



wwPDB EM Validation Summary Report ⓘ

Mar 12, 2026 – 11:41 PM UTC

PDB ID : 9BMW / pdb_00009bmw
EMDB ID : EMD-44713
Title : State-7b-post2 of motor domain from full-length human dynein-1 in 5 mM ADP
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

A user guide is available at
<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

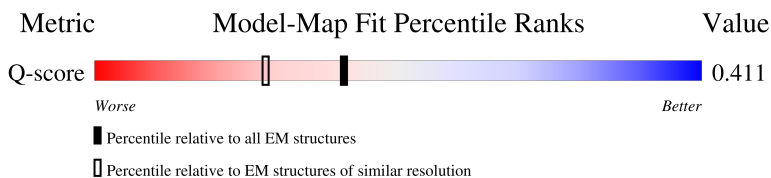
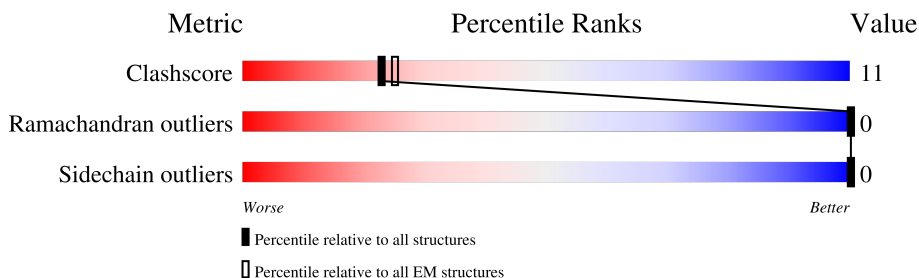
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4646	

2 Entry composition [i](#)

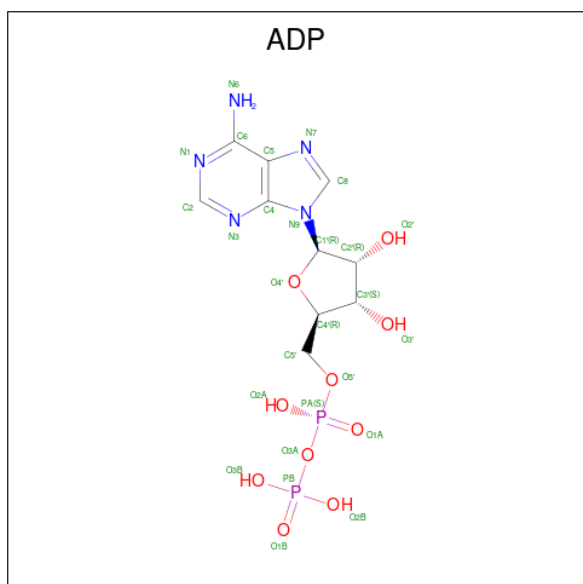
There are 4 unique types of molecules in this entry. The entry contains 24617 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

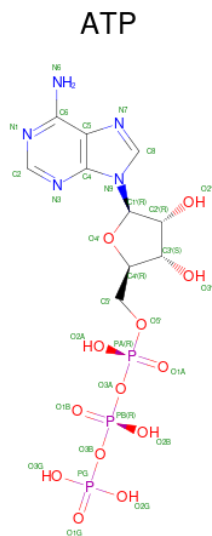
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3043	24503	15606	4234	4541	122	0	0

- 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

Y1990	L1811	E1683	S1583	M1507	K1441	A1381	VAL	GLN	ARG	GLU	ALA	ASN	GLU	THR	ASP	ASN	PHE
D1991	I1812	V1684	K1584	L1508	N1442	S1382	ALA	THR	PHE	LEU	LEU	LYS	LEU	ARG	ILE	LEU	ASN
K1992	L1815	H1695	M1589	L1509	E1443	Y1383	GLU	THR	PHE	GLN	GLU	GLN	THR	ILE	ASP	GLN	LYS
T1993	V1816	L1698	D1590	S1510	A1444	E1384	LEU	THR	PRO	ASN	GLN	GLN	VAL	GLN	GLY	VAL	LYS
S1994	L1831	I1699	V1591	P1511	I1445	F1385	Q1327	VAL	PRO	SER	TRP	TRP	VAL	GLN	PRO	MET	GLY
A1995	N1832	M1698	L1592	Y1512	V1446	V1386	D1328	THR	THR	GLY	GLY	GLY	ASP	VAL	GLU	ILE	ASN
M2018	M1845	N1699	N1593	Y1513	K1447	Q1387	L1329	THR	LEU	LEU	ASP	GLY	ASP	VAL	GLU	ILE	ASN
N2019	L1842	E1700	I1594	K1514	D1448	R1388	K1330	ASN	TYR	GLN	TYR	GLN	ARG	VAL	LEU	GLY	LEU
G2020	L1843	W1701	I1596	V1515	V1449	L1389	G1331	GLY	ASP	GLU	THR	THR	PHE	LEU	GLY	ILE	ILE
C2021	F1844	L1713	G1596	F1516	L1450	L1390	V1332	PRO	ASN	LEU	ASP	GLU	PRO	VAL	VAL	VAL	GLU
THR	Y1845	L1717	R1599	E1517	L1451	K1391	W1333	GLU	ILE	GLU	ASP	GLU	PRO	ARG	ARG	GLU	GLU
ALA	K1849	S1720	S1600	E1518	V1452	G1392	S1334	GLU	GLY	GLN	ASN	GLU	ILE	LEU	LEU	GLY	GLY
GLY	V1721	V1721	L1601	D1519	A1453	Y1393	E1335	ALA	GLY	GLN	TRP	TYR	GLY	ALA	ALA	ILE	ILE
ARG	L1857	V1724	L1604	A1520	Q1454	M1394	L1336	ALA	GLY	ASP	ALA	VAL	ARG	LEU	LEU	GLY	ASP
S2026	A1864	E1725	L1607	L1521	G1455	K1395	S1337	LEU	ALA	THR	LYS	LYS	TYR	ARG	ARG	LEU	LEU
D2030	Y1868	I1726	L1607	S1522	E1456	I1396	K1338	THR	PHE	ALA	GLU	GLU	LYS	VAL	ALA	ALA	VAL
K2033	Y1872	F1727	K1610	W1523	M1457	M1397	V1339	THR	ASN	THR	PHE	GLY	THR	TRP	TRP	THR	THR
L2039	Y1872	G1728	K1610	E1524	A1458	M1398	W1340	GLY	ILE	THR	ASP	PRO	VAL	GLN	GLN	GLY	GLY
A2040	Y1872	K1729	I1611	D1525	L1459	L1399	E1341	GLY	ILE	GLY	VAL	VAL	VAL	VAL	VAL	VAL	VAL
M2041	V1880	W1741	R1623	K1526	E1460	V1400	Q1342	LYS	ARG	ALA	VAL	VAL	VAL	GLY	GLY	GLY	GLY
D2045	C1888	K1744	S1624	L1527	E1461	I1401	I1343	PHE	ARG	VAL	ILE	VAL	VAL	VAL	VAL	VAL	VAL
I2049	M1892	Y1745	S1625	N1528	F1462	A1402	D1344	LYS	LYS	THR	THR	ASP	ASP	GLY	GLY	GLY	GLY
V2052	E1897	Q1748	F1626	R1529	L1463	L1403	Q1345	ILE	SER	THR	ILE	LYS	LYS	TYR	TYR	TYR	TYR
M2053	G1902	L1749	F1627	I1530	K1464	K1404	M1346	LYS	ALA	THR	THR	VAL	VAL	VAL	VAL	VAL	VAL
L2054	G1902	V1750	V1632	M1531	Q1465	S1405	K1347	ASP	GLN	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
S2055	P1907	M1769	G1633	F1534	R1467	A1407	E1348	GLU	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN
S2056	G1770	G1770	D1634	D1535	E1468	L1408	Q1349	ASP	ASP	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
L2065	G1771	G1771	E1635	W1536	V1469	K1409	P1350	CYS	ALA	ALA	ASN	ASN	ASN	ASN	ASN	ASN	ASN
A2066	L1912	G1772	L1636	W1537	W1470	D1410	W1351	ALA	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
I2069	K1917	G1773	L1637	I1538	E1474	R1411	S1352	LYS	LEU	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS
G1920	G1920	D1774	I1641	D1540	L1475	H1412	S1353	LYS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
H1921	H1921	A1775	K1645	Q1541	E1476	K1413	Q1355	ALA	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
Q1922	Q1922	L1778	N1646	R1542	D1476	W1414	P1356	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
L1927	L1927	E1786	V1647	Y1546	L1477	Q1415	R1357	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU
Y2086	L1928	L1789	L1650	L1547	N1482	L1416	K1358	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
L2090	D1937	L1792	F1658	I1550	K1483	M1417	L1359	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
K2094	A1940	A1793	V1658	F1551	C1484	K1418	R1360	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
S2095	L1948	V1796	V1661	T1552	R1485	R1419	Q1361	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
V2096	V1954	Q1800	I1665	G1553	L1486	L1420	N1362	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
L2097	W1954	Q1800	I1668	S1554	R1488	H1421	L1363	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
N2102	N1961	L1803	E1668	L1561	G1489	V1422	D1364	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
R2105	P1988	R1804	L1674	L1561	W1490	N1423	A1365	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
E2106	N1989	K1807	G1675	E1564	D1491	W1424	L1366	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
R2107	N1989	L1808	I1676	F1568	D1492	V1425	L1367	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
K2110	N1989	L1808	S1678	I1571	N1495	S1427	N1368	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41042	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.144	Depositor
Minimum map value	-0.610	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	329.984, 329.984, 329.984	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0312, 1.0312, 1.0312	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, MG, 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	0.16	0/25022	0.34	1/33900 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1409	LYS	CB-CA-C	-5.03	110.39	117.23

