



wwPDB EM Validation Summary Report ⓘ

Apr 24, 2025 – 11:14 AM EDT

PDB ID : 9BN6 / pdb_00009bn6
EMDB ID : EMD-44723
Title : The alpha registry-locked dynein motor domain mutant in 5mM ATPVi condition, class2
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.40 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.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

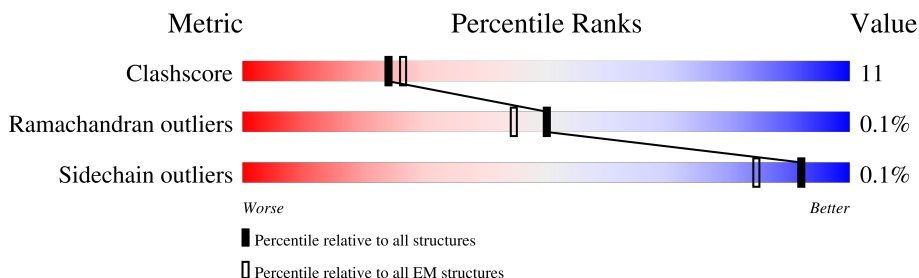
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	A	4646	<div> <div>11%</div> <div>45%</div> <div>16%</div> <div>39%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 23078 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.

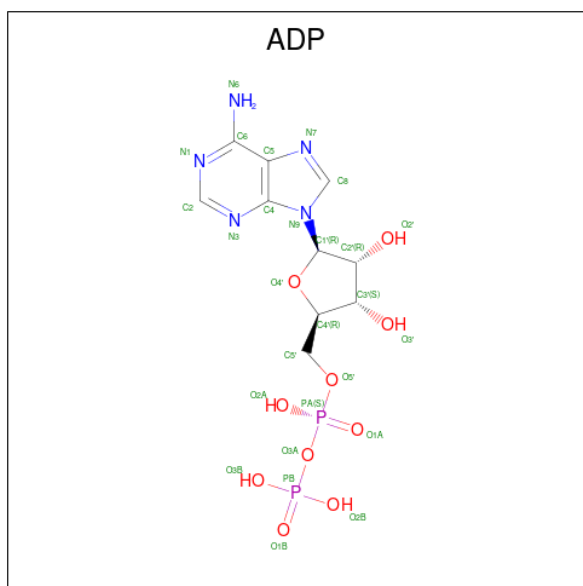
- Molecule 1 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2855	Total	C	N	O	S	0	0
			22962	14643	3963	4241	115		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2389	ASP	GLU	conflict	UNP Q14204

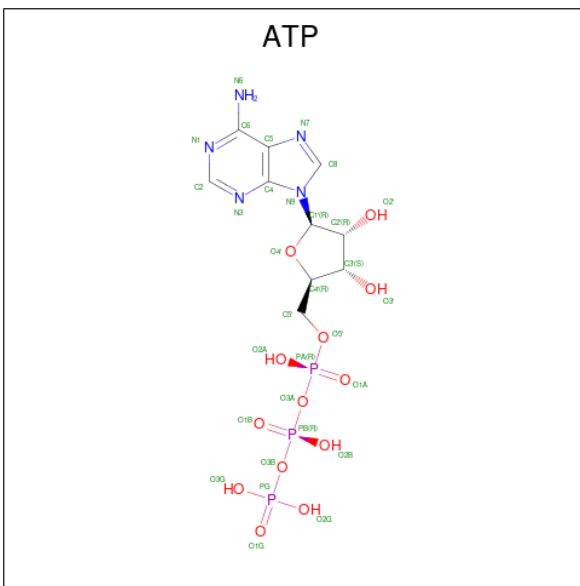
- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$)

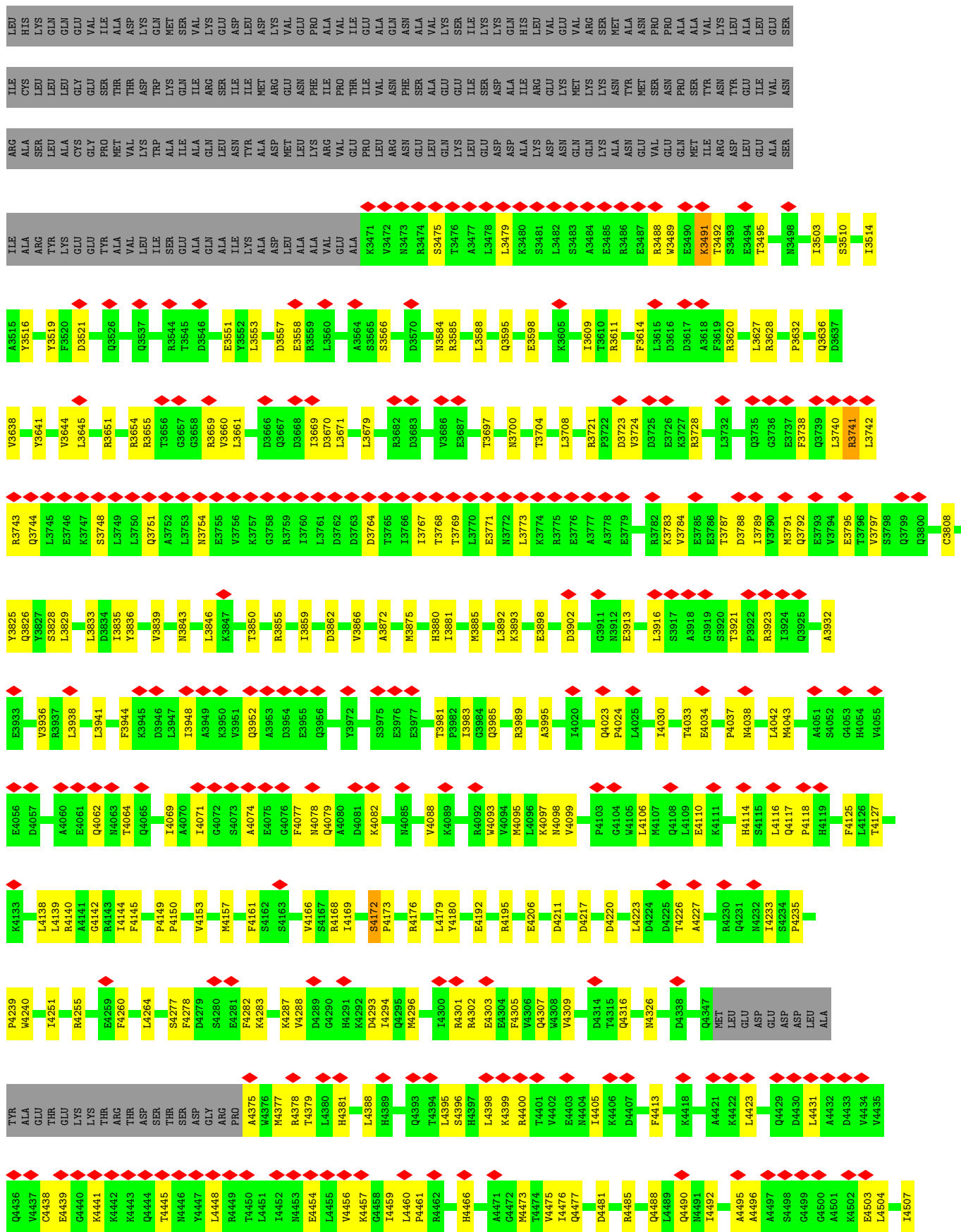
(labeled as "Ligand of Interest" by depositor).

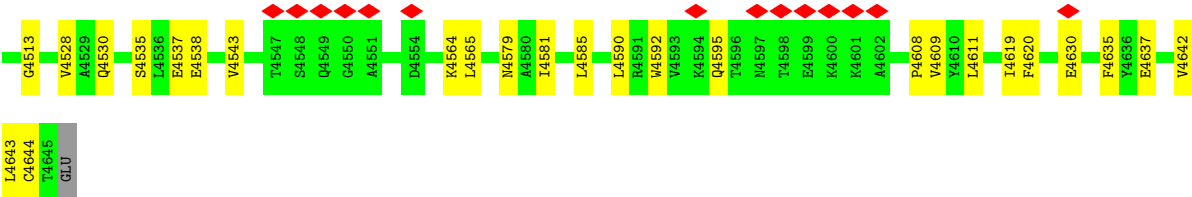


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0
3	A	1	Total 31	C 10	N 5	O 13	P 3	0

