



## wwPDB EM Validation Summary Report ⓘ

Apr 24, 2025 – 01:21 PM EDT

PDB ID : 9BMM / pdb\_00009bmm  
EMDB ID : EMD-44703  
Title : State-4 of the motor domain from full-length human dynein-1 in 5mM AMPPNP  
Authors : Chai, P.; Zhang, K.  
Deposited on : 2024-05-02  
Resolution : 3.10 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

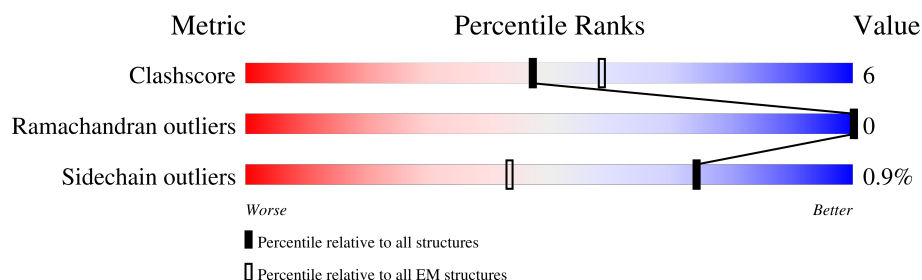
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	4646	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 23038 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	2859	22925	14595	3960	4257	113	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	

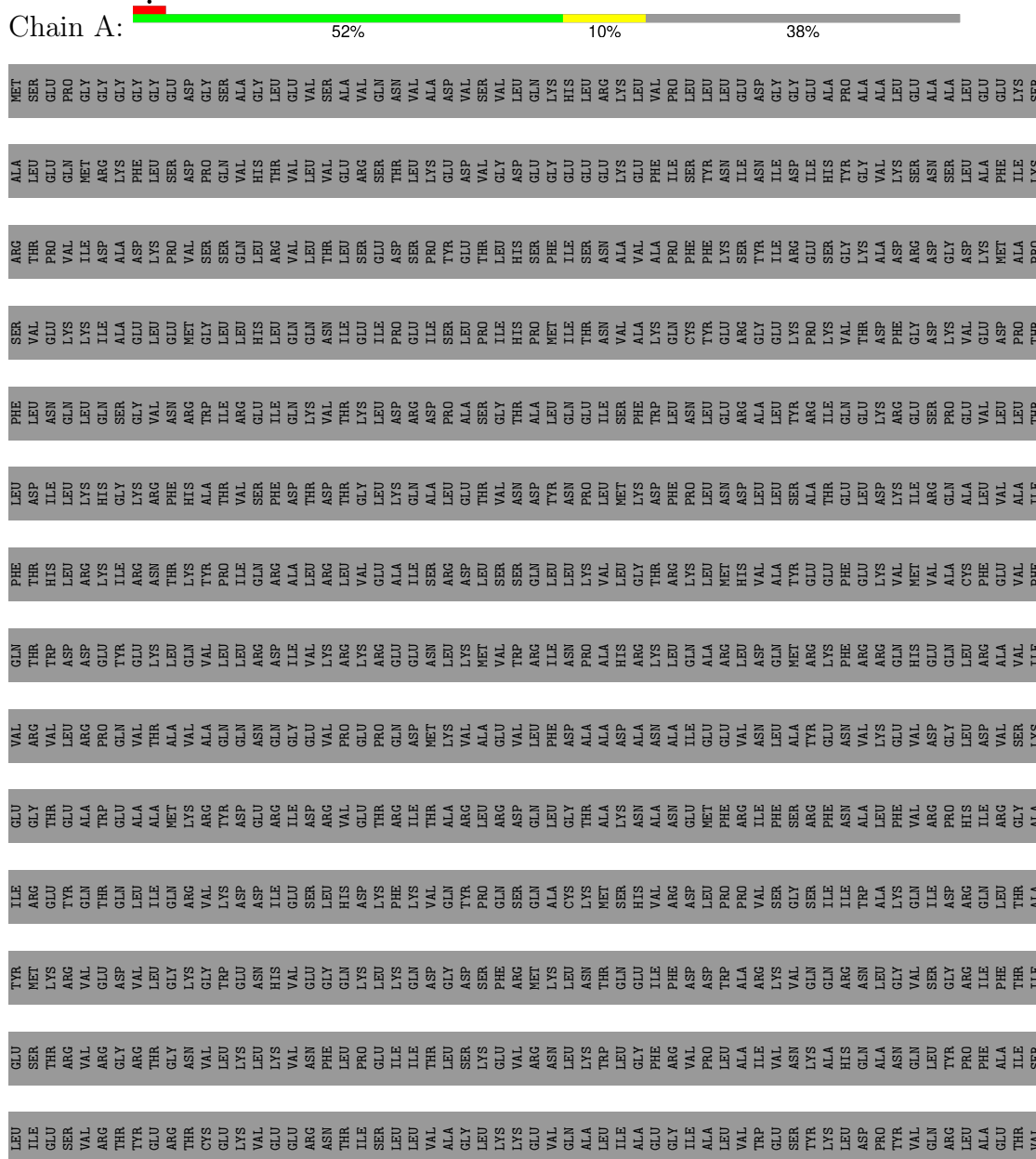
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

### 3 Residue-property plots

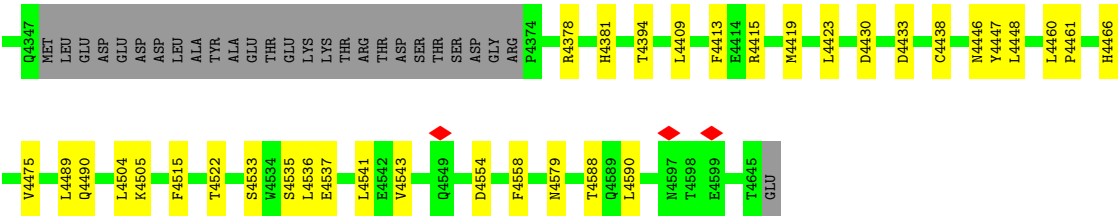
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Cytoplasmic dynein 1 heavy chain 1