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	24503	0	24573	550	0
2	A	81	0	36	4	0
3	A	31	0	12	2	0
4	A	2	0	0	0	0
All	All	24617	0	24621	550	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 550 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:1698:ILE:HD13	1:A:1701:TRP:HE1	1.44	0.82
1:A:3601:MET:HE2	1:A:3634:LEU:HD23	1.64	0.79
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	1.65	0.77
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.66	0.77
1:A:4153:VAL:HG12	1:A:4157:MET:HE2	1.69	0.75

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	3035/4646 (65%)	2967 (98%)	68 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	2706/4125 (66%)	2706 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	2588	HIS
1	A	2685	GLN
1	A	4508	HIS
1	A	2637	HIS
1	A	2913	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	$\# Z > 2$
3	ATP	A	4702	4	32,33,33	0.37	0	48,52,52	0.28	0
2	ADP	A	4701	-	28,29,29	1.39	5 (17%)	43,45,45	1.81	10 (23%)
2	ADP	A	4703	-	28,29,29	1.42	4 (14%)	43,45,45	1.91	8 (18%)
2	ADP	A	4704	-	28,29,29	1.40	4 (14%)	43,45,45	1.83	9 (20%)

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
3	ATP	A	4702	4	-	3/22/38/38	0/3/3/3
2	ADP	A	4701	-	-	3/16/32/32	0/3/3/3
2	ADP	A	4703	-	-	7/16/32/32	0/3/3/3
2	ADP	A	4704	-	-	4/16/32/32	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4703	ADP	C5-C4	4.92	1.47	1.39
2	A	4704	ADP	C5-C4	4.63	1.47	1.39
2	A	4701	ADP	C5-C4	4.56	1.47	1.39
2	A	4703	ADP	C5-C6	2.73	1.48	1.41
2	A	4704	ADP	C5-C6	2.57	1.48	1.41

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4703	ADP	C5-C4-N3	-6.44	117.84	126.72
2	A	4704	ADP	C5-C4-N3	-5.65	118.93	126.72
2	A	4701	ADP	C5-C4-N3	-5.50	119.14	126.72
2	A	4703	ADP	N3-C4-N9	5.14	135.91	127.17
2	A	4704	ADP	N3-C4-N9	4.52	134.85	127.17

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

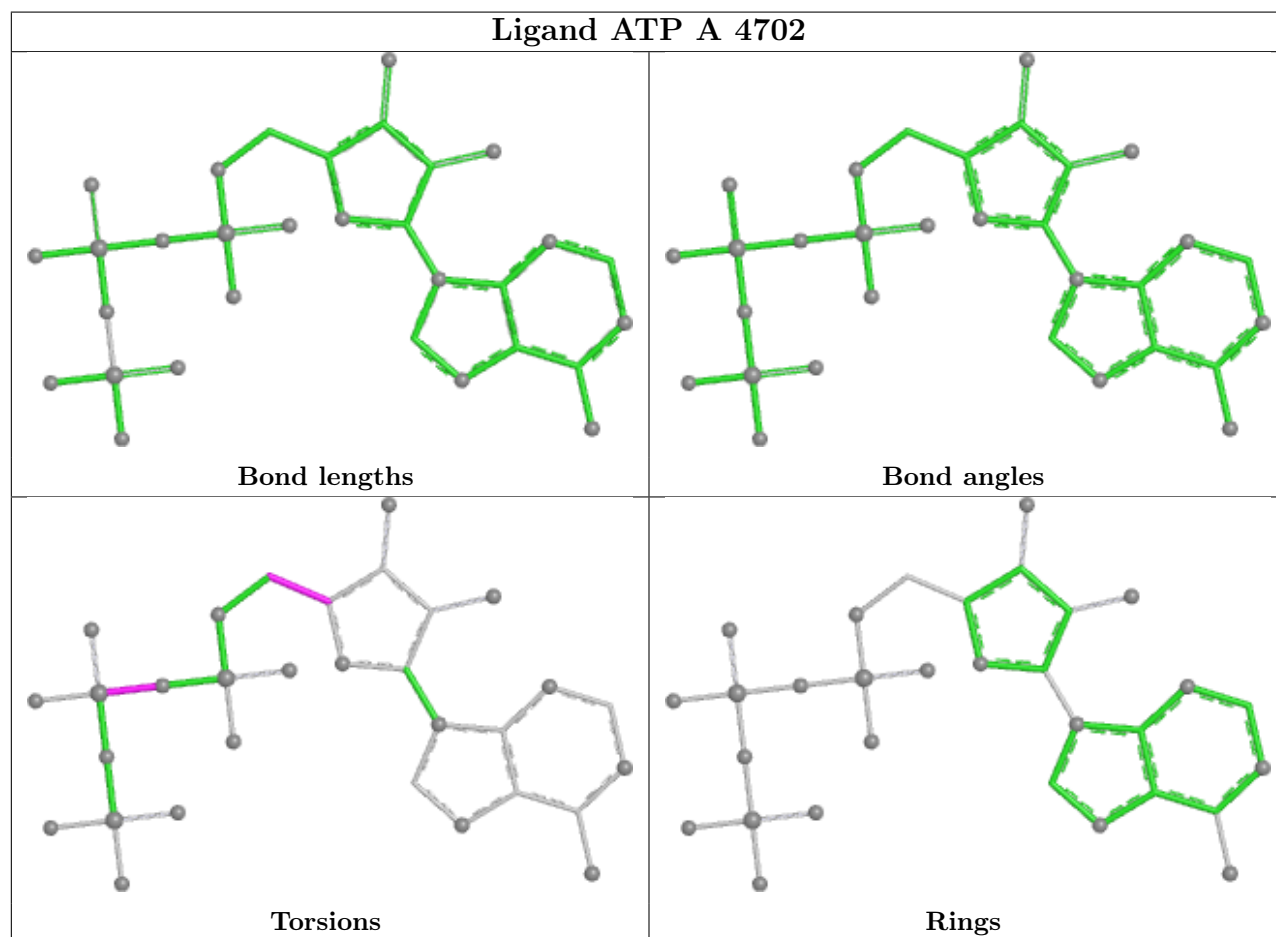
Mol	Chain	Res	Type	Atoms
2	A	4703	ADP	C5'-O5'-PA-O1A
2	A	4703	ADP	C5'-O5'-PA-O2A
2	A	4703	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O3A