P1907	L1803	V1672	M1579	L1505	LYS	ALA	VAL	TRP	ARG	GLU	GLU	ALA	ASN	GLU	ASN	PHE
E1914	R1806	G1675	K1580	S1506	ASN	TRP	ALA	GLU	PHE	GLN	PHE	LEU	LEU	ASN	ASN	PHE
K1917	R1807		K1581	A1506	GLU	GLU	GLU	LYS	PHE	THR	THR	ILE	ASP	GLN	GLN	PHE
Q1922	L1808	R1678	V1582	M1507	ILE	VAL	VAL	PRO	PRO	GLN	THR	GLN	MET	GLY	LYS	GLY
V1929	E1809	R1679	K1584	S1508	VAL	GLN	GLN	LEU	TRP	SER	VAL	VAL	PRO	ASN	ASN	VAL
N1930	H1810	E1680		L1509	LYS	ASP	ASP	THR	TRP	THR	THR	THR	ASP	GLY	GLY	ASP
C1932	I1811		L1587	S1510	VAL	VAL	VAL	ASN	TYR	LEU	LEU	LEU	GLY	ILE	ILE	ASP
E1934	I1812	S1691	V1588	P1511	LEU	LEU	LYS	GLY	TYR	ASN	GLY	VAL	VAL	LEU	GLY	LEU
D1937	T1822	E1694	M1589	Y1512	VAL	VAL	VAL	ARG	ASN	ASN	THR	THR	LEU	ASN	ILE	ILE
F1938	R1823		D1590	Y1513	ALA	ALA	TRP	PRO	ILE	GLY	GLU	ASP	GLU	PRO	VAL	VAL
C1939	S1824	I1698	V1591	K1514	GLN	GLN	SER	GLU	ILE	ASN	GLU	ASP	GLU	ARG	ARG	GLU
D1939	I1825		L1592	V1515	GLY	GLY	GLU	GLY	GLY	GLY	GLU	ASN	GLU	ILE	ILE	GLY
F1946	H1826	H1701	N1593	F1516	MET	ASN	SER	ALA	GLY	GLY	THR	THR	TYR	ALA	ALA	GLY
G1947	K1827	V1711	I1594	E1517	LEU	LEU	LEU	GLN	TRP	GLY	VAL	THR	GLY	VAL	LEU	LEU
V1951	S1828	A1714	Q1595	E1518	ALA	ALA	VAL	ALA	GLY	GLY	ASP	LYS	ALA	VAL	ARG	GLU
D1958	K1829	K1715	G1596	D1519	LEU	TRP	TRP	LEU	ALA	THR	THR	LYS	VAL	VAL	LEU	GLU
E1959	I1830		V1597	A1520	GLU	GLU	GLU	ILE	PHE	ALA	ALA	LYS	VAL	ALA	ARG	VAL
R1962	D1831	V1721	Q1598	L1521	PHE	ASN	ILE	ILE	ASN	THR	THR	GLN	GLY	GLY	TRP	VAL
L1963	F1836	V1724	R1599	S1522	L1463	LYS	LYS	GLY	ILE	ASP	ASP	ASP	GLY	VAL	VAL	GLY
E1964	E1837	E1725	S1600	W1523	K1464	ASN	GLN	THR	ASP	GLY	THR	GLY	GLY	GLY	ALA	GLY
R1965	W1838	I1726	L1601	E1524	Q1465	GLU	MET	LYS	ARG	VAL	VAL	VAL	VAL	VAL	VAL	THR
R1966	L1839	F1727	E1602	D1525	I1466	ALA	LYS	PHE	ARG	ALA	ALA	THR	GLY	GLY	GLY	THR
M1967	S1840		R1603	K1526	R1467	LEU	GLU	ARG	ASP	THR	THR	THR	GLN	TYR	ALA	GLY
V1971	F1844	G1728	L1604	L1527	E1468	LYS	PRO	LEU	ALA	ILE	THR	LYS	VAL	VAL	VAL	GLY
I1978	Y1845	K1729	A1605	N1528	V1469	ASP	TRP	GLY	ALA	GLN	VAL	VAL	VAL	VAL	VAL	THR
Q1979	F1846	A1730	D1606	R1529	W1470	ARG	VAL	ASP	ILE	ASN	VAL	VAL	VAL	ASP	ASP	THR
E1980	D1852	T1731	L1608	A1532	N1471	TRP	SER	ASP	GLN	GLN	THR	VAL	VAL	TRP	TRP	THR
A1981	V1853	S1732	I1611	F1533	T1472	LYS	GLN	ARG	GLN	GLN	GLN	GLN	TRP	ALA	ALA	PHE
N1987	L1854	D1734	A1614	F1534	F1473	LEU	PRO	GLY	VAL	VAL	VAL	VAL	GLY	VAL	VAL	GLY
P1988	F1866	P1735	E1617	D1535	E1474	MET	ARG	CYS	ALA	ALA	ASN	ASN	GLY	GLY	GLY	GLY
N1989	Y1867	N1736		W1536	L1475	LYS	LYS	ALA	ASN	LEU	LEU	LEU	TYR	PRO	PRO	VAL
Y1990	Y1868	T1737	E1617	W1537	D1476	ARG	LEU	LYS	MET	CYS	GLN	GLN	TRP	ALA	ALA	VAL
D1991	Y1872	Q1746	R1623	T1538	L1477	HIS	VAL	LYS	LYS	ASN	ASN	ASN	ASP	GLN	GLN	GLN
K1992	L1873	A1747	F1626	Q1541	Y1480	ASN	TRP	ALA	ILE	ILE	TRP	TRP	MET	ARG	ARG	VAL
T1993	G1874	Q1748	P1627	R1542	Q1481	TRP	VAL	GLU	VAL	VAL	GLU	GLU	GLY	GLN	GLN	VAL
A1995	V1875	L1749	R1628	R1543	N1482	VAL	VAL	LEU	GLU	GLU	GLY	GLY	ASP	GLY	GLY	VAL
P1996	L1752		V1632	W1544	K1483	SER	LEU	THR	ASP	ARG	VAL	VAL	ILE	VAL	VAL	VAL
I1997	L1756	I1756		Y1545	C1484	GLU	ASN	ASP	ARG	GLY	GLY	GLY	ILE	GLY	GLY	GLY
T1998	L1879		L1638	Y1546	R1485	LEU	GLN	THR	ALA	VAL	VAL	VAL	TYR	ASN	ASN	ASN
C1999	Q1881	H1769	I1641	Y1550	L1486	LEU	LYS	GLY	GLY	GLY	GLY	GLY	ASN	GLY	GLY	GLY
E2000	T1882	G1770	V1641	F1551	I1487	THR	SER	LEU	SER	GLY	GLY	GLY	ARG	GLY	GLY	GLY
L2001	P1883	G1771	I1647	T1552	R1488	GLY	PHE	LEU	ARG	GLY	GLY	GLY	GLY	GLY	GLY	GLY
L2002	L1884	G1772	A1648	G1553	G1489	ILE	PRO	GLY	THR	THR	GLN	GLN	MET	GLY	GLY	GLY
N2003	R1887	G1773	K1649	S1554	D1492	TRP	ALA	SER	THR	THR	THR	THR	ASP	LEU	LYS	LYS
V2006	T1893	D1774	Q1650	A1555	L1493	ASP	VAL	GLU	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY
	S1903	A1775	Q1651	K1558	F1494	VAL	ASP	GLU	LEU	LEU	LEU	LEU	ASN	ASN	ASN	ASN
	P1904	A1776	K1652	H1559	N1495	GLN	GLN	ARG	LEU	LEU	LEU	LEU	LYS	LYS	LYS	LYS
	F1905	P1777	H1653	K1567	K1496	TYR	ARG	VAL	THR	THR	THR	THR	TRP	TRP	TRP	TRP
	G1906		F1654	R1567	V1497	GLN	GLN	VAL	ASP	THR	THR	THR	GLN	GLN	GLN	GLN
		E1786	I1665	S1572	K1498											
		L1792	L1666	E1574	E1499											
				T1573	H1500											
				F1575	I1501											
				L1576	N1502											

WORLDWIDE
PDB
PROTEIN DATA BANK





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	72335	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	36000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.597	Depositor
Minimum map value	-1.141	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	411.48, 411.48, 411.48	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.143, 1.143, 1.143	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

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	0.25	0/23454	0.49	0/31791

There are no bond length outliers.

There are no bond angle outliers.

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	22962	0	23030	490	0
2	A	54	0	24	2	0
3	A	62	0	24	5	0
All	All	23078	0	23078	490	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 490 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:4037:PRO:HG2	1:A:4117:GLN:HE21	1.40	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3151:HIS:HD1	1:A:3516:TYR:HH	1.18	0.86
1:A:2929:PRO:HB3	1:A:3060:ARG:HA	1.61	0.83
1:A:2453:ARG:HB2	1:A:2729:ARG:HA	1.64	0.79
1:A:2930:GLN:HE21	1:A:3059:ILE:HA	1.45	0.79

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	2841/4646 (61%)	2759 (97%)	78 (3%)	4 (0%)	48 78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4172	SER
1	A	4251	ILE
1	A	1730	ALA
1	A	2871	ILE

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	2540/4125 (62%)	2538 (100%)	2 (0%)	92 97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3491	LYS
1	A	3741	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4595	GLN
1	A	4530	GLN
1	A	4079	GLN
1	A	4038	ASN
1	A	4117	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	$\# Z > 2$
2	ADP	A	4704	-	24,29,29	0.88	0	29,45,45	1.25	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	A	4703	-	28,33,33	0.65	0	34,52,52	0.60	1 (2%)
3	ATP	A	4702	-	28,33,33	0.64	0	34,52,52	0.59	1 (2%)
2	ADP	A	4701	-	24,29,29	0.89	0	29,45,45	1.22	2 (6%)

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	4704	-	-	4/12/32/32	0/3/3/3
3	ATP	A	4703	-	-	3/18/38/38	0/3/3/3
3	ATP	A	4702	-	-	9/18/38/38	0/3/3/3
2	ADP	A	4701	-	-	4/12/32/32	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	4704	ADP	N3-C2-N1	-3.68	123.68	128.67
2	A	4701	ADP	N3-C2-N1	-3.62	123.75	128.67
2	A	4701	ADP	C4-C5-N7	-2.60	106.59	109.34
2	A	4704	ADP	C4-C5-N7	-2.56	106.63	109.34
3	A	4702	ATP	C5-C6-N6	2.33	123.86	120.31