P4149	S3939	13766	M3584	A3452	THR	ALA	T3211	Q3057	D2847	A2651	R2451	R2273
P4150	C3940	13767	T3600	V3453	THR	ASP	V3212	E3073	H2857	L2688	S2290	S2290
N4156	L3941	E3776	T3607	L3454	TRP	GLN	D3213	R3077	F2858	M2671	C2454	E2294
K3945	F3944	E3779	R3614	S3456	GLN	SER	E3217	D3078	E2864	T2676	M2481	R2298
D3946	K3945	E3457	F3614	E3457	ILE	VAL	R3218	T3081	K2865	Q2677	Q2482	G2305
L3947	V3638	A3458	A3460	A3458	ARG	LYS	R3219	R3088	R2869	F2682	I2483	D2306
K3950	V3638	A3459	A3460	A3459	SER	GLU	R3220	R3088	R2869	F2682	Q2485	L2486
L4179	V3644	ILE	A3460	ILE	ILE	ASP	R3221	R3088	R2869	F2682	V2307	D2308
L4183	V3644	ALA	A3461	ALA	MET	ASP	L3091	L3091	E2903	R2684	E2487	E2313
H4187	V3648	ASP	I3461	ASP	ARG	LYS	L3222	K3092	E2904	Q2685	I2498	L2319
R4196	L3649	MET	K3462	K3462	GLU	VAL	R3223	W3093	L2905	R2686	L2502	L2325
D4217	K3650	LEU	A3463	A3463	ASN	GLU	K3224	F3094	D2906	V2687	F2692	L2333
D4220	R3651	LYS	D3464	D3464	PHE	PRO	K3225	G3095	V2907	E2688	M2510	F2343
L4223	E3652	ARG	L3465	L3465	ILE	ALA	S3226	D3096	V2907	E2688	T2522	Q2346
L4224	R3653	VAL	A3466	A3466	PRO	VAL	K3227	V3097	I2925	F2692	S2506	L2346
A4227	R3654	GLU	E3469	E3469	THR	ILE	Q3228	F3109	L2933	D2717	M2510	L2333
L4233	L3661	PRO	E3469	E3469	ILE	GLU	K3229	T3110	L2933	D2717	M2510	L2333
S4234	T3662	LEU	E3469	E3469	VAL	ALA	L3229	T3110	L2933	D2717	M2510	L2333
L4237	T3663	ARG	E3469	E3469	ASN	GLN	E3230	M3113	I2936	K2721	I2518	F2343
L4238	L3664	GLU	E3469	E3469	PHE	ASN	V3231	M3113	I2936	K2721	I2518	F2343
L4239	G3665	LEU	E3469	E3469	SER	ALA	K3232	L3115	K2943	P2732	T2522	Q2346
L4240	D3666	GLN	E3469	E3469	ALA	VAL	N3233	E3116	K2943	P2732	T2522	Q2346
L4241	L3671	LYS	E3469	E3469	GLU	LYS	A3234	V3129	I2961	F2751	D2536	T2355
L4242	L3671	LEU	E3469	E3469	GLU	SER	A3235	Q3135	K2962	R2751	D2536	T2355
L4243	T3671	LYS	E3469	E3469	ILE	ILE	A3236	F3136	V2963	N2752	E2537	C2359
L4244	T3671	ASP	E3469	E3469	SER	LYS	N3237	F3137	H2964	R2753	E2537	C2359
L4245	S3680	GLU	E3469	E3469	ASP	GLN	A3238	R2965	R2965	R2763	S2542	E2366
L4246	T3681	ALA	E3469	E3469	ILE	GLN	K3239	K2966	K2966	R2773	W2548	L2369
L4247	T3681	LYS	E3469	E3469	ARG	HIS	D3238	Y2967	Y2967	V2774	W2548	L2369
L4248	S3694	ASP	E3469	E3469	GLU	VAL	K3239	R2968	T2968	V2774	W2548	L2369
L4249	R3695	ASP	E3469	E3469	LYS	VAL	L3240	R3140	C2969	E2775	V2562	D2388
L4250	L3708	GLN	E3469	E3469	MET	VAL	K3241	I3143	D2975	F2784	T2571	GLY
L4251	V3716	LYS	E3469	E3469	LYS	ARG	K3242	F3149	N2987	Y2792	L2572	GLU
L4252	T3723	ALA	E3469	E3469	ASN	MET	MET	F3149	N2987	Y2792	L2572	GLU
L4253	T3723	ASN	E3469	E3469	MET	ASN	VAL	L3154	D2995	I2793	D2573	ASP
L4254	S3729	VAL	E3469	E3469	SER	ASN	LYS	L3154	E2996	Y2794	T2574	ALA
L4255	D3730	GLU	E3469	E3469	ASN	PRO	ASP	R3160	S2997	V2803	R2576	GLN
L4256	L3731	GLN	E3469	E3469	PRO	ALA	GLN	L3161	N2998	R2804	R2576	ARG
L4257	A3517	MET	E3469	E3469	SER	ALA	ALA	A3162	V2999	L2816	L2581	ARG
L4258	L3521	ILE	E3469	E3469	TYR	VAL	VAL	K3163	L3000	L2816	L2581	ARG
L4259	R3525	ASP	E3469	E3469	ASN	LYS	GLU	T3168	G3003	L2821	P2590	LYS
L4260	R3525	GLU	E3469	E3469	TYR	LYS	LYS	T3171	E3006	L2822	L2593	GLY
L4261	Q3542	GLU	E3469	E3469	ILE	ALA	LYS	T3172	R3007	W2825	F2606	ASP
L4262	F3543	ALA	E3469	E3469	VAL	GLU	VAL	V3017	V2617	Q2834	V2617	GLY
L4263	F3543	SER	E3469	E3469	ASN	SER	MET	I3180	D2835	D2835	S2623	GLU
L4264	T3545	ILE	E3469	E3469	ARG	ILE	SER	I3180	R2836	R2836	S2623	GLU
L4265	D3546	ARG	E3469	E3469	ALA	CYS	GLU	A3184	L3020	L2837	P2628	ALA
L4266	L3547	SER	E3469	E3469	SER	LEU	ILE	A3184	L3020	L2837	P2628	ALA
L4267	L3553	LEU	E3469	E3469	LEU	LEU	GLN	S3192	M3043	V2838	K2633	ALA
L4268	D3557	TYR	E3469	E3469	ALA	LEU	GLN	S3192	M3043	V2838	K2633	ALA
L4269	L3557	LYS	E3469	E3469	GLY	GLY	GLN	N3202	L3044	E2840	R2642	ALA
L4270	L3557	LYS	E3469	E3469	CYS	GLY	GLN	N3202	L3044	E2840	R2642	ALA
L4271	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4272	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4273	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4274	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4275	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4276	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4277	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4278	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4279	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4280	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4281	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4282	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4283	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4284	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4285	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4286	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4287	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4288	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4289	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4290	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4291	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4292	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4293	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4294	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4295	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4296	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4297	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4298	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4299	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4300	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4301	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4302	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4303	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4304	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4305	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4306	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4307	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4308	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4309	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4310	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4311	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4312	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4313	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4314	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4315	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4316	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4317	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4318	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4319	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4320	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4321	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4322	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4323	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4324	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4325	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4326	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4327	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4328	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4329	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4330	L3557	PRO	E3469	E3469	PRO	SER	LEU	K3207	L3050	E2842	V2433	ALA
L4331	L3557											





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	92310	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	2.145	Depositor
Minimum map value	-1.237	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.25	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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ADP, 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	0.26	0/23409	0.46	1/31728 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	3788	ASP	CB-CG-OD2	5.25	123.03	118.30

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	22925	0	22998	265	0
2	A	81	0	36	2	0
3	A	31	0	12	0	0
4	A	1	0	0	0	0
All	All	23038	0	23046	265	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 265 close contacts within the same asymmetric unit are listed below, sorted by

their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.63	0.81
1:A:2115:LYS:HD2	1:A:2118:ARG:HH21	1.46	0.79
1:A:1914:GLU:HG3	2:A:4701:ADP:H2'	1.62	0.79
1:A:1879:LEU:HD11	1:A:1914:GLU:HB3	1.66	0.76
1:A:2834:GLN:NE2	1:A:2847:ASP:OD2	2.21	0.74

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	2851/4646 (61%)	2809 (98%)	42 (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	2532/4125 (61%)	2510 (99%)	22 (1%)	75	88

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3661	LEU
1	A	3793	GLU
1	A	3729	SER
1	A	3925	GLN
1	A	2573	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2752	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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	ADP	A	4704	-	24,29,29	0.88	0	29,45,45	1.18	2 (6%)
3	ATP	A	4702	4	28,33,33	0.75	0	34,52,52	0.80	1 (2%)
2	ADP	A	4703	-	24,29,29	0.89	0	29,45,45	1.23	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ADP	A	4701	-	24,29,29	0.73	0	29,45,45	0.78	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	4704	-	-	1/12/32/32	0/3/3/3
3	ATP	A	4702	4	-	0/18/38/38	0/3/3/3
2	ADP	A	4703	-	-	5/12/32/32	0/3/3/3
2	ADP	A	4701	-	-	0/12/32/32	0/3/3/3

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4703	ADP	N3-C2-N1	-3.69	123.66	128.67
2	A	4704	ADP	N3-C2-N1	-3.56	123.83	128.67
2	A	4704	ADP	C4-C5-N7	-2.55	106.64	109.34
2	A	4703	ADP	C4-C5-N7	-2.47	106.72	109.34
3	A	4702	ATP	C5-C6-N6	2.34	123.88	120.31

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

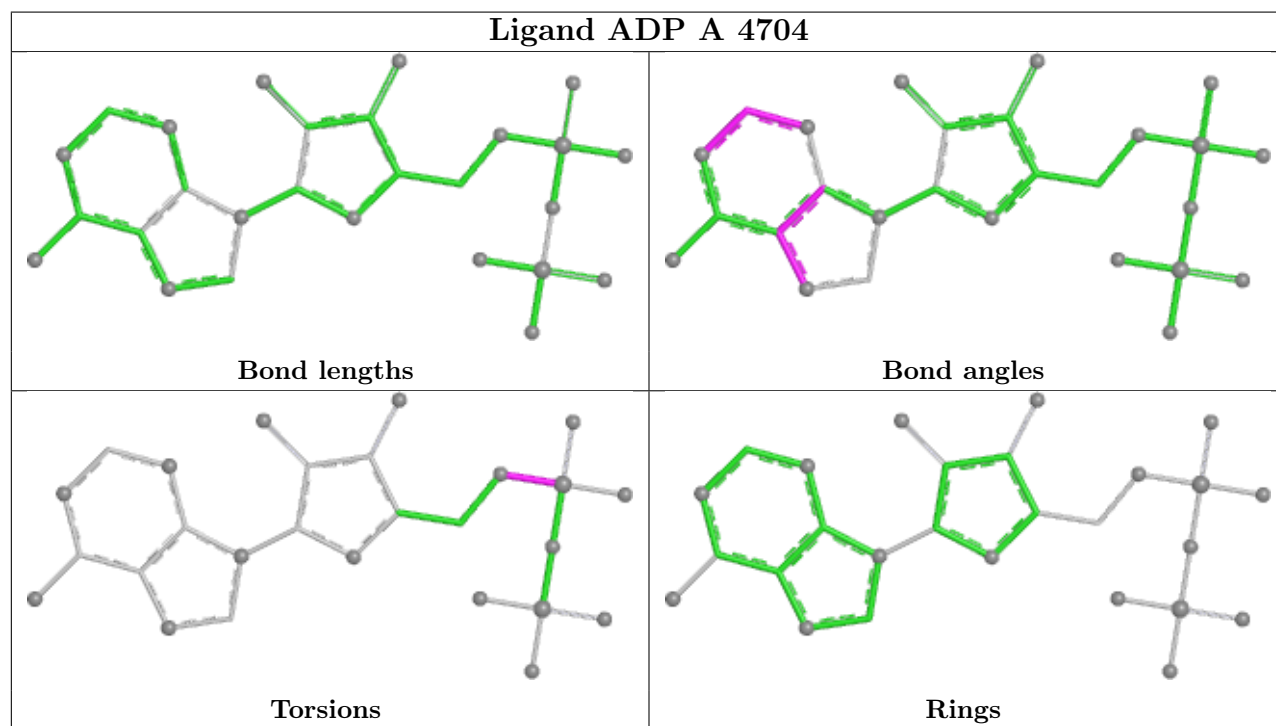
Mol	Chain	Res	Type	Atoms
2	A	4703	ADP	C5'-O5'-PA-O1A
2	A	4703	ADP	C5'-O5'-PA-O3A
2	A	4703	ADP	O4'-C4'-C5'-O5'
2	A	4703	ADP	C3'-C4'-C5'-O5'
2	A	4703	ADP	C5'-O5'-PA-O2A