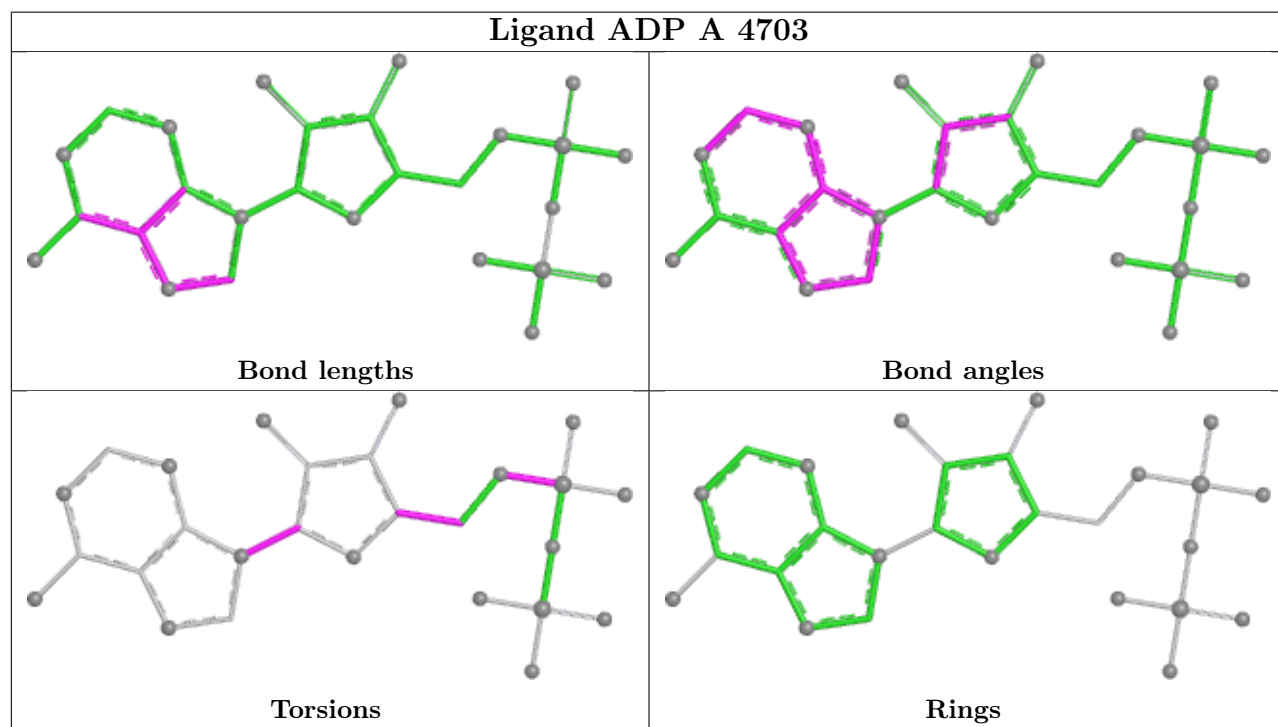
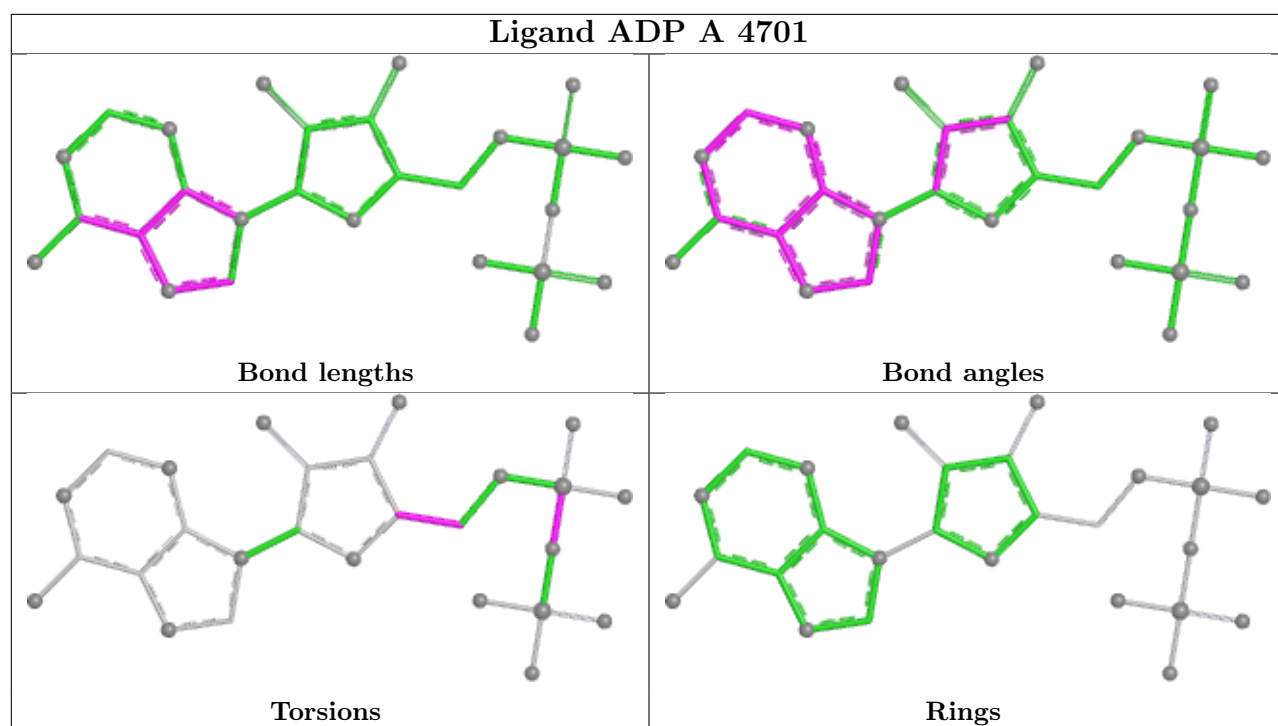
There are no ring outliers.

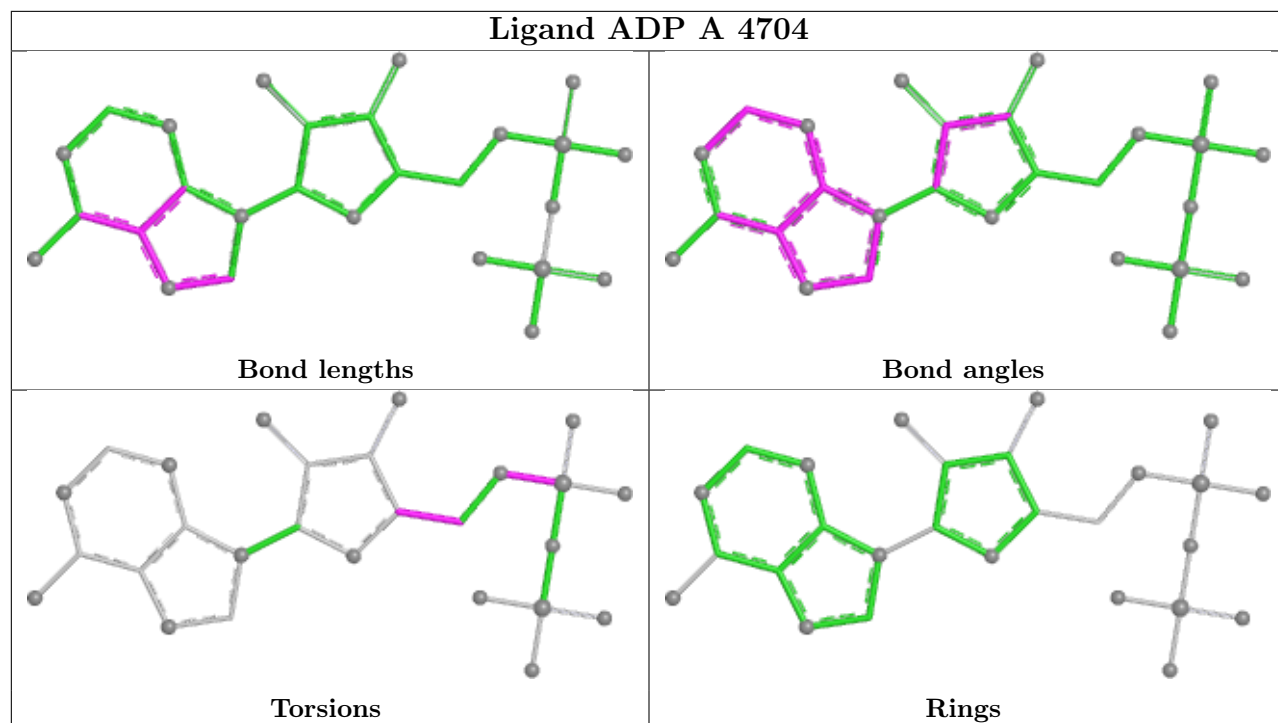
4 monomers are involved in 6 short contacts:

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

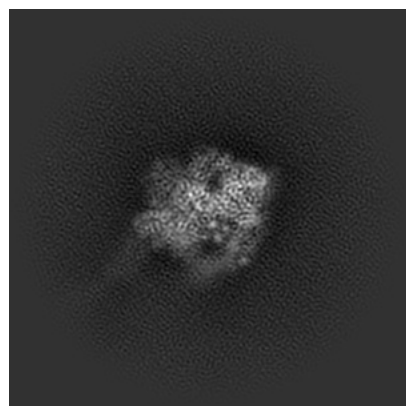
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44713. These allow visual inspection of the internal detail of the map and identification of artifacts.

