



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 09:13 PM UTC

PDB ID : 9BM3 / pdb_00009bm3
EMDB ID : EMD-44686
Title : State-5a of motor domain from full-length human dynein-1 in 5 mM ATP
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.49 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

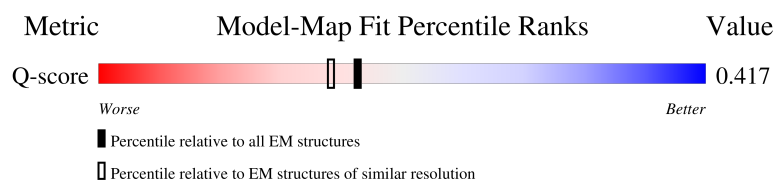
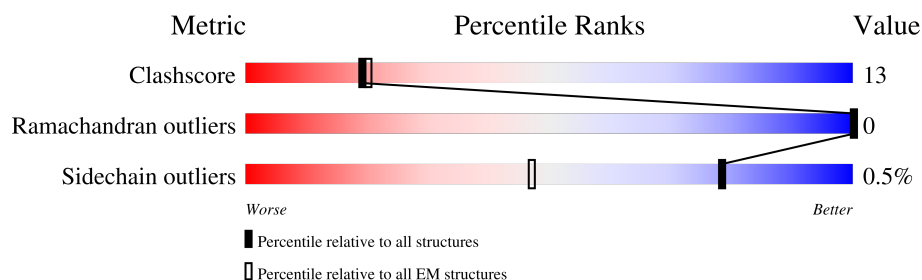
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

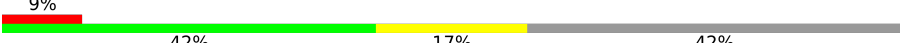
The reported resolution of this entry is 3.49 Å.

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	13600 (2.99 - 3.99)

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 3 unique types of molecules in this entry. The entry contains 21867 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	2711	21755	13852	3757	4035	111	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).

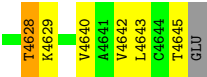


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	



LEU	VAL	L3091	N3014	L2909	T2800	F2606	Y2495	ALA	D2277	E2126	L2028
VAL	ASP	F3094	G3015	V2910	R2801	R2610	A2497	GLN	G2278	I2127	F2029
VAL	GLN	G3095	E3016	V2911	W2802	A2611	L2498	ARG	T2281	E2135	D2030
ARG	GLN	D3096	V3017	N2912	R2803	L2612	L2499	ARG	H2282	I2136	L2031
SER	GLU	D3096	V3017	N2913	R2804	M2615	W2500	LYS	L2137	L2137	L2032
MET	ALA	T3099	L3020	L2920	R2811	M2615	L2501	GLY	K2286	L2138	R2037
ALA	GLU	F3021	F3021	L2920	P2812	L2620	G2504	LYS	I2287	Q2139	R2041
ASN	LYS	E3100	E3022	D2923	L2816	N2621	D2505	ASP	S2290	R2179	T2042
PRO	LYS	A3101	G3023	R2924	P2817	F2622	M2510	GLU	V2291	E2180	K2043
PRO	LYS	L3102	D3024	L2925	W2818	S2623	R2511	GLY	E2181	P2044	P2044
ALA	VAL	Y3103	D3025	F2926	E2819	S2623	L2502	GLU	L2182	D2045	D2045
ALA	MET	Q3104	E3026	F2926	G2820	T2626	S2503	GLU	K2183	K2046	K2046
VAL	SER	Y3105	Y3026	L2933	L2821	T2626	G2504	ALA	E2294	Q2047	Q2047
LYS	GLN	G3106	A3027	L2933	L2822	L2631	D2505	ALA	L2191	L2048	L2048
LEU	LEU	K3107	T3028	L2936	A2826	L2631	G2505	ALA	L2191	L2048	L2048
ALA	ILE	T3110	L3029	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
LEU	GLU	M3111	M3030	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
SER	GLN	M3113	M3031	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
ILE	LEU	D3114	Q3032	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
CYS	HIS	L3115	C3033	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
LEU	LYS	E3116	K3034	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
LEU	GLN	K3117	E3035	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
LEU	GLN	P3118	Q3038	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
GLY	GLU	N3119	K3039	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
GLU	VAL	N3119	E3040	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
SER	ILE	D3124	Q3040	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
THR	ALA	Y3125	G3041	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
ASP	ASP	K3126	L3042	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
ASP	LYS	T3211	M3043	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
TRP	GLN	T3212	L3044	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
LYS	MET	D3213	D3045	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
GLN	SER	Q3214	Q3046	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
ILE	VAL	Y3215	H3047	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
ARG	LYS	E3216	E3048	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
ILE	ASP	E3217	E3049	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
MET	ASP	L3218	K3052	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
ARG	VAL	R3220	W3053	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
ASN	PRO	ASP	S3056	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
ILE	ALA	LEU	L3154	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
PRO	VAL	ARG	T3059	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
THR	VAL	ILE	R3060	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
ILE	GLU	LYS	N3061	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
VAL	ALA	SER	L3062	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
ASN	GLN	GLU	H3063	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
PHE	ASN	LEU	V3064	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
SER	ALA	LEU	V3065	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
ALA	VAL	GLU	P3070	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
VAL	LYS	VAL	S3071	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
GLU	SER	LYS	K3169	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
GLU	ILE	ILE	A3170	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
SER	LYS	LYS	T3171	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
ASP	LYS	ASP	T3172	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
ALA	GLN	ALA	H3175	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
ILE	HIS	HIS	D3178	L2936	A2826	L2631	D2505	ALA	L2191	L2048	L2048
ASP	GLU	ASP	E2274	L2605	L2605	L2605	L2605	ASP	E2274	L2605	L2605
GLU	GLU	GLU	E2274	L2605	L2605	L2605	L2605	GLU	E2274	L2605	L2605
ASP	ASP	ASP	E2274	L2605	L2605	L2605	L2605	ASP	E2274	L2605	L2605
LYS	LYS	LYS	E2274	L2605	L2605	L2605	L2605	LYS	E2274	L2605	L2605
LEU	LEU	LEU	E2274	L2605	L2605	L2605	L2605	LEU	E2274	L2605	L2605
LYS	LYS	LYS	E2274	L2605	L2605	L2605	L2605	LYS	E2274	L2605	L2605
MET	MET	MET	E2274	L2605	L2605	L2605	L2605	MET	E2274	L2605	L2605





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65824	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	0.644	Depositor
Minimum map value	-0.354	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.12	Depositor
Map size ($\text{\AA}$)	332.80002, 332.80002, 332.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.832, 0.832, 0.832	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0/22220	0.36	3/30121 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2812	PRO	CA-N-CD	-8.91	99.53	112.00
1	A	1848	PRO	CA-N-CD	-6.17	103.36	112.00
1	A	2020	PRO	CA-N-CD	-5.04	104.95	112.00

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	21755	0	21789	555	0
2	A	81	0	36	7	0
3	A	31	0	12	0	0
All	All	21867	0	21837	555	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 13.

The worst 5 of 555 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:3662:ILE:HD11	1:A:3671:LEU:HB2	1.54	0.87
1:A:3790:VAL:HG13	1:A:3794:VAL:HB	1.56	0.87
1:A:3661:LEU:HD11	1:A:3668:ASP:HB3	1.61	0.83
1:A:3731:LEU:HD12	1:A:3790:VAL:HG21	1.66	0.78
1:A:2053:MET:HE1	1:A:2094:LYS:HA	1.66	0.78

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	2699/4646 (58%)	2635 (98%)	64 (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	2407/4125 (58%)	2395 (100%)	12 (0%)	81	80

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1964	GLU
1	A	2043	LYS
1	A	4628	THR
1	A	2090	LEU
1	A	1884	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4397	HIS
1	A	4466	HIS
1	A	2549	GLN
1	A	2482	GLN
1	A	4490	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	4701	-	28,29,29	0.44	0	43,45,45	0.45	0
2	ADP	A	4704	-	28,29,29	1.38	4 (14%)	43,45,45	1.79	8 (18%)
2	ADP	A	4703	-	28,29,29	1.40	4 (14%)	43,45,45	1.90	8 (18%)
3	ATP	A	4702	-	32,33,33	0.51	0	48,52,52	0.56	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	4701	-	-	2/16/32/32	0/3/3/3
2	ADP	A	4704	-	-	4/16/32/32	0/3/3/3
2	ADP	A	4703	-	-	4/16/32/32	0/3/3/3
3	ATP	A	4702	-	-	1/22/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4703	ADP	C5-C4	4.70	1.47	1.39
2	A	4704	ADP	C5-C4	4.51	1.47	1.39
2	A	4703	ADP	C5-C6	2.66	1.48	1.41
2	A	4704	ADP	C5-C6	2.56	1.48	1.41
2	A	4704	ADP	C5-N7	-2.41	1.34	1.39

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4703	ADP	C5-C4-N3	-6.11	118.30	126.72
2	A	4704	ADP	C5-C4-N3	-5.64	118.95	126.72
2	A	4703	ADP	N3-C4-N9	4.98	135.64	127.17
2	A	4704	ADP	N3-C4-N9	4.43	134.71	127.17
2	A	4703	ADP	C2-N3-C4	3.89	121.33	111.83

There are no chirality outliers.