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

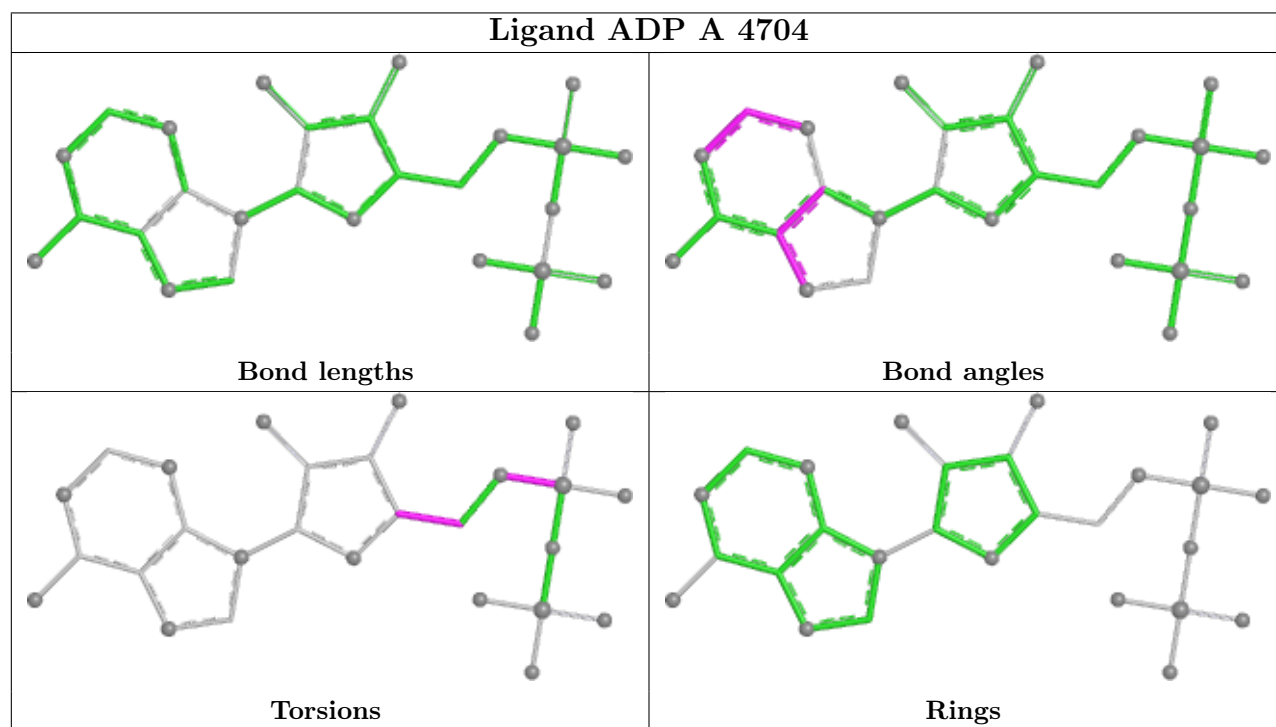
Mol	Chain	Res	Type	Atoms
2	A	4701	ADP	C5'-O5'-PA-O1A
2	A	4701	ADP	C5'-O5'-PA-O2A
2	A	4701	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	O4'-C4'-C5'-O5'

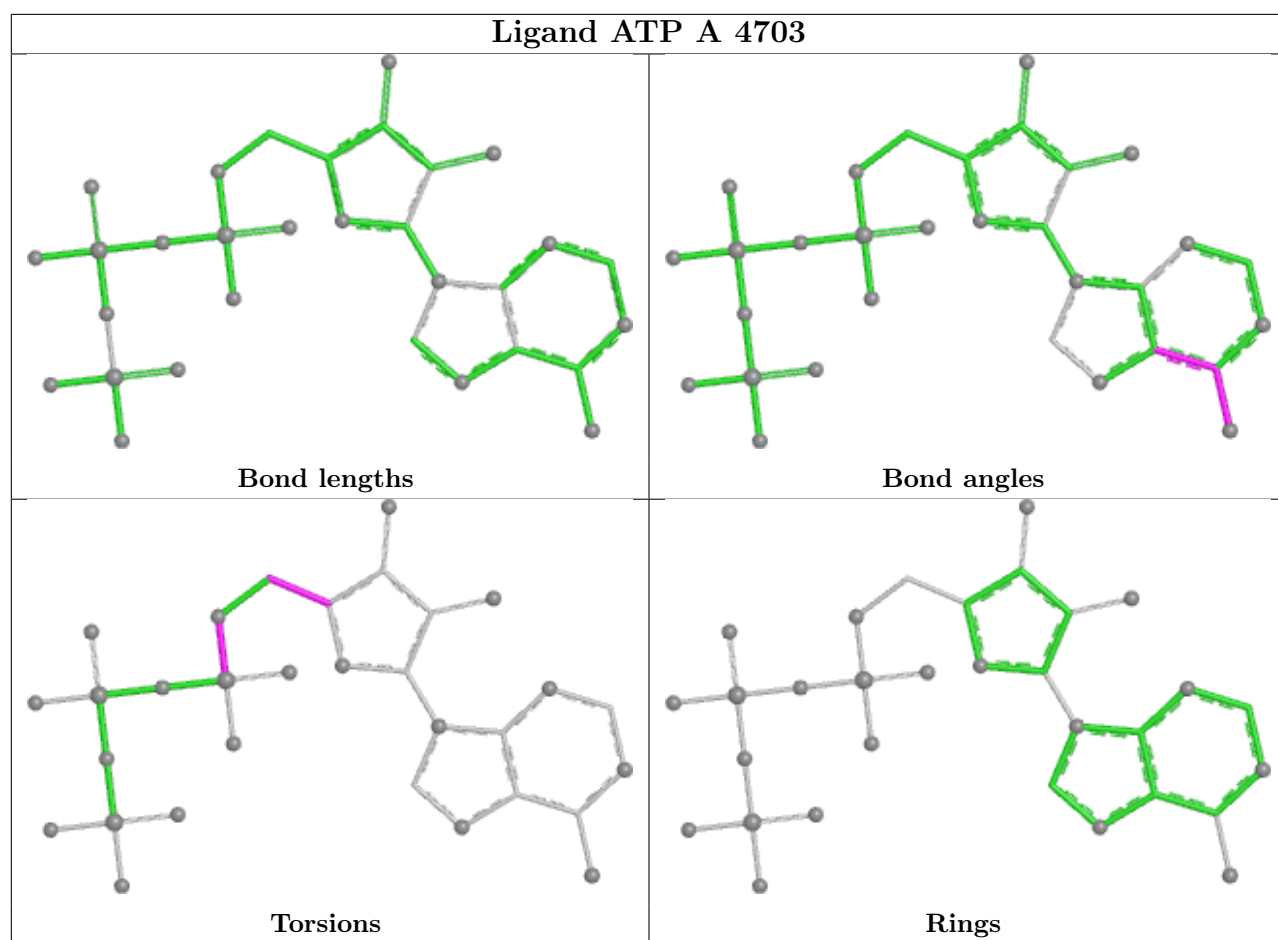
There are no ring outliers.