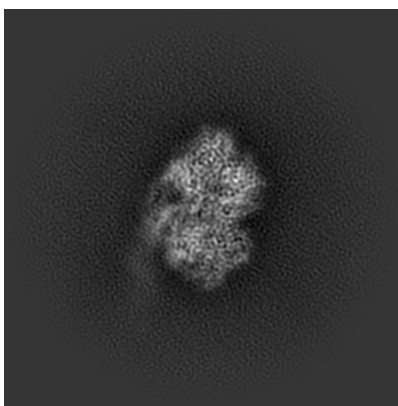
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

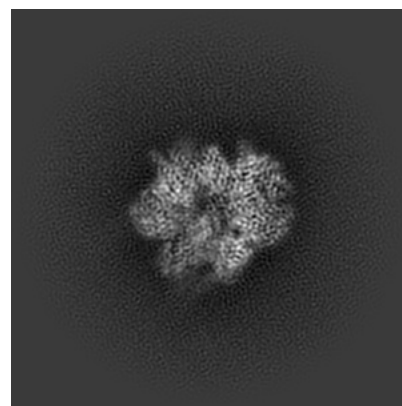
6.1.1 Primary map



X

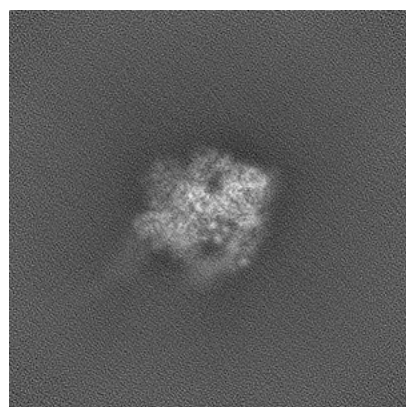


Y

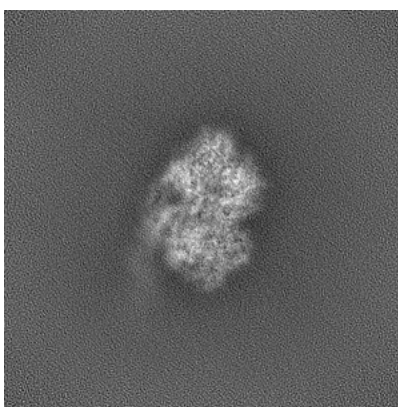


Z

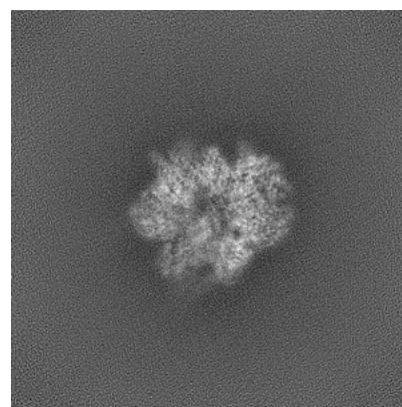
6.1.2 Raw map



X



Y

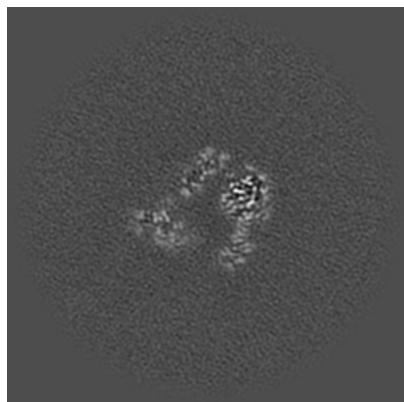


Z

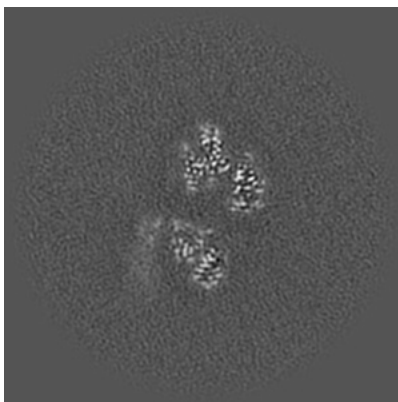
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

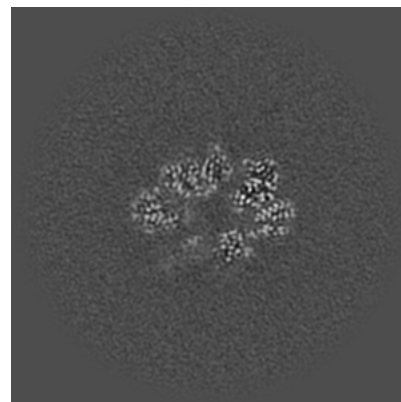
6.2.1 Primary map



X Index: 160

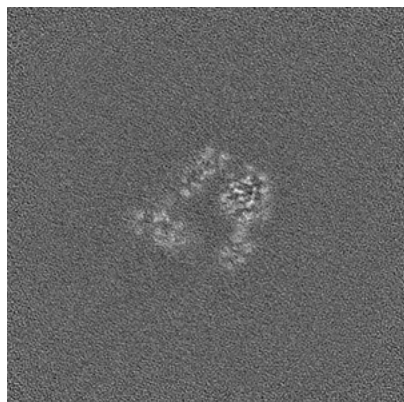


Y Index: 160

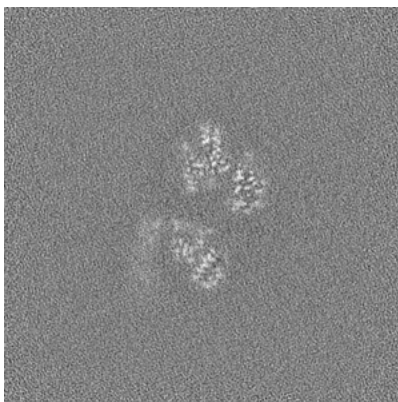


Z Index: 160

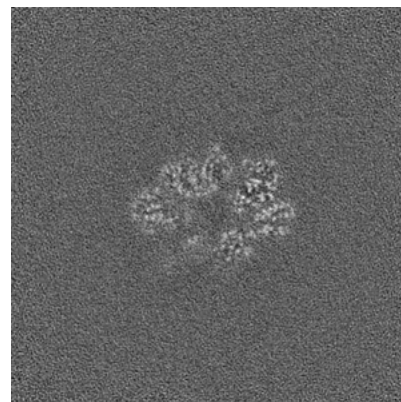
6.2.2 Raw map



X Index: 160



Y Index: 160

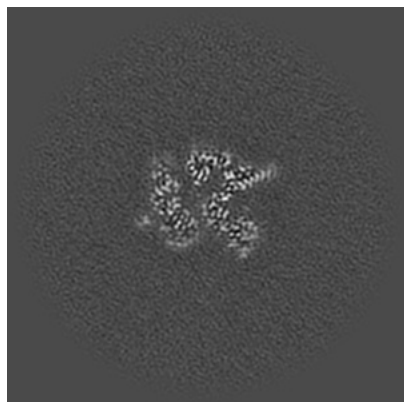


Z Index: 160

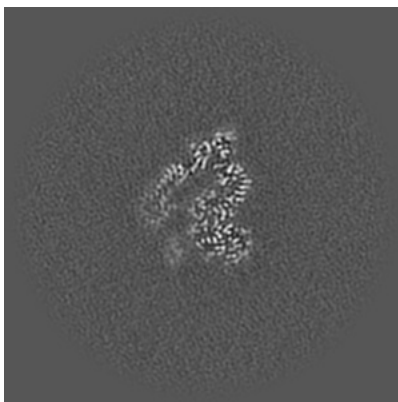
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

