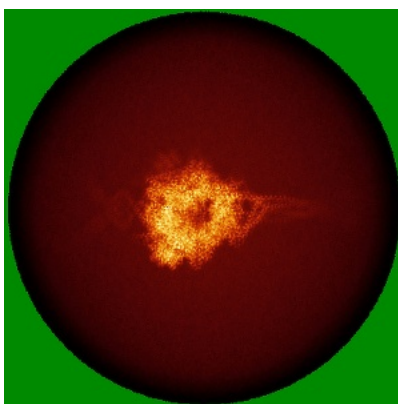
The images above show the largest variance slices of the map in three orthogonal directions.

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

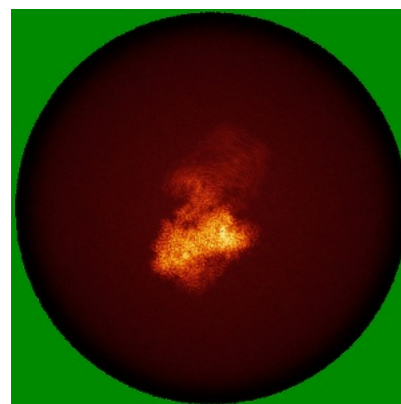
### 6.4.1 Primary map



X

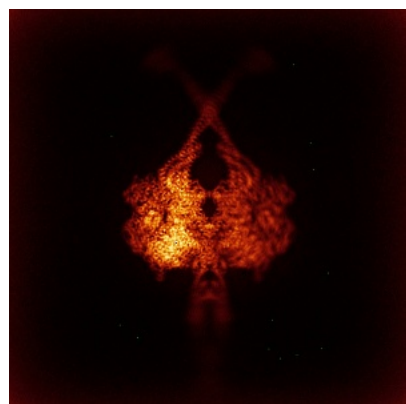


Y

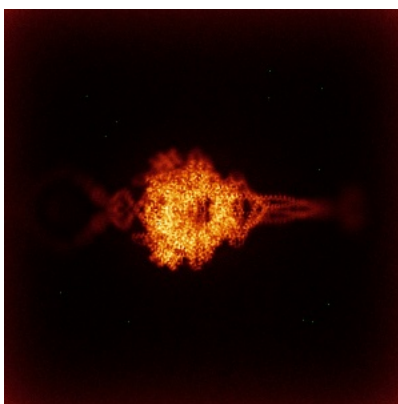


Z

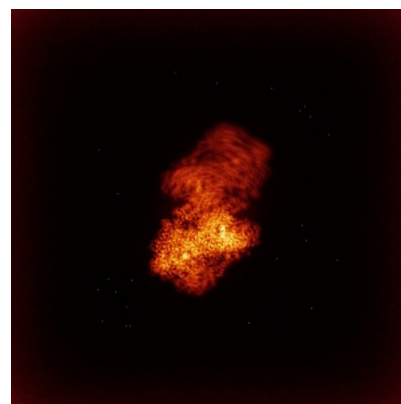
### 6.4.2 Raw map



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 0.4. 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.



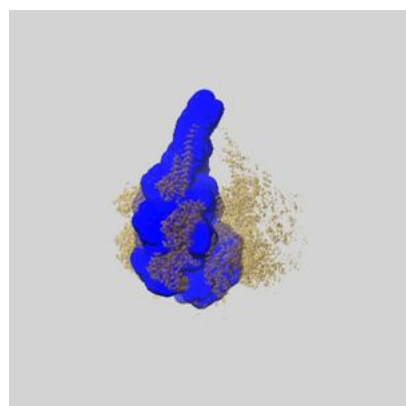
## 6.6 Mask visualisation [i](#)

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

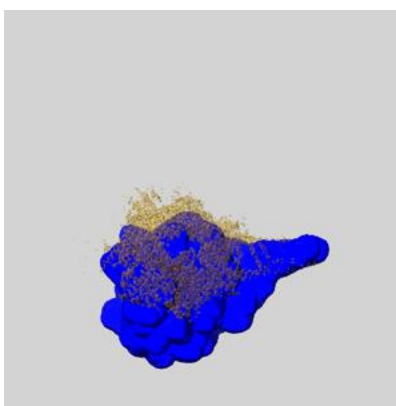
A mask typically either:

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

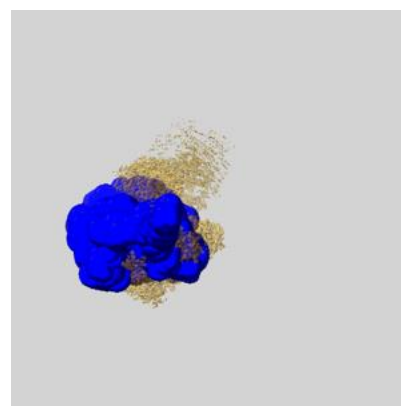
### 6.6.1 emd\_46856\_msk\_1.map [i](#)



X



Y

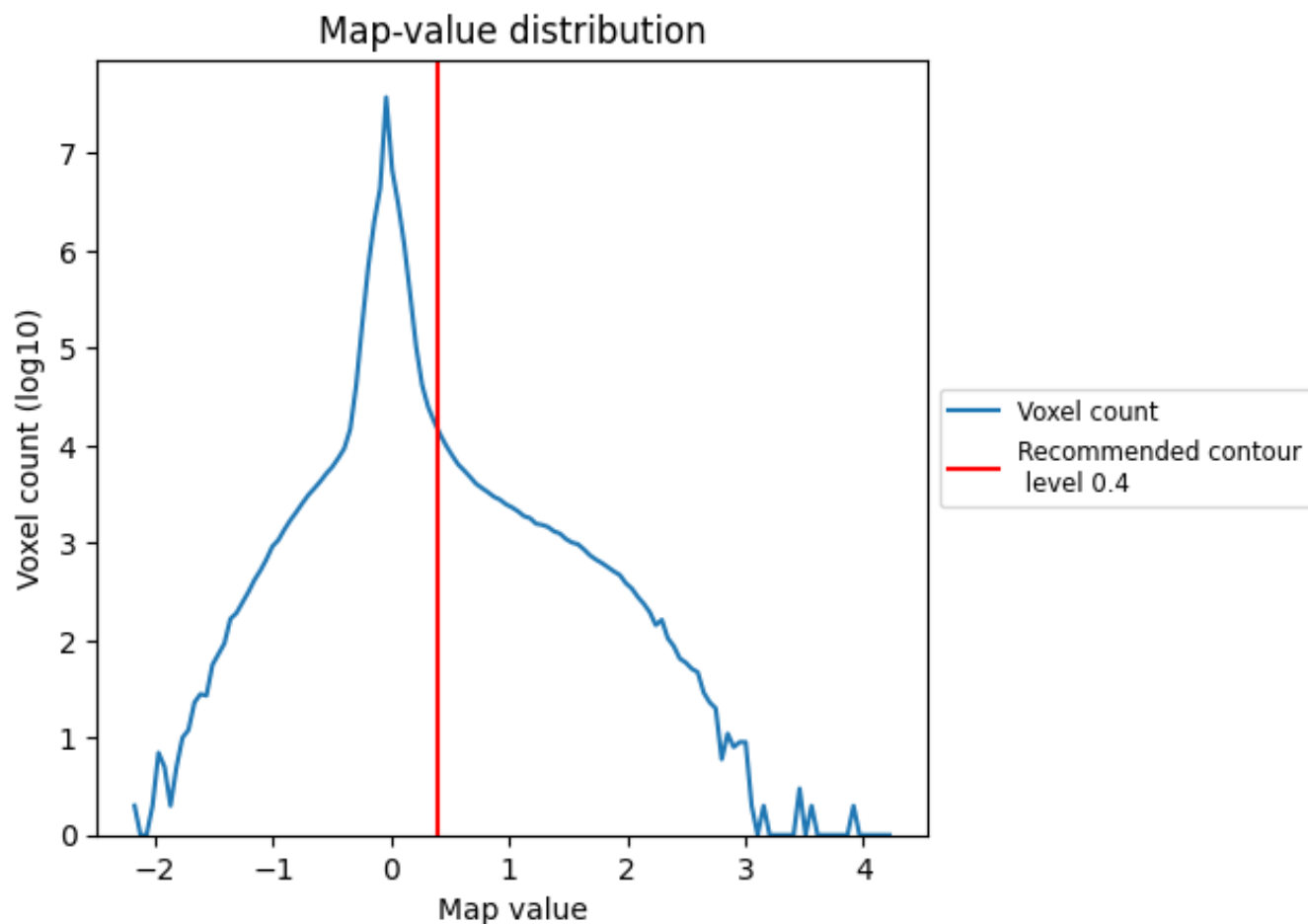


Z

## 7 Map analysis [i](#)

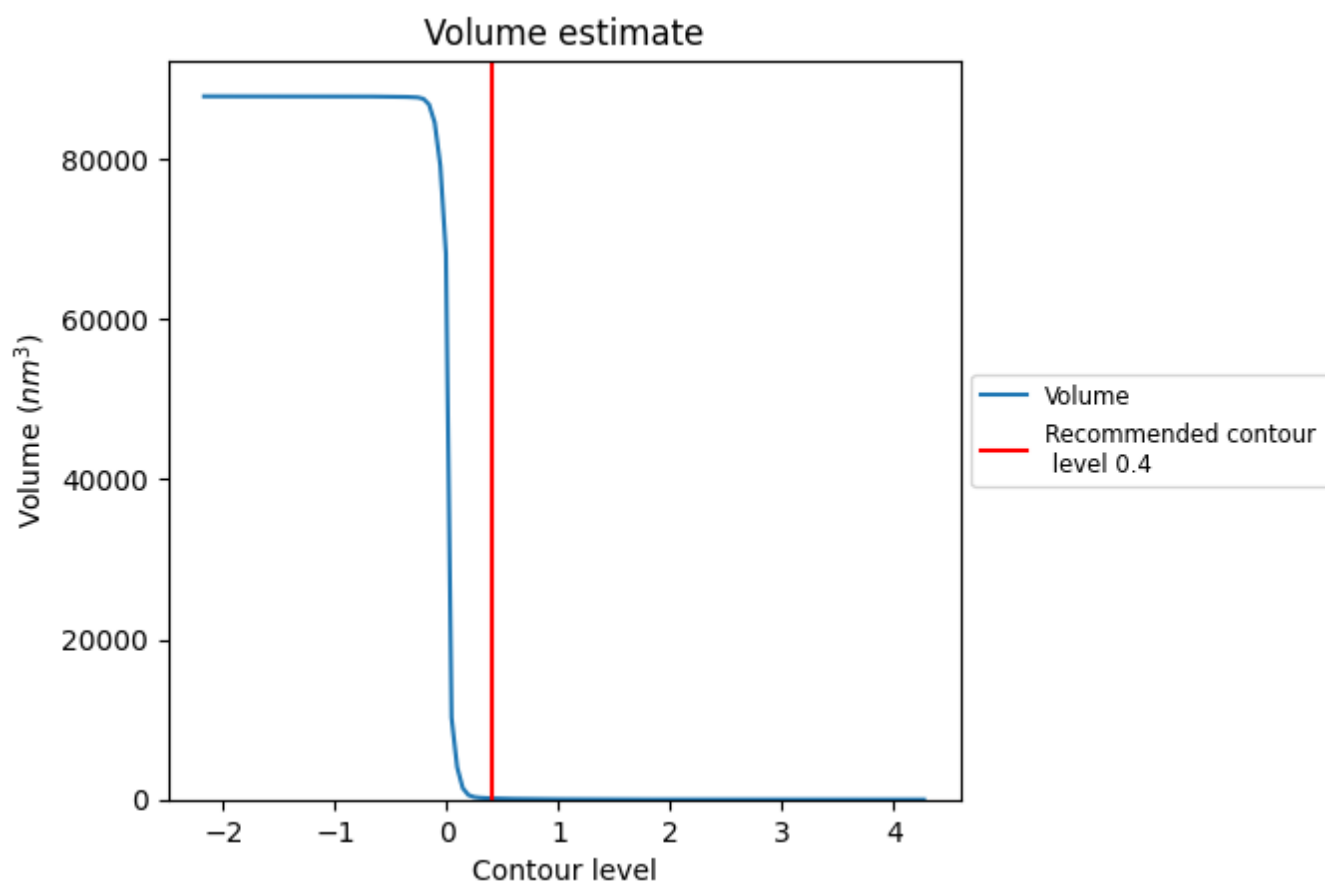
This section contains the results of statistical analysis of the map.