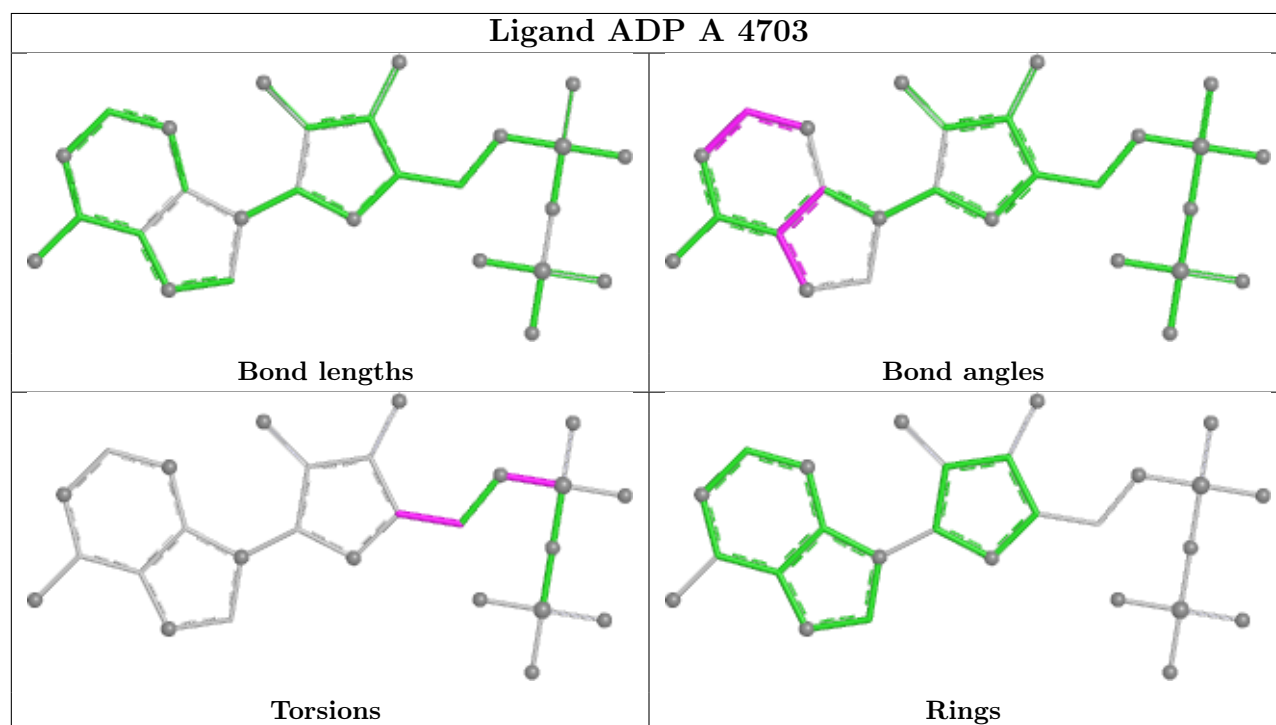
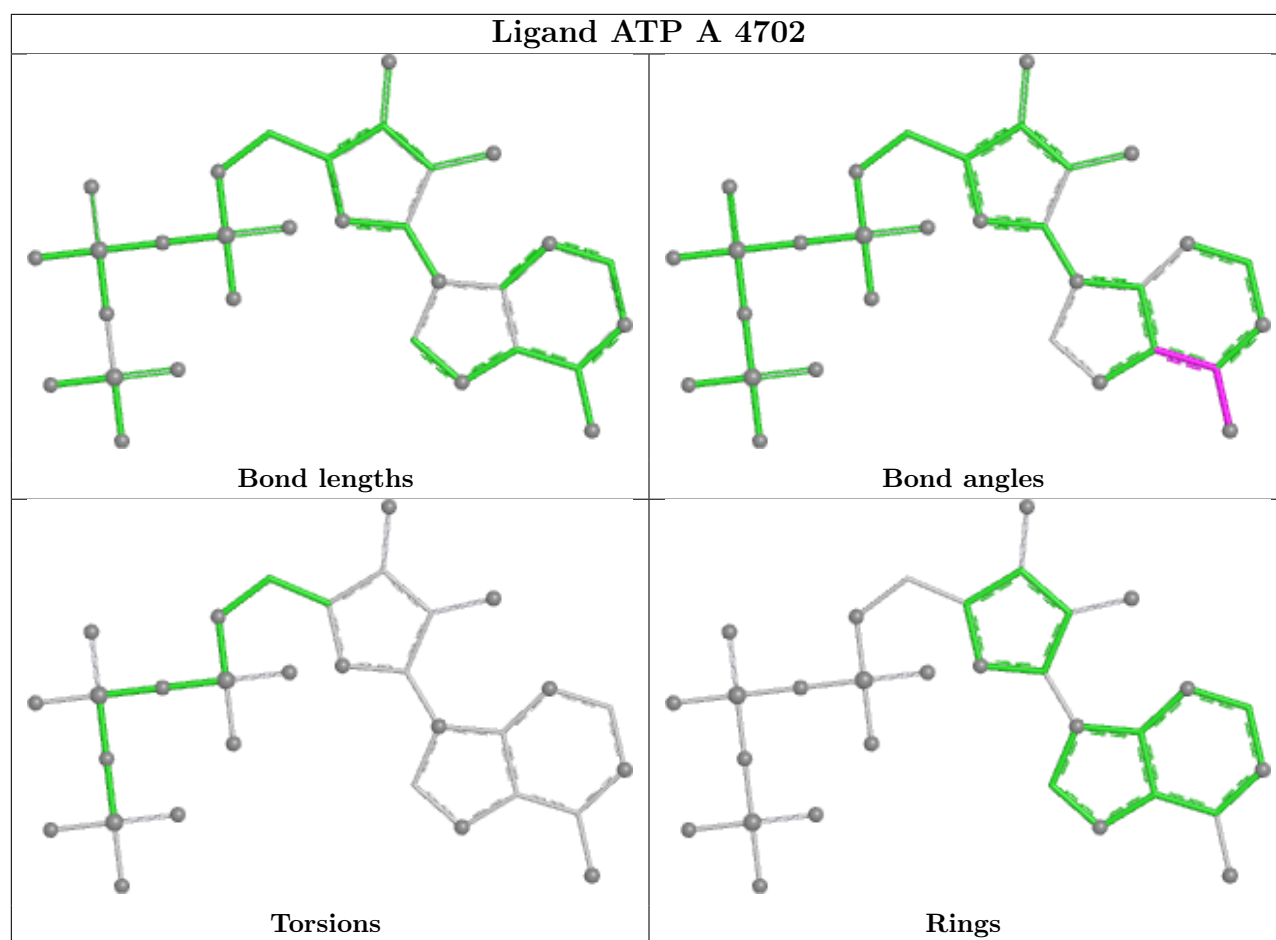
There are no ring outliers.

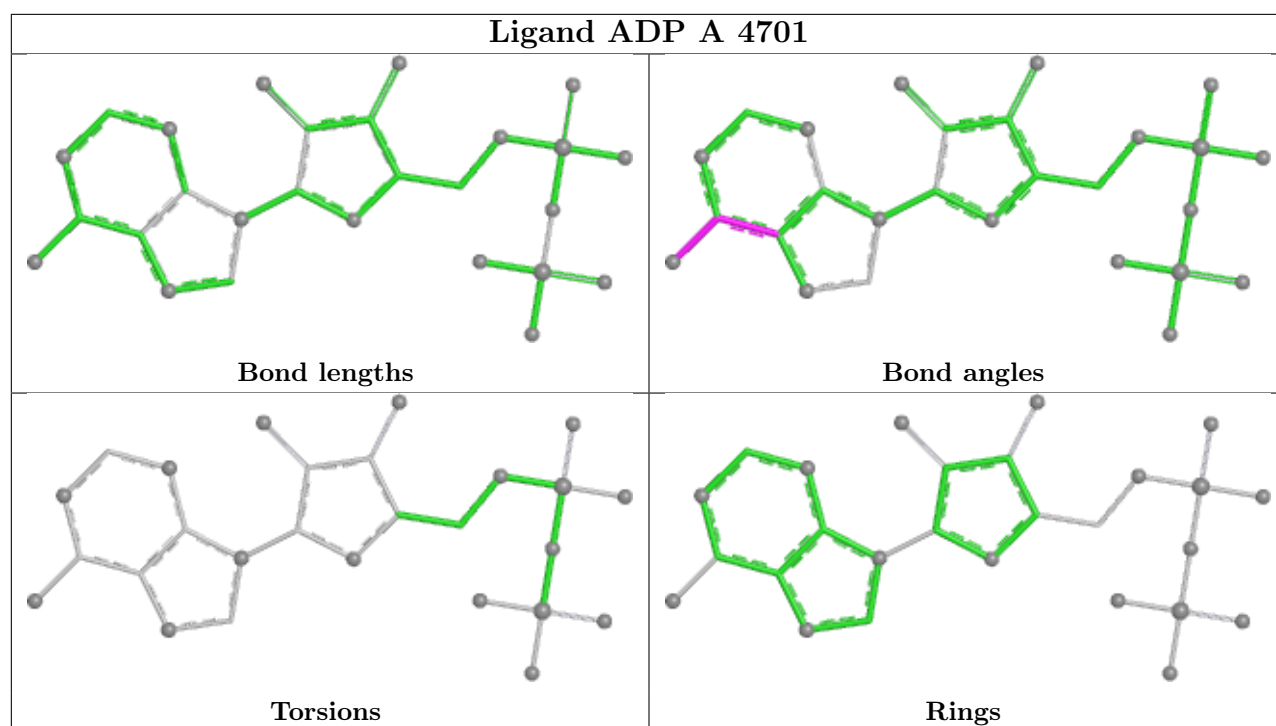
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4704	ADP	1	0
2	A	4701	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