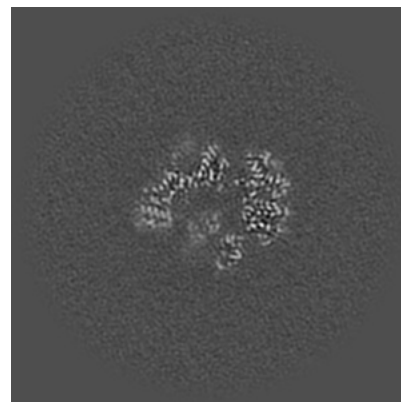
6.3.1 Primary map



X Index: 183

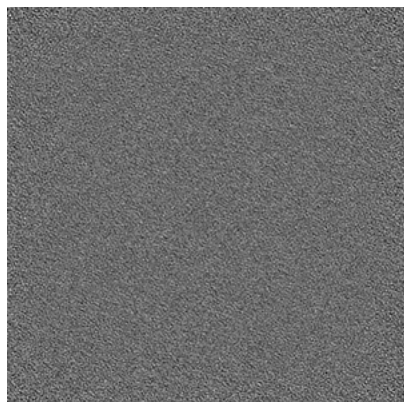


Y Index: 181

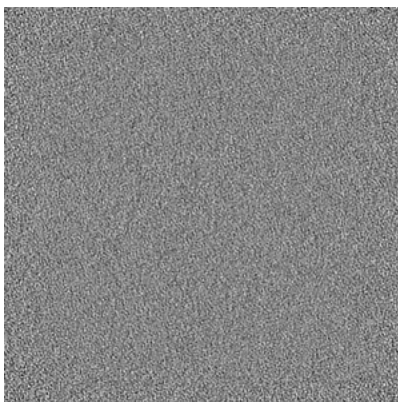


Z Index: 172

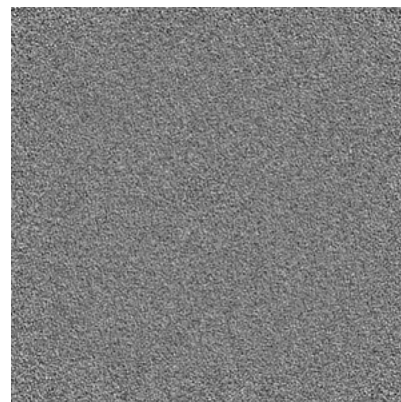
6.3.2 Raw map



X Index: 0



Y Index: 0

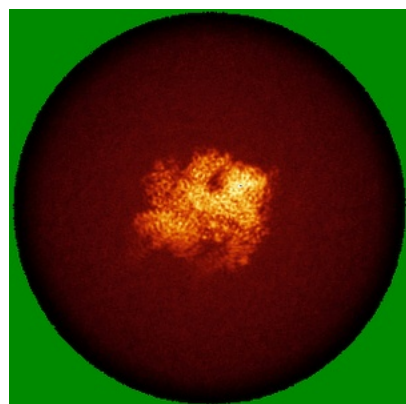


Z Index: 0

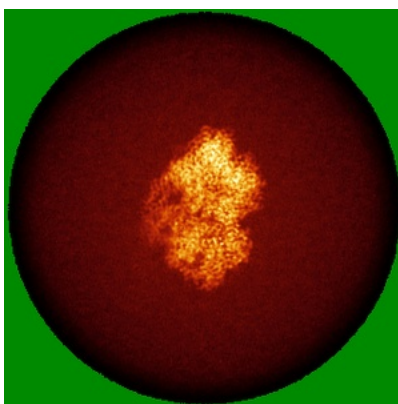
The images above show the largest variance slices of the map in three orthogonal directions.

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

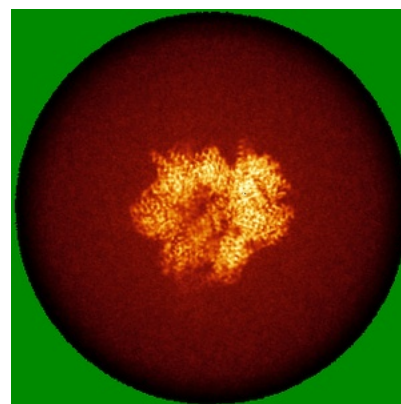
6.4.1 Primary map



X

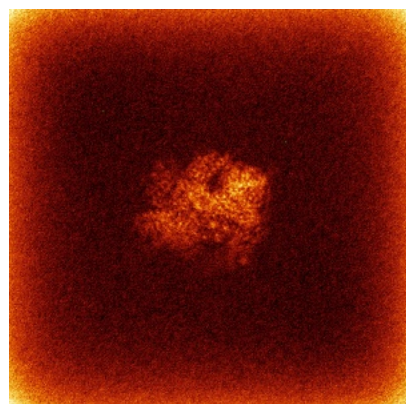


Y

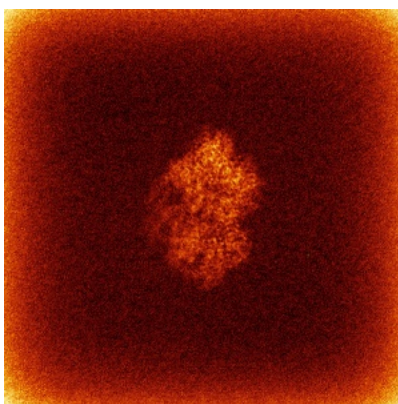


Z

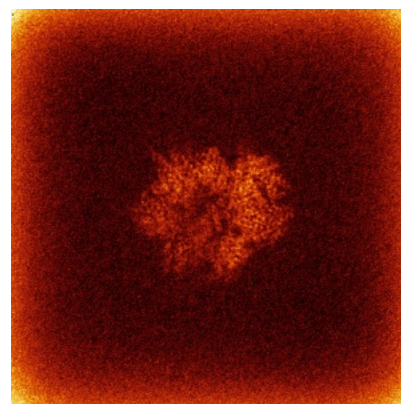
6.4.2 Raw map



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](#)

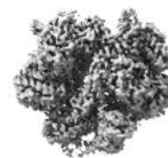
6.5.1 Primary map



X



Y



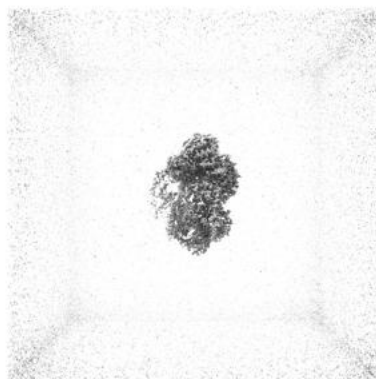
Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

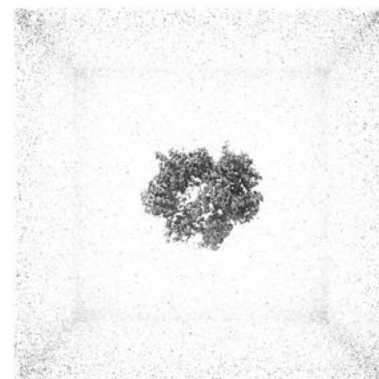
6.5.2 Raw map



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.

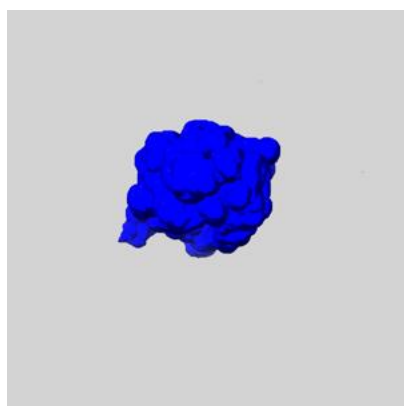
6.6 Mask visualisation [i](#)

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

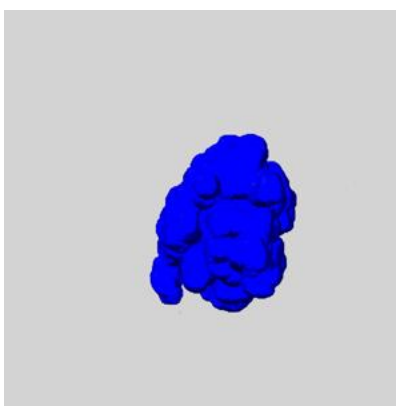
A mask typically either:

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

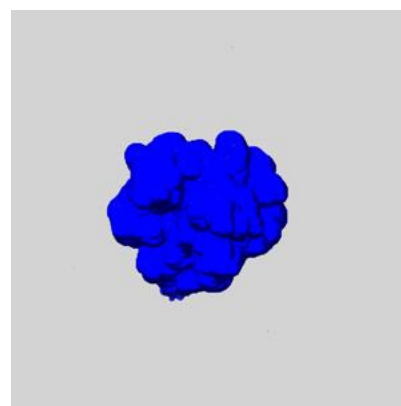
6.6.1 emd_44713_msk_1.map [i](#)