5 of 11 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

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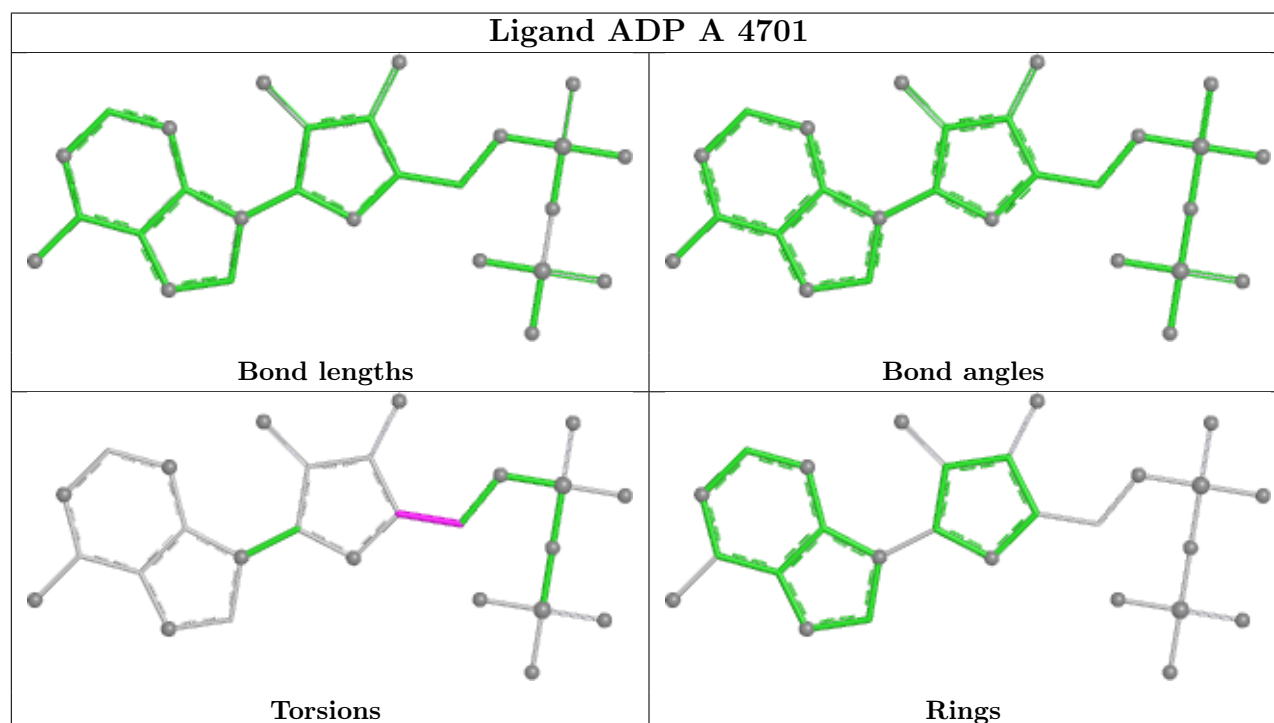
Mol	Chain	Res	Type	Atoms
2	A	4703	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	PA-O3A-PB-O2B
2	A	4704	ADP	PA-O3A-PB-O3B

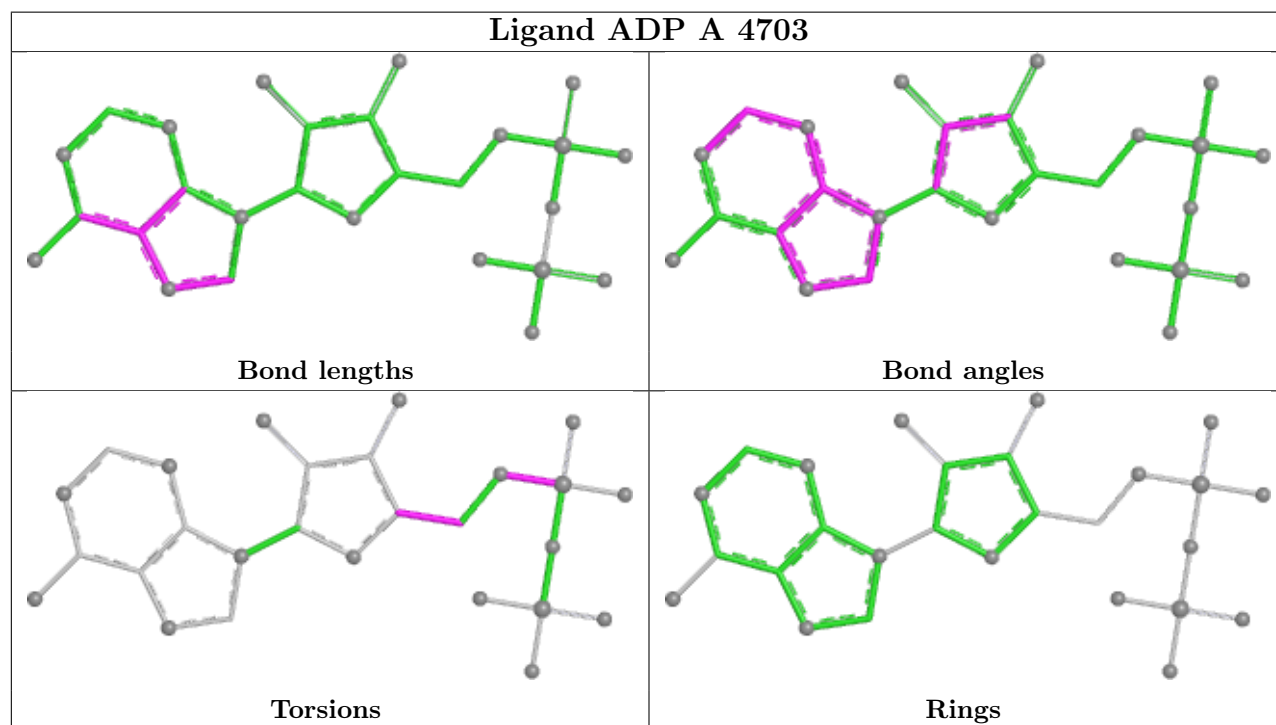
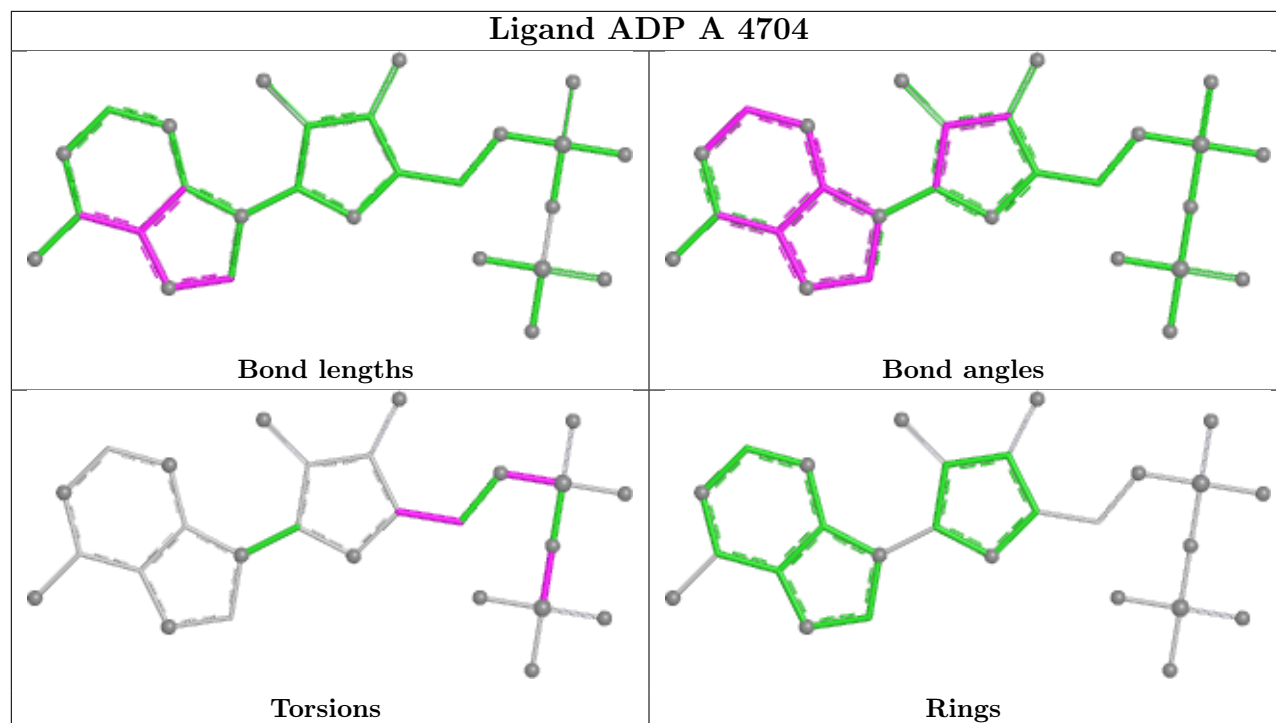
There are no ring outliers.