### 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](#)

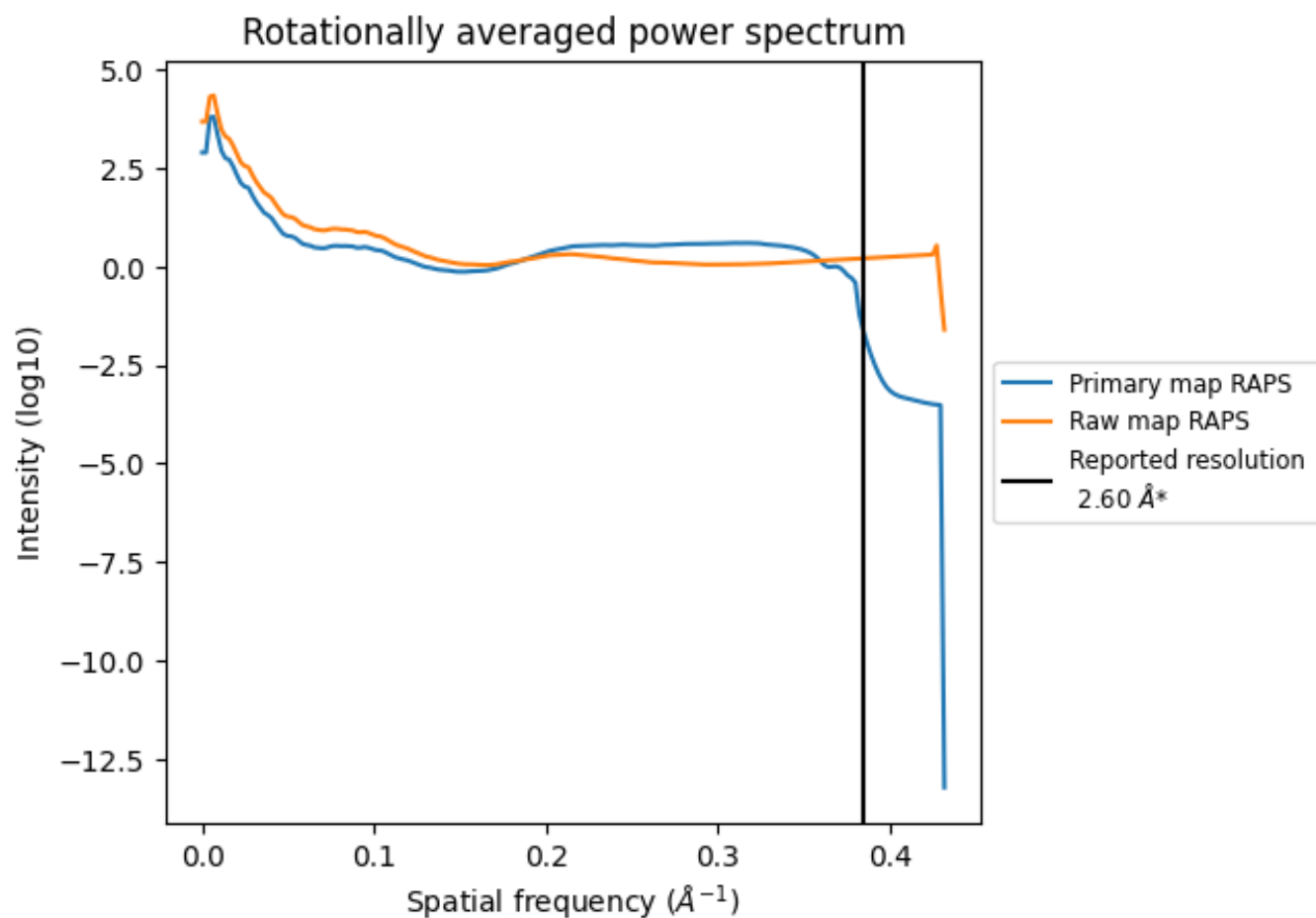


The volume at the recommended contour level is 150 nm<sup>3</sup>; this corresponds to an approximate mass of 136 kDa.