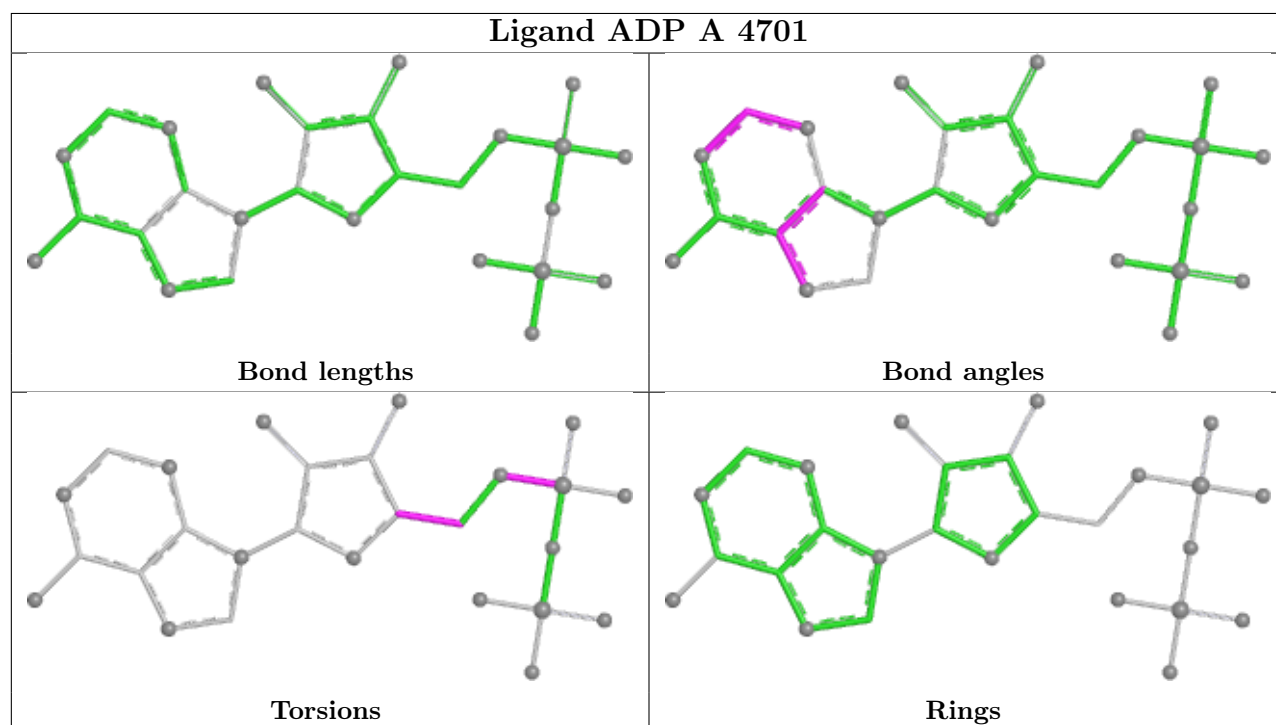
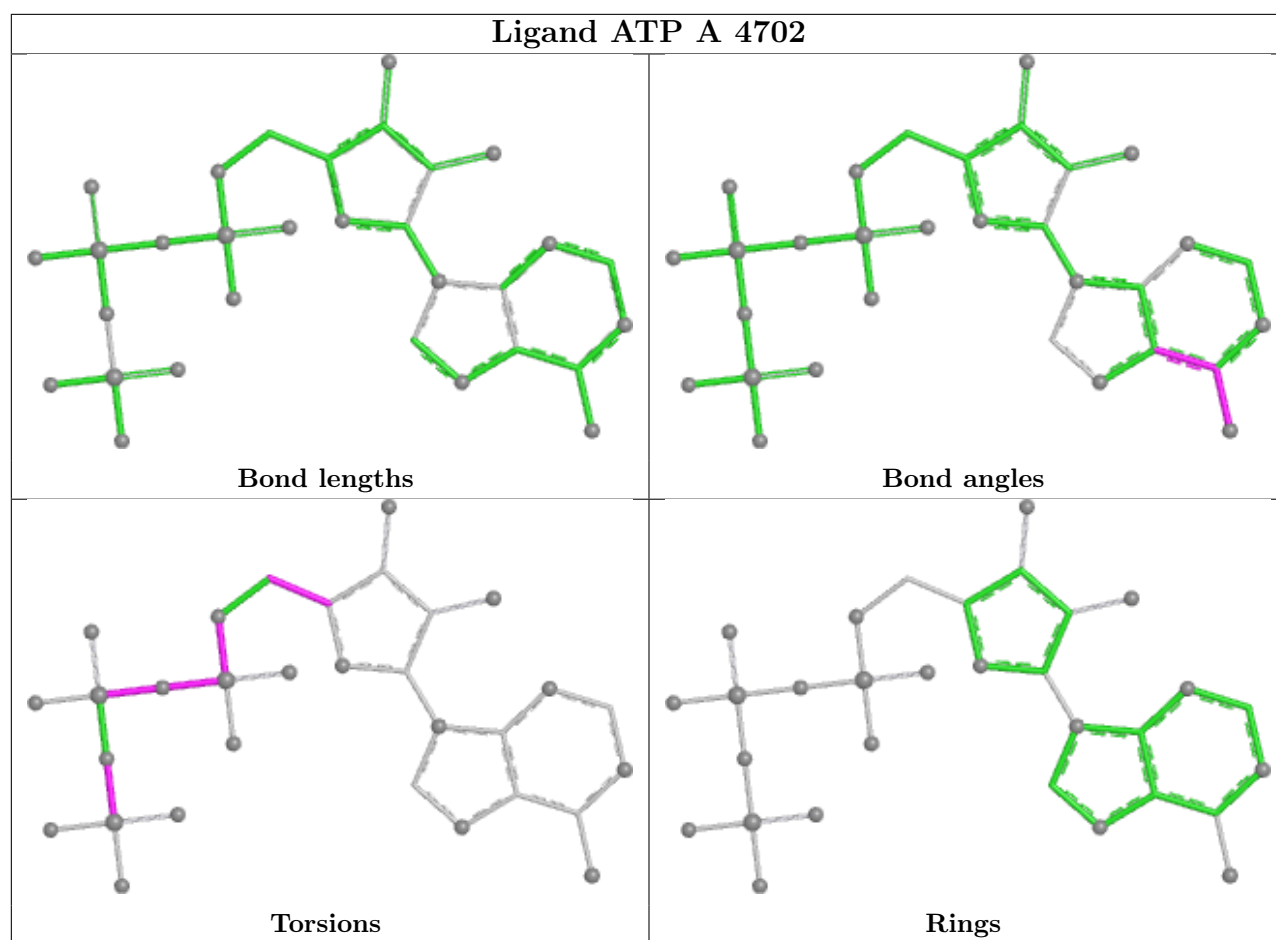
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4704	ADP	1	0
3	A	4703	ATP	1	0
3	A	4702	ATP	4	0
2	A	4701	ADP	1	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.

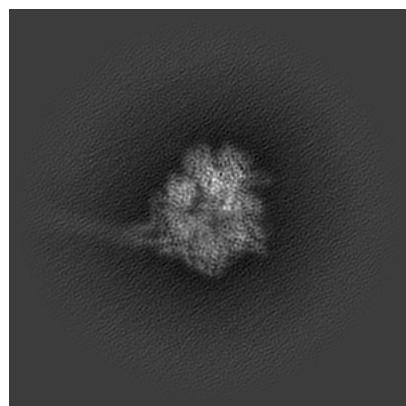
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44723. These allow visual inspection of the internal detail of the map and identification of artifacts.

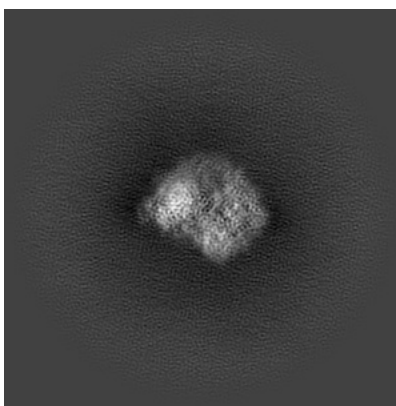
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

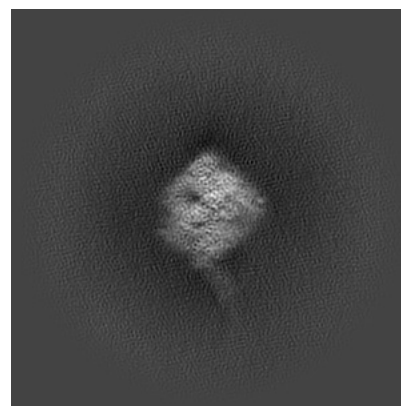
6.1.1 Primary map



X

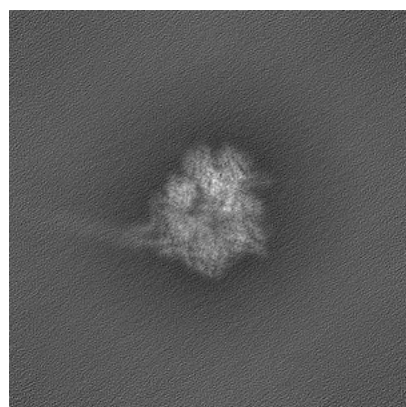


Y

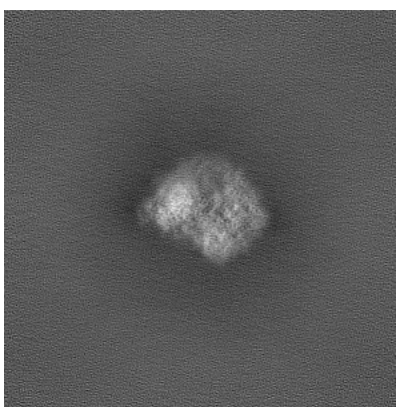


Z

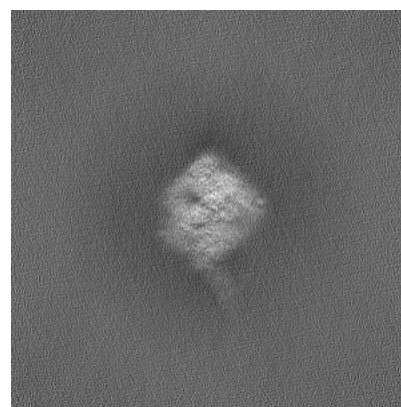
6.1.2 Raw map



X



Y

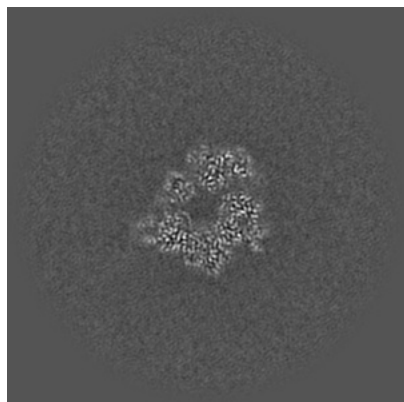


Z

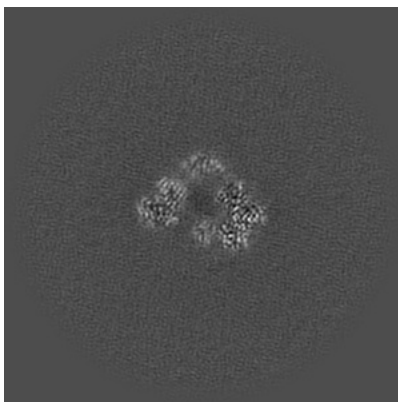
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