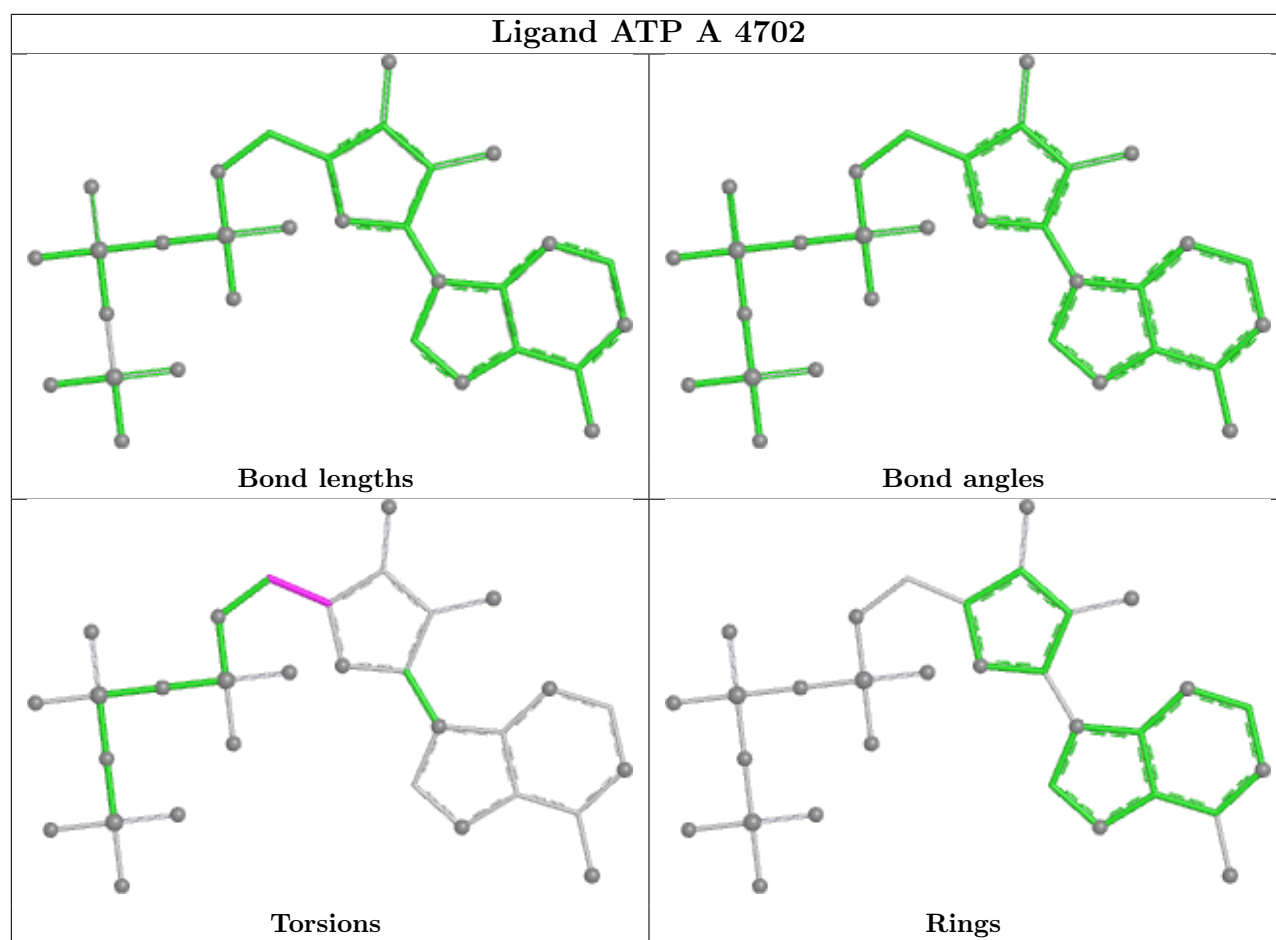
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4701	ADP	2	0
2	A	4703	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.

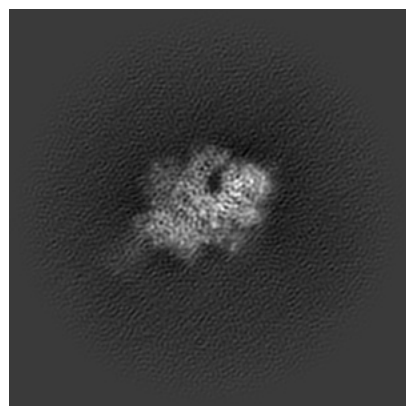
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44686. These allow visual inspection of the internal detail of the map and identification of artifacts.

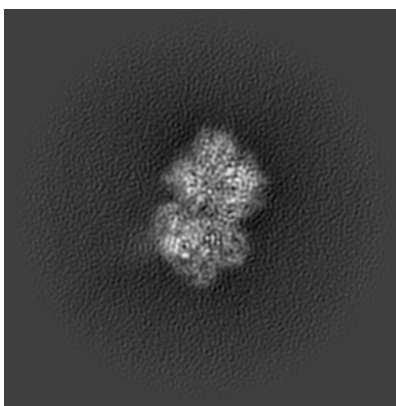
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