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 ⓘ

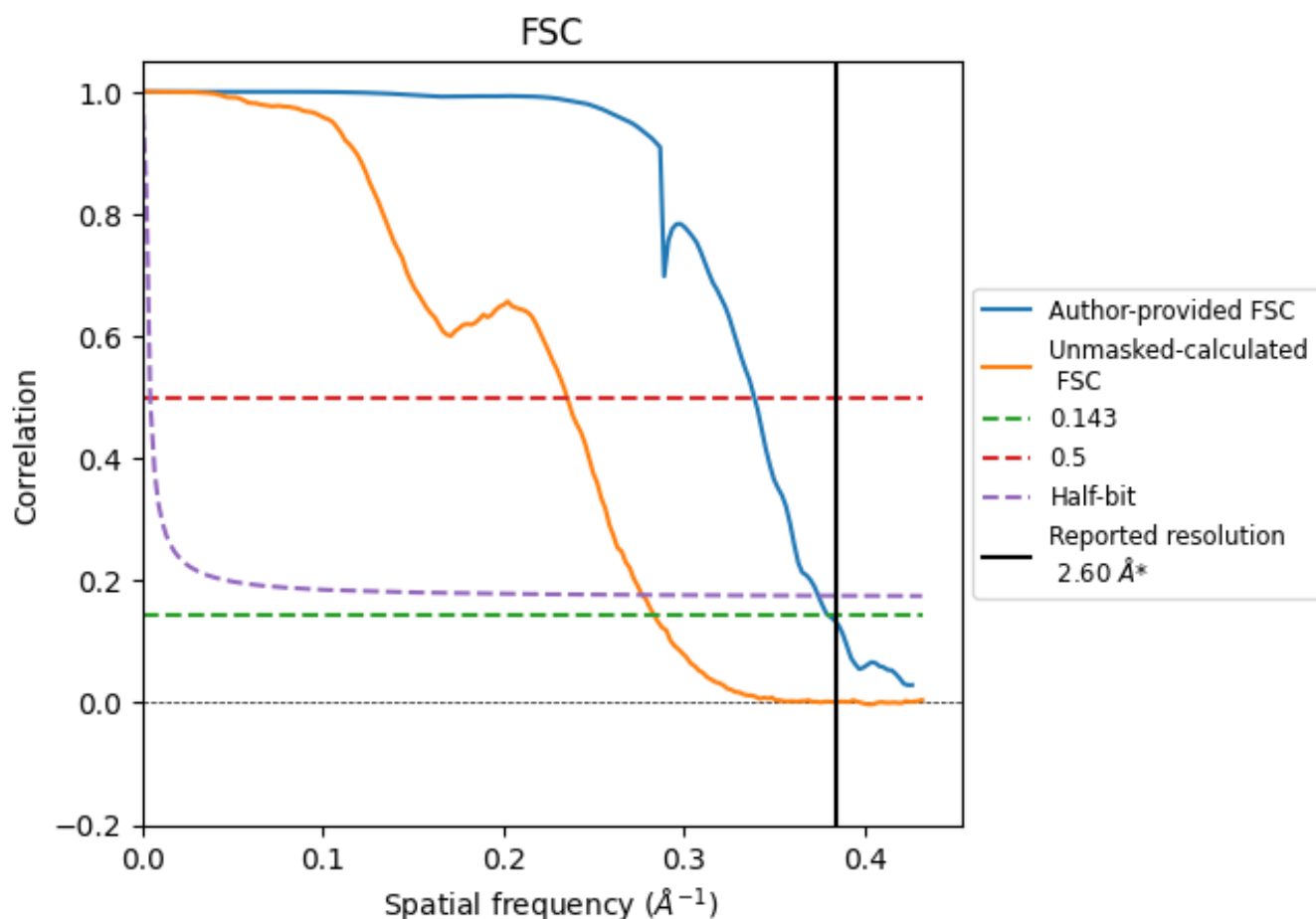


\*Reported resolution corresponds to spatial frequency of 0.385  $\text{\AA}^{-1}$

