



## wwPDB EM Validation Summary Report ⓘ

Sep 2, 2025 – 02:18 PM EDT

PDB ID : 9DGP / pdb\_00009dgp  
EMDB ID : EMD-46843  
Title : Motor domain of dynein-1 complex on microtubules  
Authors : Rao, Q.; Chai, P.; Zhang, K.  
Deposited on : 2024-09-03  
Resolution : 3.50 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.dev126  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
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) : 2.45.1

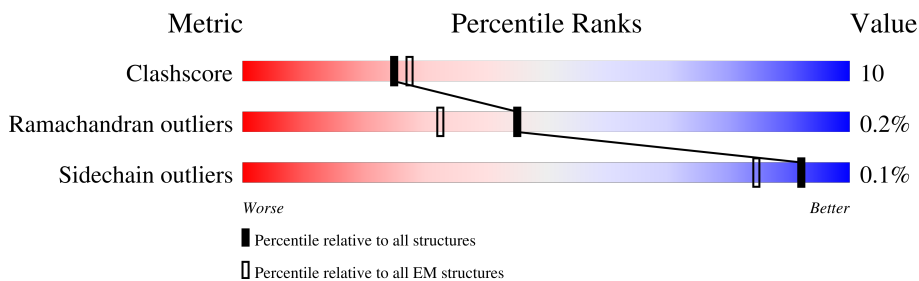
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 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 5 unique types of molecules in this entry. The entry contains 24585 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	3037	24461	15582	4227	4533	119	1	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).



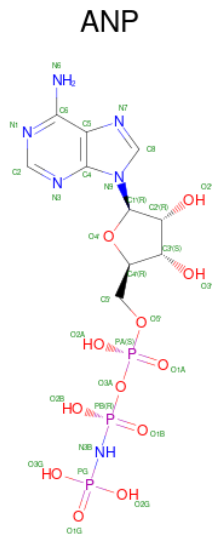
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	27	10	5	10	2	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula:  $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 31	C 10	N 6	O 12	P 3	0
4	A	1	Total 31	C 10	N 6	O 12	P 3	0

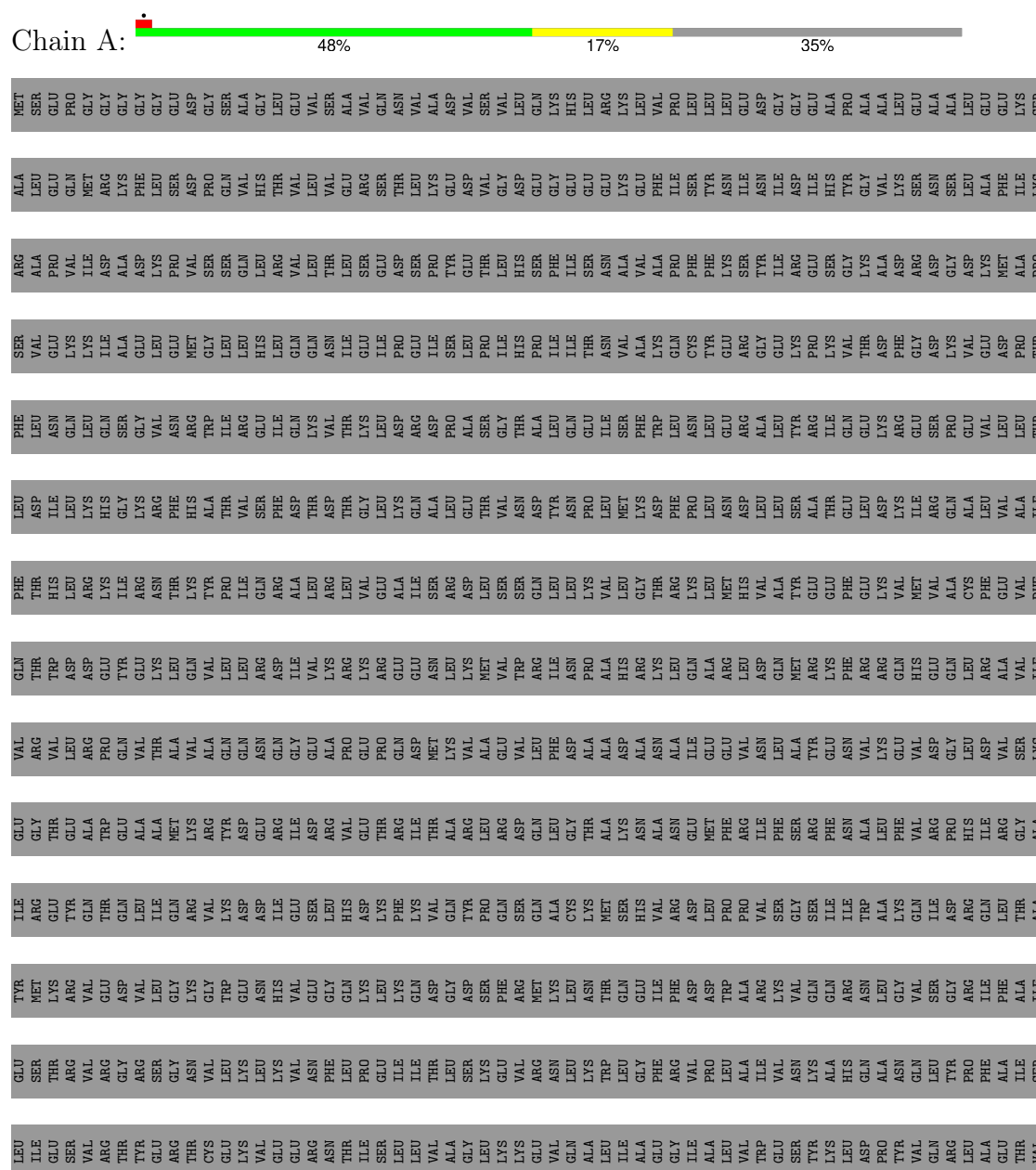
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	4	Total 4	Mg 4	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









