



wwPDB EM Validation Summary Report ⓘ

Mar 14, 2026 – 08:10 AM UTC

PDB ID : 9BN1 / pdb_00009bn1
EMDB ID : EMD-44718
Title : State-8 of motor domain from full-length human dynein-1 in apo condition
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.80 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

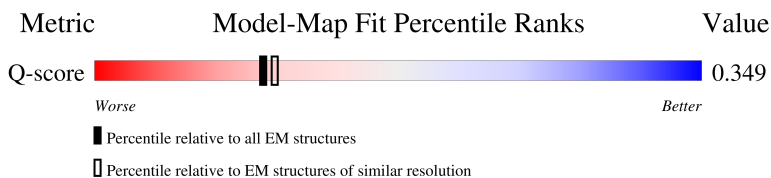
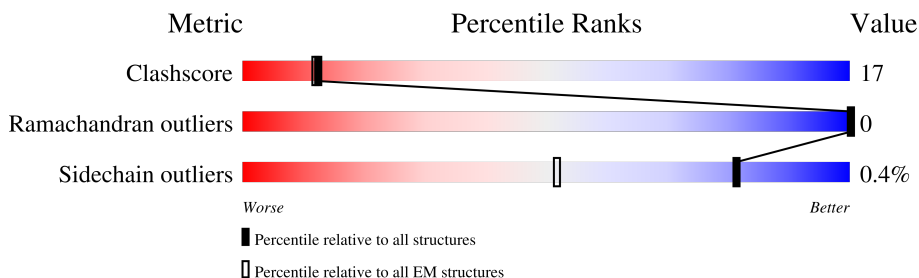
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

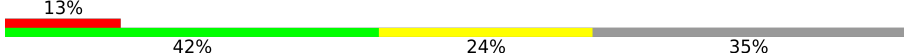
The reported resolution of this entry is 3.80 Å.

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	10198 (3.30 - 4.30)

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 24476 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	3029	24390	15542	4208	4518	122	0	0

- Molecule 2 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
			Total	C	N	O	P	
2	A	1	31	10	5	13	3	0

- Molecule 3 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
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

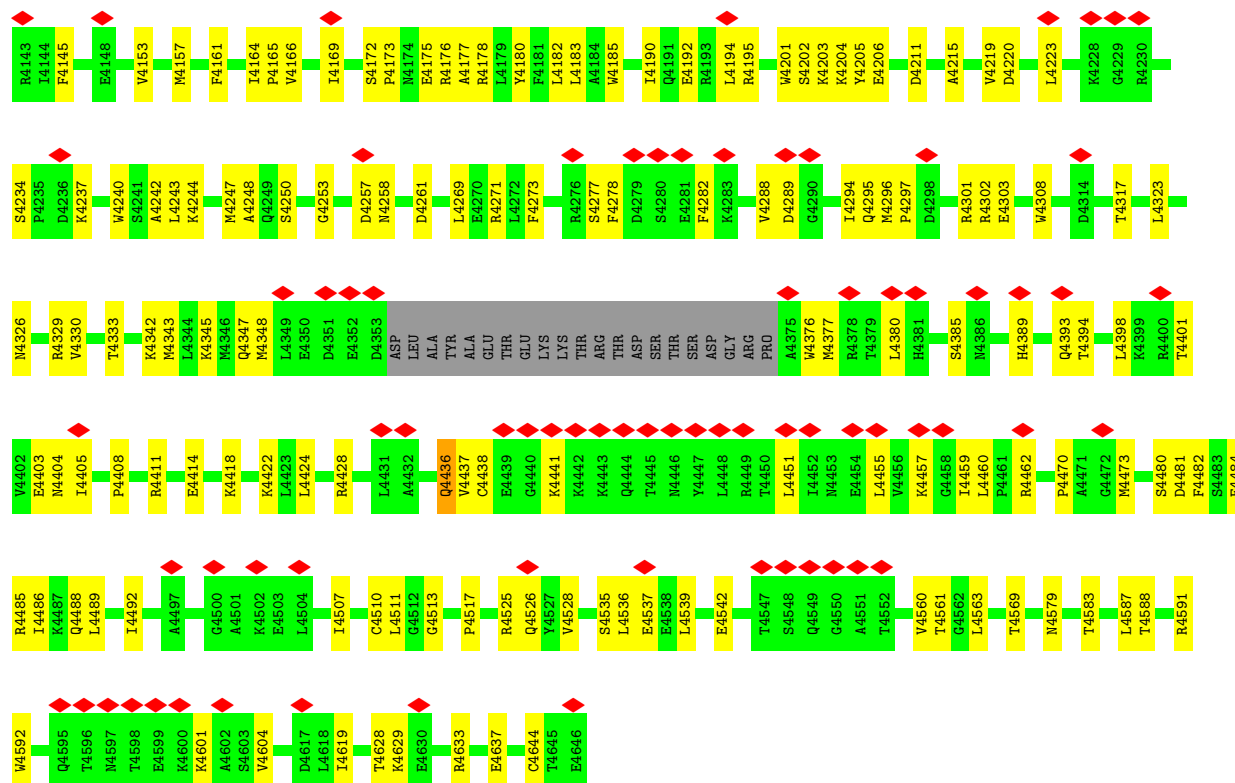
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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