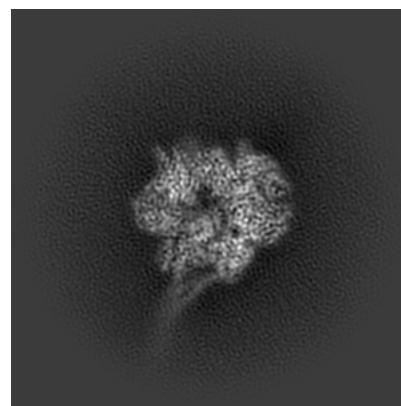
6.1.1 Primary map



X

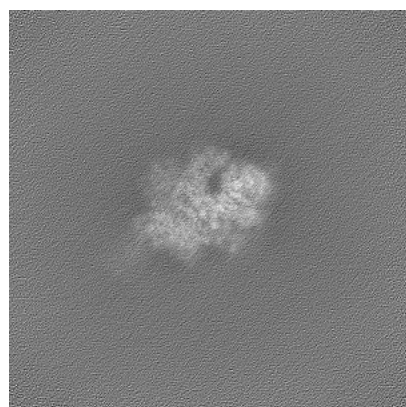


Y

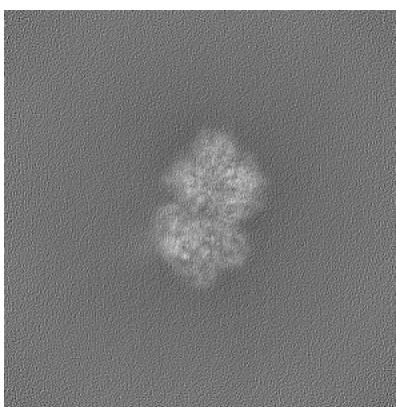


Z

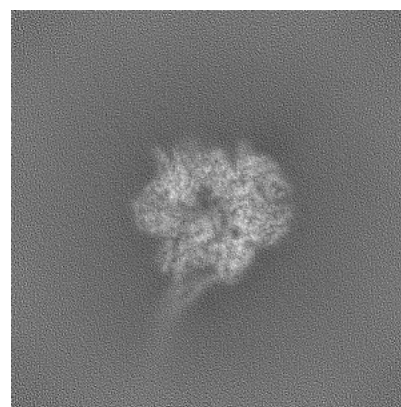
6.1.2 Raw map



X



Y

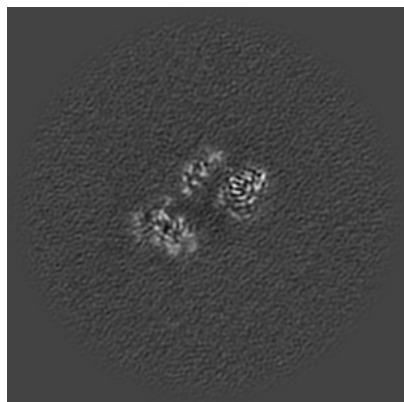


Z

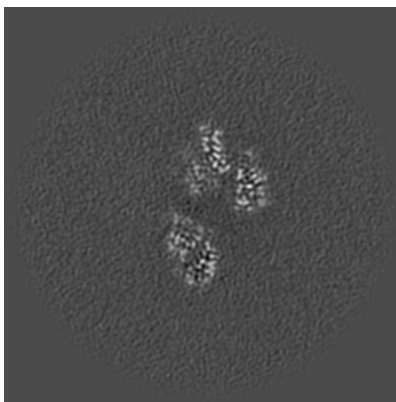
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

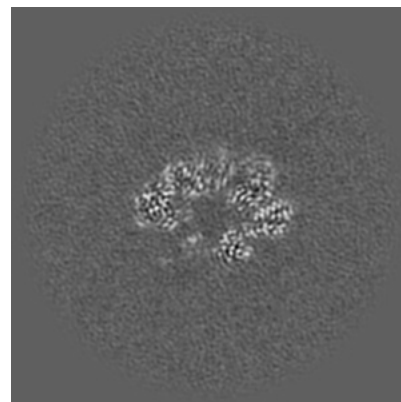
6.2.1 Primary map



X Index: 200

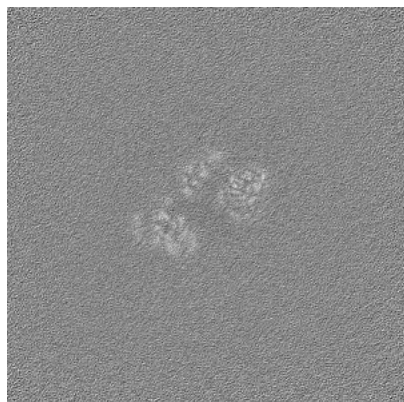


Y Index: 200

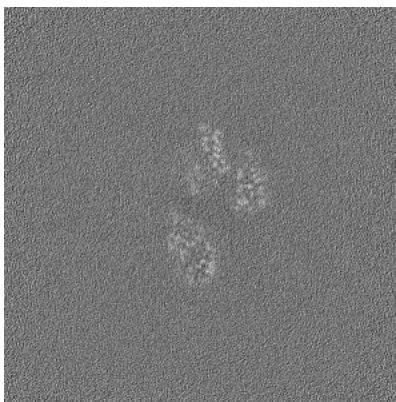


Z Index: 200

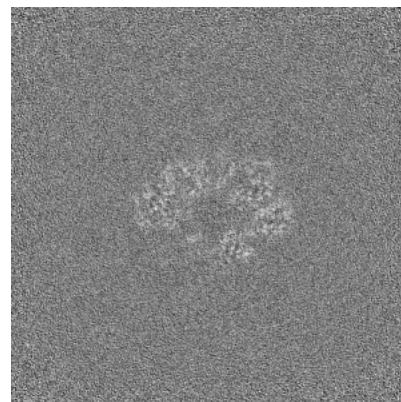
6.2.2 Raw map



X Index: 200



Y Index: 200

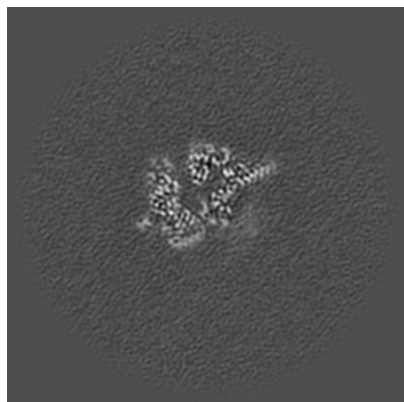


Z Index: 200

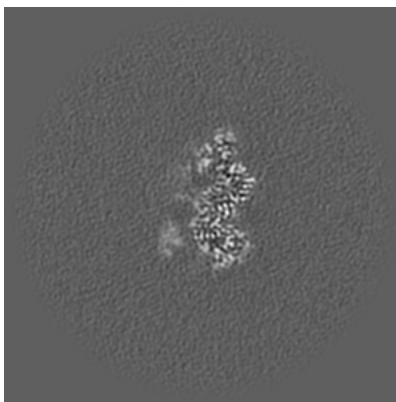
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