E4538	N4404	R4301	F4147	A3752	◆	S4548	Q4429	D4433	L4448	◆	T4569	K4574	S4578	T4583	P4586	L4587	T4588	Q4589	L4590	◆	N4597	◆	A4598	K4601	V4604	V4605	V4609	I4619	F4620	T4621	V4622	I4626	A4627	E4630	Y4636	E4637	V4642	◆	E4646
L4539	I4405	R4302	T4160	A3753	◆	Q4549	L4423	F4558	L4460	◆	K4564	K4574	S4578	T4583	P4586	L4587	T4588	Q4589	L4590	◆	N4597	◆	A4598	K4601	V4604	V4605	V4609	I4619	F4620	T4621	V4622	I4626	A4627	E4630	Y4636	E4637	V4642	◆	E4646
C4540	P4408	Q4307	T4160	A3754	◆	S4548	L4423	F4558	L4460	◆	K4564	K4574	S4578	T4583	P4586	L4587	T4588	Q4589	L4590	◆	N4597	◆	A4598	K4601	V4604	V4605	V4609	I4619	F4620	T4621	V4622	I4626	A4627	E4630	Y4636	E4637	V4642	◆	E4646
E4542	R4411	L4311	R4168	A3755	◆	Q4549	L4423	F4558	L4460	◆	K4564	K4574	S4578	T4583	P4586	L4587	T4588	Q4589	L4590	◆	N4597	◆	A4598	K4601	V4604	V4605	V4609	I4619	F4620	T4621	V4622	I4626	A4627	E4630	Y4636	E4637	V4642	◆	E4646
V4543	F4412	L4311	I4169	A3756	◆	Q4549	L4423	F4558	L4460	◆	K4564	K4574	S4578	T4583	P4586	L4587	T4588	Q4589	L4590	◆	N4597	◆	A4598	K4601	V4604	V4605	V4609	I4619	F4620	T4621	V4622	I4626	A4627	E4630	Y4636	E4637	V4642	◆	E4646
◆	V4417	P4324	S4172	A3757	◆	Q4549	L4423	F4558	L4460	◆	K4564	K4574	S4578	T4583	P4586	L4587	T4588	Q4589	L4590	◆	N4597	◆	A4598	K4601	V4604	V4605	V4609	I4619	F4620	T4621	V4622	I4626	A4627	E4630	Y4636	E4637	V4642	◆	E4646
◆	L4424	V4330	A4177	A3758	◆	Q4549	L4423	F4558	L4460	◆	K4564	K4574	S4578	T4583	P4586	L4587	T4588	Q4589	L4590	◆	N4597	◆	A4598	K4601	V4604	V4605	V4609	I4619	F4620	T4621	V4622	I4626	A4627	E4630	Y4636	E4637	V4642	◆	E4646
A4551	L4424	V4330	A4177	A3759	◆	Q4549	L4423	F4558	L4460	◆	K4564	K4574	S4578	T4583	P4586	L4587	T4588	Q4589	L4590	◆	N4597	◆	A4598	K4601	V4604	V4605	V4609	I4619	F4620	T4621	V4622	I4626	A4627	E4630	Y4636	E4637	V4642	◆	E4646
◆	Q4429	T4333	R4178	A3760	◆	Q4549	L4423	F4558	L4460	◆	K4564	K4574	S4578	T4583	P4586	L4587	T4588	Q4589	L4590	◆	N4597	◆	A4598	K4601	V4604	V4605	V4609	I4619	F4620	T4621	V4622	I4626	A4627	E4630	Y4636	E4637	V4642	◆	E4646
D4554	Q4429	T4333	R4178	A3761	◆	Q4549	L4423	F4558	L4460	◆	K4564	K4574	S4578	T4583	P4586	L4587	T4588	Q4589	L4590	◆	N4597	◆	A4598	K4601	V4604	V4605	V4609	I4619	F4620	T4621	V4622	I4626	A4627	E4630	Y4636	E4637	V4642	◆	E4646
S4557	D4433	K4342	F4192	A3762	◆	Q4549	L4423	F4558	L4460	◆	K4564	K4574	S4578	T4583	P4586	L4587	T4588	Q4589	L4590	◆	N4597	◆	A4598	K4601	V4604	V4605	V4609	I4619	F4620	T4621	V4622	I4626	A4627	E4630	Y4636	E4637	V4642	◆	E4646
F4558	D4433	K4342	F4192	A3763	◆	Q4549	L4423	F4558	L4460	◆	K4564	K4574	S4578	T4583	P4586	L4587	T4588	Q4589	L4590	◆	N4597	◆	A4598	K4601	V4604	V4605	V4609	I4619	F4620	T4621	V4622	I4626	A4627	E4630	Y4636	E4637	V4642	◆	E4646
◆	C4438	L4344	R4193	A3764	◆	Q4549	L4423	F4558	L4460	◆	K4564	K4574	S4578	T4583	P4586	L4587	T4588	Q4589	L4590	◆	N4597	◆	A4598	K4601	V4604	V4605	V4609	I4619	F4620	T4621	V4622	I4626	A4627	E4630	Y4636	E4637	V4642	◆	E4646
K4564	C4438	L4344	R4193	A3765	◆	Q4549	L4423	F4558	L4460	◆	K4564	K4574	S4578	T4583	P4586	L4587	T4588	Q4589	L4590	◆	N4597	◆	A4598	K4601	V4604	V4605	V4609	I4619	F4620	T4621	V4622	I4626	A4627	E4630	Y4636	E4637	V4642	◆	E4646
T4569	K4442	M4346	E4209	A3766	◆	Q4549	L4423	F4558	L4460	◆	K4564	K4574	S4578	T4583	P4586	L4587	T4588	Q4589	L4590	◆	N4597	◆	A4598	K4601	V4604	V4605	V4609	I4619	F4620	T4621	V4622	I4626	A4627	E4630	Y4636	E4637	V4642	◆	E4646
◆	L4448	L4349	L4212	A3767	◆	Q4549	L4423	F4558	L4460	◆	K4564	K4574	S4578	T4583	P4586	L4587	T4588	Q4589	L4590	◆	N4597	◆	A4598	K4601	V4604	V4605	V4609	I4619	F4620	T4621	V4622	I4626	A4627	E4630	Y4636	E4637	V4642	◆	E4646
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T4583	S4463	D4351	D4217	A3770	◆	Q4549	L4423	F4558	L4460	◆	K4564	K4574	S4578	T4583	P4586	L4587	T4588	Q4589	L4590	◆	N4597	◆	A4598	K4601	V4604	V4605	V4609	I4619	F4620	T4621	V4622	I4626	A4627	E4630	Y4636	E4637	V4642	◆	E4646
P4586	S4463	D4351	D4217	A3771	◆	Q4549	L4423	F4558	L4460	◆	K4564	K4574	S4578	T4583	P4586	L4587	T4588	Q4589	L4590	◆	N4597	◆	A4598	K4601	V4604	V4605	V4609	I4619	F4620	T4621	V4622	I4626	A4627	E4630	Y4636	E4637	V4642	◆	E4646
L4587	S4463	D4351	D4217	A3772	◆	Q4549	L4423	F4558	L4460	◆	K4564	K4574	S4578	T4583	P4586	L4587	T4588	Q4589	L4590	◆	N4597	◆	A4598	K4601	V4604	V4605	V4609	I4619	F4620	T4621	V4622	I4626	A4627	E4630	Y4636	E4637	V4642	◆	E4646
Q4589	S4463	D4351	D4217	A3773	◆	Q4549	L4423	F4558	L4460	◆	K4564	K4574	S4578	T4583	P4586	L4587	T4588	Q4589	L4590	◆	N4597	◆	A4598	K4601	V4604	V4605	V4609	I4619	F4620	T4621	V4622	I4626	A4627	E4630	Y4636	E4637	V4642	◆	E4646
L4590	S4463	D4351	D4217	A3774	◆	Q4549	L4423	F4558	L4460	◆	K4564	K4574	S4578	T4583	P4586	L4587	T4588	Q4589	L4590	◆	N4597	◆	A4598	K4601	V4604	V4605	V4609	I4619	F4620	T4621	V4622	I4626	A4627	E4630	Y4636	E4637	V4642	◆	E4646
◆	V4475	ALA	P4239	A3787	◆	Q4549	L4423	F4558	L4460	◆	K4564	K4574	S4578	T4583	P4586	L4587	T4588	Q4589	L4590	◆	N4597	◆	A4598	K4601	V4604	V4605	V4609	I4619	F4620	T4621	V4622	I4626	A4627	E4630	Y4636	E4637	V4642	◆	E4646
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◆	V4478	GLU	A4248	A3809	◆	Q4549	L4423	F4558	L4460	◆	K4564	K4574	S4578	T4583	P4586	L4587	T4588	Q4589	L4590	◆	N4597	◆	A4598	K4601	V4604	V4605	V4609	I4619	F4620	T4621	V4622	I4626	A4627	E4630	Y4636	E4637	V4642	◆	E4646
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◆	R4485	LYS	I4251	A3820	◆	Q4549	L4423	F4558	L4460	◆	K4564	K4574	S4578	T4583	P4586	L4587	T4588	Q4589	L4590	◆	N4597	◆	A4598	K4601	V4604	V4605	V4609	I4619	F4620	T4621	V4622	I4626	A4627	E4630	Y4636	E4637	V4642	◆	E4646
A4598	I4486	THR	G4253	A3821	◆	Q4549	L4423	F4558	L4460	◆	K4564	K4574	S4578	T4583	P4586	L4587	T4588	Q4589	L4590	◆	N4597	◆	A4598	K4601	V4604	V4605	V4609	I4619	F4620	T4621	V4622	I4626	A4627	E4630	Y4636	E4637	V4642	◆	E4646
◆	S4493	THR	G4253	A3829	◆	Q4549	L4423	F4558	L4460	◆	K4564	K4574	S4578	T4583	P4586	L4587	T4588	Q4589	L4590	◆	N4597	◆	A4598	K4601	V4604	V4605	V4609	I4619	F4620	T4621	V4622	I4626	A4627	E4630	Y4636	E4637	V4642	◆	E4646
K4601	S4493	THR	G4253	A3829	◆	Q4549	L4423	F4558	L4460	◆	K4564	K4574	S4578	T4583	P4586	L4587	T4588	Q4589	L4590	◆	N4597	◆	A4598	K4601	V4604	V4605	V4609	I4619	F4620	T4621	V4622	I4626	A4627	E4630	Y4636	E4637	V4642	◆	E4646
◆	V4604	ASP	T4267	A3835	◆	Q4549	L4423	F4558	L4460	◆	K4564	K4574	S4578																										

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	106660	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	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.813	Depositor
Minimum map value	-1.093	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.15	Depositor
Map size ( $\text{\AA}$ )	333.312, 333.312, 333.312	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	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: ANP, MG, 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	0.37	0/24982	0.49	0/33848

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	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1360	ARG	Sidechain
1	A	2292	ARG	Sidechain
1	A	2757	ARG	Sidechain
1	A	4123	ARG	Sidechain
1	A	4302	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	24461	0	24528	508	0
2	A	27	0	12	2	0
3	A	31	0	12	2	0
4	A	62	0	26	4	0
5	A	4	0	0	0	0
All	All	24585	0	24578	508	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 10.