Q3057	M2953	V2853	F2652	L2577	Q2482	ARG	K2323	V2236	E2133	Y2055	S1986
V3065	V2958	L2855	C2663	E2578	L2483	LYS	L2324	L2237	Q2134	S2056	N1987
F3066	R2757	L2755	E2664	A2579	E2484	GLY	L2325	L2238	E2135	Q2057	P1988
T3067	P2760	H2857	I2665	L2580	Q2485	LYS	L2326	L2244	L2136	R2060	N1989
N3068	R2763	R2863	N2667	Y2493	Y2493	ASP	L2327	G2249	L2137	L2085	Y1990
N3069	R2766	E2864	T2668	T2583	L2494	GLU	P2328	K2257	E2143	T2069	D1991
F3070	A2766	R2869	L2671	L2498	I2498	GLY	N2329	K2261	E2144	V2070	K1992
S3071	T2770	P2870	K2672	L2499	L2499	GLU	G2330	K2271	M2145	P2071	T1993
S3072	M2773	L2871	G2675	L2591	W2500	K2408	E2331	K2287	Y2146	F2072	S1994
G3073	E2775	S2874	Q2676	P2596	S2503	A2409	R2332	T2287	P2147	L2075	A1995
G3074	E2779	S2874	Q2677	G2598	G2504	L2413	L2333	L2268	L2148	C2076	P1996
N3078	E2775	S2874	Q2678	L2585	D2505	Q2414	L2335	L2269	L2149	D2077	I1997
T3081	M2779	K2879	V2679	P2597	S2503	T2415	P2336	P2270	E2152	E2000	E2000
F3086	D2787	D2880	I2680	G2598	G2504	Q2416	P2336	N2271	V2164	E2078	E2000
F3094	H2791	L2881	L2680	G2598	G2504	T2417	P2336	M2271	Q2169	Q2079	L2001
G3095	Y2792	L2881	L2680	G2598	G2504	R2418	P2336	M2271	Q2169	Q2079	L2001
N3096	D2787	L2881	L2680	G2598	G2504	R2419	P2336	M2271	Q2169	Q2079	L2001
N3097	H2791	L2881	L2680	G2598	G2504	R2420	P2336	M2271	Q2169	Q2079	L2001
N3098	Y2792	L2881	L2680	G2598	G2504	T2421	P2336	M2271	Q2169	Q2079	L2001
N3099	D2787	L2881	L2680	G2598	G2504	R2422	P2336	M2271	Q2169	Q2079	L2001
N3100	Y2792	L2881	L2680	G2598	G2504	T2423	P2336	M2271	Q2169	Q2079	L2001
A3101	D2787	L2881	L2680	G2598	G2504	R2424	P2336	M2271	Q2169	Q2079	L2001
A3102	Y2792	L2881	L2680	G2598	G2504	T2425	P2336	M2271	Q2169	Q2079	L2001
A3103	D2787	L2881	L2680	G2598	G2504	R2426	P2336	M2271	Q2169	Q2079	L2001
A3104	Y2792	L2881	L2680	G2598	G2504	T2427	P2336	M2271	Q2169	Q2079	L2001
A3105	D2787	L2881	L2680	G2598	G2504	R2428	P2336	M2271	Q2169	Q2079	L2001
A3106	Y2792	L2881	L2680	G2598	G2504	T2429	P2336	M2271	Q2169	Q2079	L2001
A3107	D2787	L2881	L2680	G2598	G2504	R2430	P2336	M2271	Q2169	Q2079	L2001
A3108	Y2792	L2881	L2680	G2598	G2504	T2431	P2336	M2271	Q2169	Q2079	L2001
A3109	D2787	L2881	L2680	G2598	G2504	R2432	P2336	M2271	Q2169	Q2079	L2001
A3110	Y2792	L2881	L2680	G2598	G2504	T2433	P2336	M2271	Q2169	Q2079	L2001
A3111	D2787	L2881	L2680	G2598	G2504	R2434	P2336	M2271	Q2169	Q2079	L2001
A3112	Y2792	L2881	L2680	G2598	G2504	T2435	P2336	M2271	Q2169	Q2079	L2001
A3113	D2787	L2881	L2680	G2598	G2504	R2436	P2336	M2271	Q2169	Q2079	L2001
A3114	Y2792	L2881	L2680	G2598	G2504	T2437	P2336	M2271	Q2169	Q2079	L2001
A3115	D2787	L2881	L2680	G2598	G2504	R2438	P2336	M2271	Q2169	Q2079	L2001
A3116	Y2792	L2881	L2680	G2598	G2504	T2439	P2336	M2271	Q2169	Q2079	L2001
A3117	D2787	L2881	L2680	G2598	G2504	R2440	P2336	M2271	Q2169	Q2079	L2001
A3118	Y2792	L2881	L2680	G2598	G2504	T2441	P2336	M2271	Q2169	Q2079	L2001
A3119	D2787	L2881	L2680	G2598	G2504	R2442	P2336	M2271	Q2169	Q2079	L2001
A3120	Y2792	L2881	L2680	G2598	G2504	T2443	P2336	M2271	Q2169	Q2079	L2001
A3121	D2787	L2881	L2680	G2598	G2504	R2444	P2336	M2271	Q2169	Q2079	L2001
A3122	Y2792	L2881	L2680	G2598	G2504	T2445	P2336	M2271	Q2169	Q2079	L2001
A3123	D2787	L2881	L2680	G2598	G2504	R2446	P2336	M2271	Q2169	Q2079	L2001
A3124	Y2792	L2881	L2680	G2598	G2504	T2447	P2336	M2271	Q2169	Q2079	L2001
A3125	D2787	L2881	L2680	G2598	G2504	R2448	P2336	M2271	Q2169	Q2079	L2001
A3126	Y2792	L2881	L2680	G2598	G2504	T2449	P2336	M2271	Q2169	Q2079	L2001
A3127	D2787	L2881	L2680	G2598	G2504	R2450	P2336	M2271	Q2169	Q2079	L2001
A3128	Y2792	L2881	L2680	G2598	G2504	T2451	P2336	M2271	Q2169	Q2079	L2001
A3129	D2787	L2881	L2680	G2598	G2504	R2452	P2336	M2271	Q2169	Q2079	L2001
A3130	Y2792	L2881	L2680	G2598	G2504	T2453	P2336	M2271	Q2169	Q2079	L2001
A3131	D2787	L2881	L2680	G2598	G2504	R2454	P2336	M2271	Q2169	Q2079	L2001
A3132	Y2792	L2881	L2680	G2598	G2504	T2455	P2336	M2271	Q2169	Q2079	L2001
A3133	D2787	L2881	L2680	G2598	G2504	R2456	P2336	M2271	Q2169	Q2079	L2001
A3134	Y2792	L2881	L2680	G2598	G2504	T2457	P2336	M2271	Q2169	Q2079	L2001
A3135	D2787	L2881	L2680	G2598	G2504	R2458	P2336	M2271	Q2169	Q2079	L2001
A3136	Y2792	L2881	L2680	G2598	G2504	T2459	P2336	M2271	Q2169	Q2079	L2001
A3137	D2787	L2881	L2680	G2598	G2504	R2460	P2336	M2271	Q2169	Q2079	L2001
A3138	Y2792	L2881	L2680	G2598	G2504	T2461	P2336	M2271	Q2169	Q2079	L2001
A3139	D2787	L2881	L2680	G2598	G2504	R2462	P2336	M2271	Q2169	Q2079	L2001
A3140	Y2792	L2881	L2680	G2598	G2504	T2463	P2336	M2271	Q2169	Q2079	L2001
A3141	D2787	L2881	L2680	G2598	G2504	R2464	P2336	M2271	Q2169	Q2079	L2001
A3142	Y2792	L2881	L2680	G2598	G2504	T2465	P2336	M2271	Q2169	Q2079	L2001





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50945	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	0.817	Depositor
Minimum map value	-0.311	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	333.312, 333.312, 333.312	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.302, 1.302, 1.302	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.18	0/24908	0.40	1/33751 (0.0%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1862	ALA	CB-CA-C	-5.13	110.68	116.63

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1603	ARG	Sidechain

5.2 Too-close contacts

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	24390	0	24462	826	0
2	A	31	0	12	4	0
3	A	54	0	24	7	0
4	A	1	0	0	0	0
All	All	24476	0	24498	826	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 17.

The worst 5 of 826 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:1457:MET:HE1	1:A:3659:ARG:HA	1.41	1.03
1:A:2444:GLU:H	1:A:2510:MET:HE1	1.33	0.92
1:A:2667:ASN:HD22	1:A:2712:CYS:HB2	1.35	0.91
1:A:1550:ILE:HG23	1:A:1638:LEU:HD21	1.51	0.90
1:A:3206:ARG:HH12	1:A:3209:LYS:HD3	1.35	0.89

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	3019/4646 (65%)	2946 (98%)	73 (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	2696/4125 (65%)	2686 (100%)	10 (0%)	84 83

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

Mol	Chain	Res	Type
1	A	4127	THR
1	A	4161	PHE
1	A	4436	GLN
1	A	2787	ASP
1	A	3572	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2960	GLN
1	A	3555	ASN
1	A	4526	GLN
1	A	3198	GLN
1	A	3584	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	ADP	A	4703	-	28,29,29	1.38	4 (14%)	43,45,45	1.82	9 (20%)
2	ATP	A	4701	4	32,33,33	0.63	1 (3%)	48,52,52	0.39	0
3	ADP	A	4702	-	28,29,29	1.36	4 (14%)	43,45,45	1.87	10 (23%)

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

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

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4703	ADP	C5-C4	4.61	1.47	1.39
3	A	4702	ADP	C5-C4	4.44	1.47	1.39
2	A	4701	ATP	PA-O3A	-2.70	1.56	1.59
3	A	4702	ADP	C5-C6	2.62	1.48	1.41
3	A	4703	ADP	C5-C6	2.62	1.48	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4702	ADP	C5-C4-N3	-5.93	118.55	126.72
3	A	4703	ADP	C5-C4-N3	-5.77	118.77	126.72
3	A	4702	ADP	N3-C4-N9	4.77	135.28	127.17
3	A	4703	ADP	N3-C4-N9	4.58	134.95	127.17
3	A	4702	ADP	C2-N3-C4	3.83	121.19	111.83