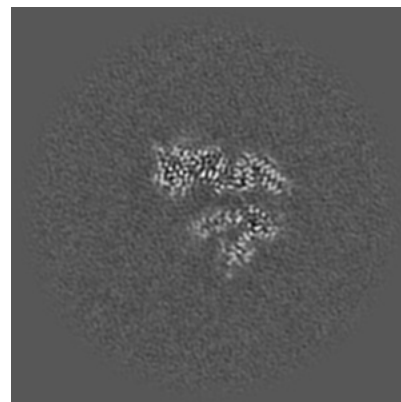
6.3.1 Primary map



X Index: 229

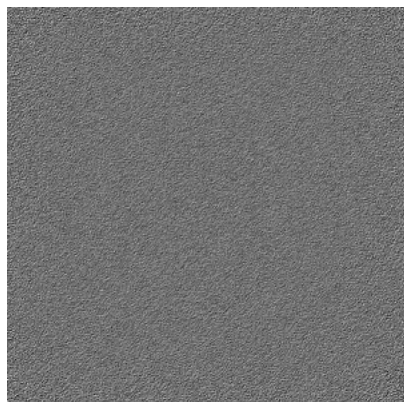


Y Index: 226

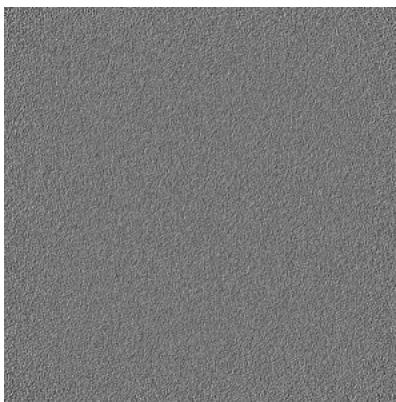


Z Index: 225

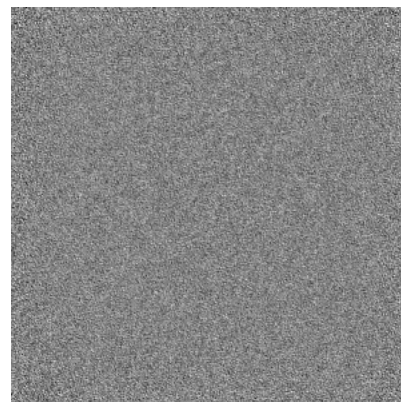
6.3.2 Raw map



X Index: 0



Y Index: 0

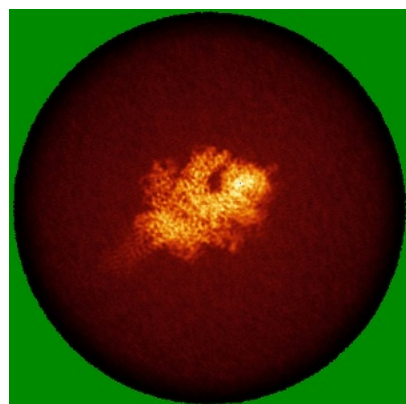


Z Index: 0

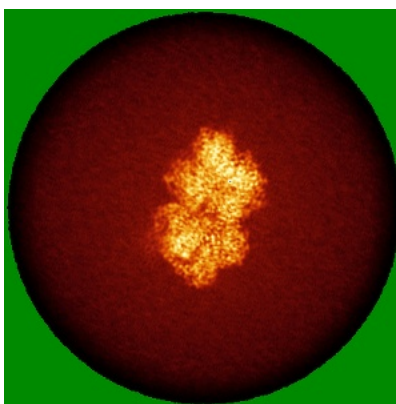
The images above show the largest variance slices of the map in three orthogonal directions.

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

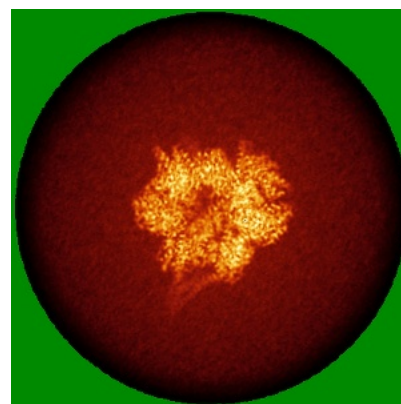
6.4.1 Primary map



X

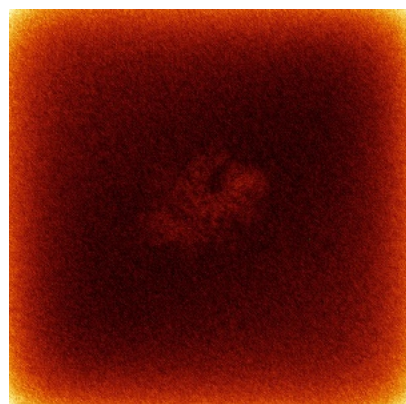


Y

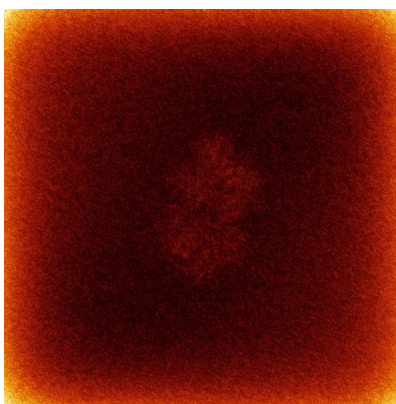


Z

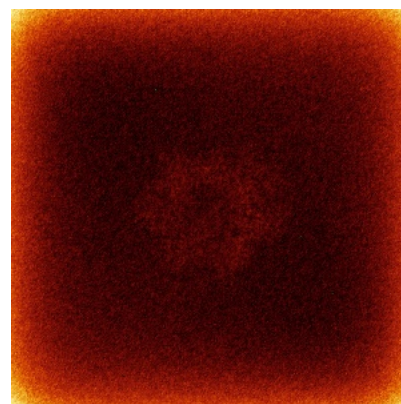
6.4.2 Raw map



X



Y



Z

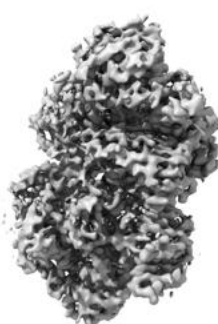
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

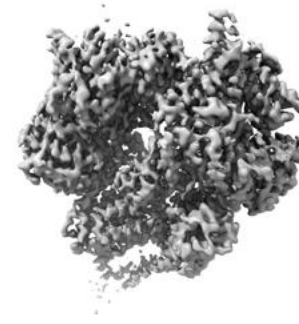
6.5.1 Primary map



X



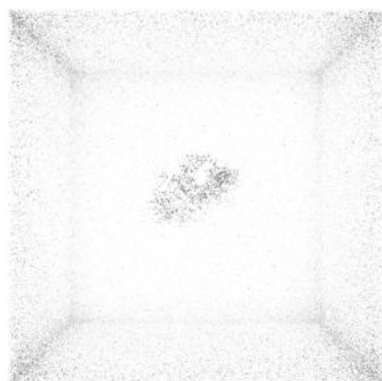
Y



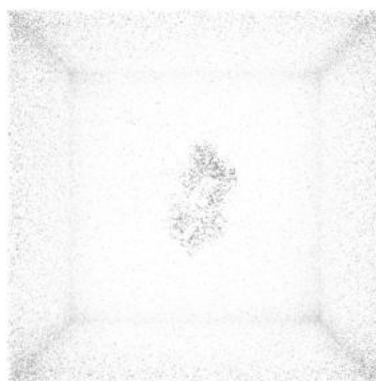
Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

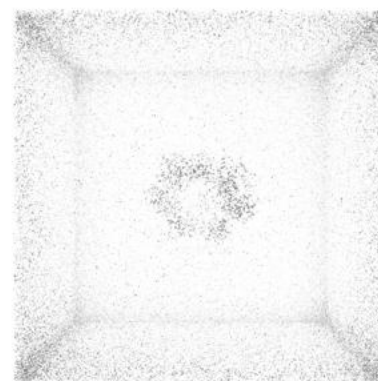
6.5.2 Raw map



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.

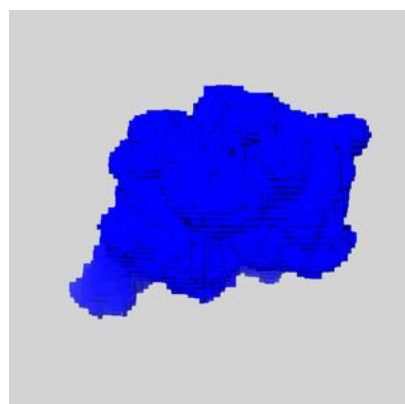
6.6 Mask visualisation [i](#)

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

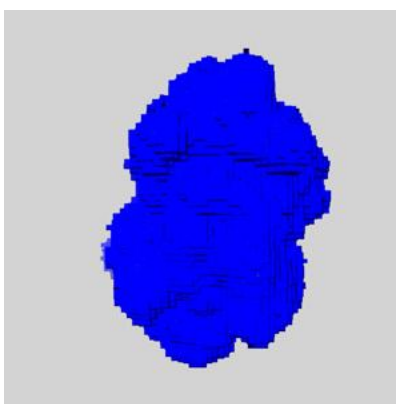
A mask typically either:

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

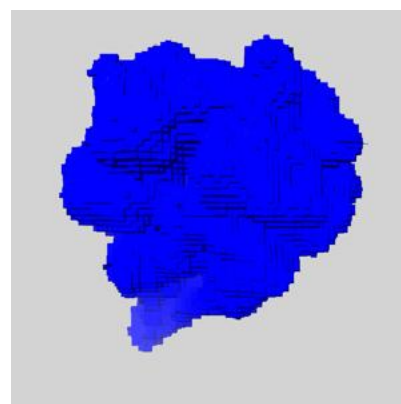
6.6.1 emd_44686_msk_1.map [i](#)