The worst 5 of 508 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:2598:GLY:H	4:A:4703:ANP:HNB1	1.23	0.85
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.64	0.79
1:A:1370:LEU:HD11	1:A:1390:LEU:HD12	1.66	0.77
1:A:2581:LEU:HD21	1:A:2605:LEU:HD23	1.68	0.75
1:A:2506:SER:HB3	1:A:2510:MET:HB2	1.71	0.70

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	3026/4646 (65%)	2968 (98%)	53 (2%)	5 (0%)	44 75

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3914	ILE
1	A	4586	PRO
1	A	4028	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	4292	LYS
1	A	4130	ILE

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2704/4122 (66%)	2702 (100%)	2 (0%)	<a href="#">92</a> <a href="#">97</a>

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

Mol	Chain	Res	Type
1	A	2295	LEU
1	A	2855	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4078	ASN
1	A	4100	HIS
1	A	4506	ASN
1	A	2282	HIS
1	A	2263	HIS

### 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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ANP	A	4704	5	29,33,33	2.51	6 (20%)	31,52,52	1.50	4 (12%)
4	ANP	A	4703	5	29,33,33	2.49	6 (20%)	31,52,52	1.45	3 (9%)
2	ADP	A	4701	-	24,29,29	0.88	0	29,45,45	1.22	2 (6%)
3	ATP	A	4702	5	28,33,33	0.72	0	34,52,52	0.58	1 (2%)

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
4	ANP	A	4704	5	-	8/14/38/38	0/3/3/3
4	ANP	A	4703	5	-	4/14/38/38	0/3/3/3
2	ADP	A	4701	-	-	3/12/32/32	0/3/3/3
3	ATP	A	4702	5	-	3/18/38/38	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	4704	ANP	PB-O3A	8.86	1.70	1.59
4	A	4703	ANP	PB-O3A	8.83	1.70	1.59
4	A	4703	ANP	PG-N3B	6.22	1.79	1.63
4	A	4704	ANP	PG-N3B	6.17	1.79	1.63
4	A	4704	ANP	PG-O1G	4.69	1.53	1.46

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	4703	ANP	O2B-PB-O1B	4.90	120.38	109.87
4	A	4704	ANP	O2B-PB-O1B	4.81	120.18	109.87
4	A	4704	ANP	O1G-PG-N3B	-4.09	105.75	111.77
4	A	4703	ANP	O1G-PG-N3B	-3.84	106.12	111.77
2	A	4701	ADP	N3-C2-N1	-3.69	123.67	128.67

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	4703	ANP	PB-N3B-PG-O1G
4	A	4703	ANP	PA-O3A-PB-O2B
4	A	4704	ANP	PB-N3B-PG-O1G
4	A	4704	ANP	PG-N3B-PB-O1B
4	A	4704	ANP	C5'-O5'-PA-O2A

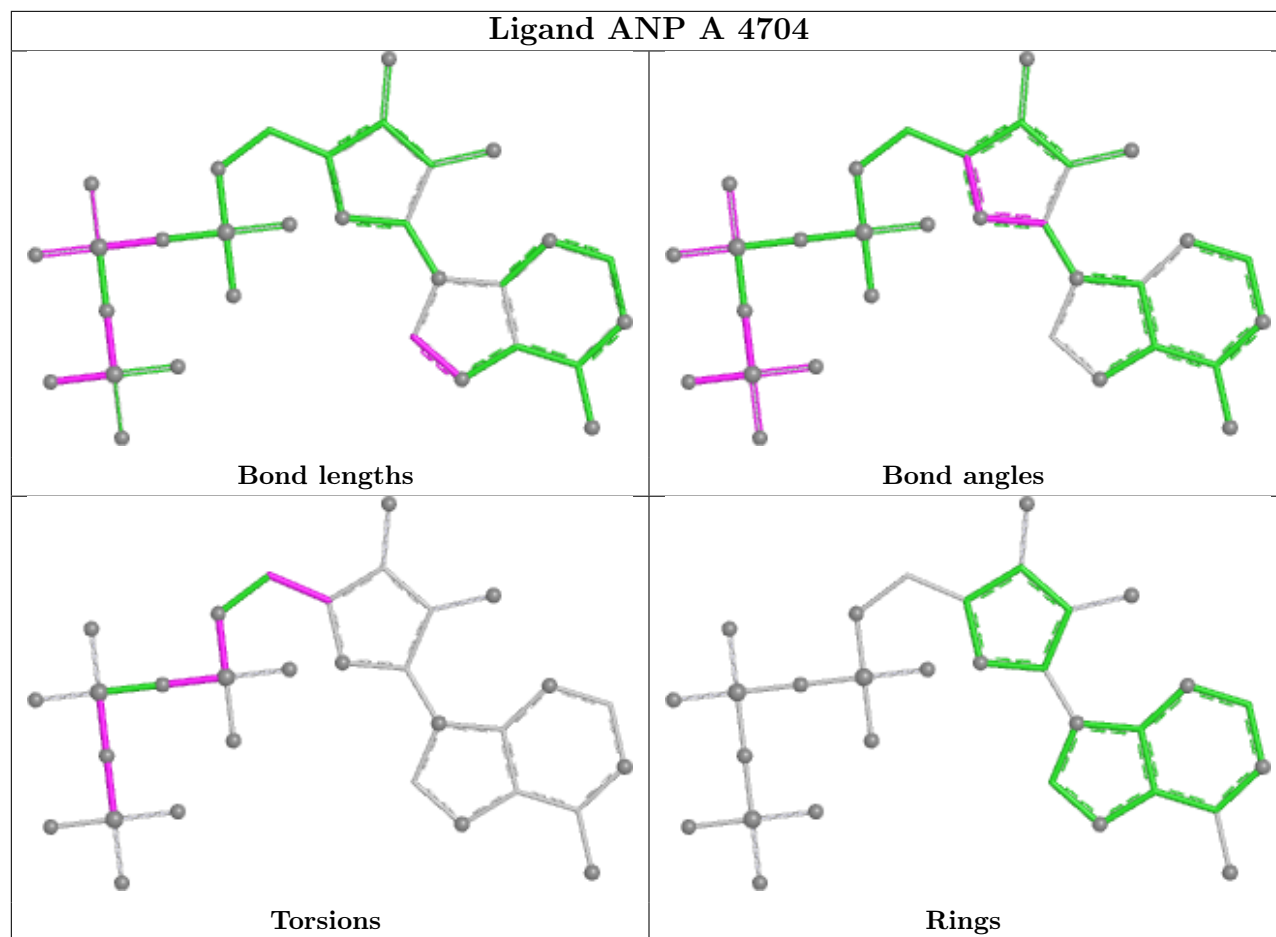
There are no ring outliers.

3 monomers are involved in 8 short contacts:

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

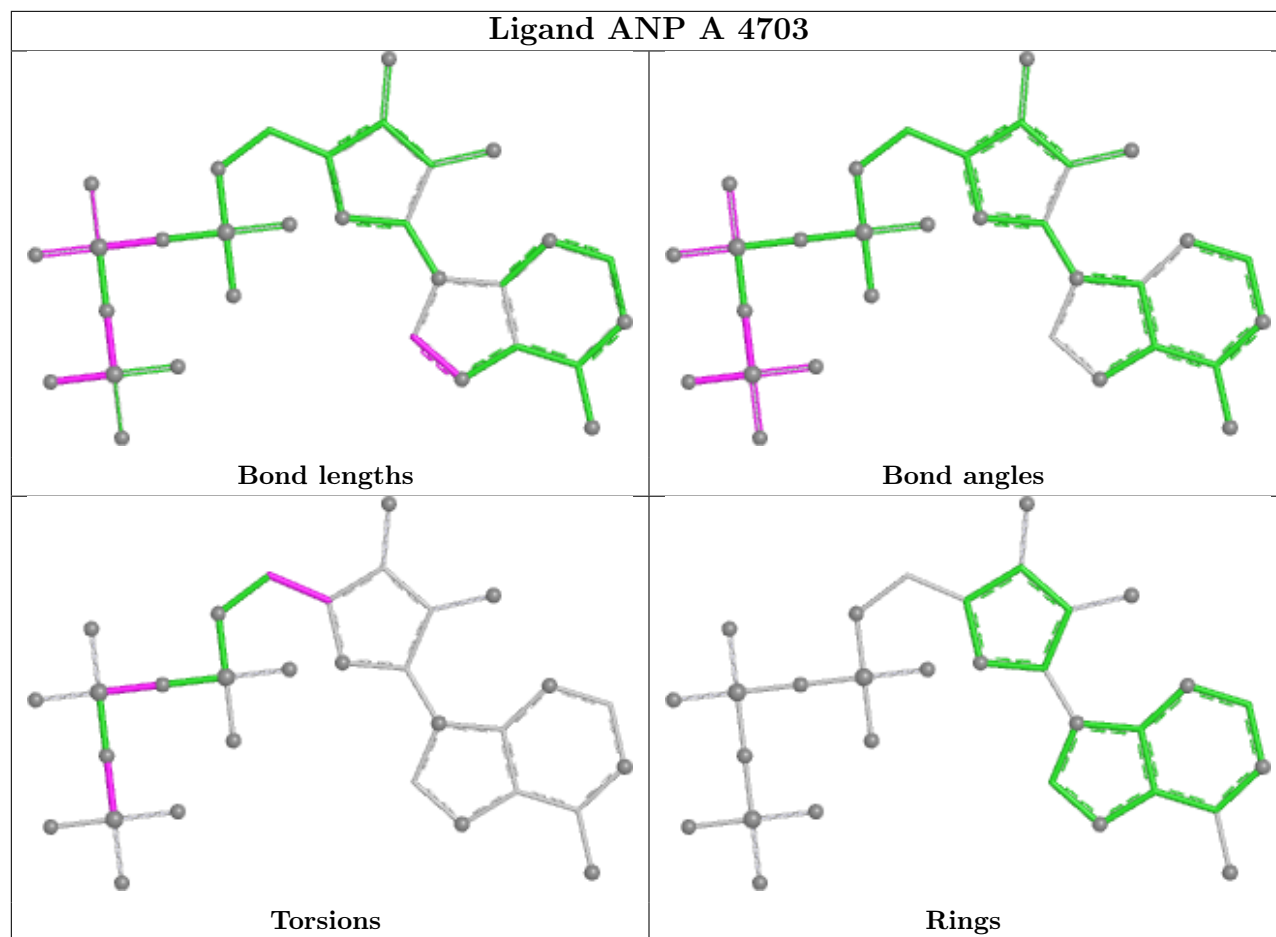
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