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

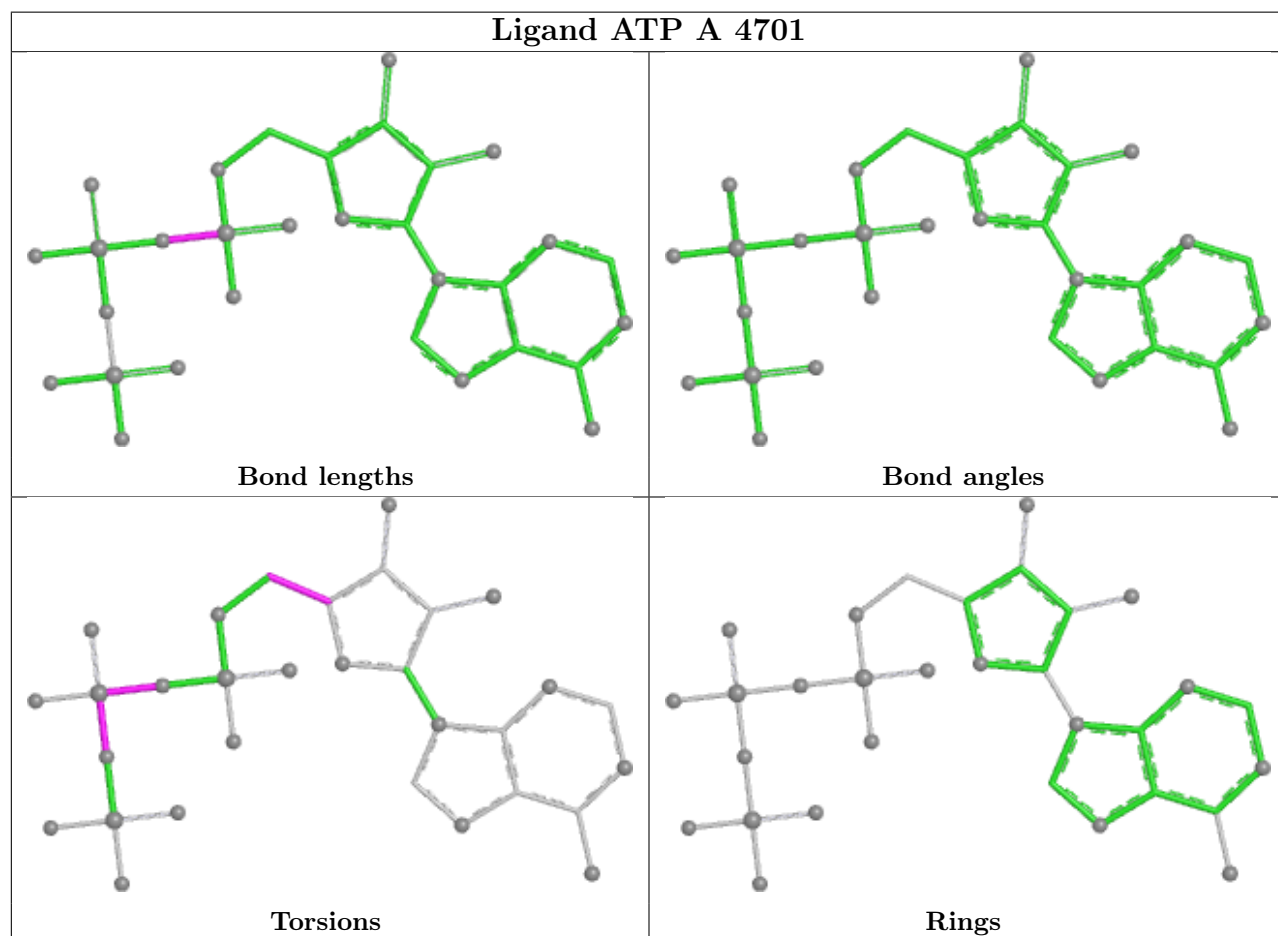
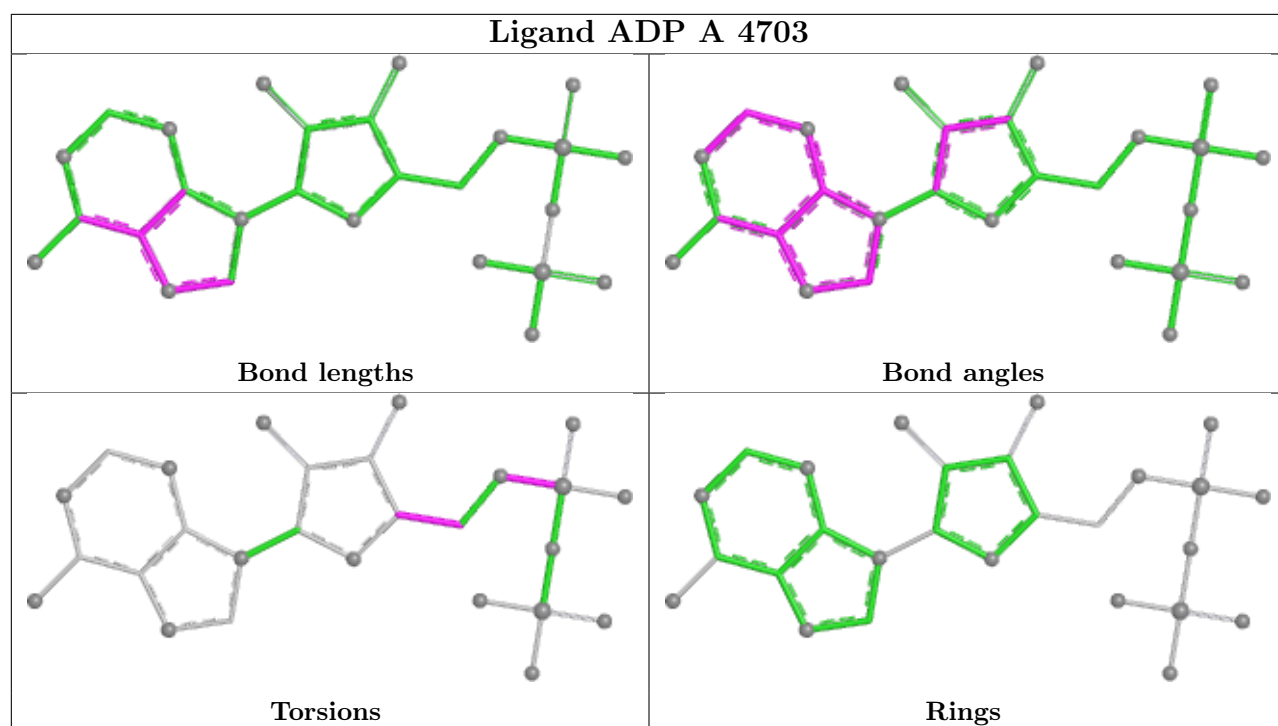
Mol	Chain	Res	Type	Atoms
2	A	4701	ATP	O4'-C4'-C5'-O5'
2	A	4701	ATP	C3'-C4'-C5'-O5'
3	A	4703	ADP	C5'-O5'-PA-O1A
2	A	4701	ATP	PG-O3B-PB-O2B
2	A	4701	ATP	PA-O3A-PB-O1B

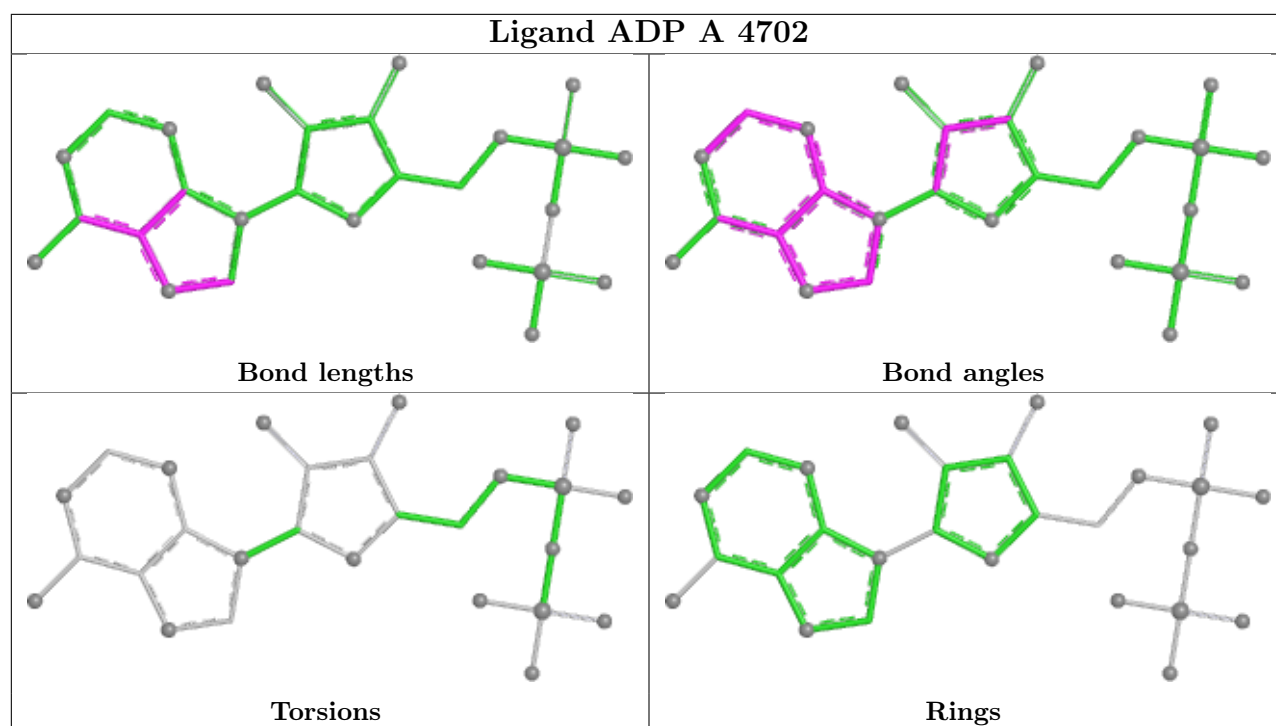
There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4703	ADP	2	0
2	A	4701	ATP	4	0
3	A	4702	ADP	5	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.