X



Y

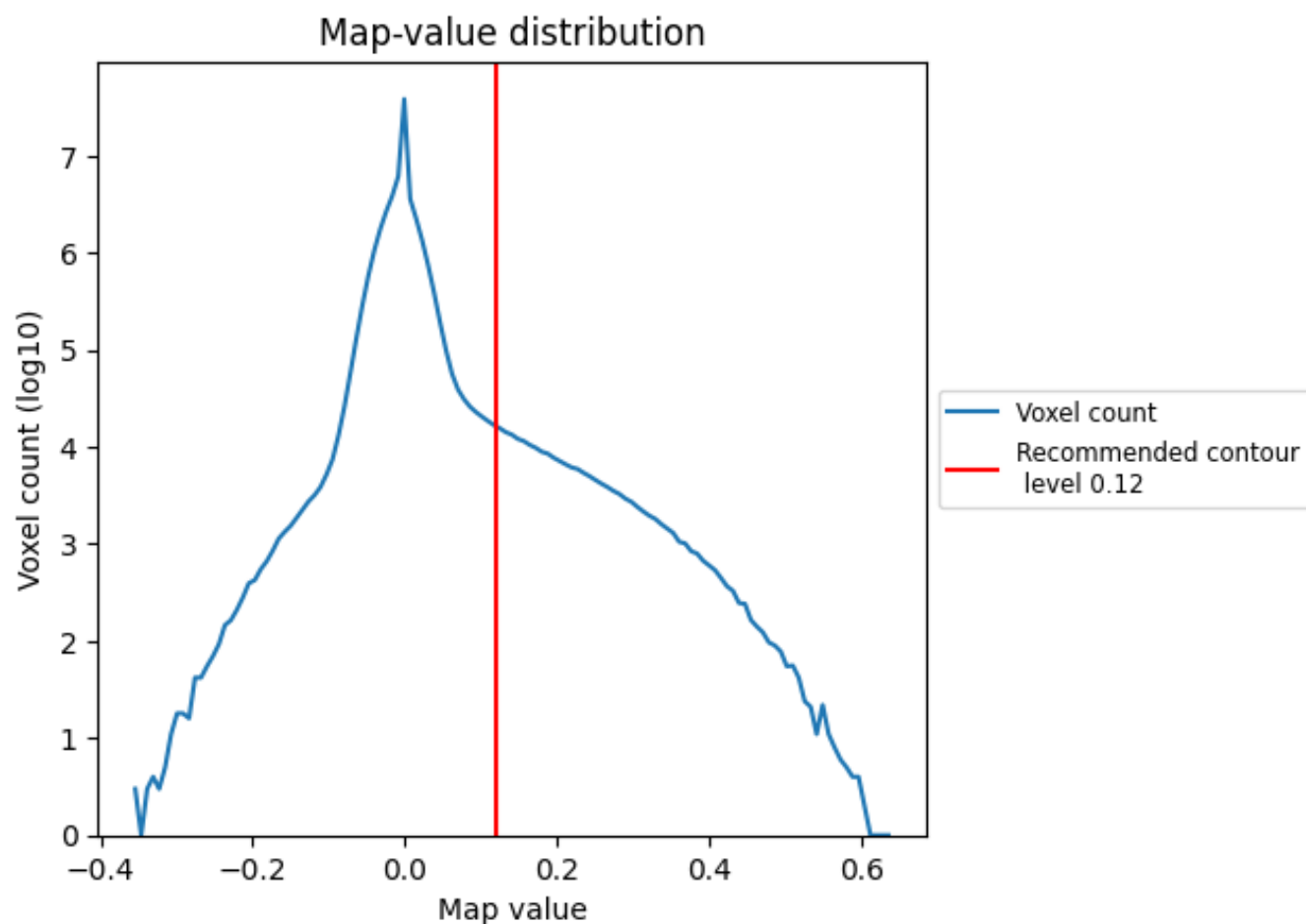


Z

7 Map analysis [i](#)

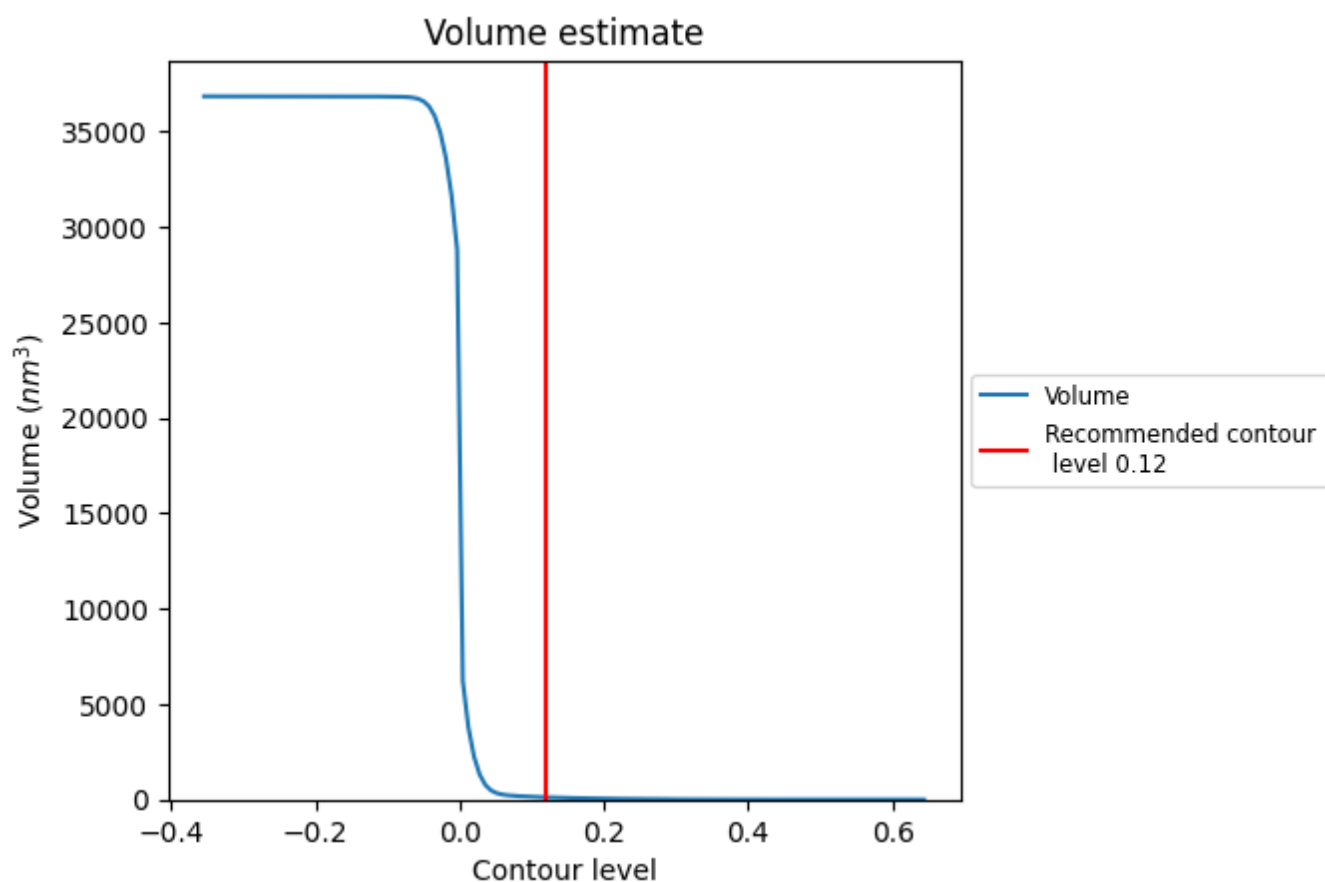
This section contains the results of statistical analysis of the map.

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.