## Ligand ANP A 4704

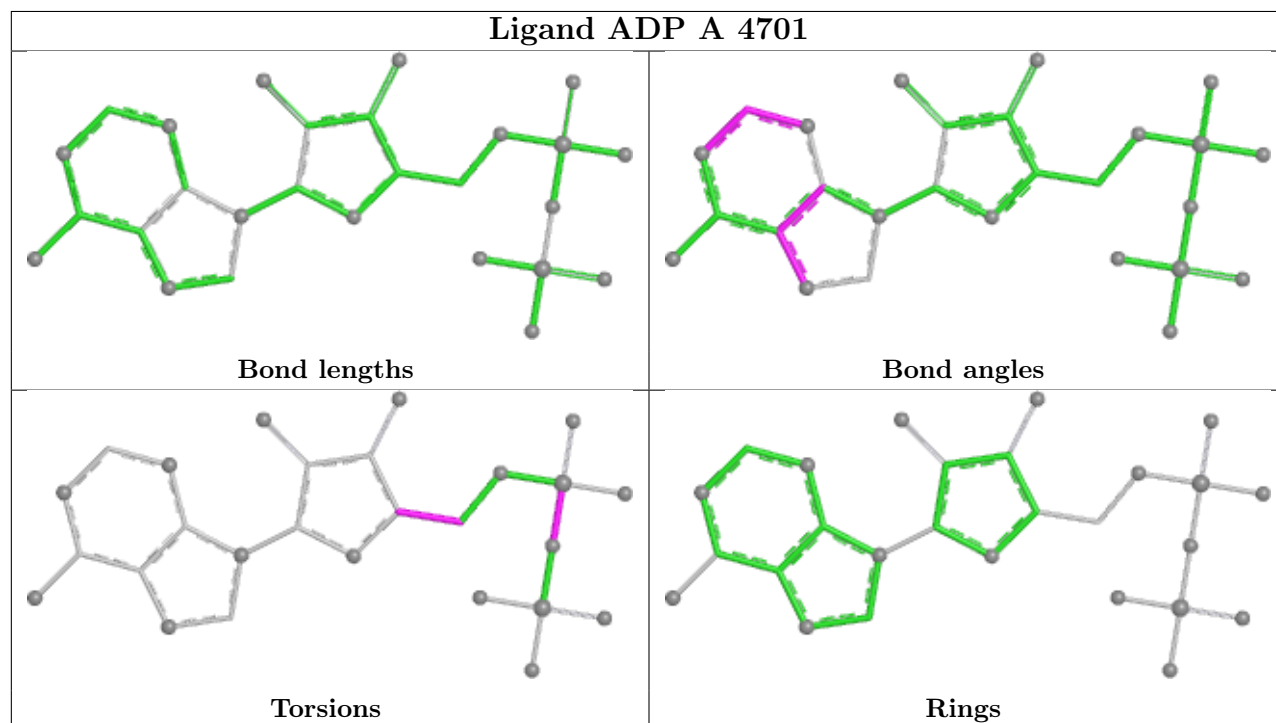


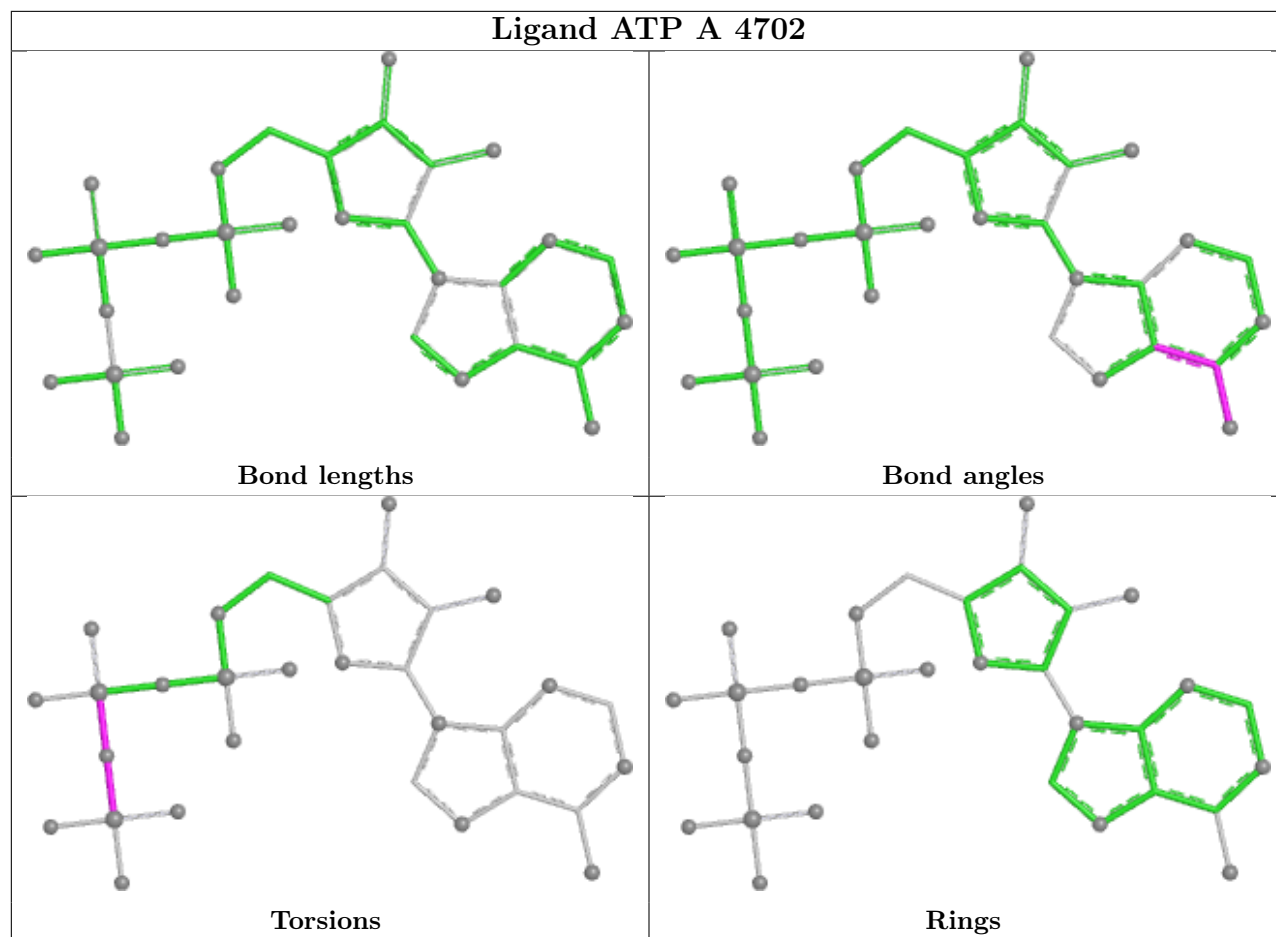


## Ligand ANP A 4703



## Ligand ADP A 4701





## 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.

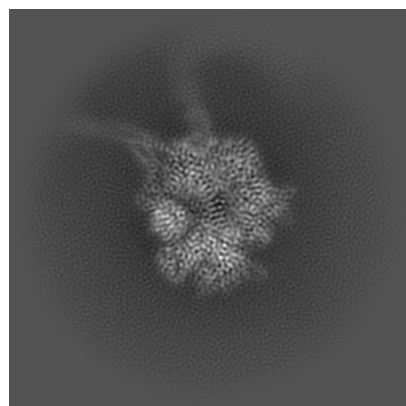
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46843. These allow visual inspection of the internal detail of the map and identification of artifacts.

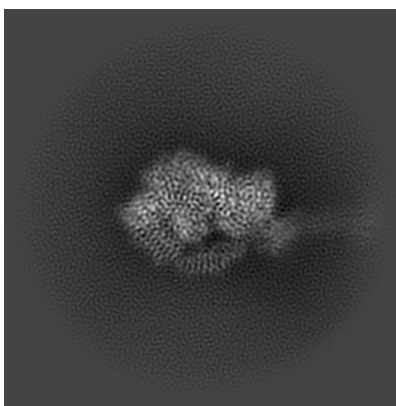
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

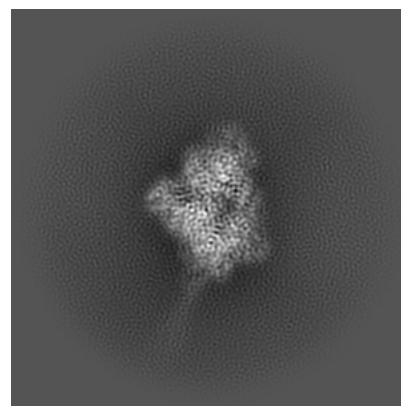
#### 6.1.1 Primary map



X

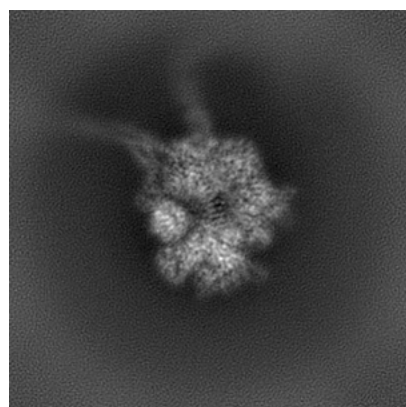


Y

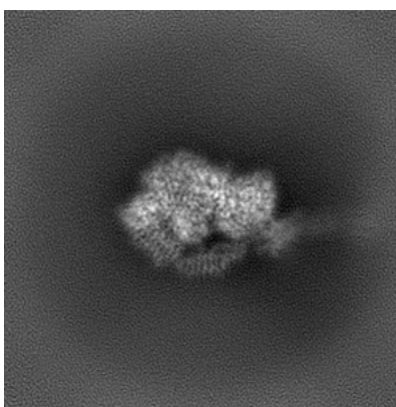


Z

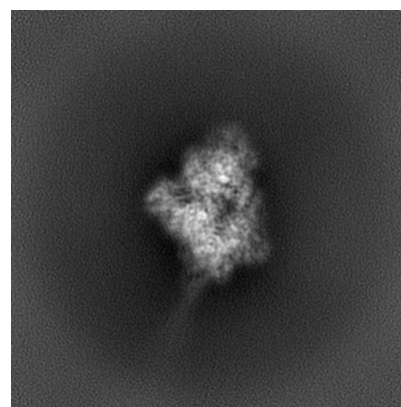
#### 6.1.2 Raw map



X



Y

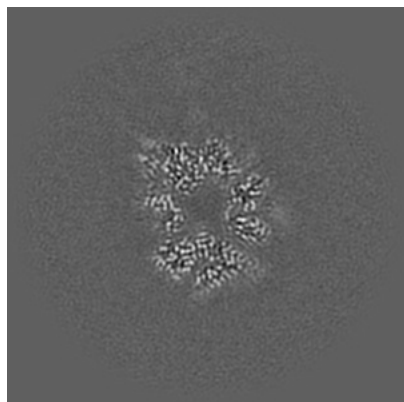


Z

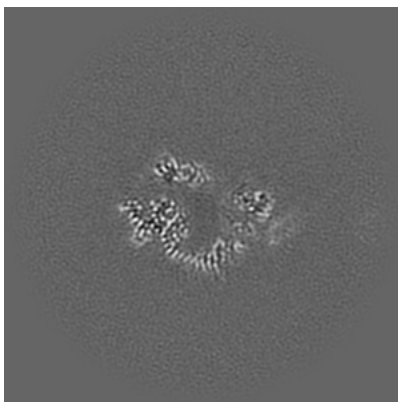
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

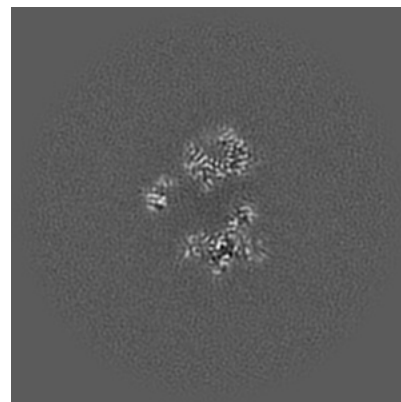
### 6.2.1 Primary map



X Index: 128

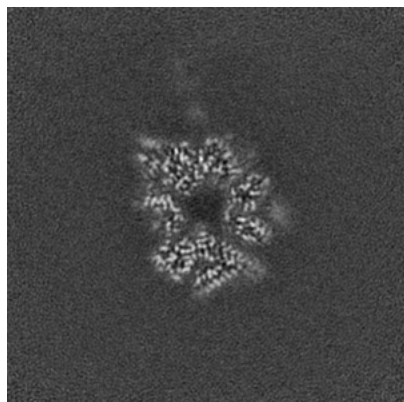


Y Index: 128

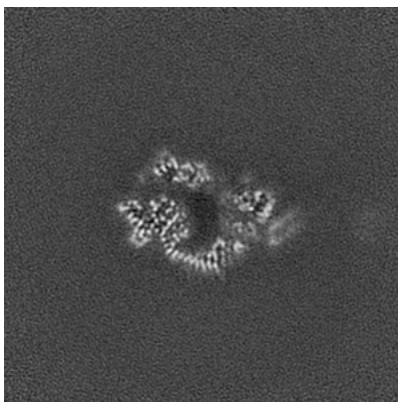


Z Index: 128

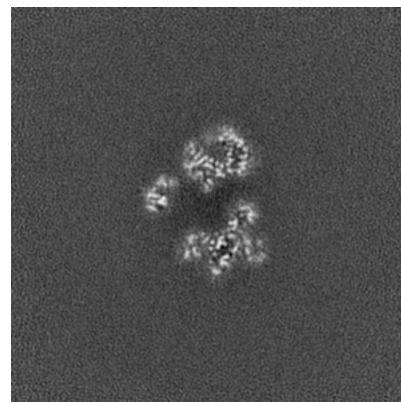
### 6.2.2 Raw map



X Index: 128



Y Index: 128

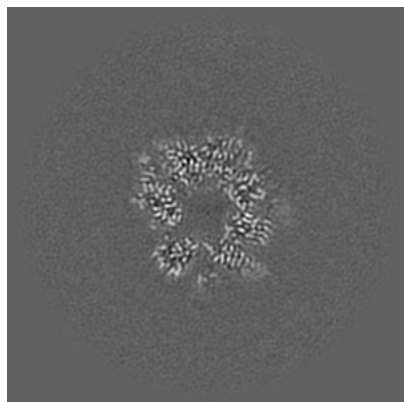


Z Index: 128

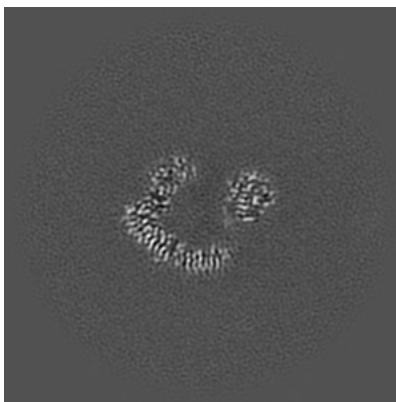
The images above show central slices of the map in three orthogonal directions.