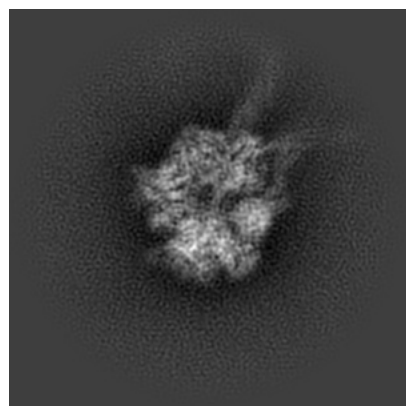
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44718. These allow visual inspection of the internal detail of the map and identification of artifacts.

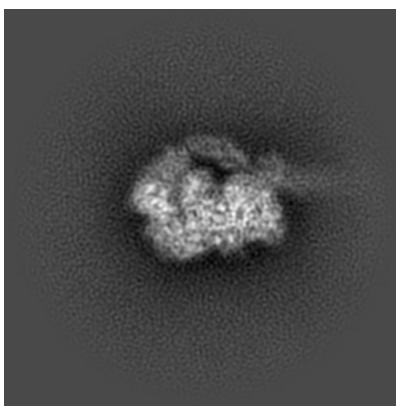
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

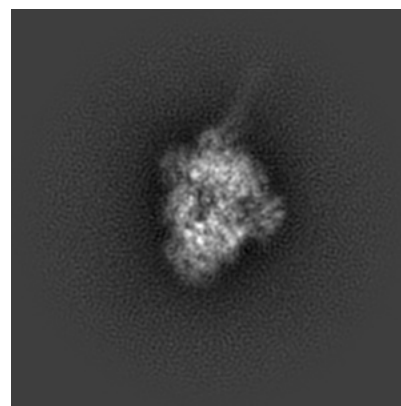
6.1.1 Primary map



X

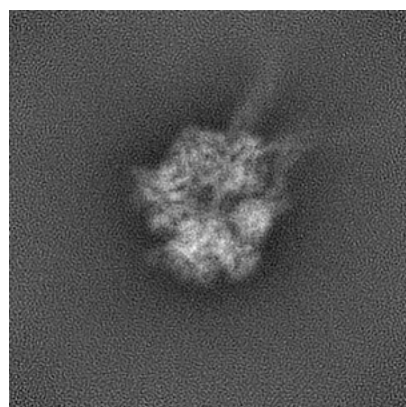


Y

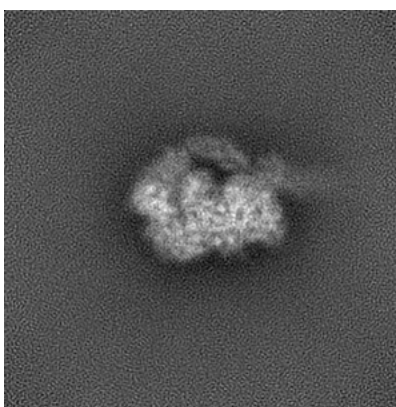


Z

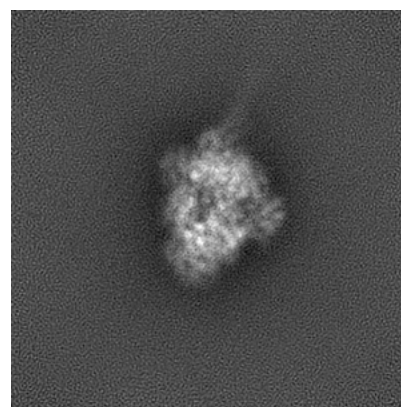
6.1.2 Raw map



X



Y

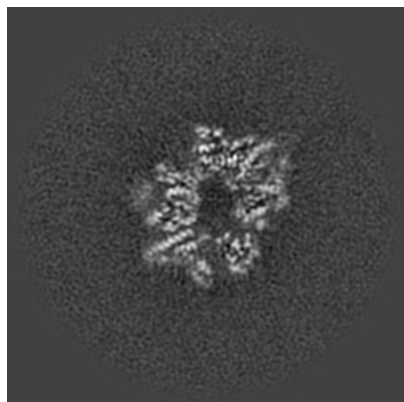


Z

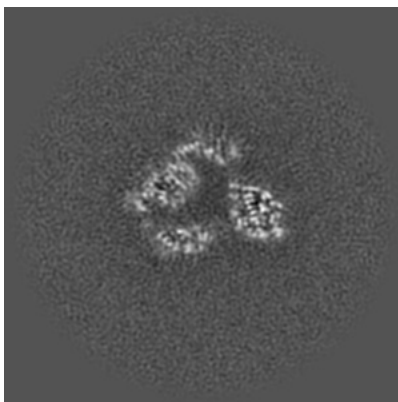
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

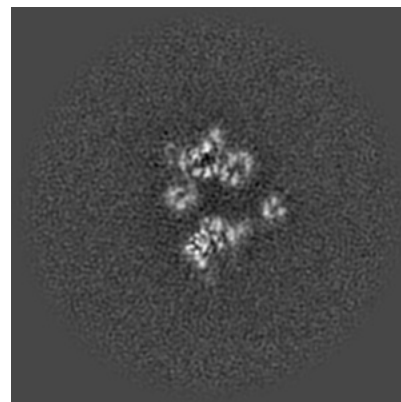
6.2.1 Primary map



X Index: 128

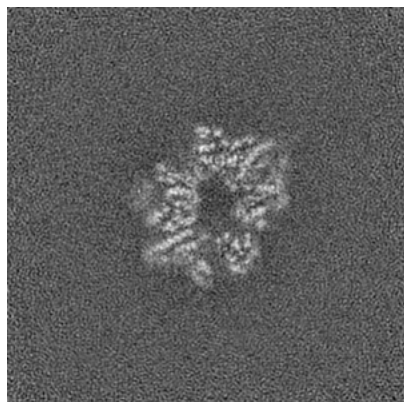


Y Index: 128



Z Index: 128

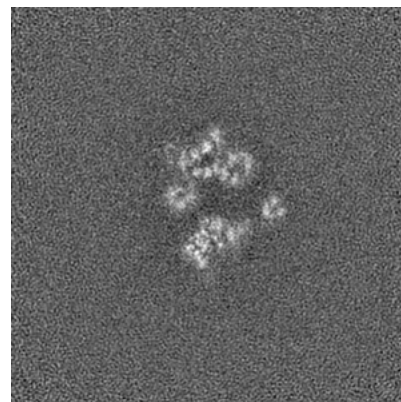
6.2.2 Raw map



X Index: 128



Y Index: 128

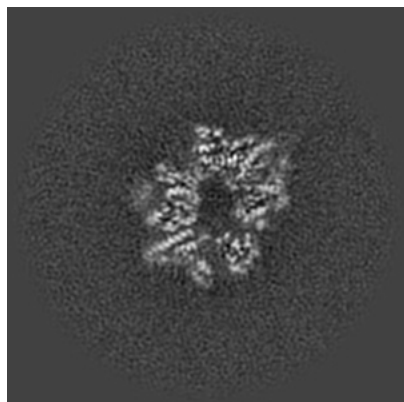


Z Index: 128

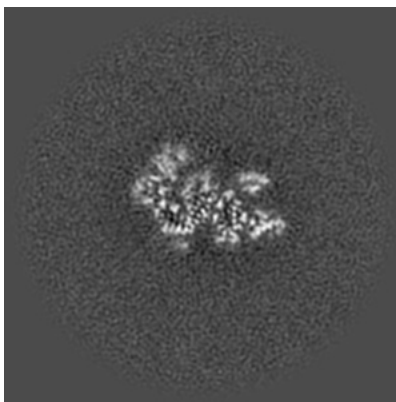
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