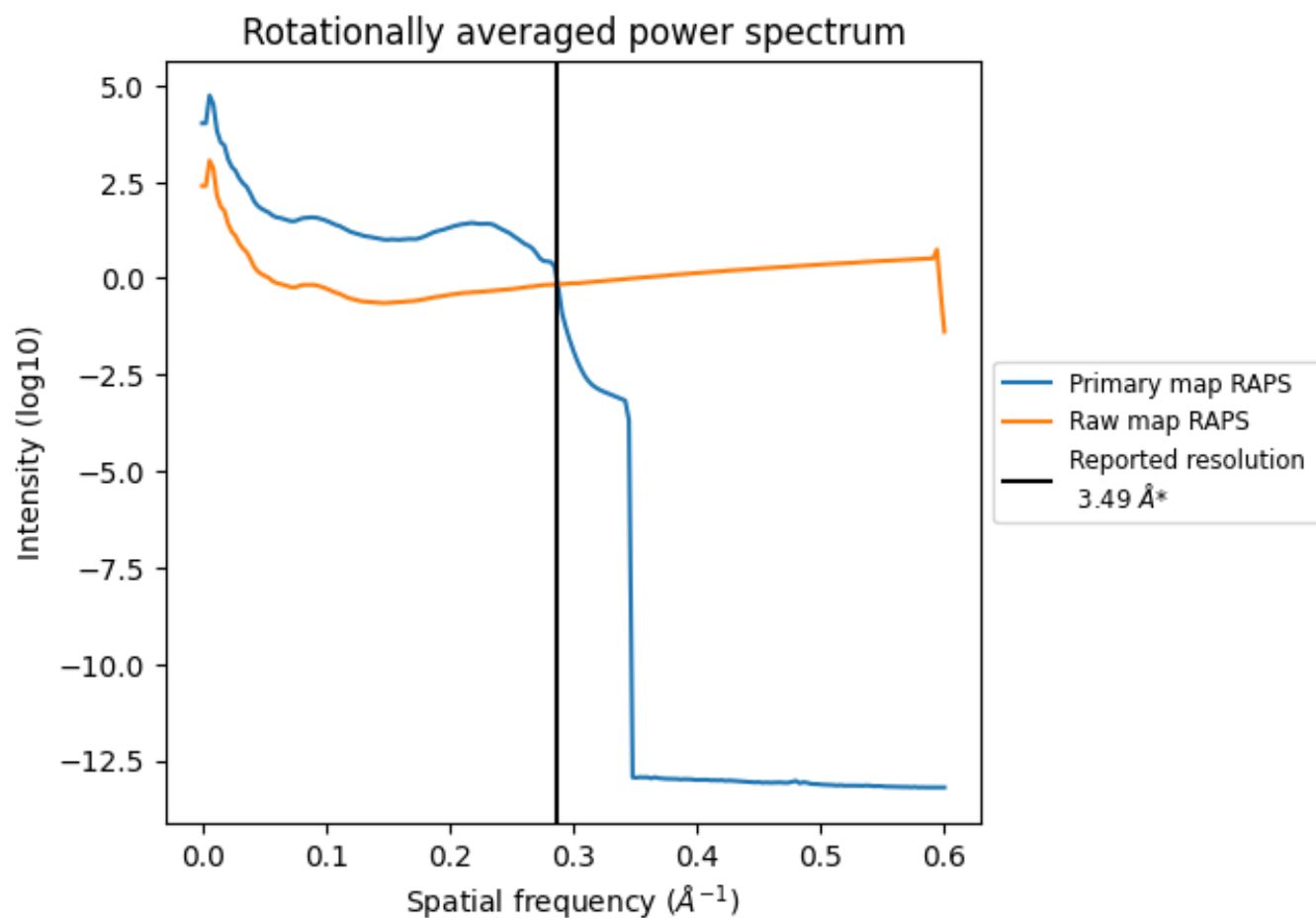
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 118 nm³; this corresponds to an approximate mass of 107 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 ⓘ

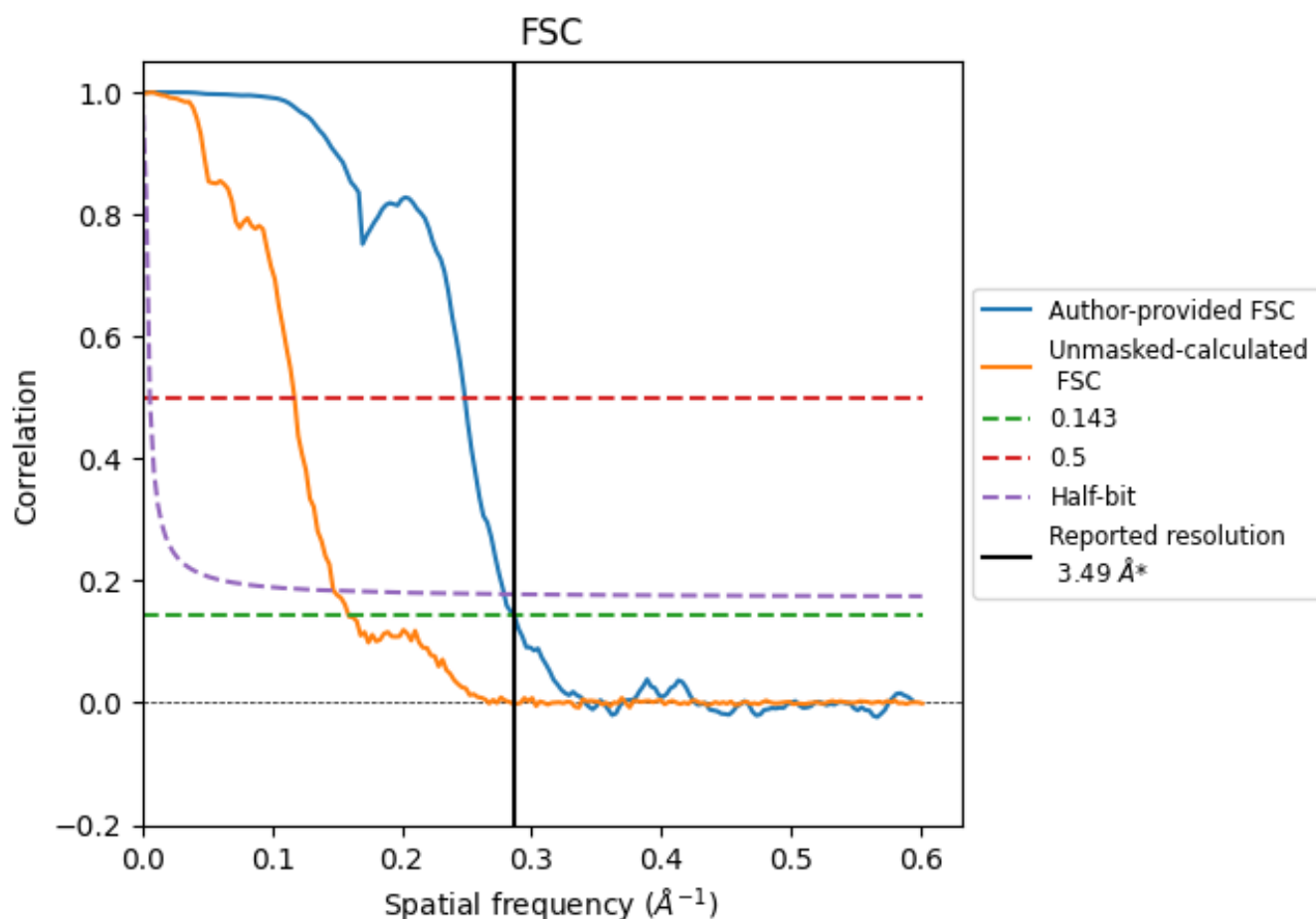


*Reported resolution corresponds to spatial frequency of 0.287 Å⁻¹

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 0.287 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

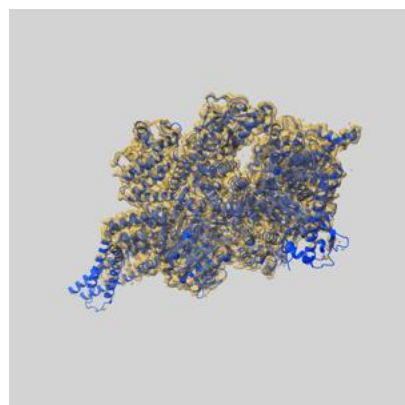
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.49	-	-
Author-provided FSC curve	3.49	4.02	3.59
Unmasked-calculated*	6.29	8.53	6.78

*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 6.29 differs from the reported value 3.49 by more than 10 %

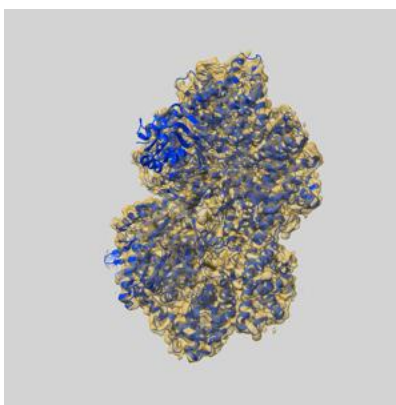
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44686 and PDB model 9BM3. Per-residue inclusion information can be found in section 3 on page 5.