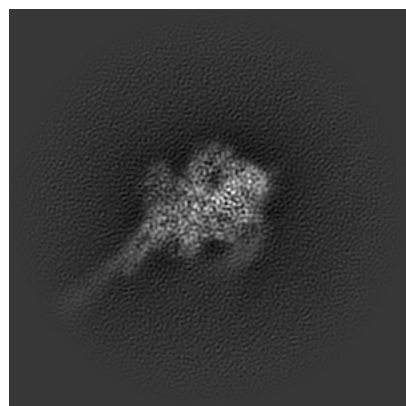
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44703. These allow visual inspection of the internal detail of the map and identification of artifacts.

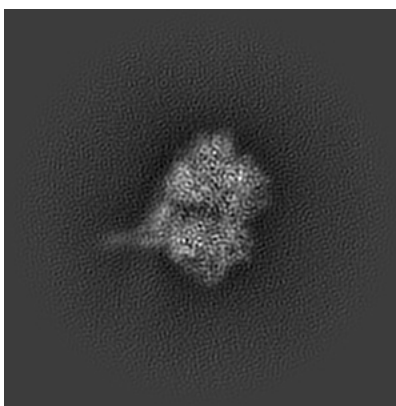
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

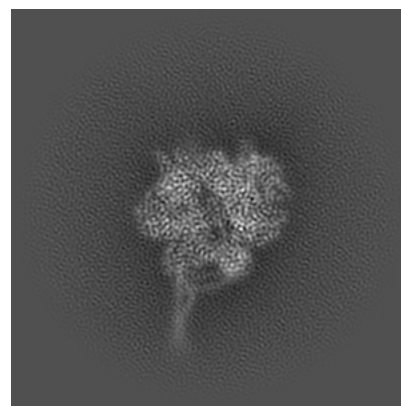
#### 6.1.1 Primary map



X

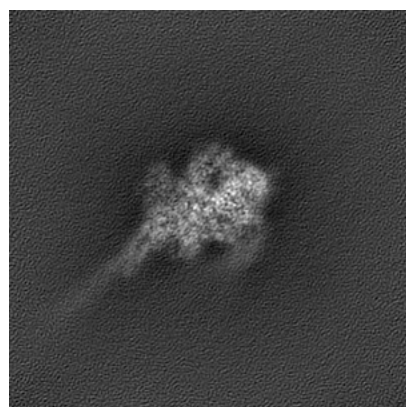


Y

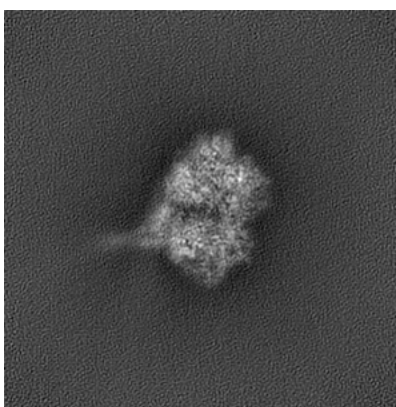


Z

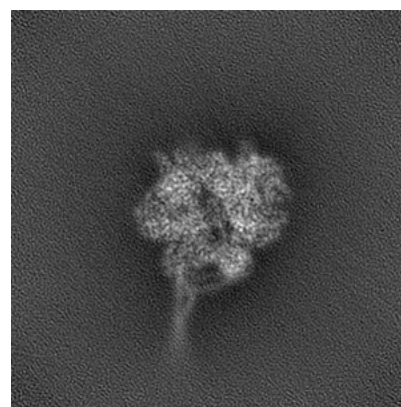
#### 6.1.2 Raw map



X



Y

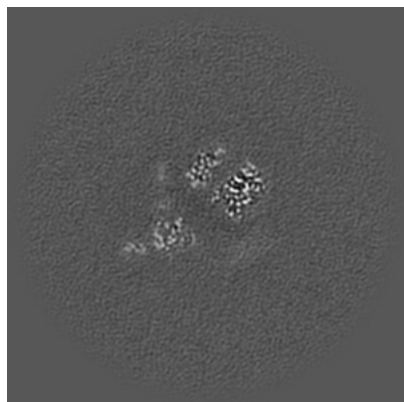


Z

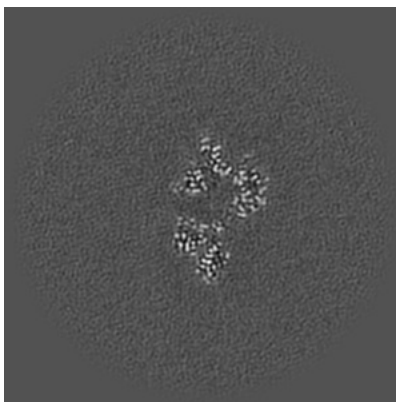
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

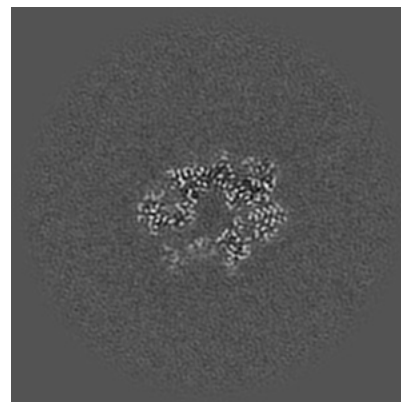
### 6.2.1 Primary map



X Index: 128

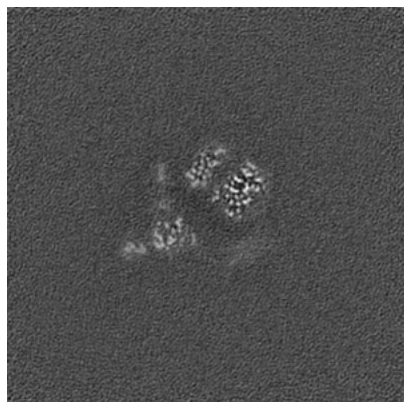


Y Index: 128

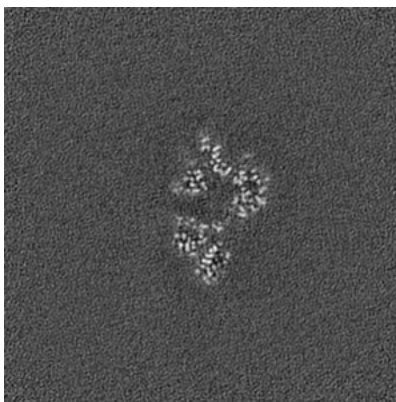


Z Index: 128

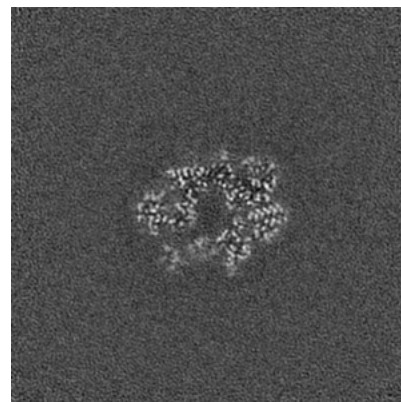
### 6.2.2 Raw map



X Index: 128



Y Index: 128

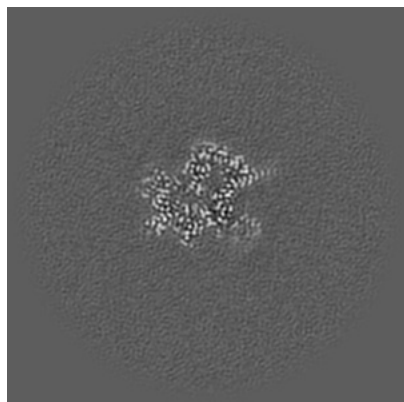


Z Index: 128

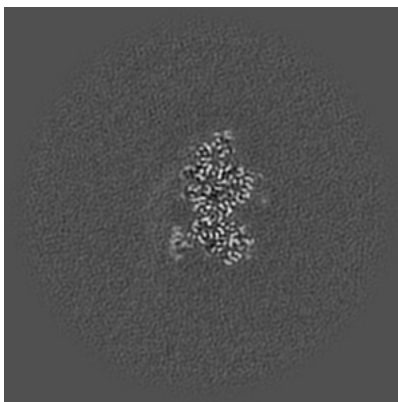
The images above show central slices of the map in three orthogonal directions.