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

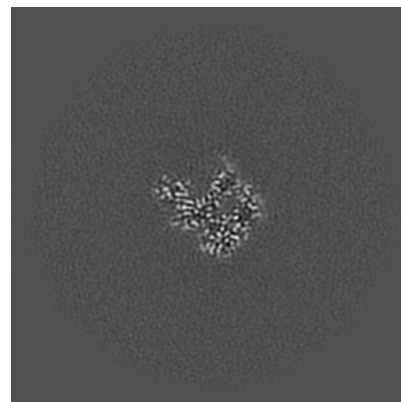
### 6.3.1 Primary map



X Index: 132

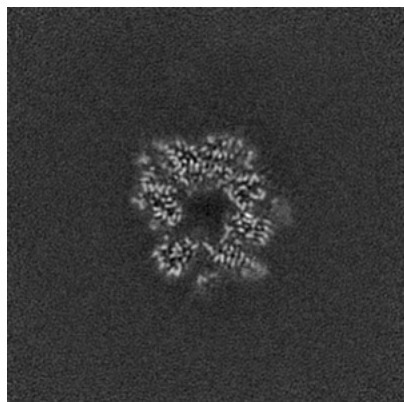


Y Index: 136

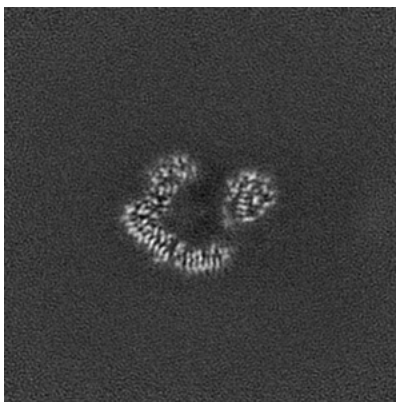


Z Index: 101

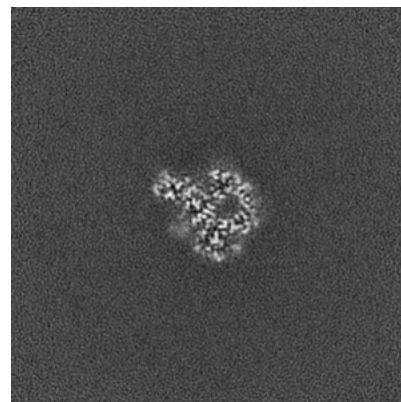
### 6.3.2 Raw map



X Index: 132



Y Index: 136



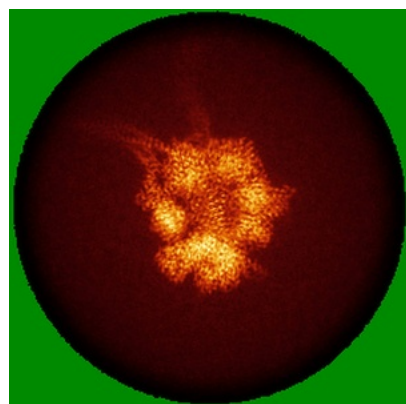
Z Index: 97

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

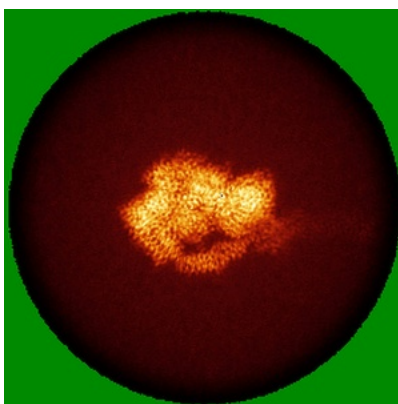


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

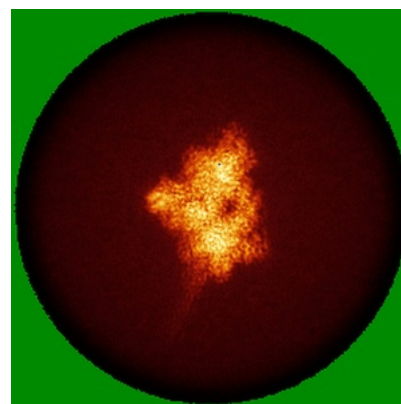
### 6.4.1 Primary map



X

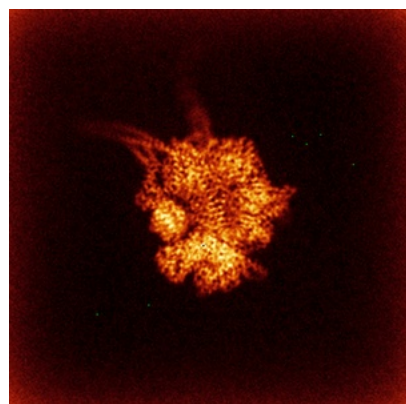


Y

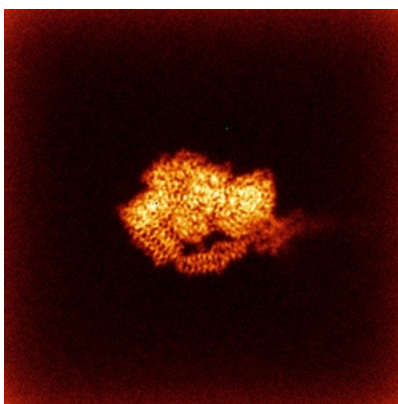


Z

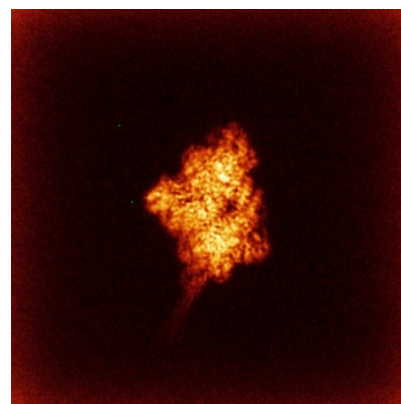
### 6.4.2 Raw map



X



Y

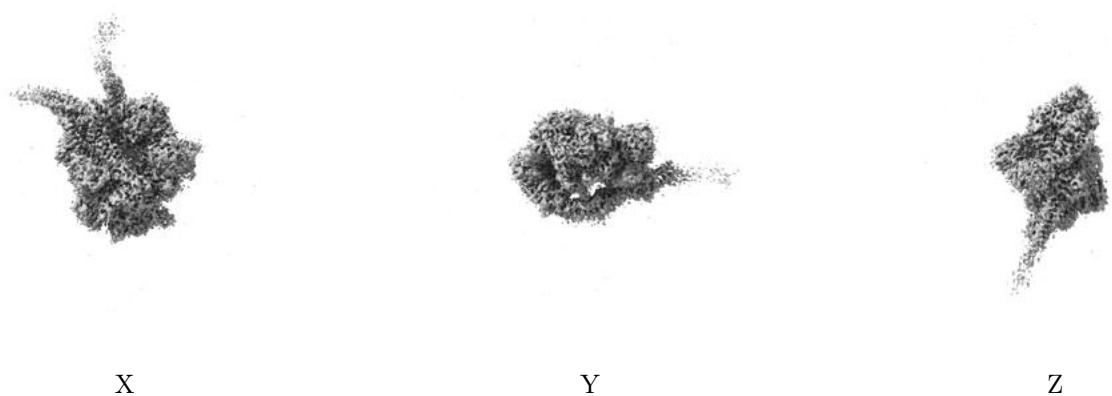


Z

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.