X



Y

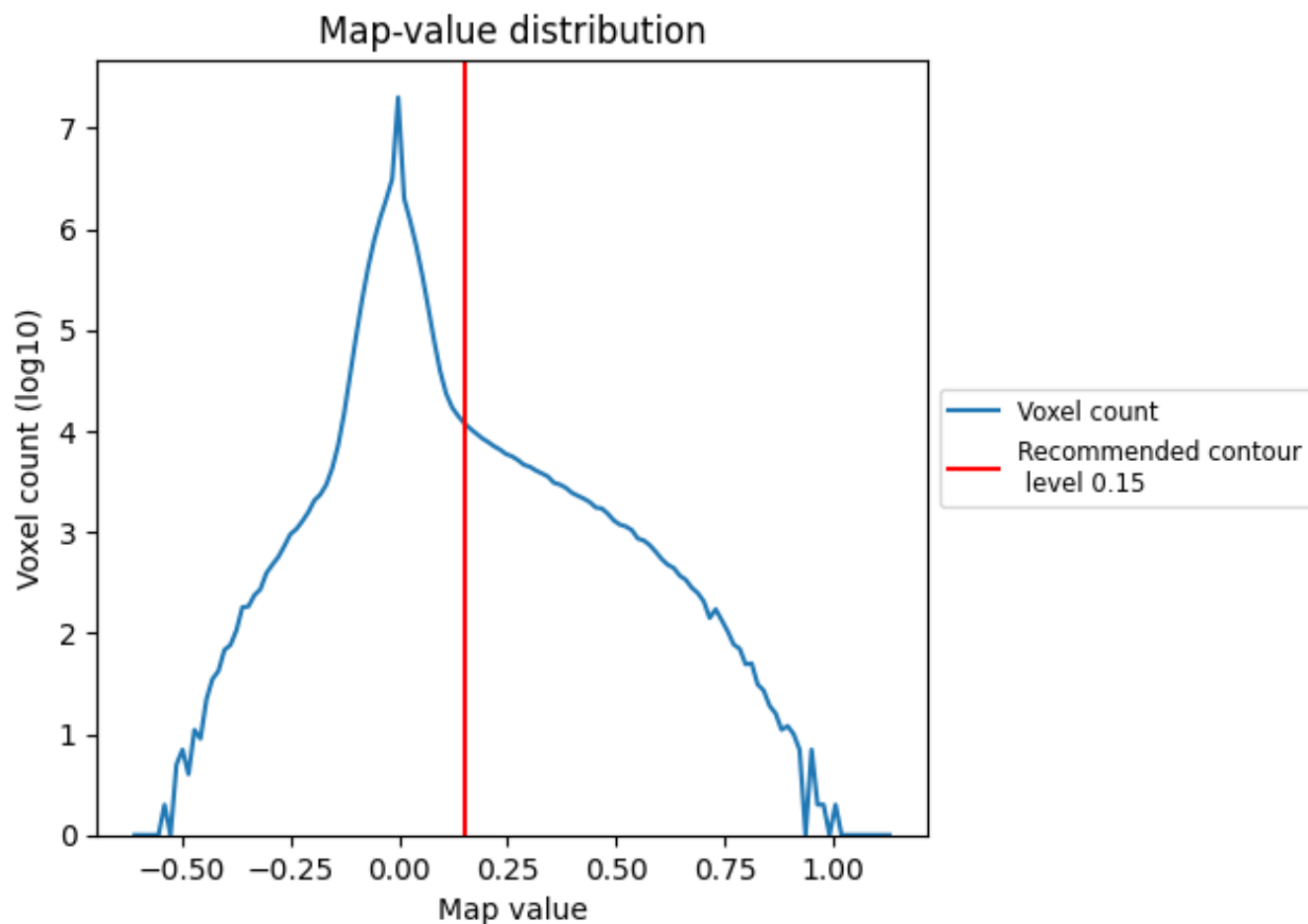


Z

7 Map analysis [i](#)

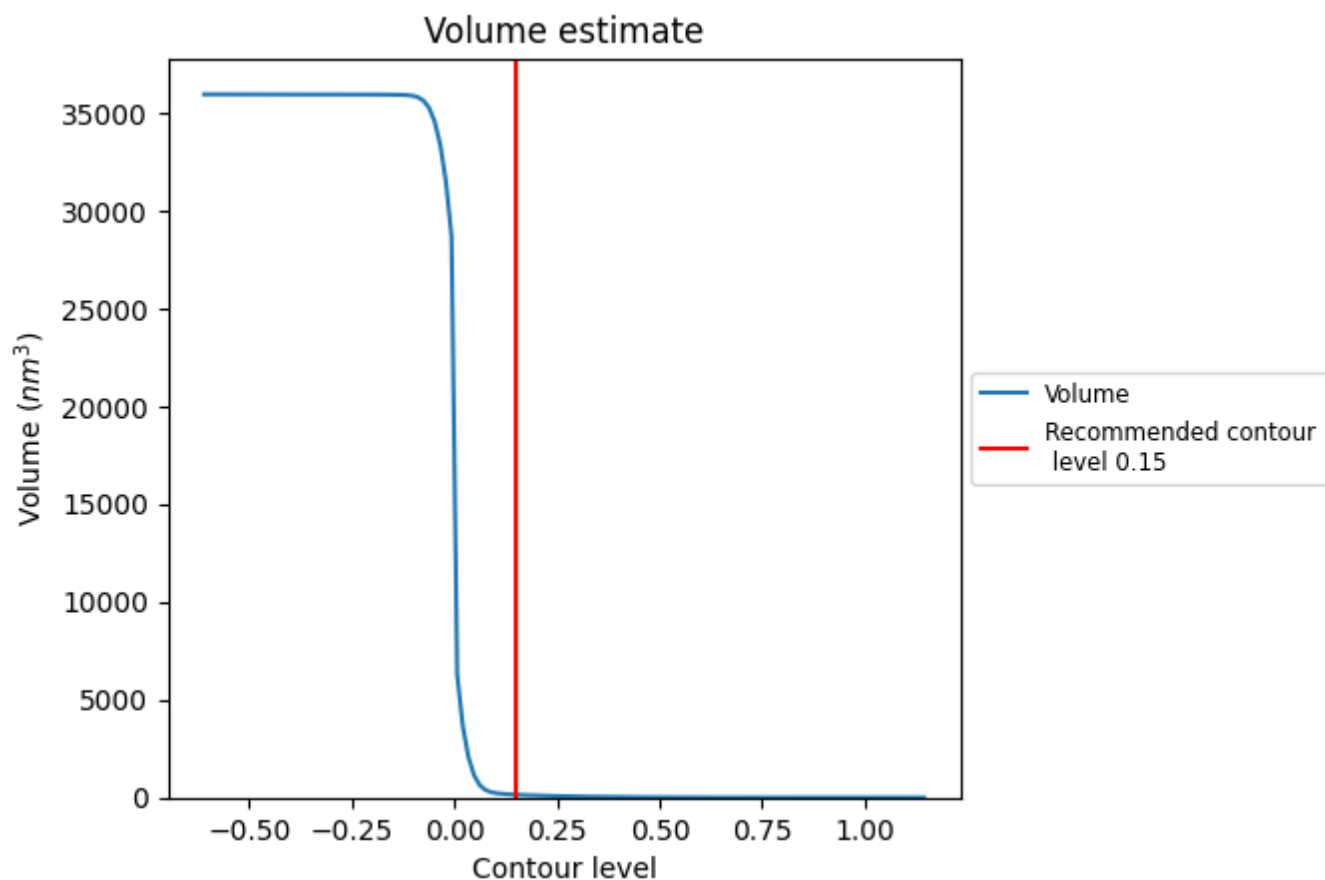
This section contains the results of statistical analysis of the map.

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.