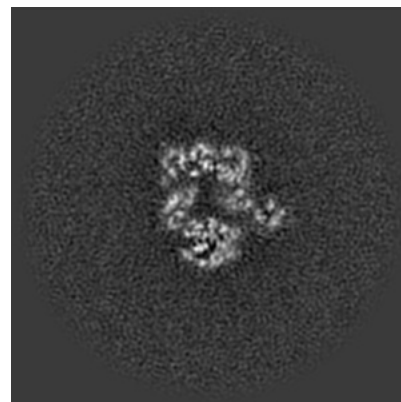
6.3.1 Primary map



X Index: 128

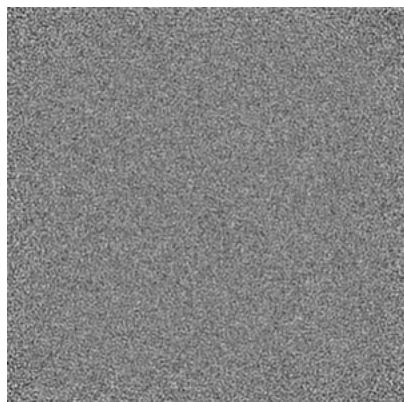


Y Index: 111

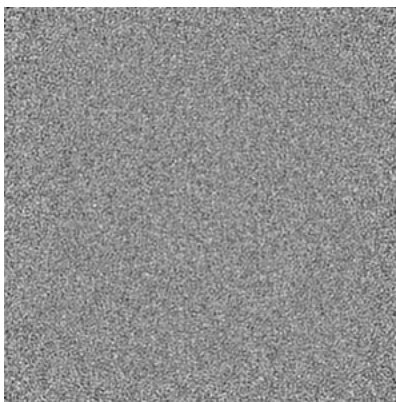


Z Index: 119

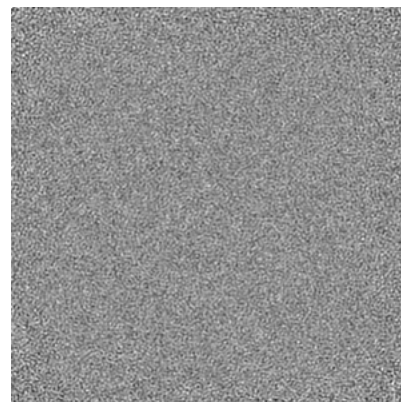
6.3.2 Raw map



X Index: 0



Y Index: 0

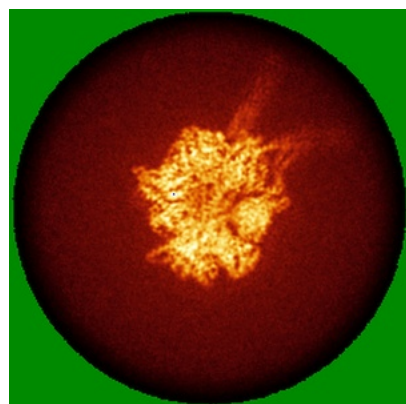


Z Index: 0

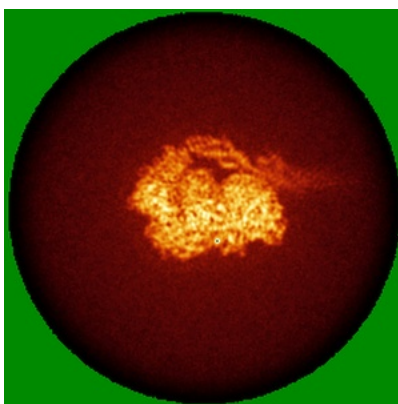
The images above show the largest variance slices of the map in three orthogonal directions.

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

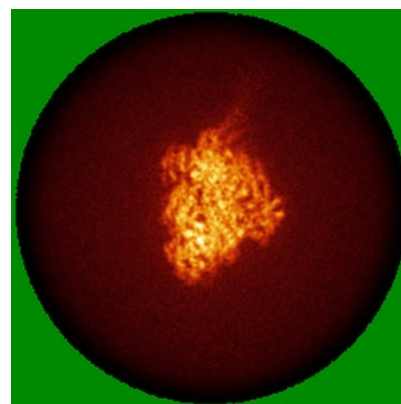
6.4.1 Primary map



X

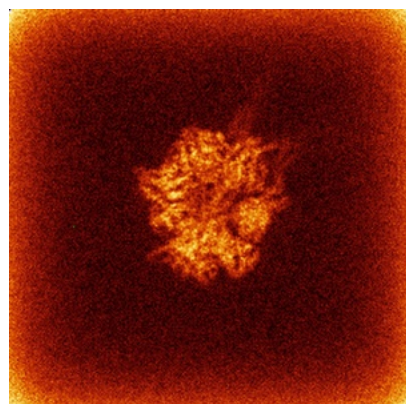


Y

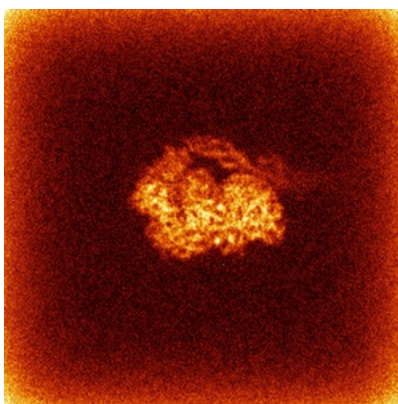


Z

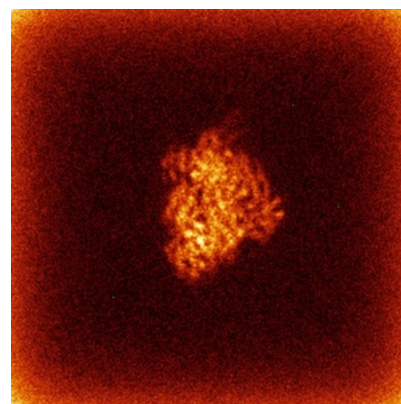
6.4.2 Raw map



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.

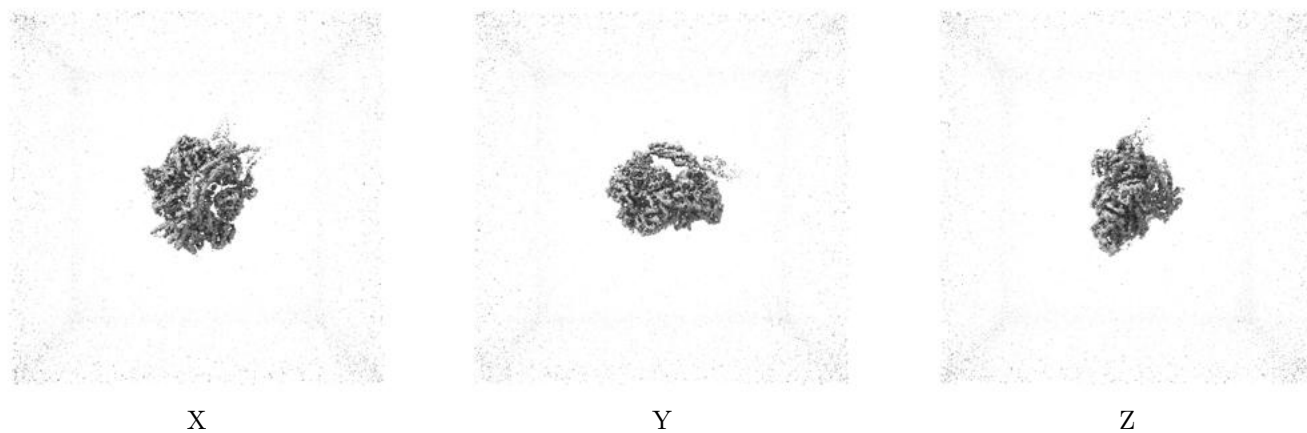
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

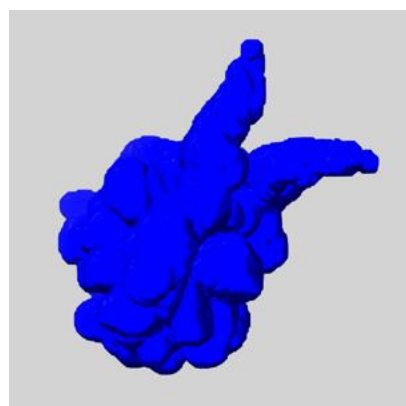
6.6 Mask visualisation [i](#)

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

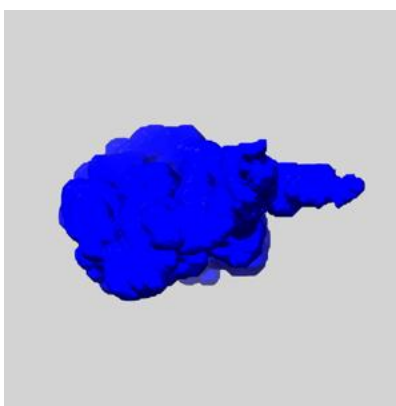
A mask typically either:

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

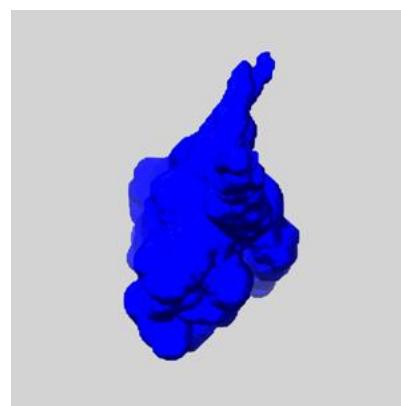
6.6.1 emd_44718_msk_1.map [i](#)



X



Y

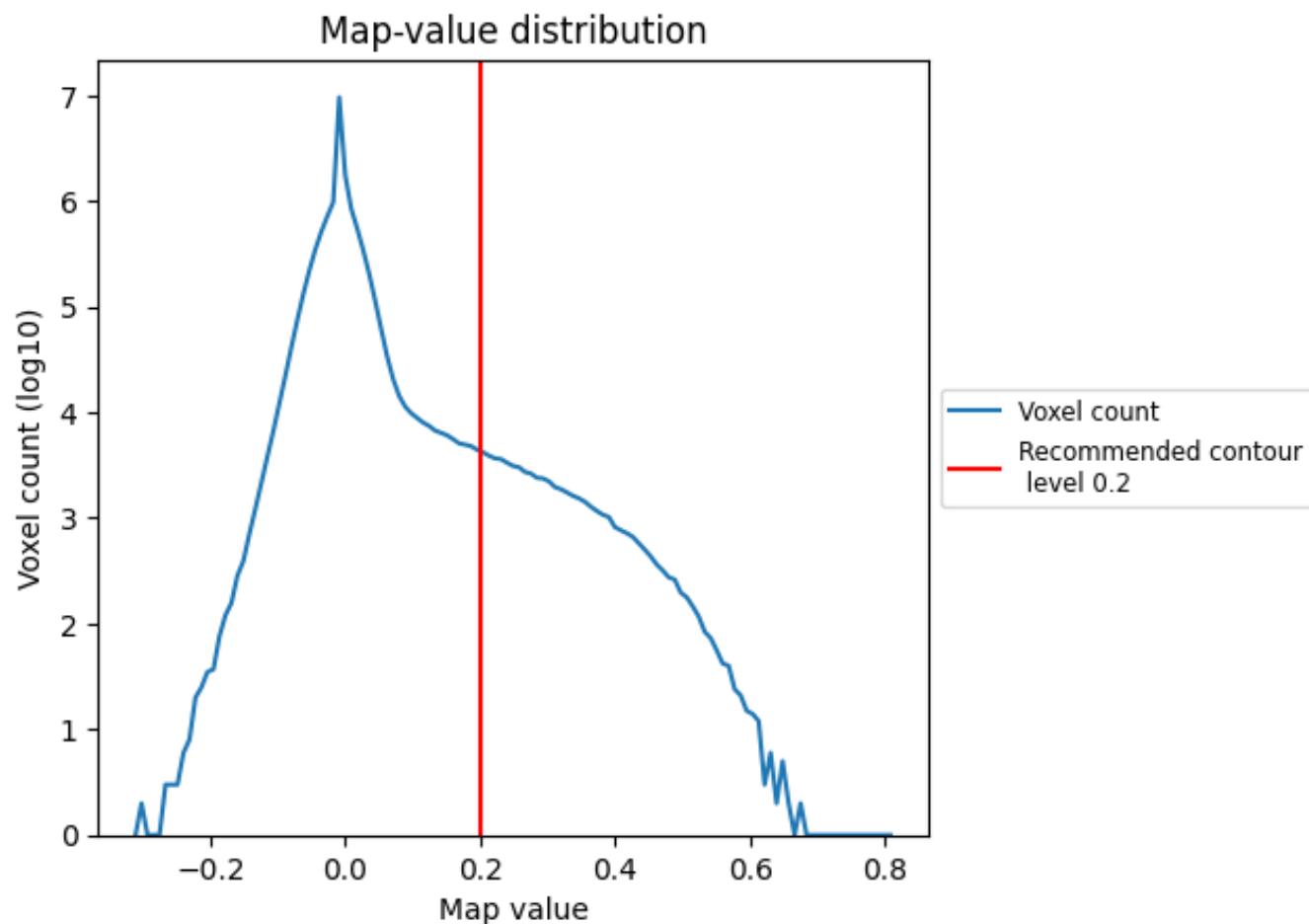


Z

7 Map analysis [i](#)

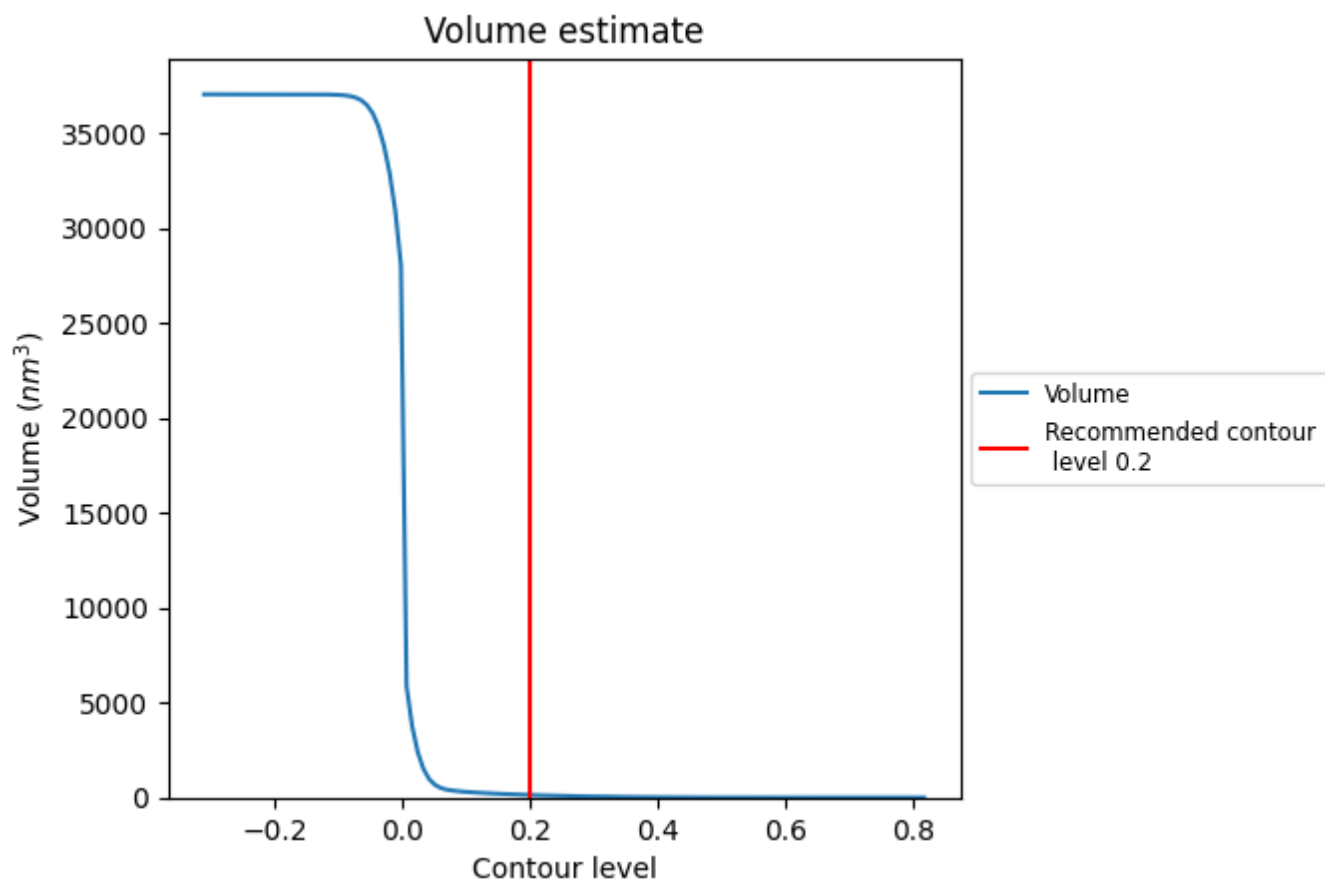
This section contains the results of statistical analysis of the map.

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.