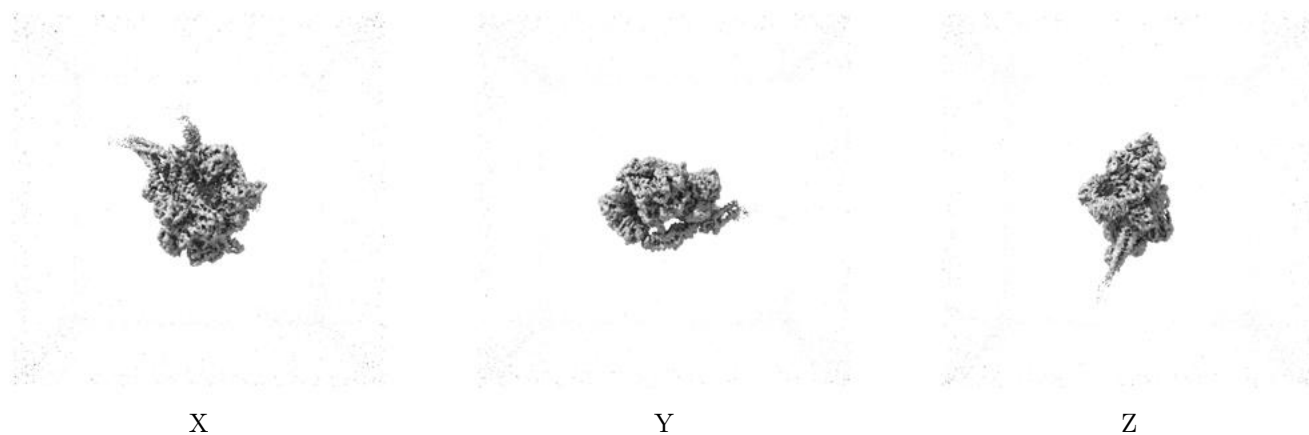
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



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

### 6.5.2 Raw map



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.

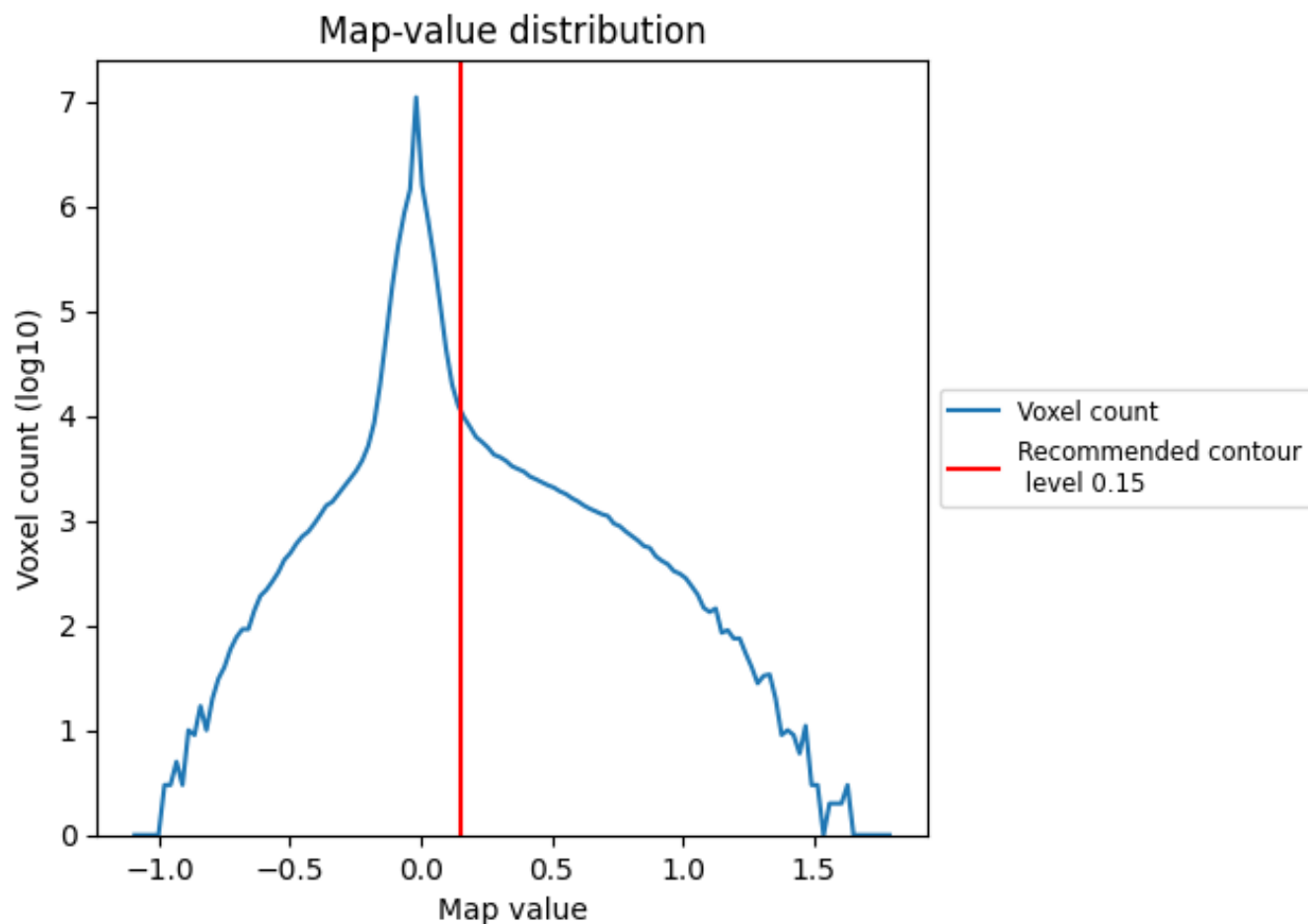
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

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

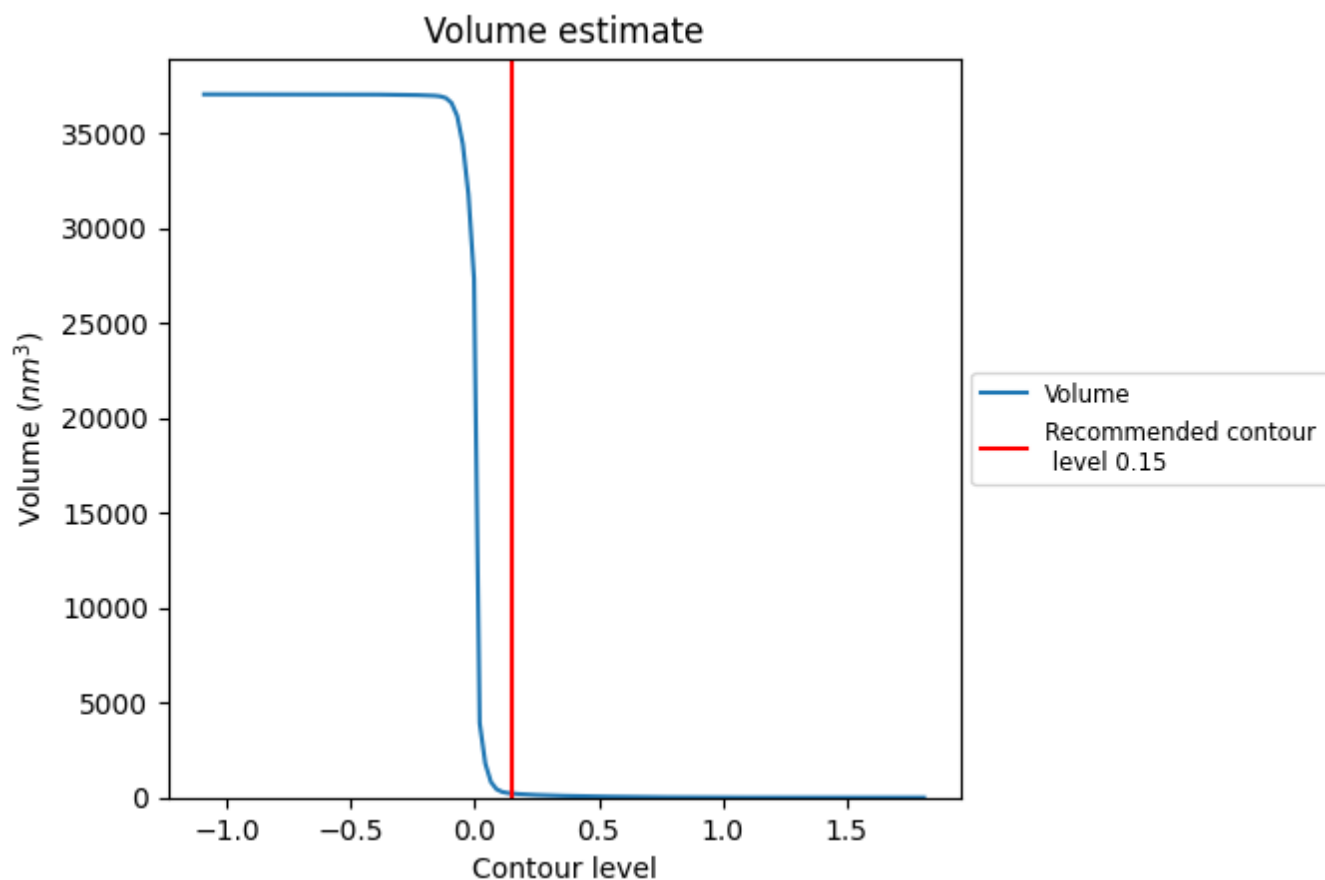
### 7.1 Map-value distribution [i](#)



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.