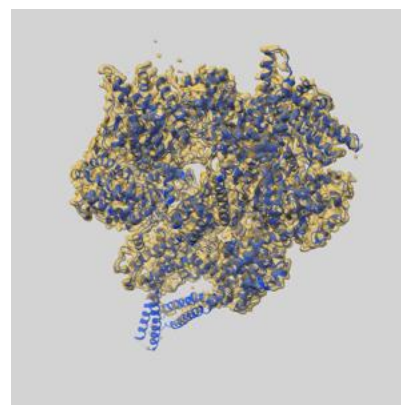
9.1 Map-model overlay [i](#)



X



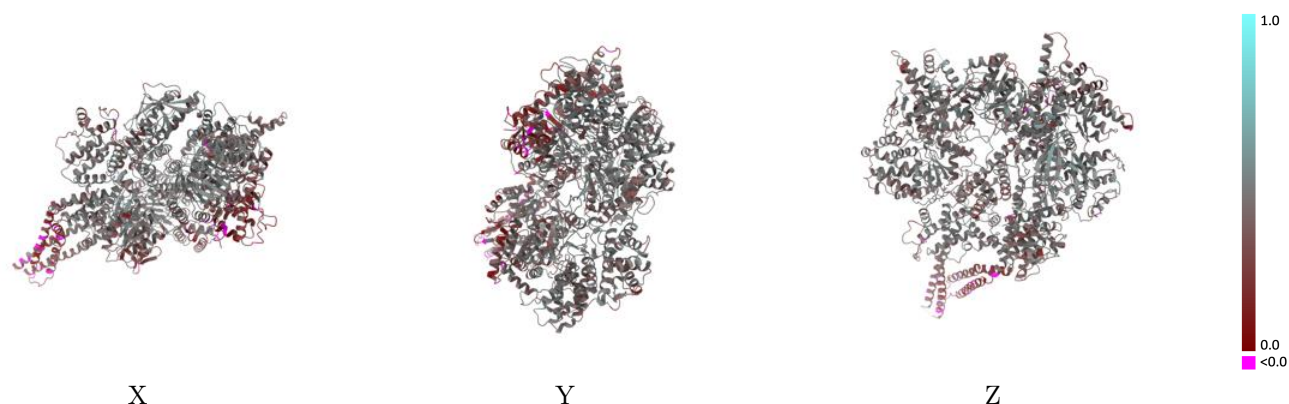
Y



Z

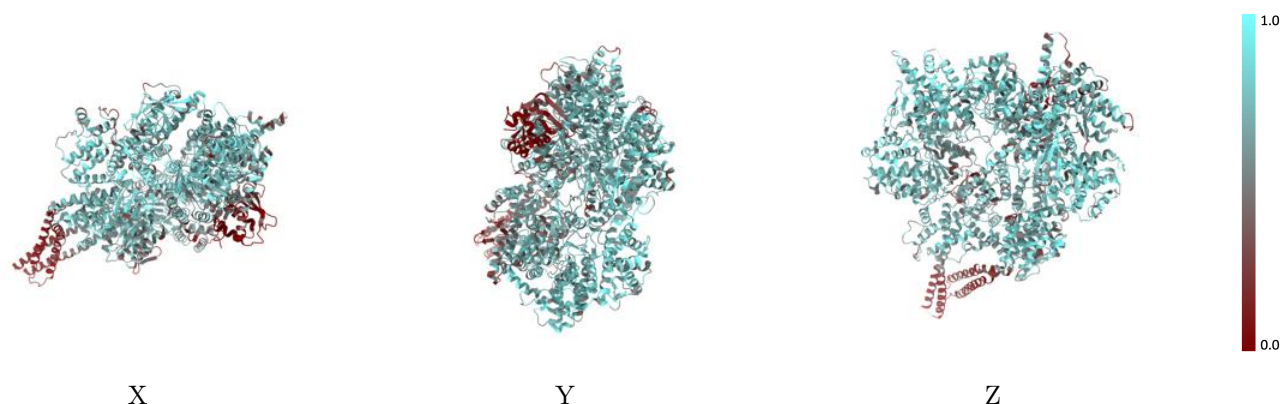
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



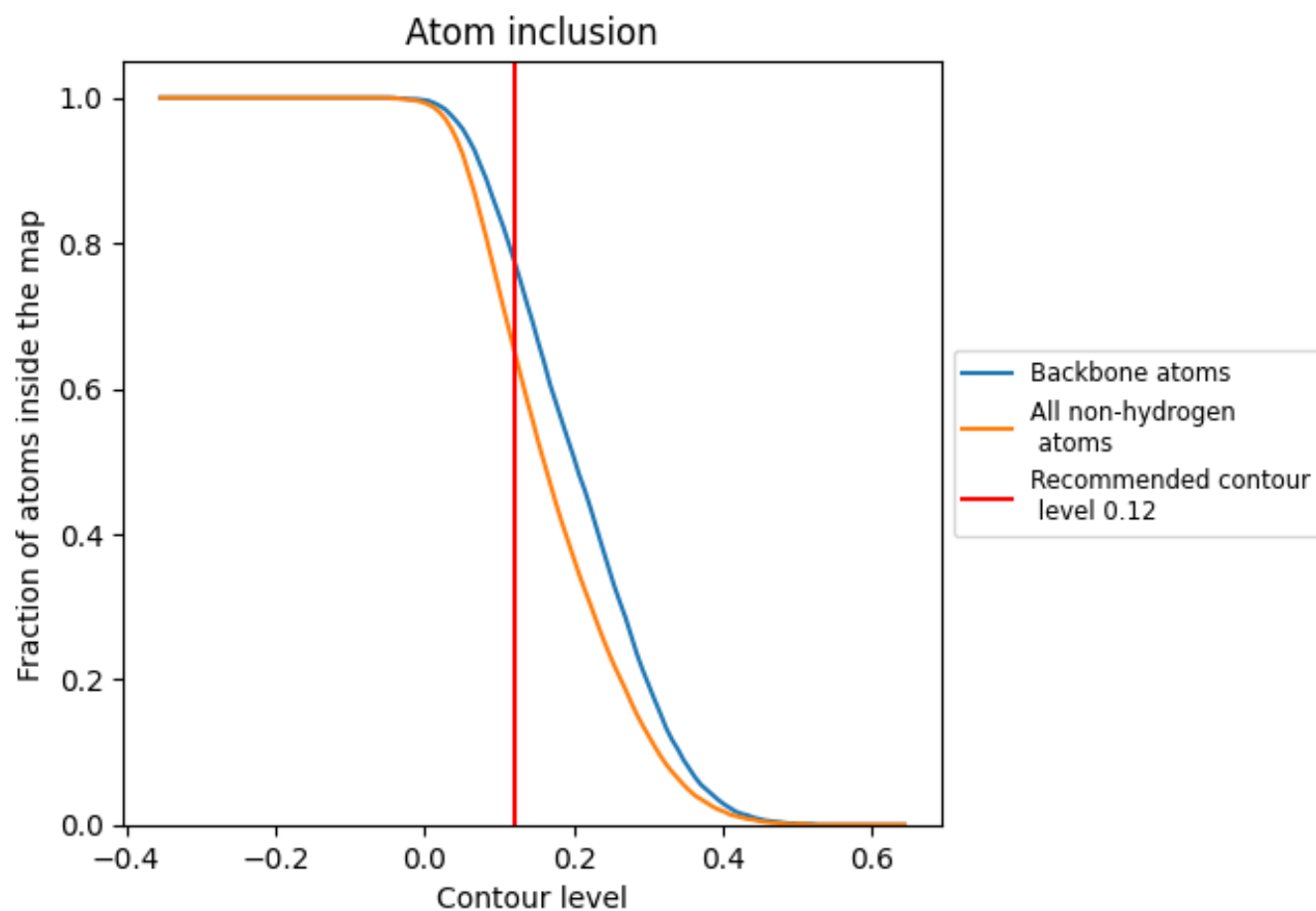
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 65% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6530	0.4170
A	0.6530	0.4170