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

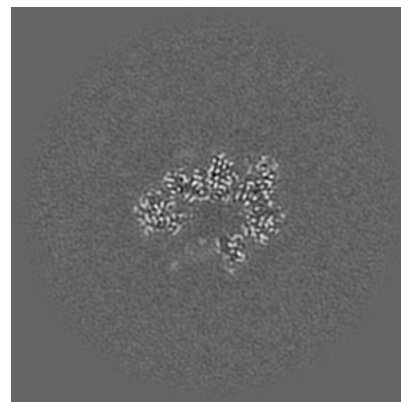
### 6.3.1 Primary map



X Index: 146

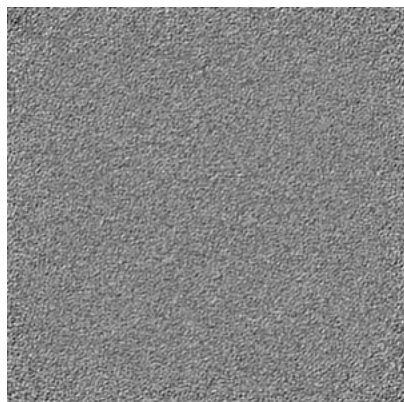


Y Index: 143

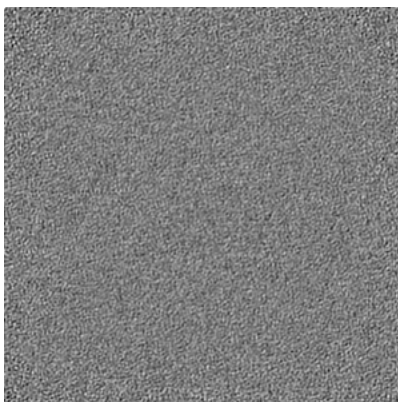


Z Index: 131

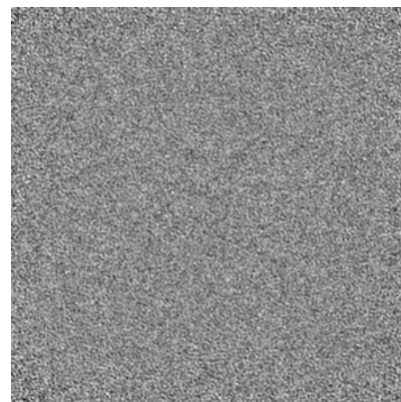
### 6.3.2 Raw map



X Index: 0



Y Index: 0



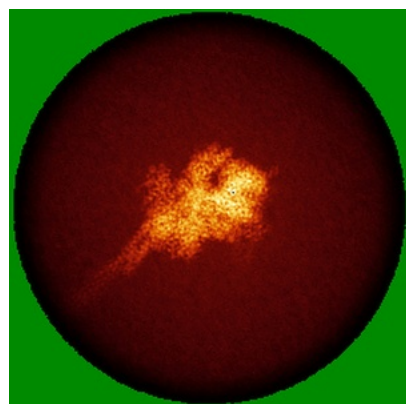
Z Index: 0

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

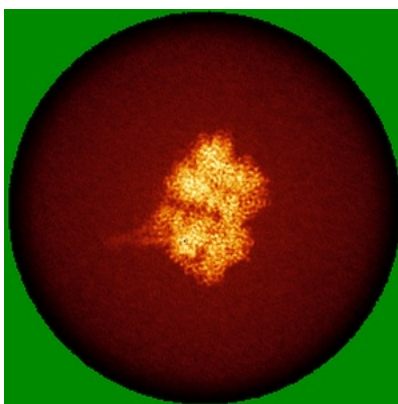


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

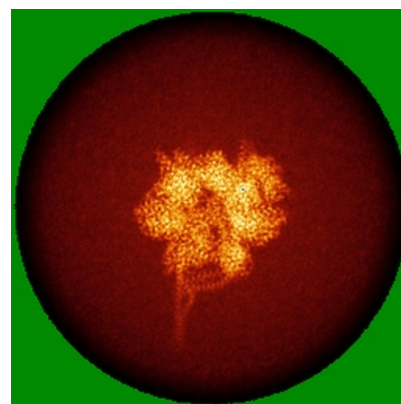
### 6.4.1 Primary map



X

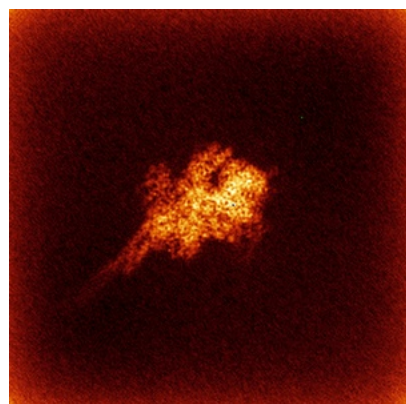


Y

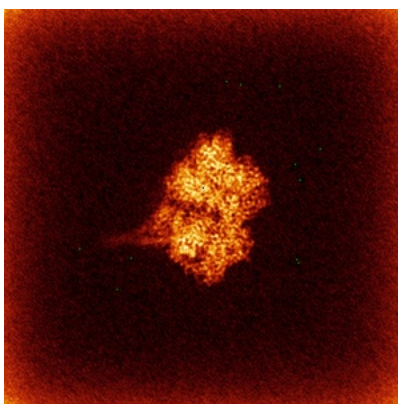


Z

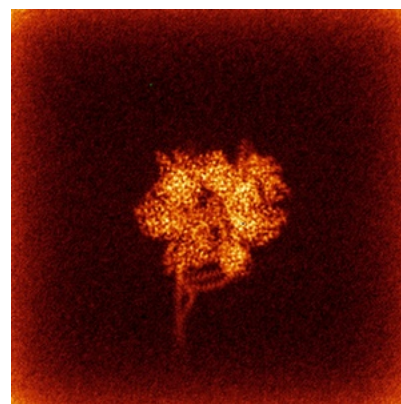
### 6.4.2 Raw map



X



Y

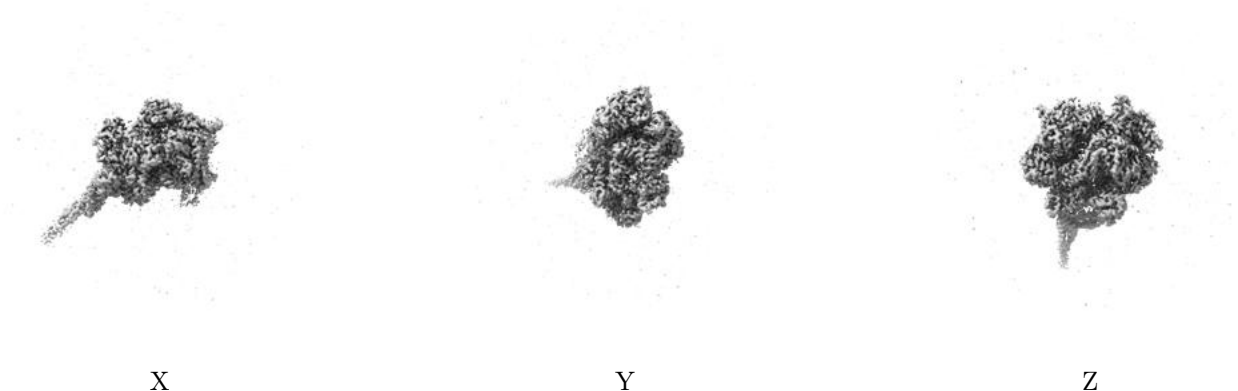


Z

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.