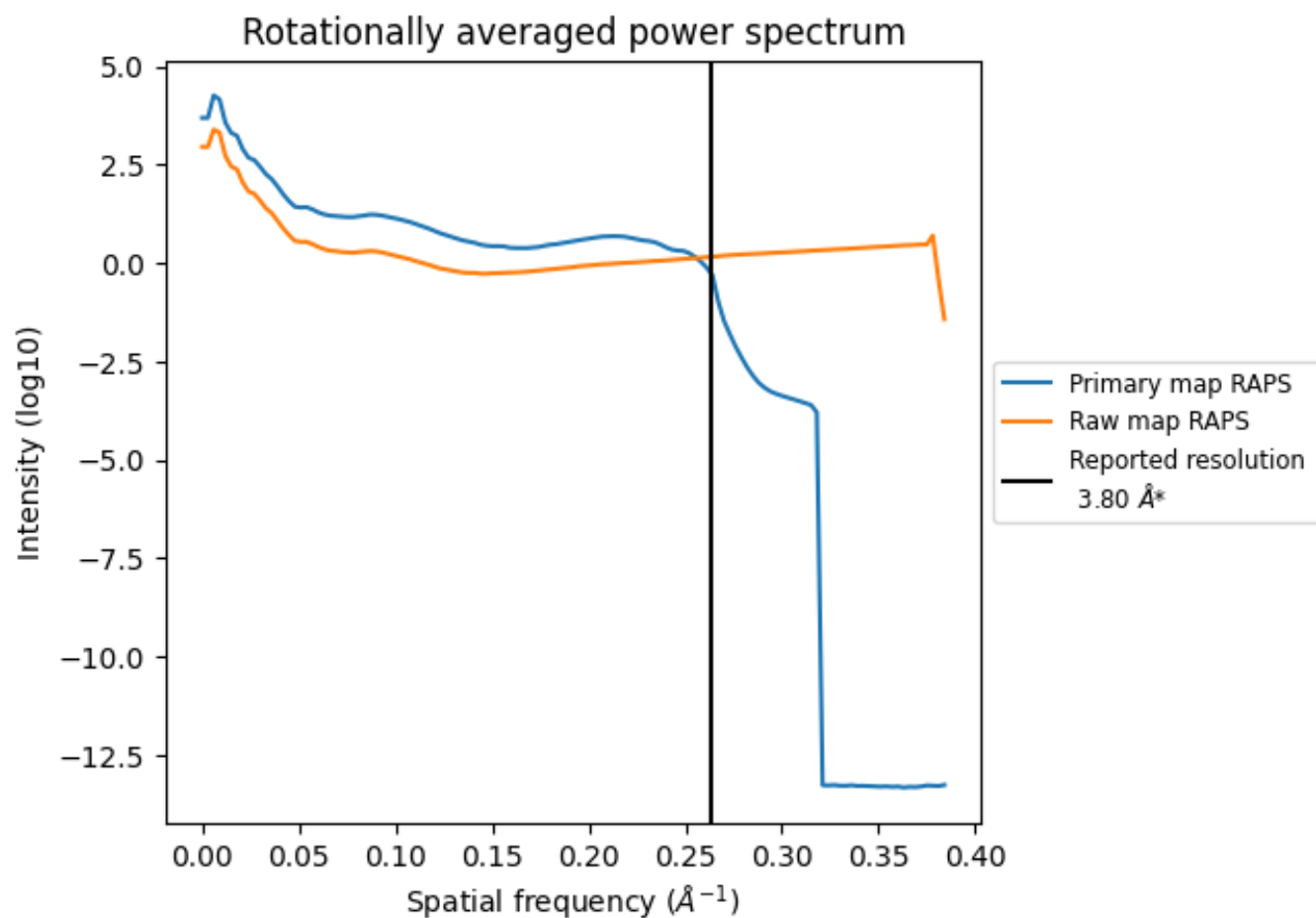
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 134 nm^3 ; this corresponds to an approximate mass of 121 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 ⓘ

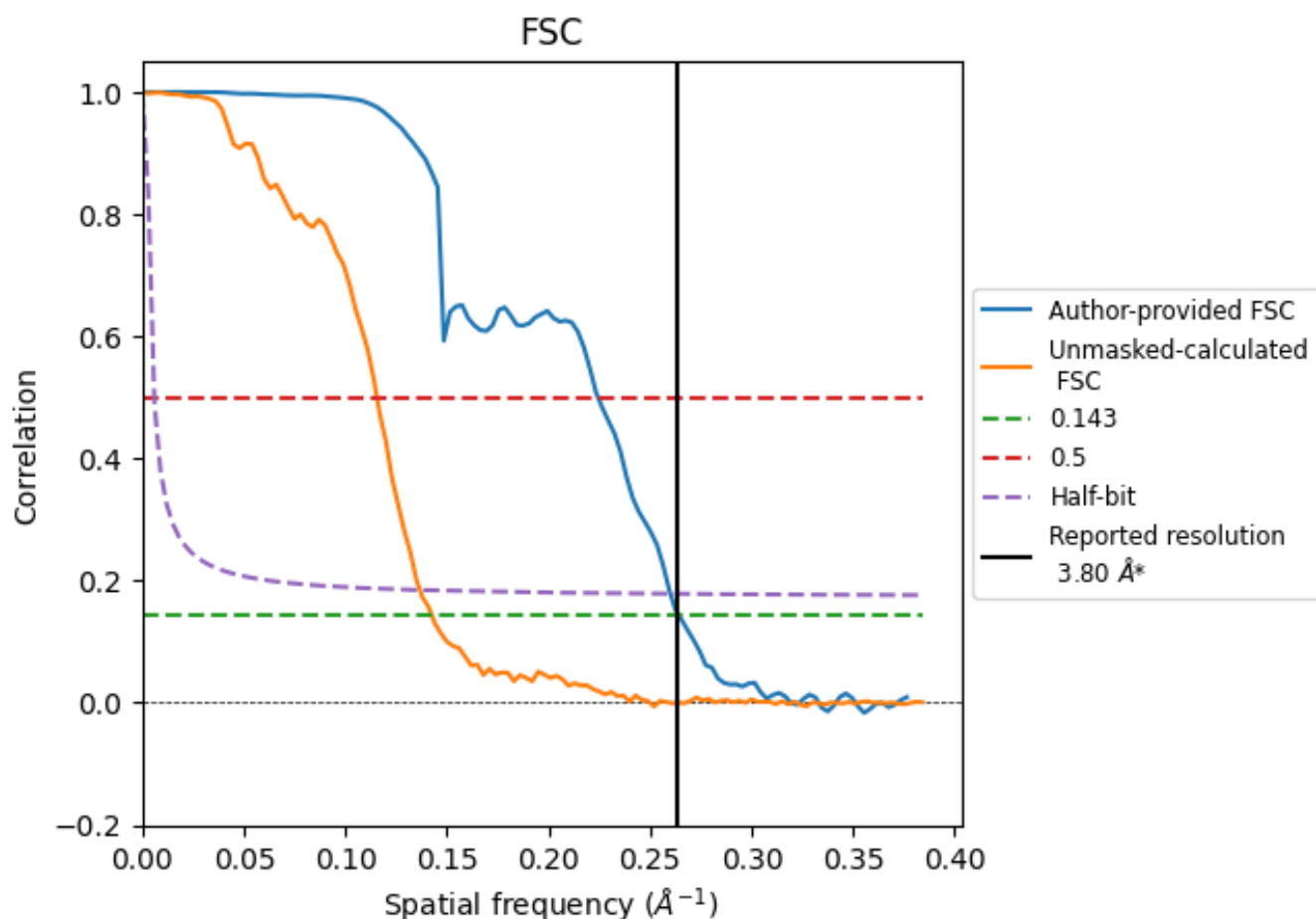


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 $0.263 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

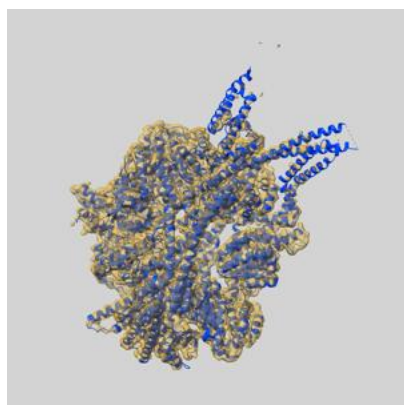
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.78	4.46	3.84
Unmasked-calculated*	7.01	8.65	7.31

*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 7.01 differs from the reported value 3.8 by more than 10 %