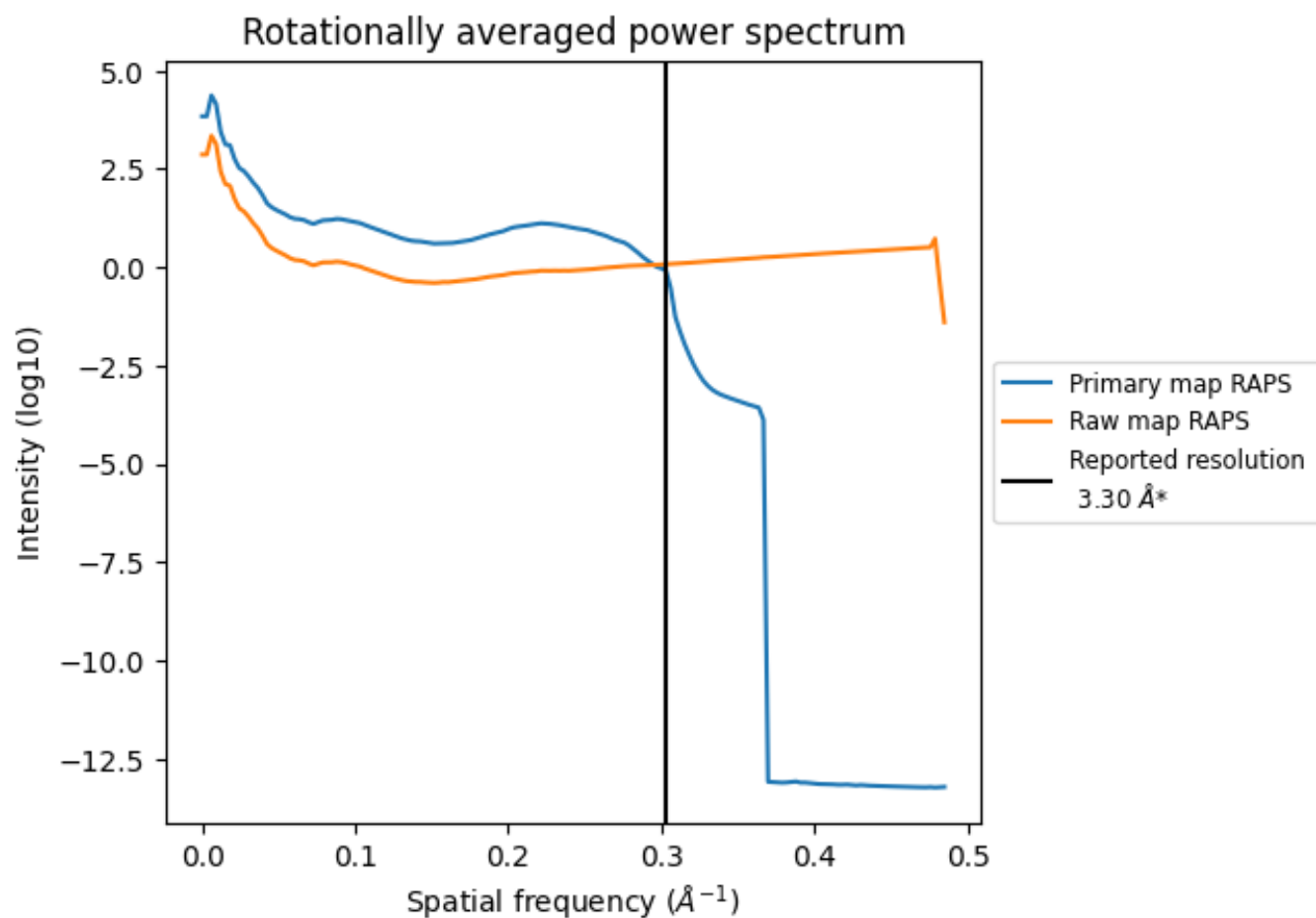
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 146 nm³; this corresponds to an approximate mass of 132 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 ⓘ

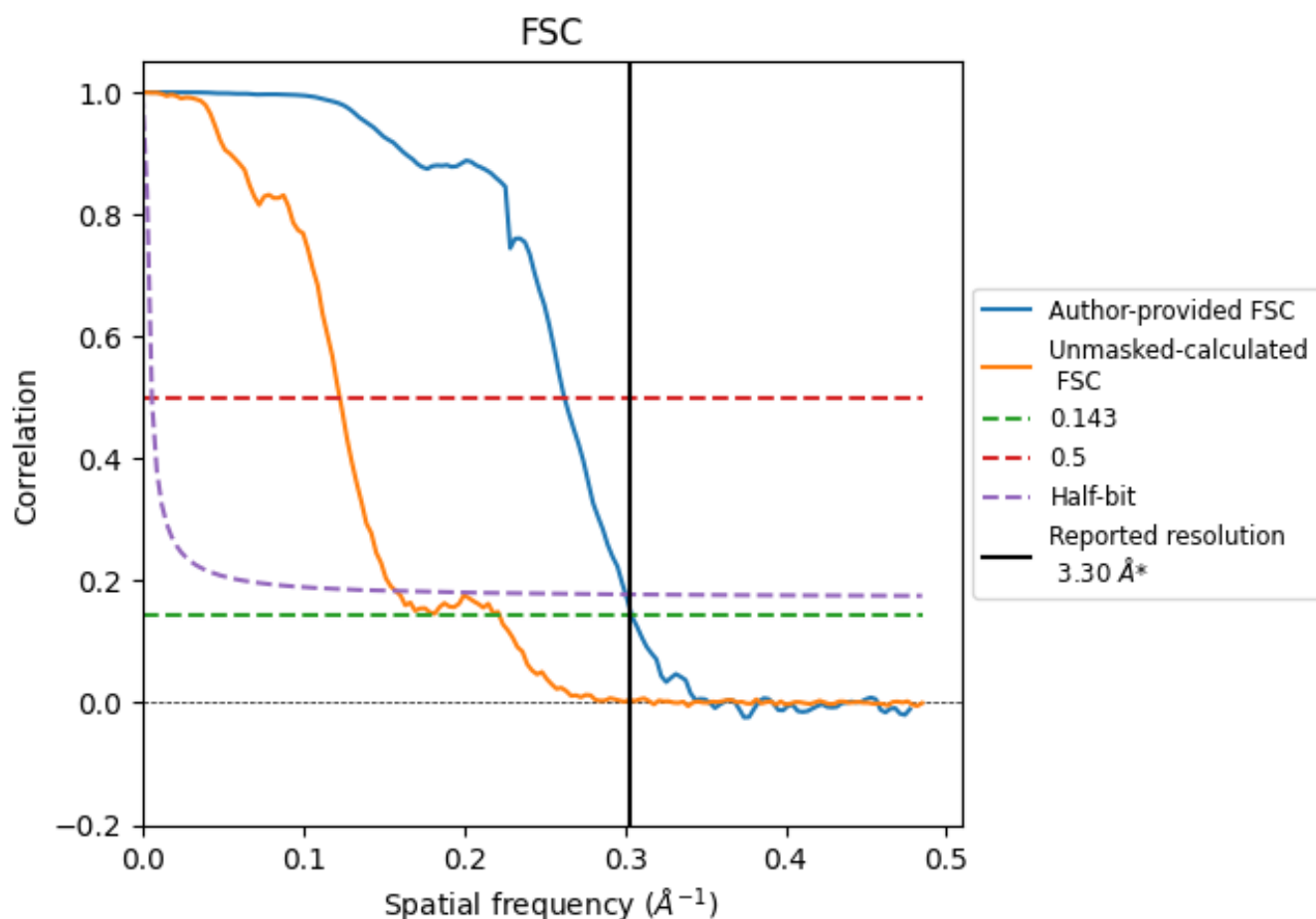


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

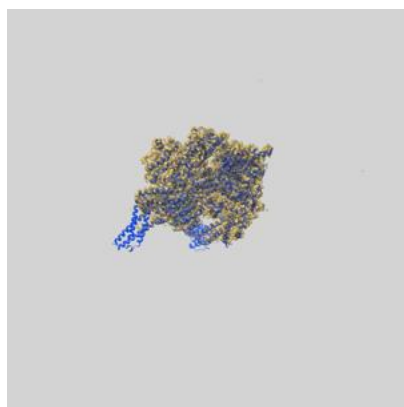
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.29	3.81	3.33
Unmasked-calculated*	4.50	8.14	6.34

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

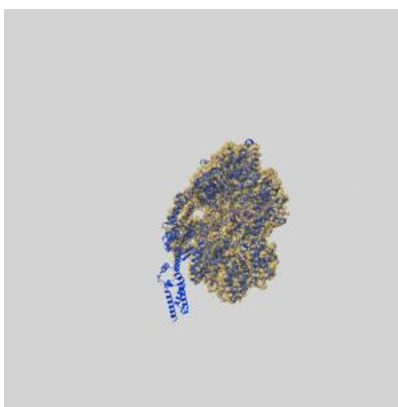
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44713 and PDB model 9BMW. Per-residue inclusion information can be found in section 3 on page 5.