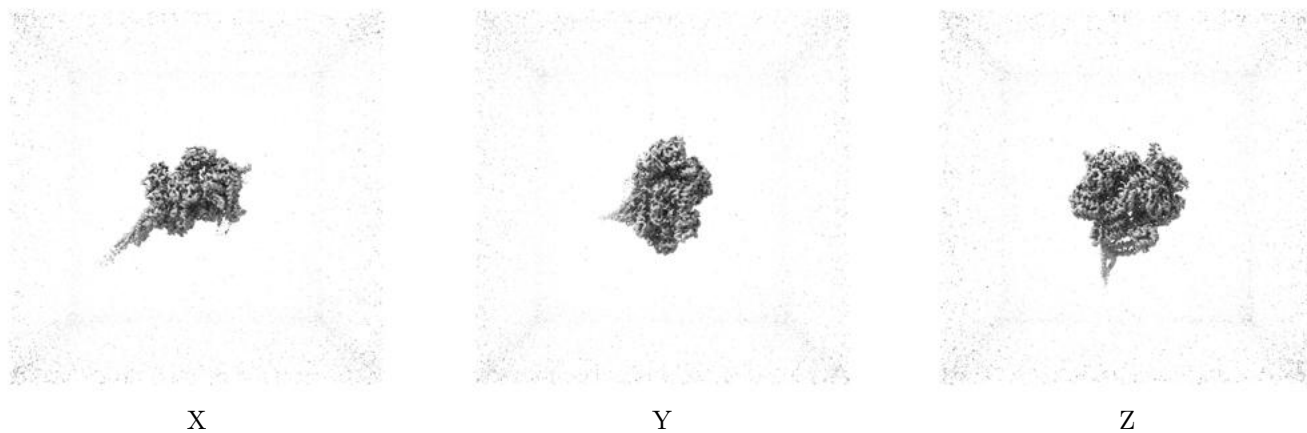
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

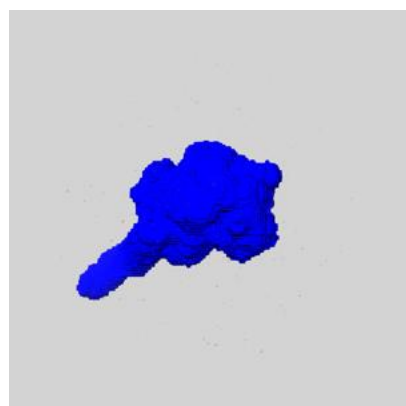
## 6.6 Mask visualisation [i](#)

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

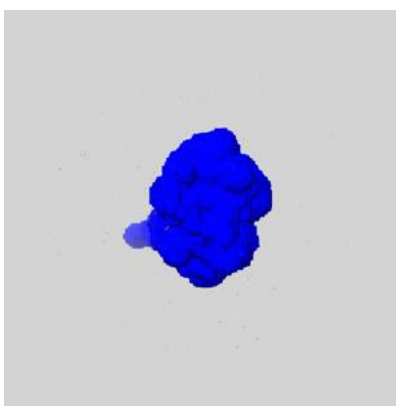
A mask typically either:

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

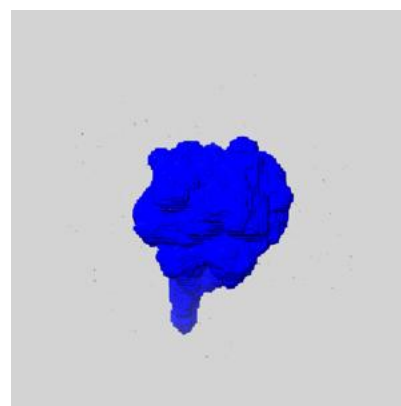
### 6.6.1 emd\_44703\_msk\_1.map [i](#)



X



Y

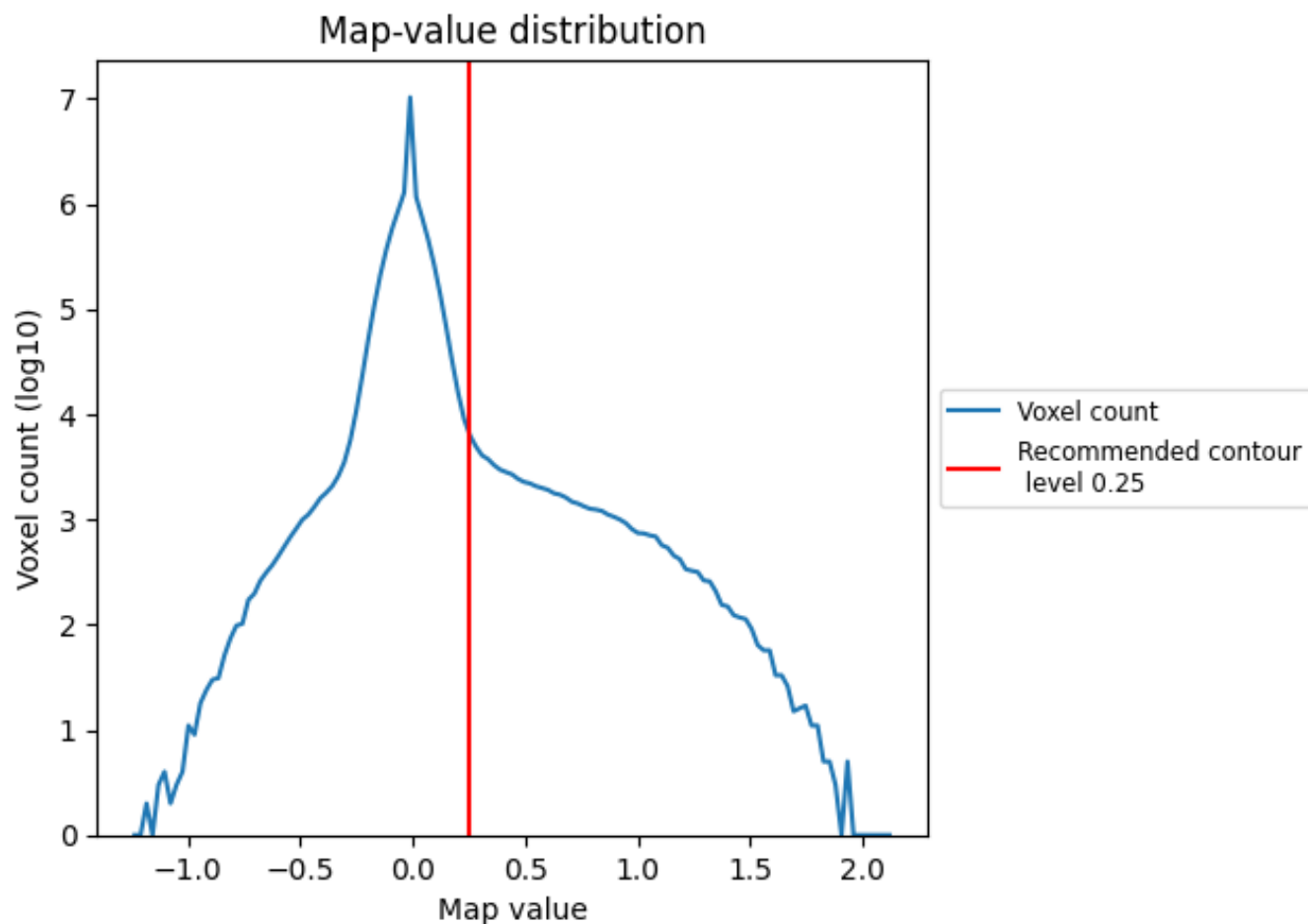


Z

## 7 Map analysis [i](#)

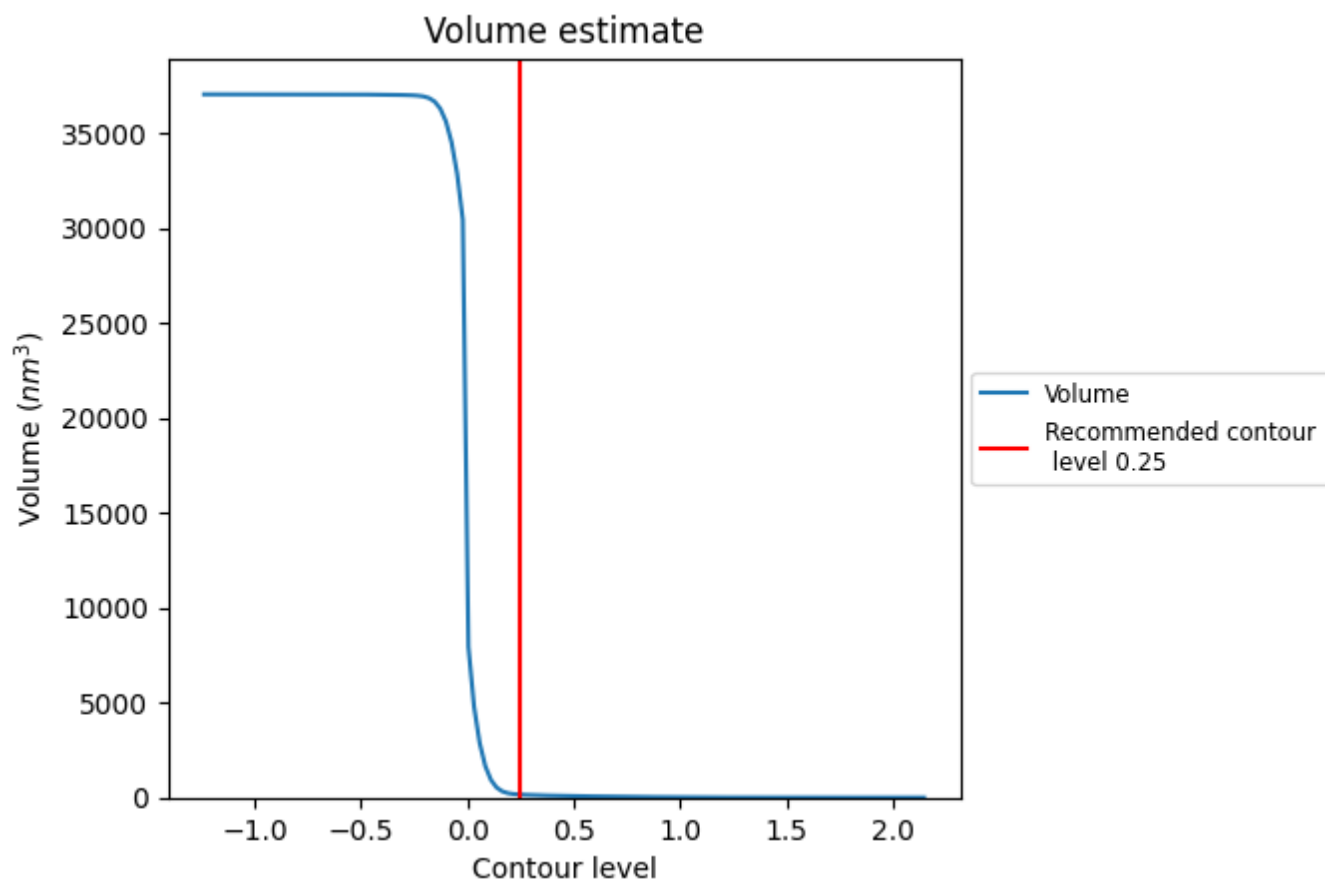
This section contains the results of statistical analysis of the map.