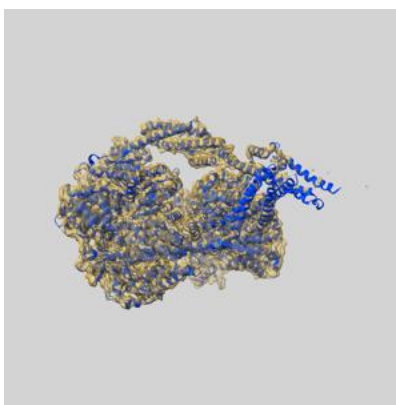
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44718 and PDB model 9BN1. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

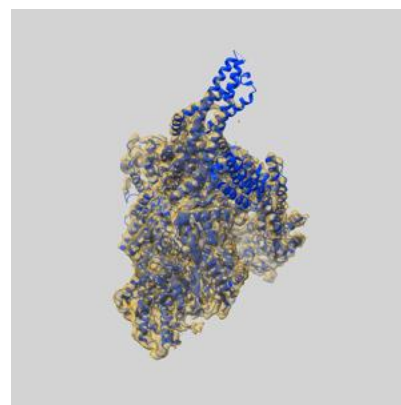
9.1 Map-model overlay [i](#)



X



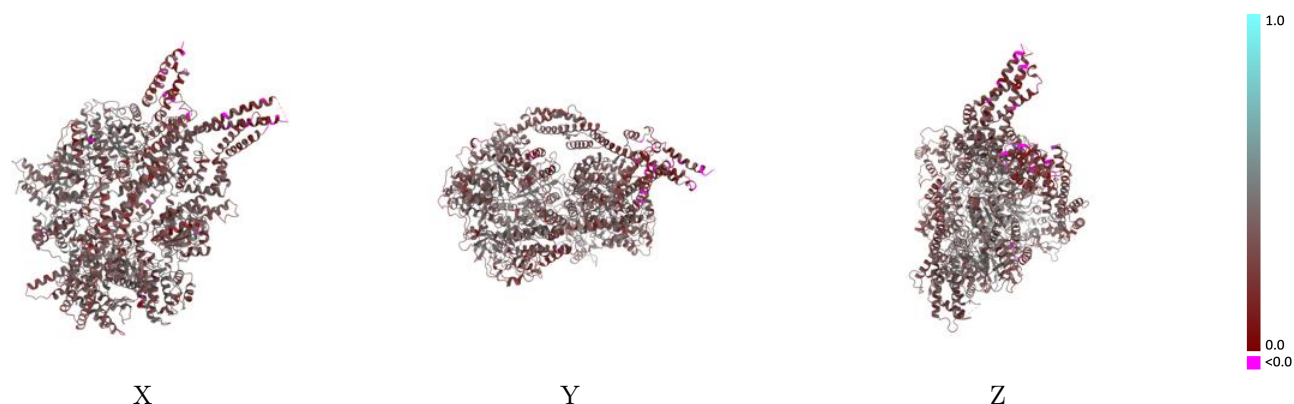
Y



Z

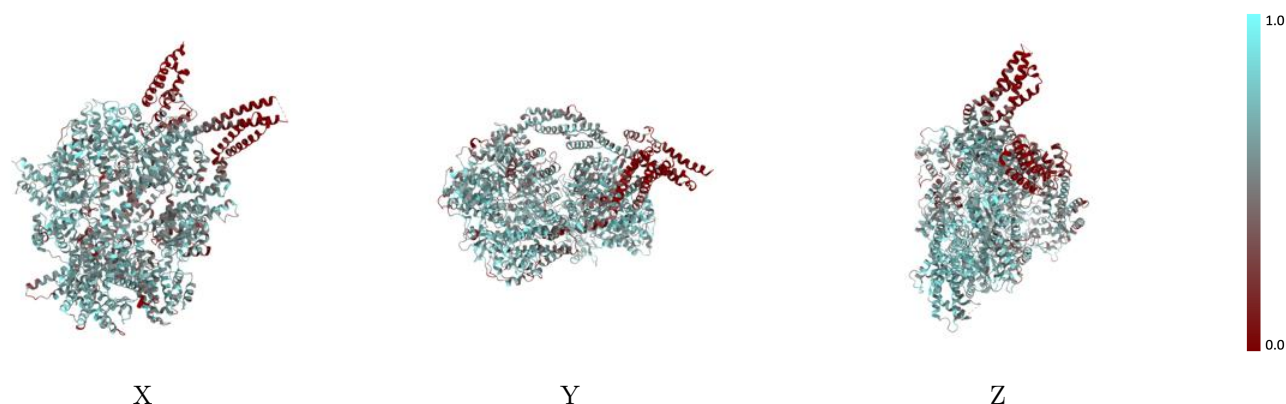
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



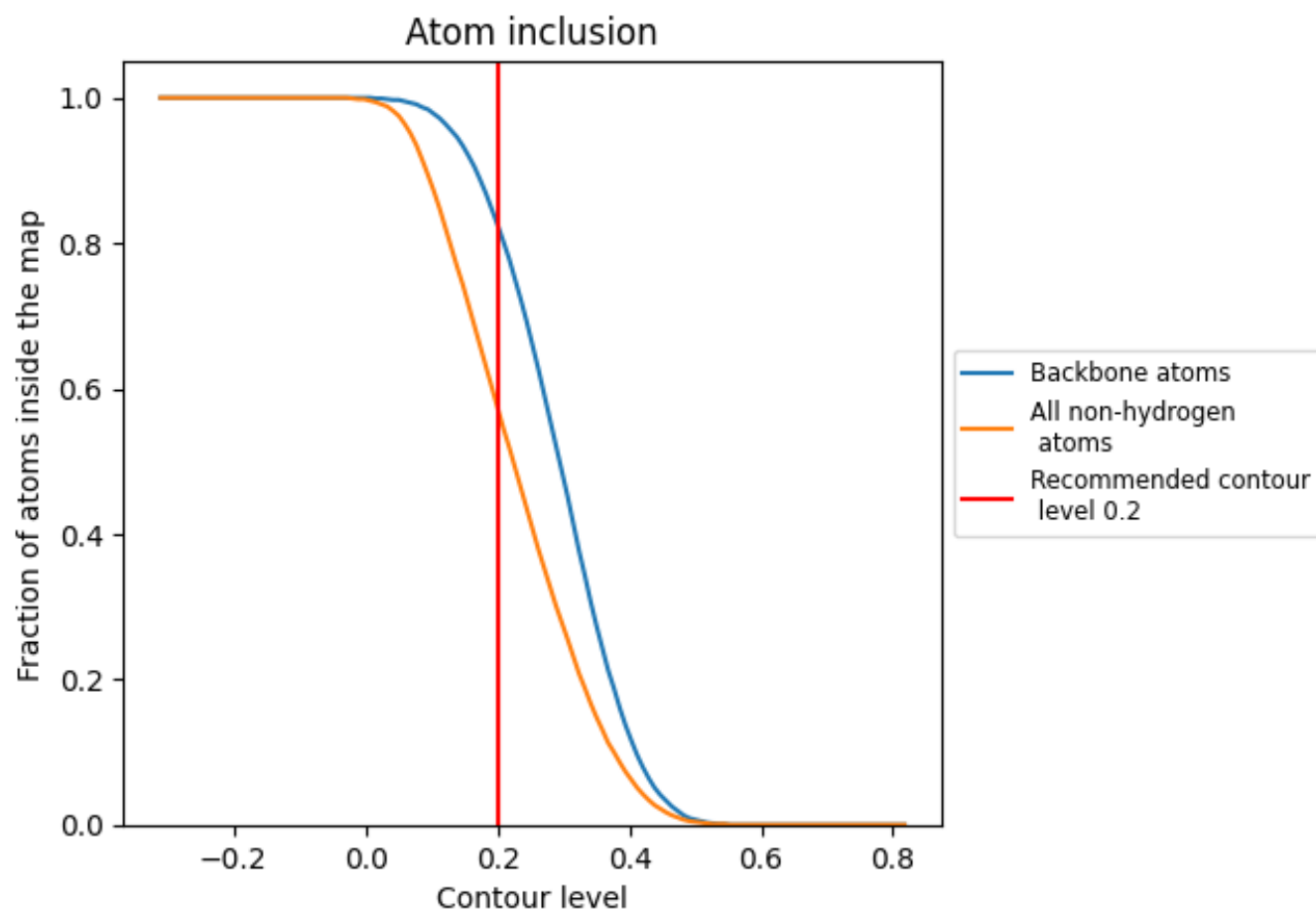
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5750	0.3490
A	0.5750	0.3490