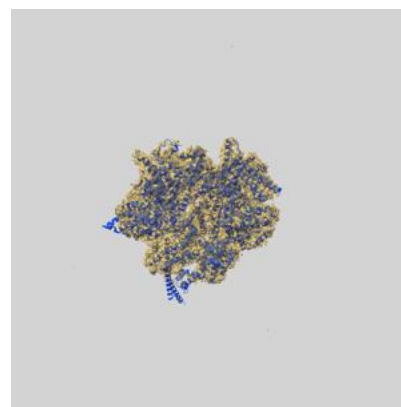
9.1 Map-model overlay [i](#)



X



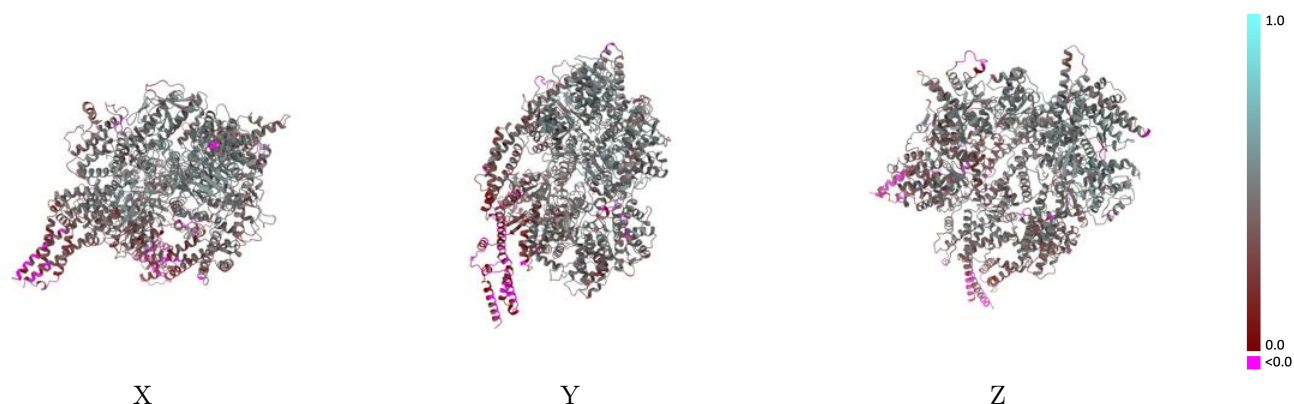
Y



Z

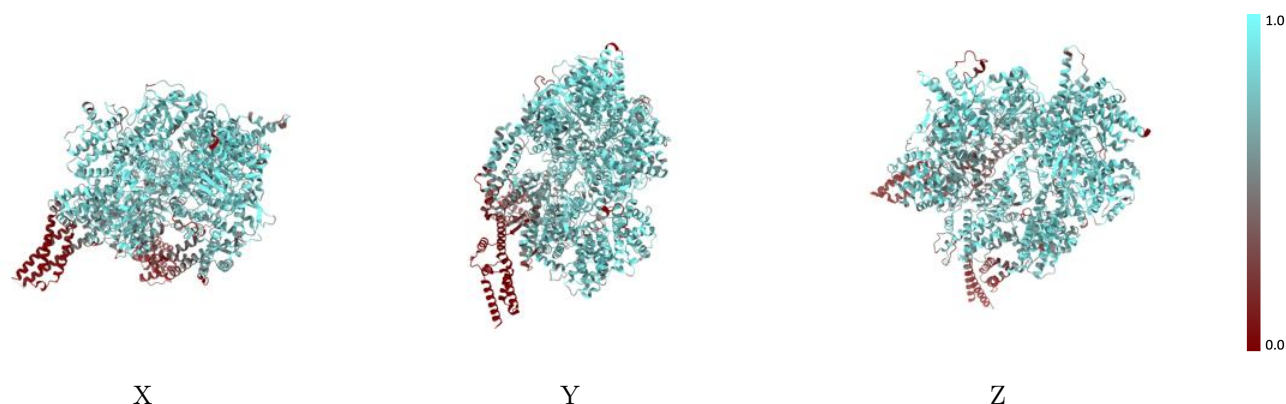
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



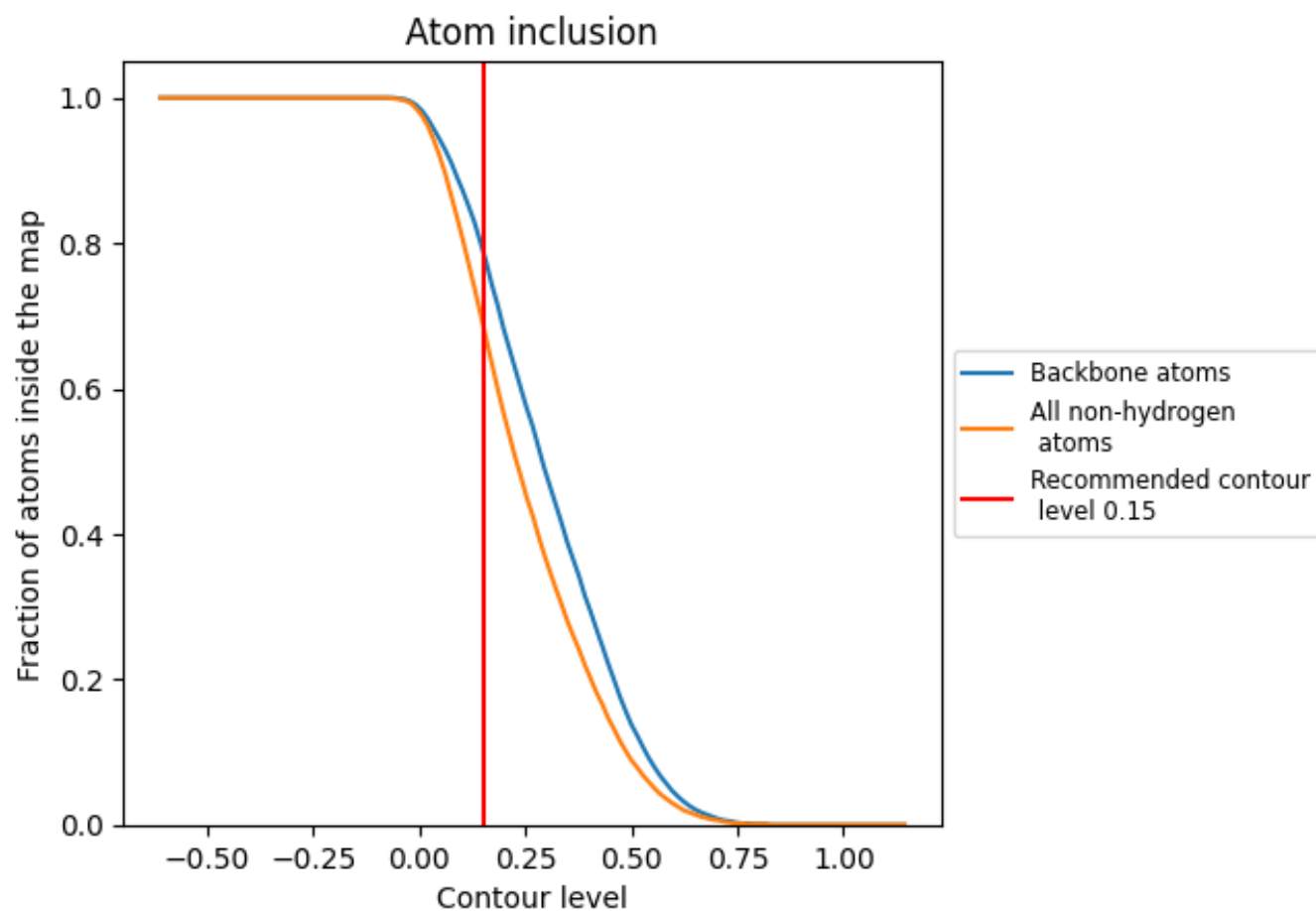
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 69% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6880	<div></div> 0.4110
A	<div></div> 0.6880	<div></div> 0.4110