### 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](#)

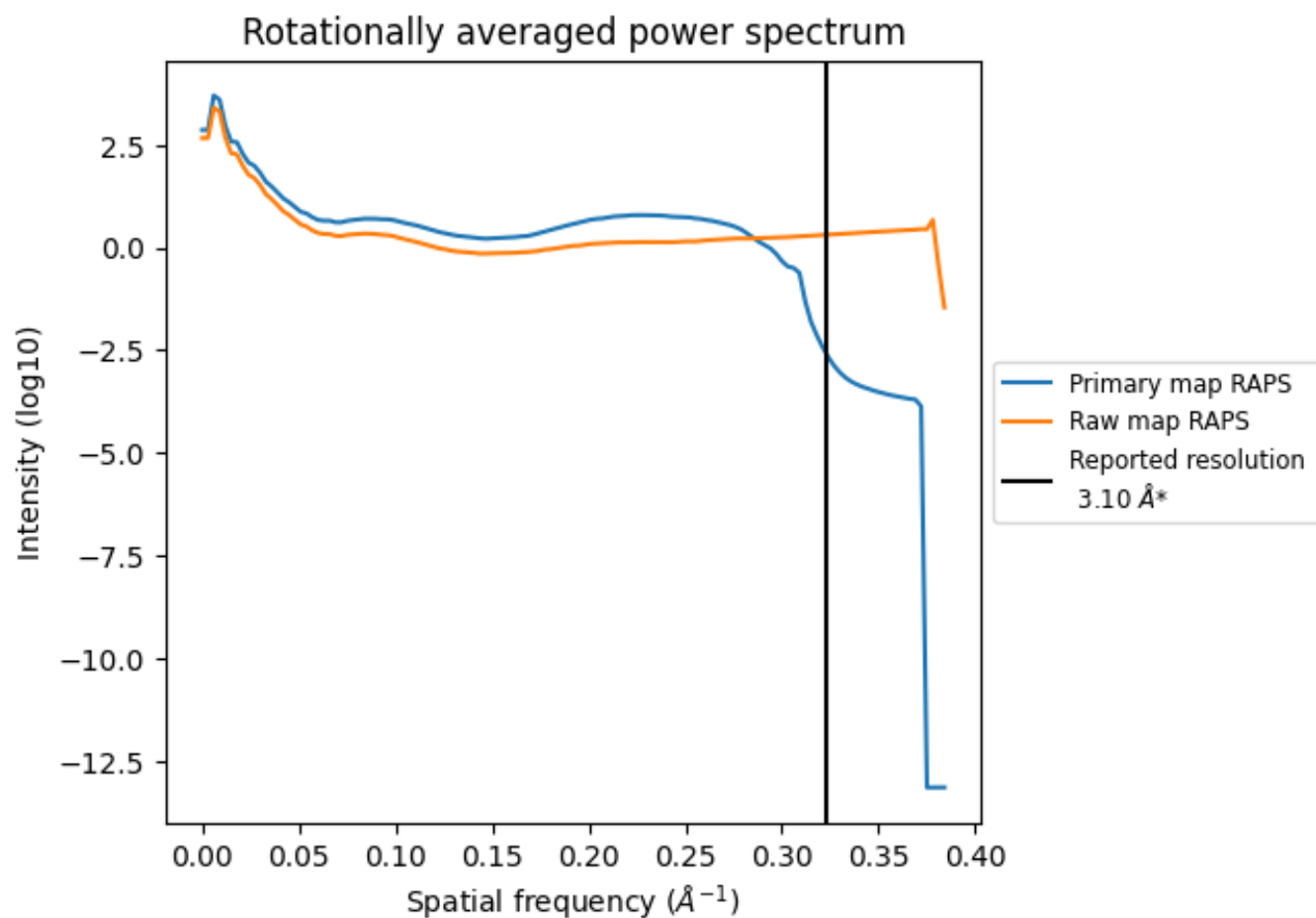


The volume at the recommended contour level is 156 nm<sup>3</sup>; this corresponds to an approximate mass of 141 kDa.