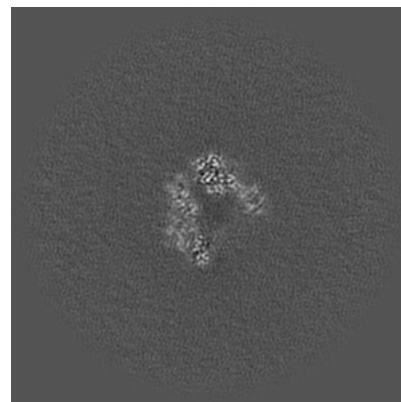
6.2.1 Primary map



X Index: 180

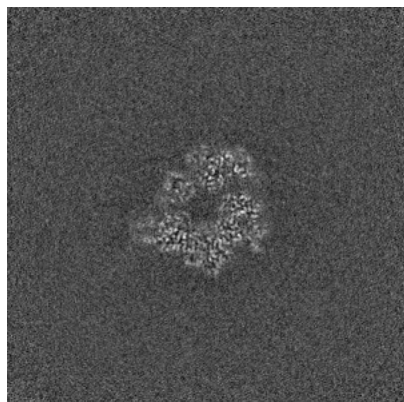


Y Index: 180

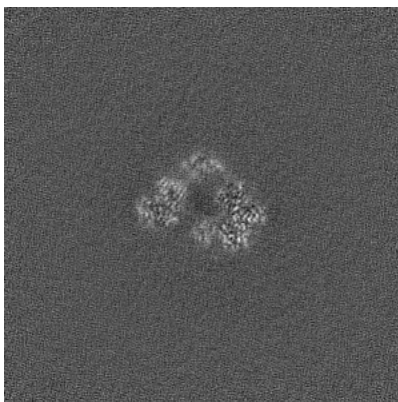


Z Index: 180

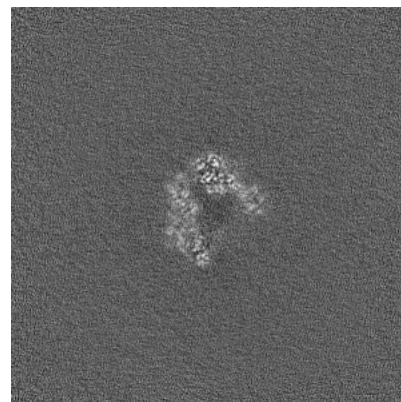
6.2.2 Raw map



X Index: 180



Y Index: 180

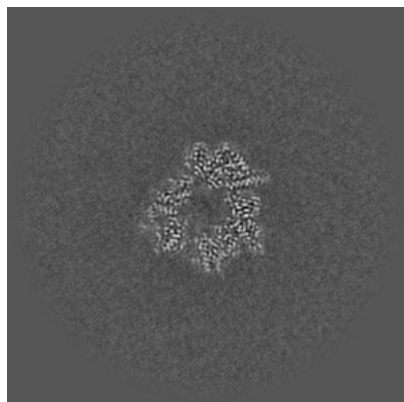


Z Index: 180

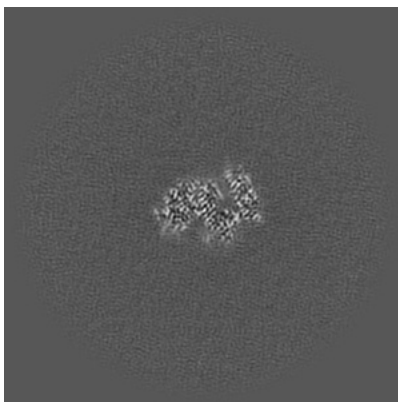
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

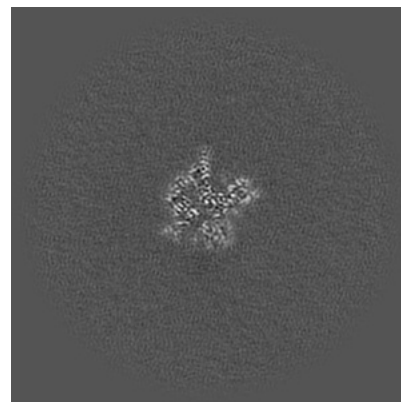
6.3.1 Primary map



X Index: 174

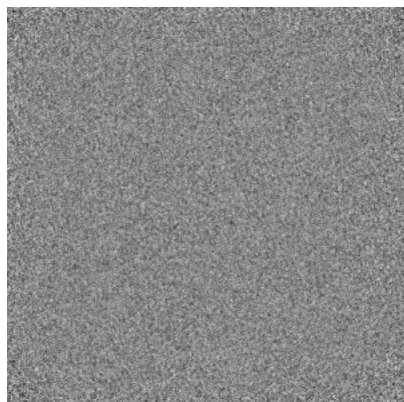


Y Index: 204

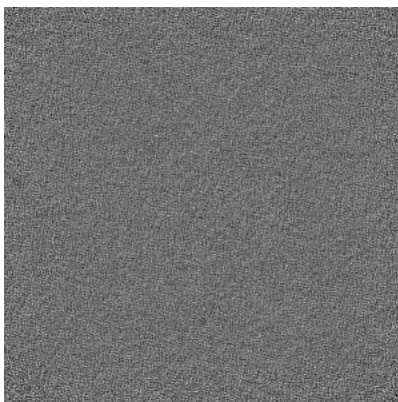


Z Index: 202

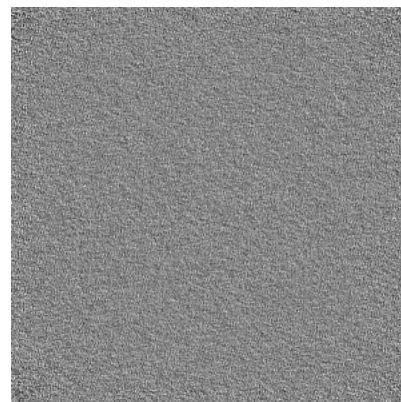
6.3.2 Raw map



X Index: 0



Y Index: 0

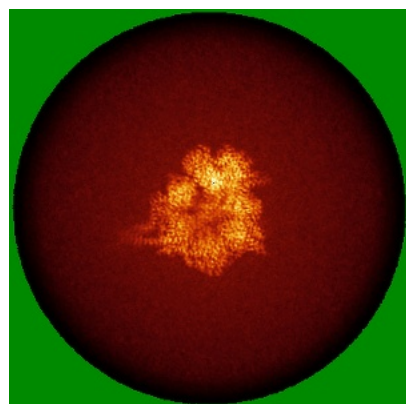


Z Index: 0

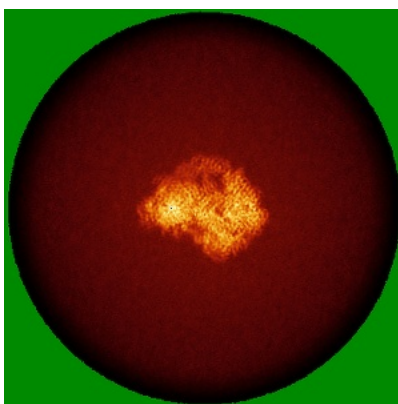
The images above show the largest variance slices of the map in three orthogonal directions.

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

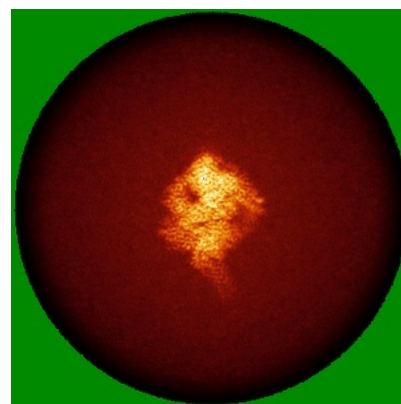
6.4.1 Primary map



X

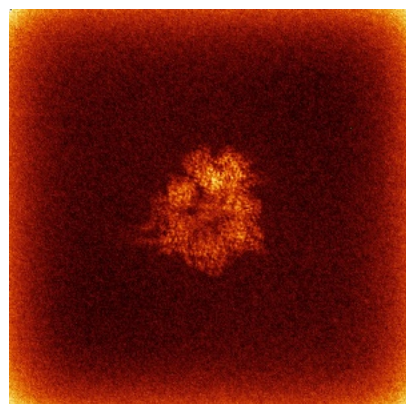


Y

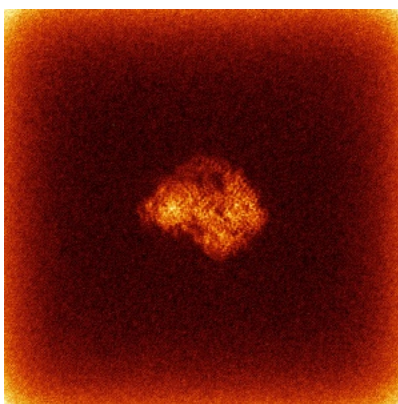


Z

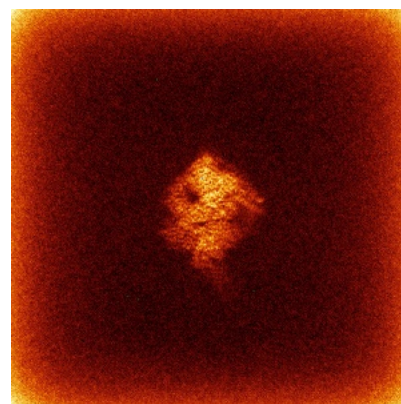
6.4.2 Raw map



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.