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

## 8.2 Resolution estimates [i](#)

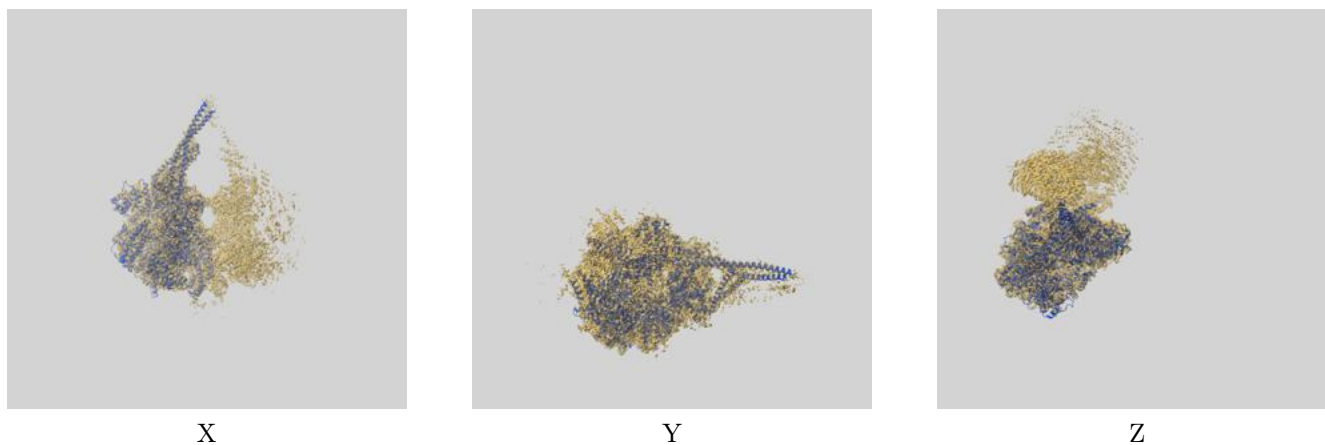
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.63	2.95	2.67
Unmasked-calculated*	3.53	4.25	3.61

\*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 3.53 differs from the reported value 2.6 by more than 10 %

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

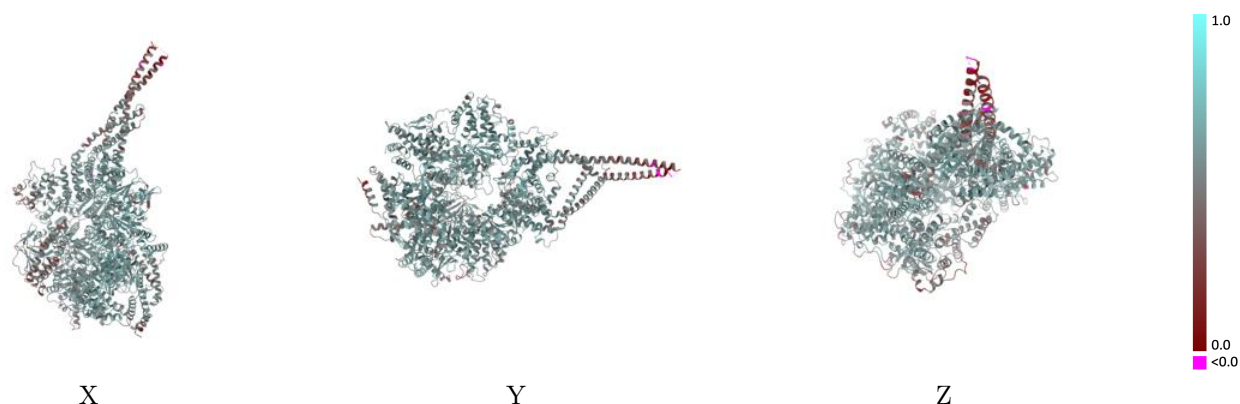
This section contains information regarding the fit between EMDB map EMD-46856 and PDB model 9DH5. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

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



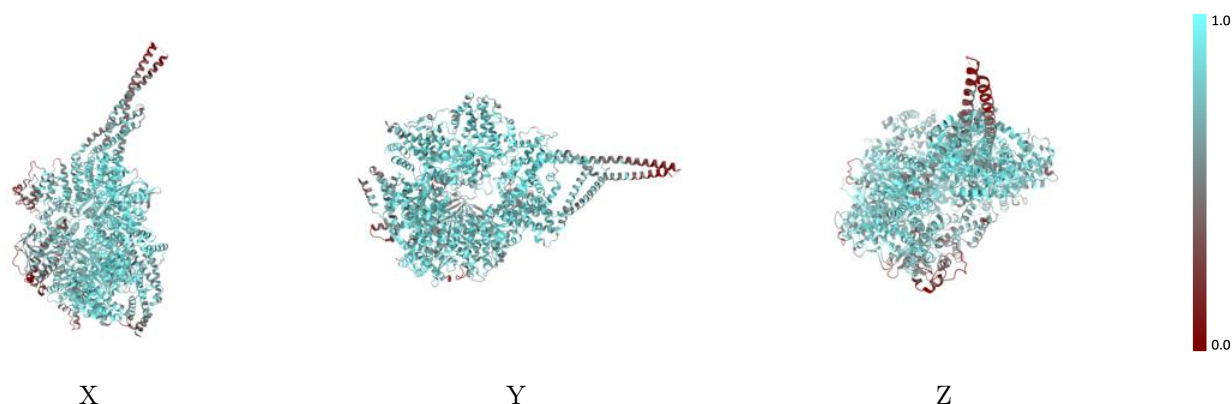
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