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 ⓘ

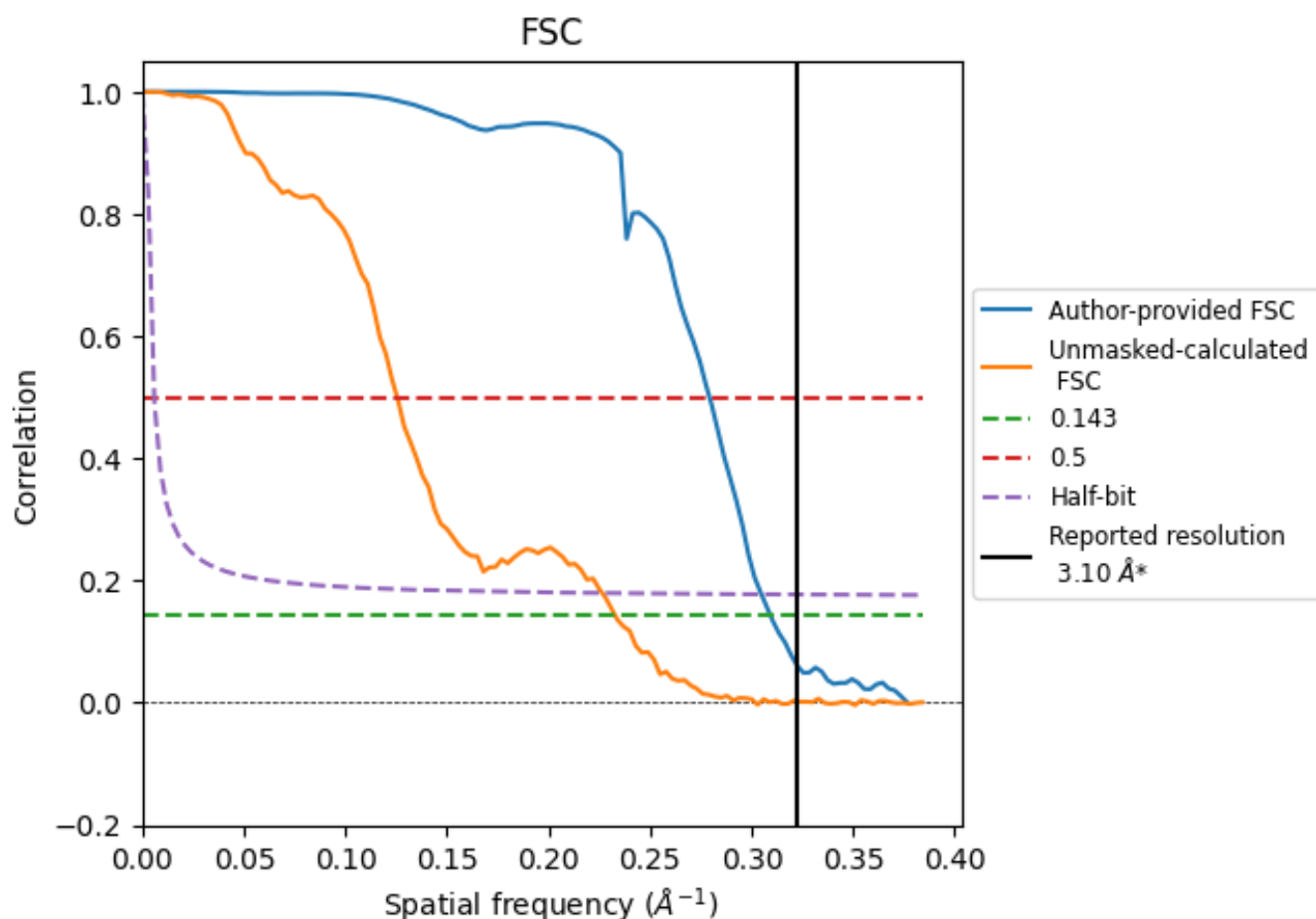


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

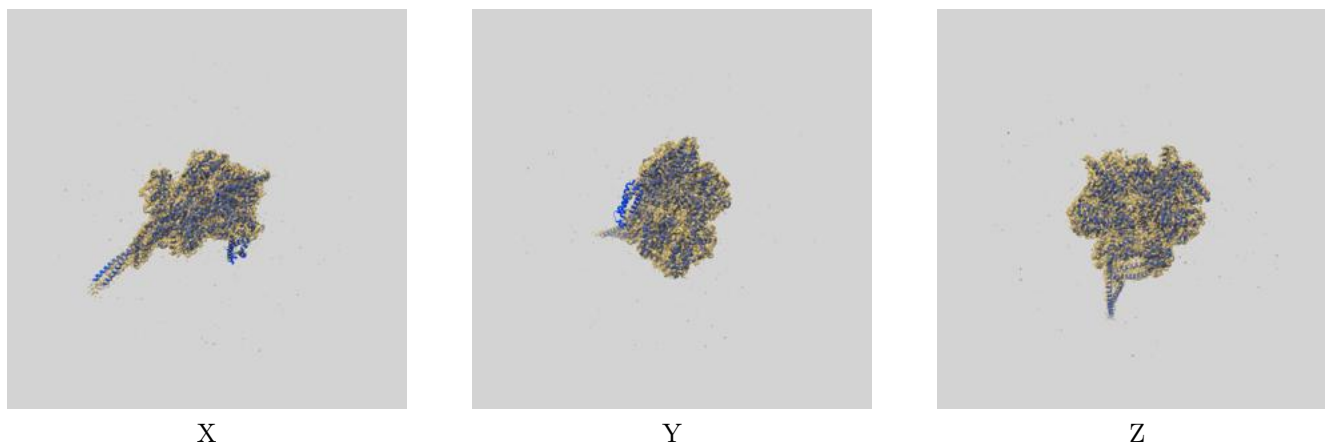
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.23	3.58	3.28
Unmasked-calculated*	4.30	7.97	4.42

\*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 4.30 differs from the reported value 3.1 by more than 10 %

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

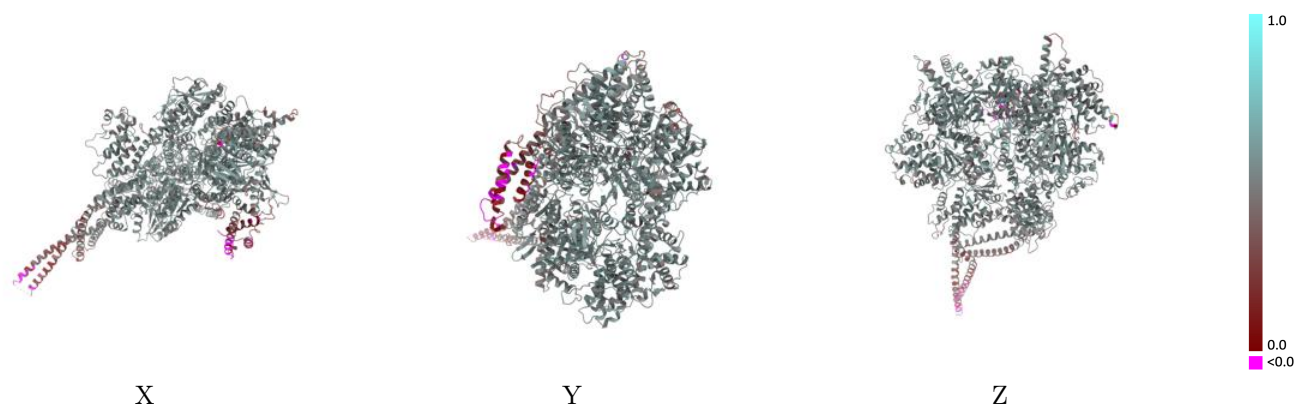
This section contains information regarding the fit between EMDB map EMD-44703 and PDB model 9BMM. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

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



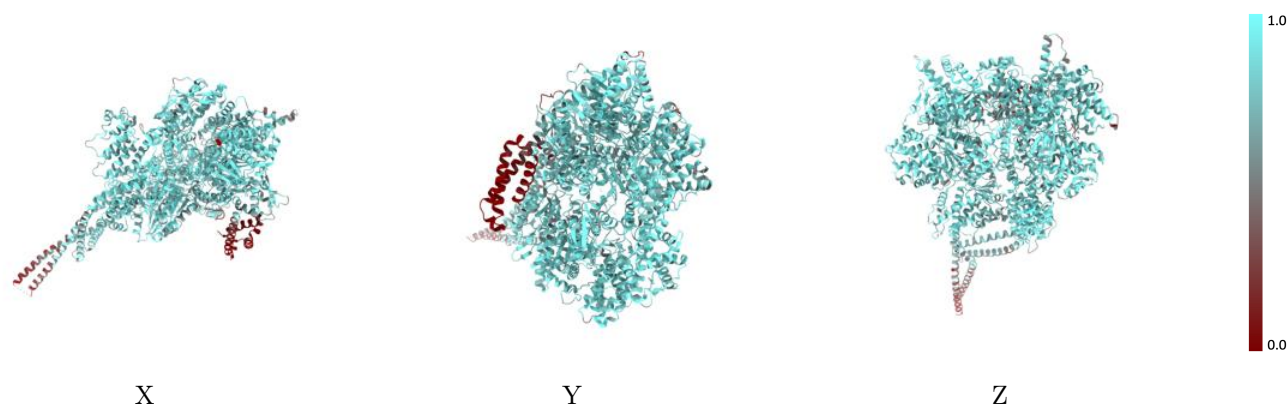
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



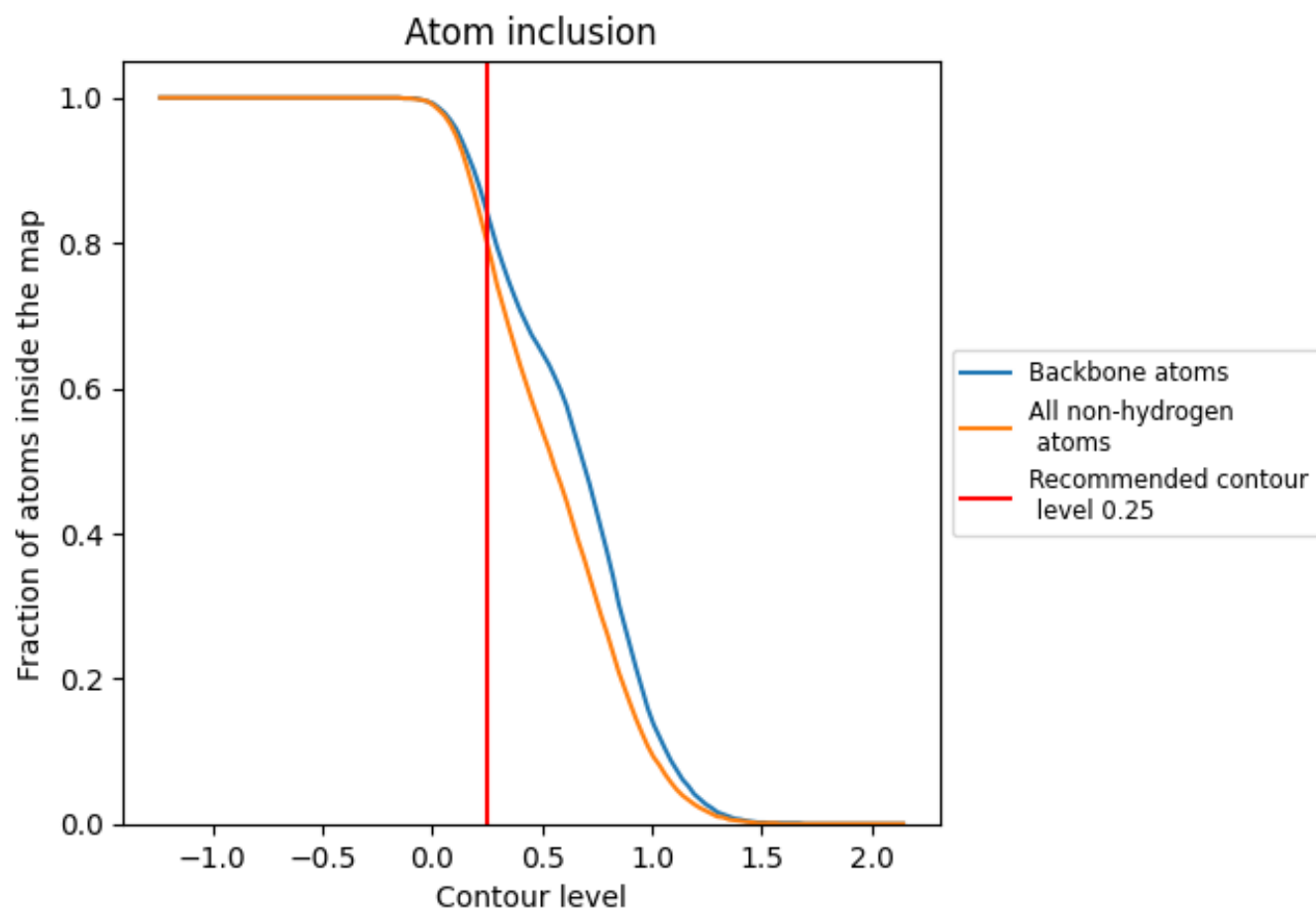
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 80% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8000	<div><div></div></div> 0.4970
A	<div><div></div></div> 0.8000	<div><div></div></div> 0.4970