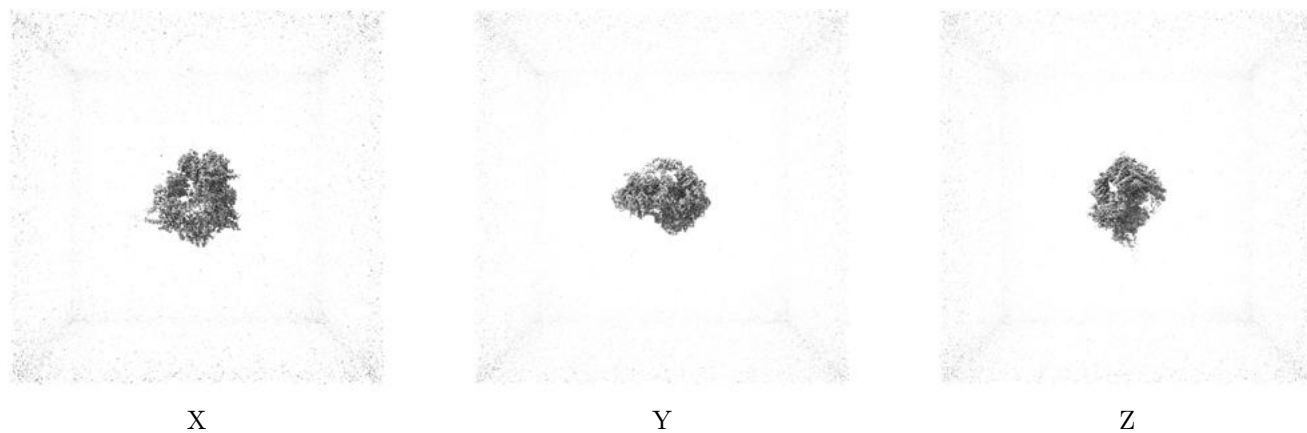
6.5 Orthogonal surface views [i](#)

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.

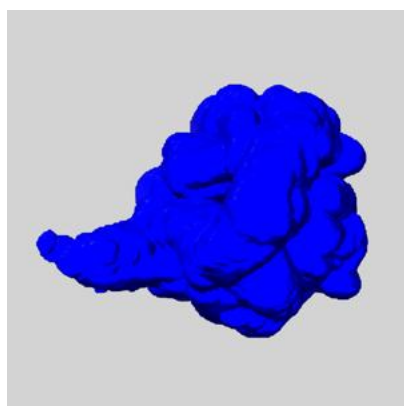
6.6 Mask visualisation [i](#)

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

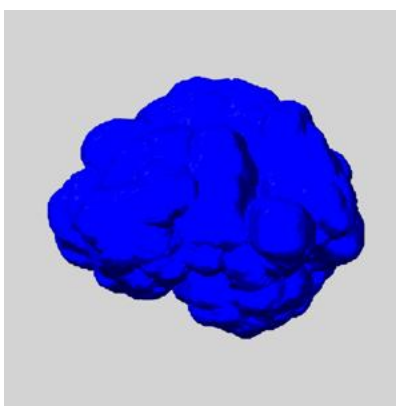
A mask typically either:

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

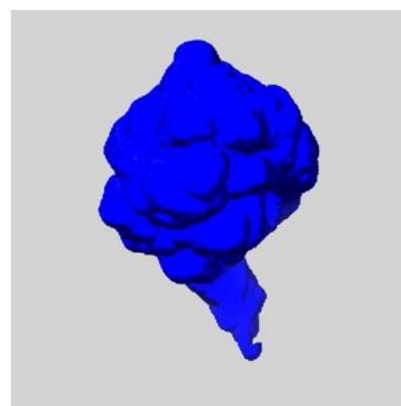
6.6.1 emd_44723_msk_1.map [i](#)



X



Y

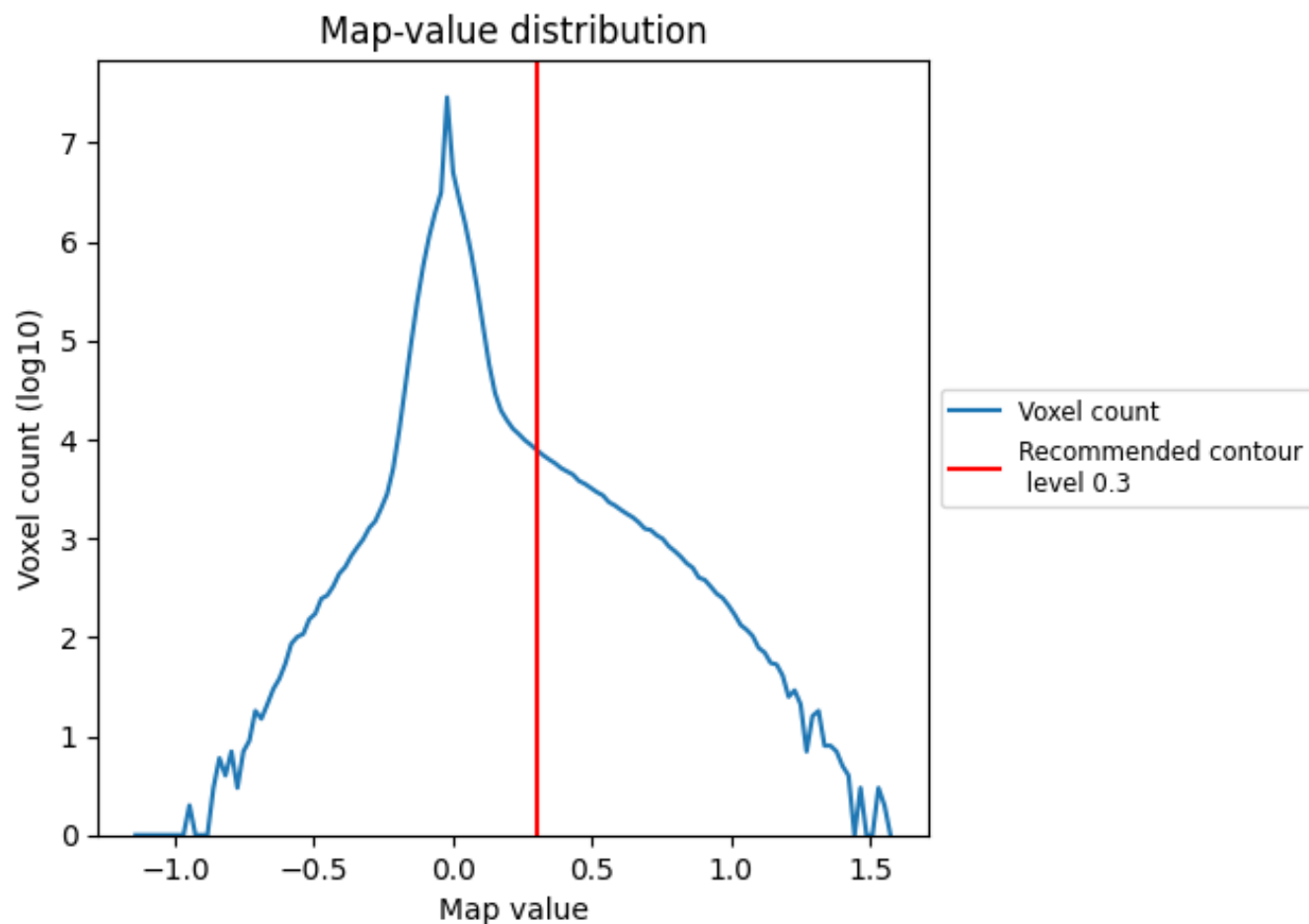


Z

7 Map analysis [i](#)

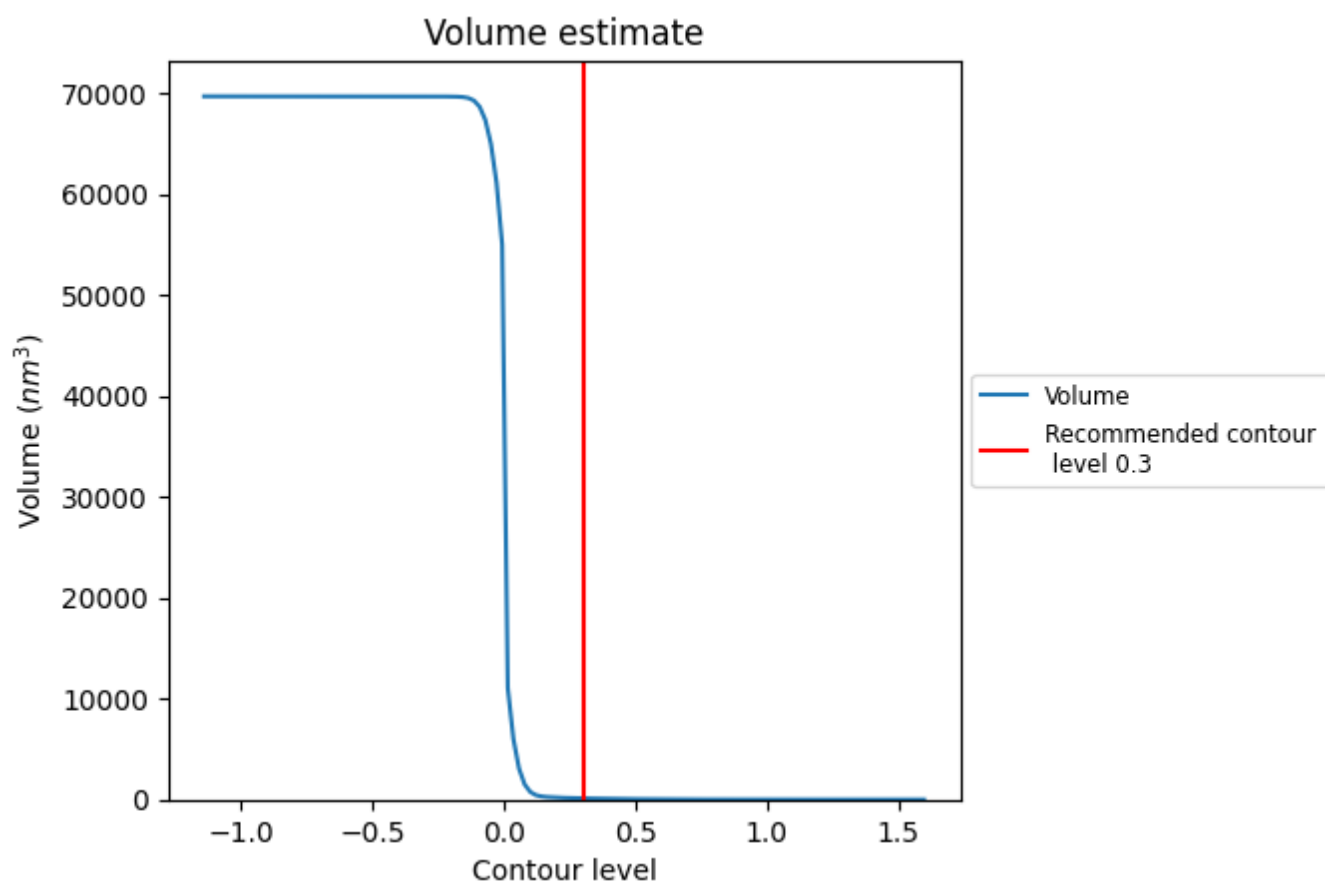
This section contains the results of statistical analysis of the map.