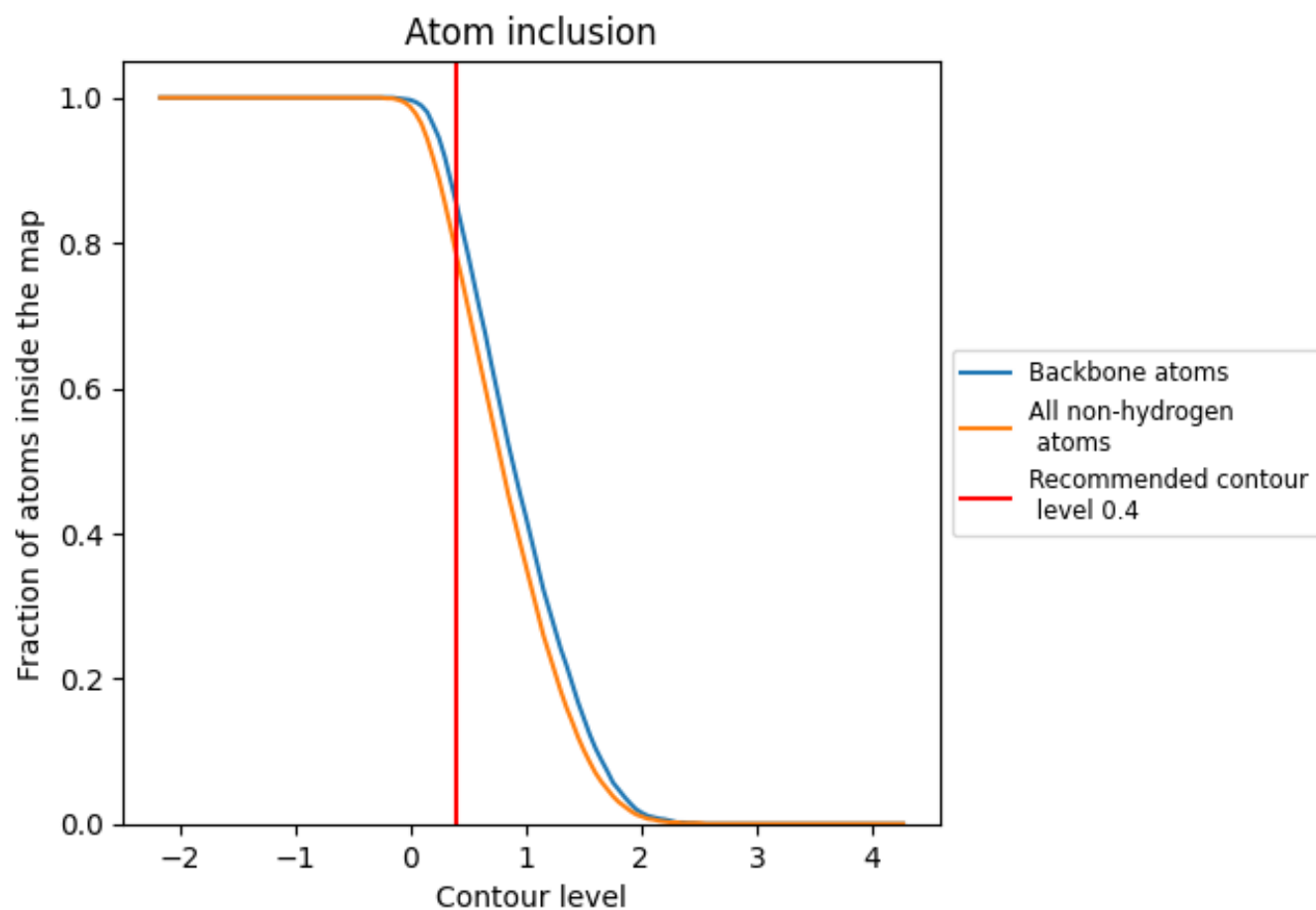
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 78% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7800	<div><div></div></div> 0.5660
A	<div><div></div></div> 0.7800	<div><div></div></div> 0.5660