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.

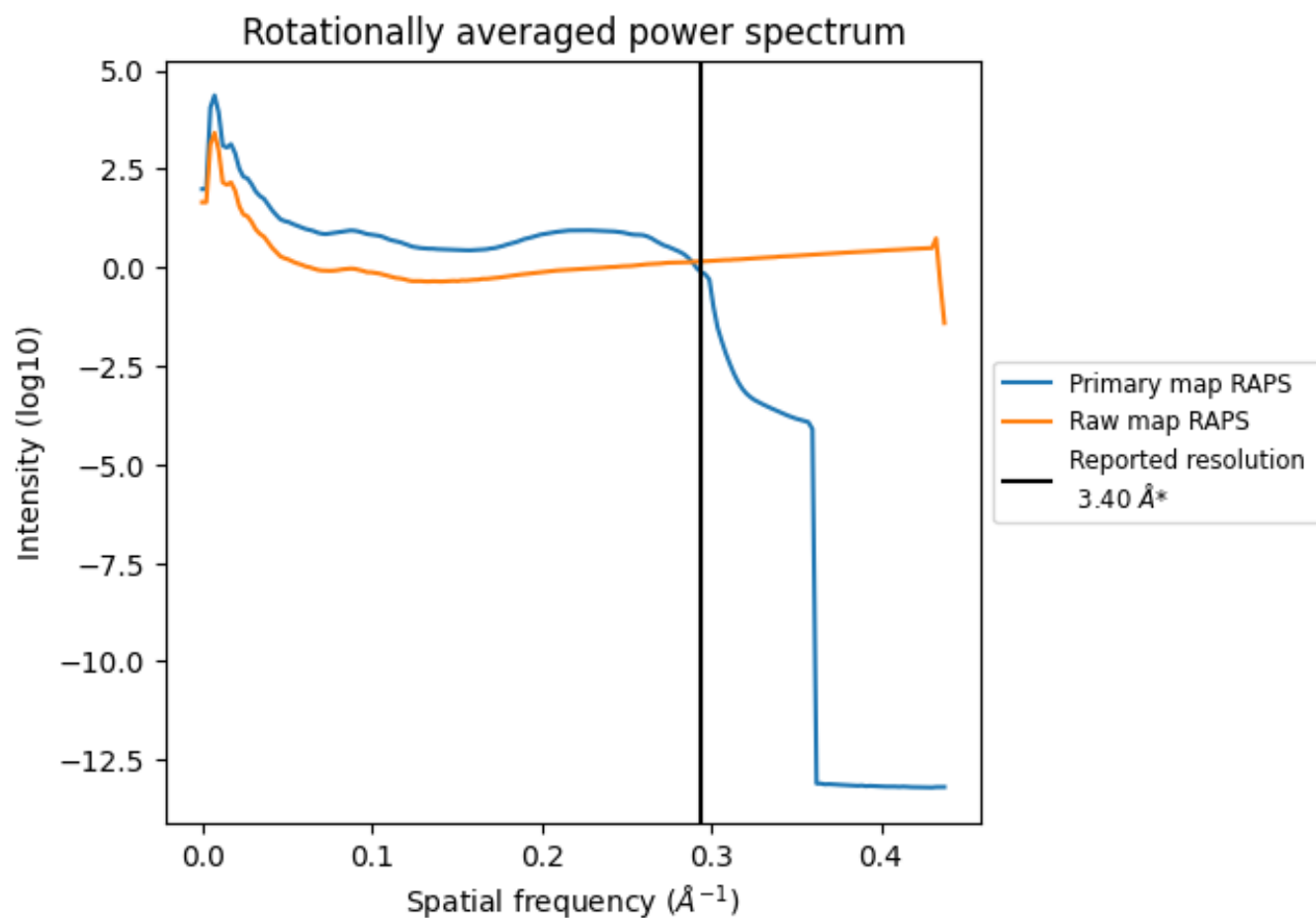
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 120 nm³; this corresponds to an approximate mass of 109 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 ⓘ

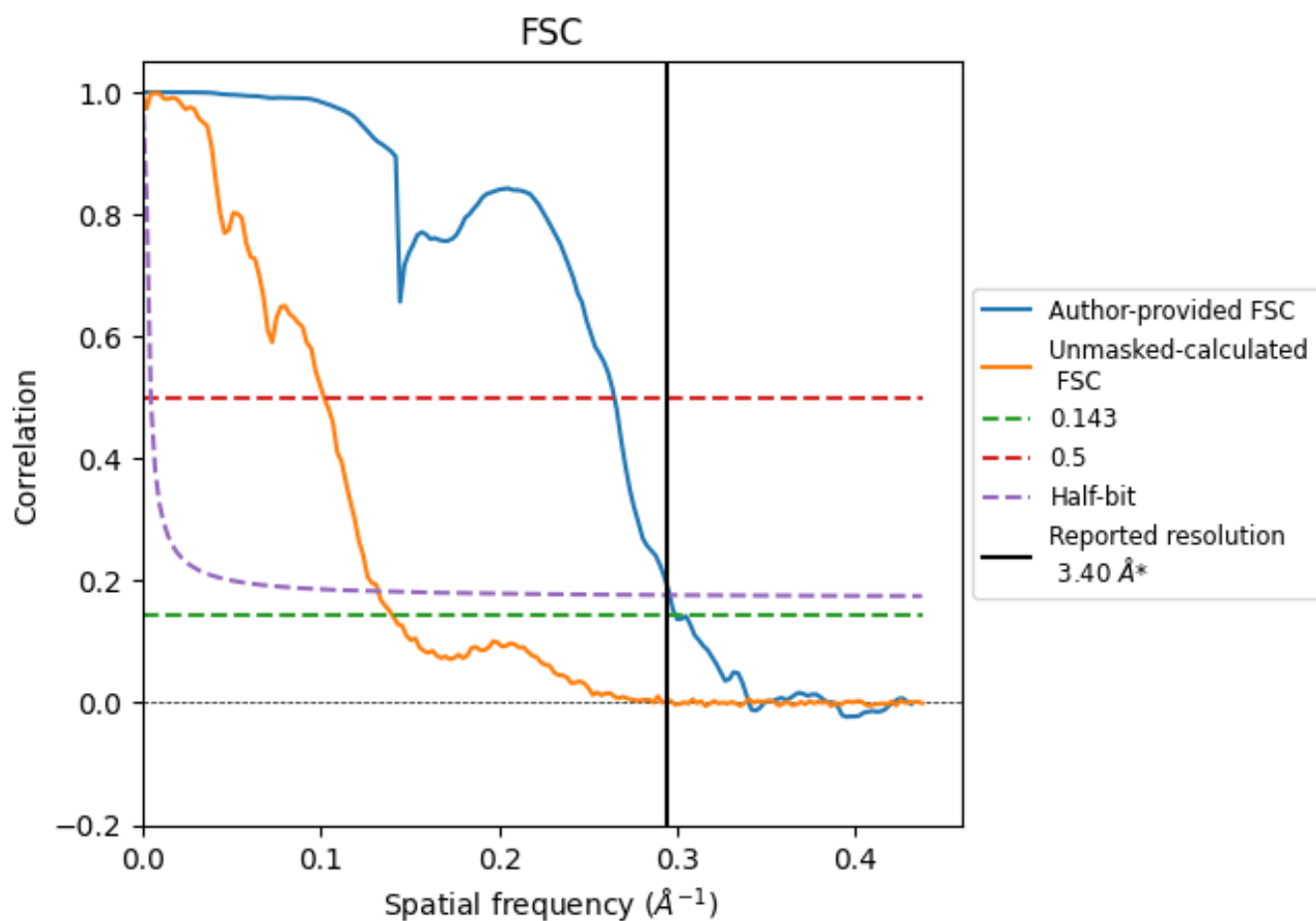


*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

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 0.294 \AA^{-1}

8.2 Resolution estimates [i](#)

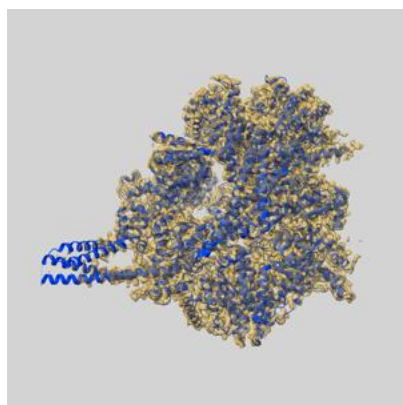
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.34	3.78	3.38
Unmasked-calculated*	7.12	9.80	7.56

*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 7.12 differs from the reported value 3.4 by more than 10 %

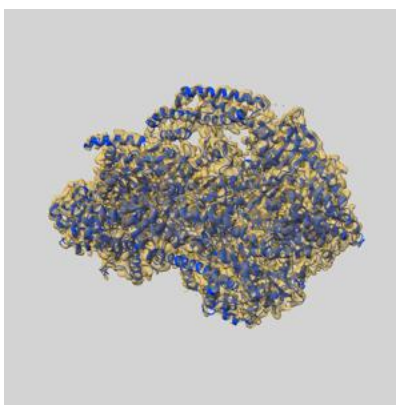
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44723 and PDB model 9BN6. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

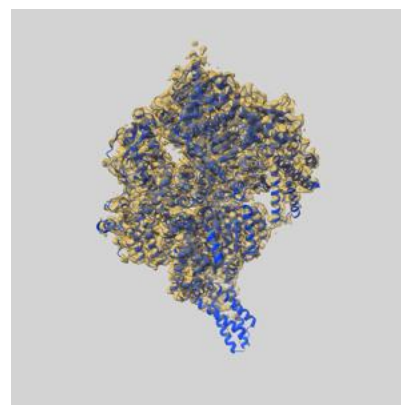
9.1 Map-model overlay [i](#)



X



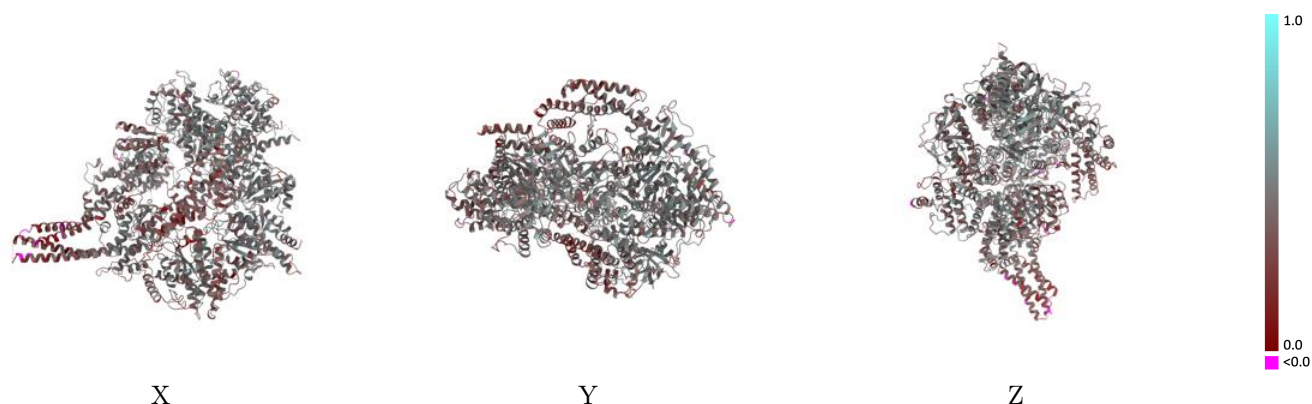
Y



Z

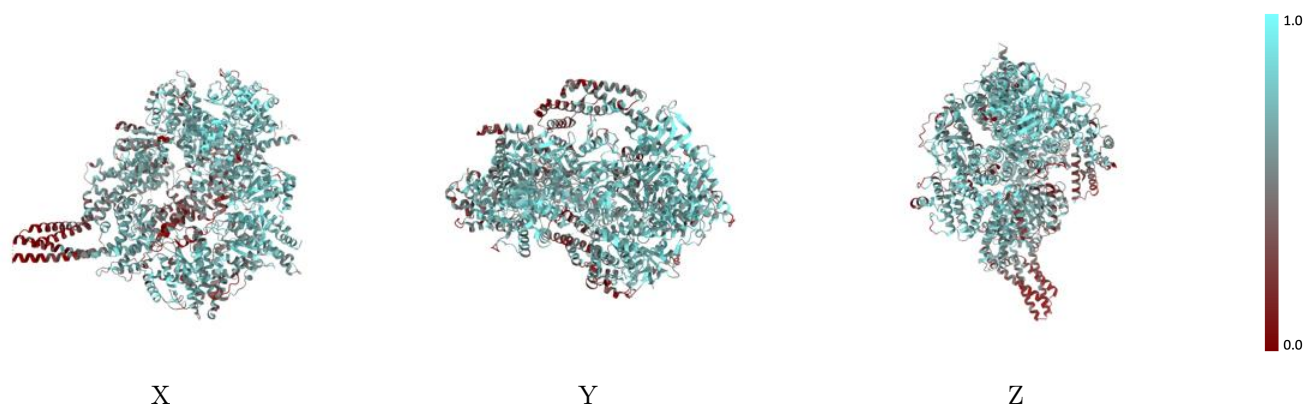
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



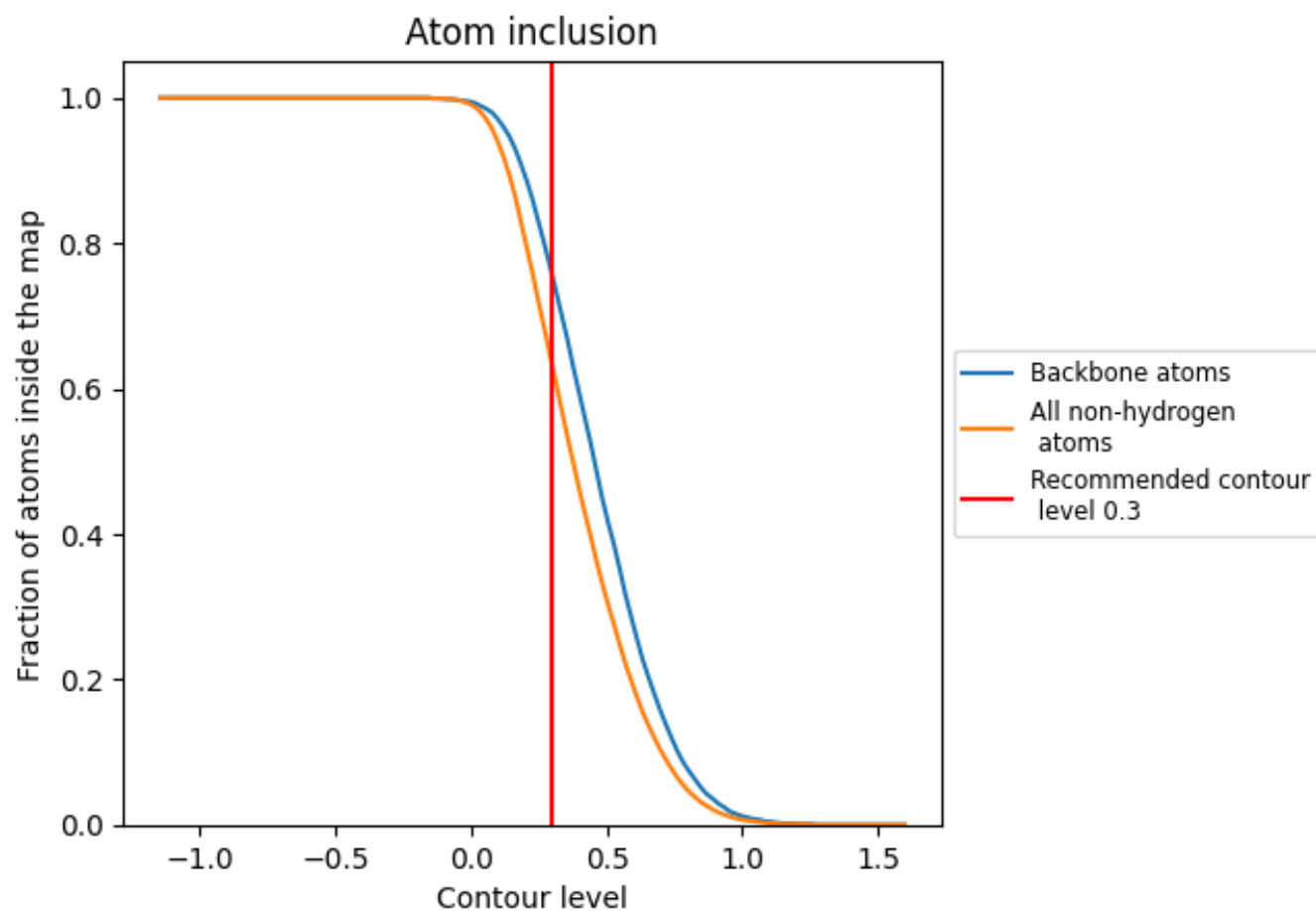
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 76% of all backbone atoms, 63% 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> 0.6320	<div></div> 0.4100
A	<div></div> 0.6320	<div></div> 0.4100