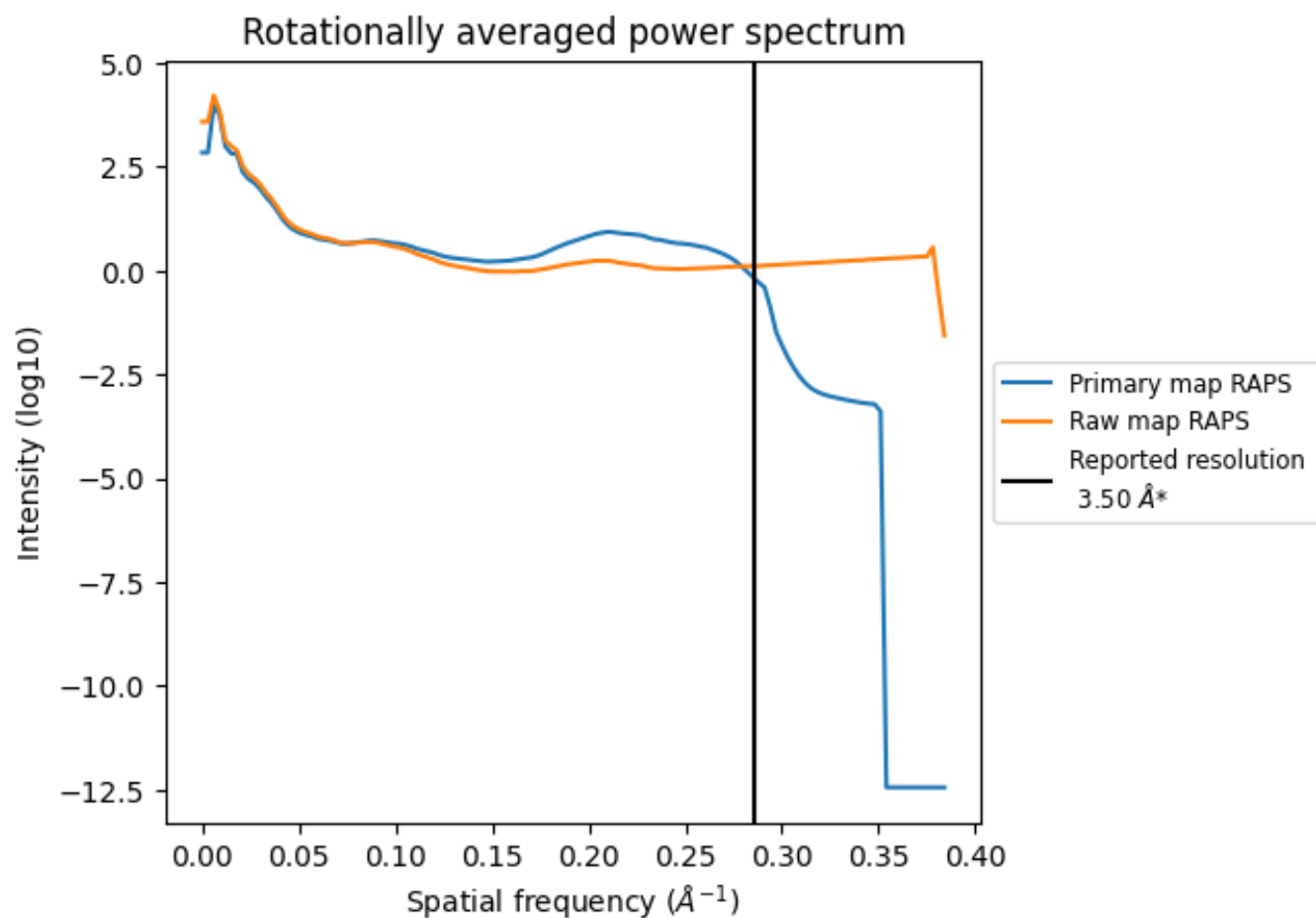
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $215 \text{ nm}^3$ ; this corresponds to an approximate mass of 194 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 ⓘ

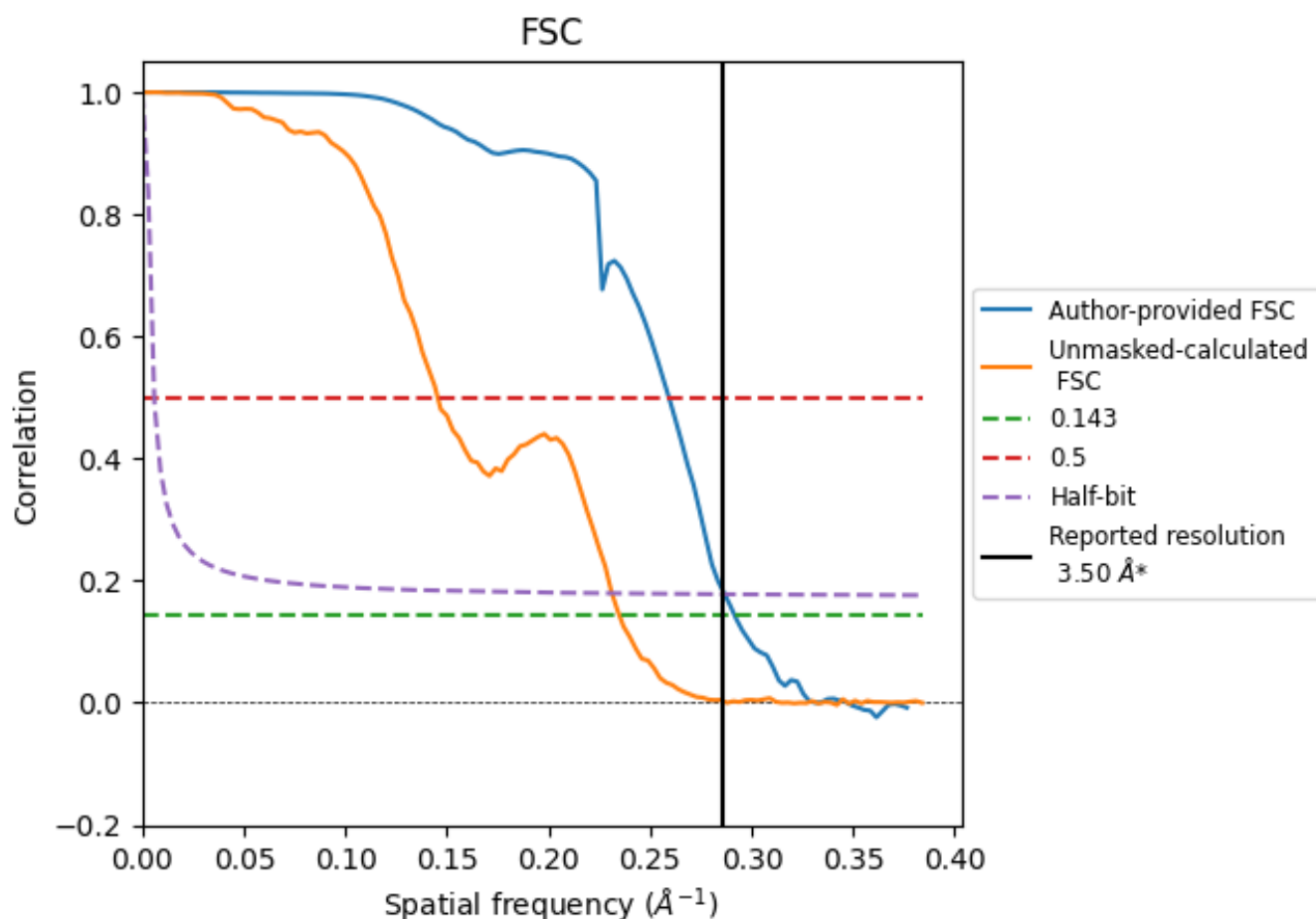


\*Reported resolution corresponds to spatial frequency of 0.286 Å<sup>-1</sup>

## 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  $0.286 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

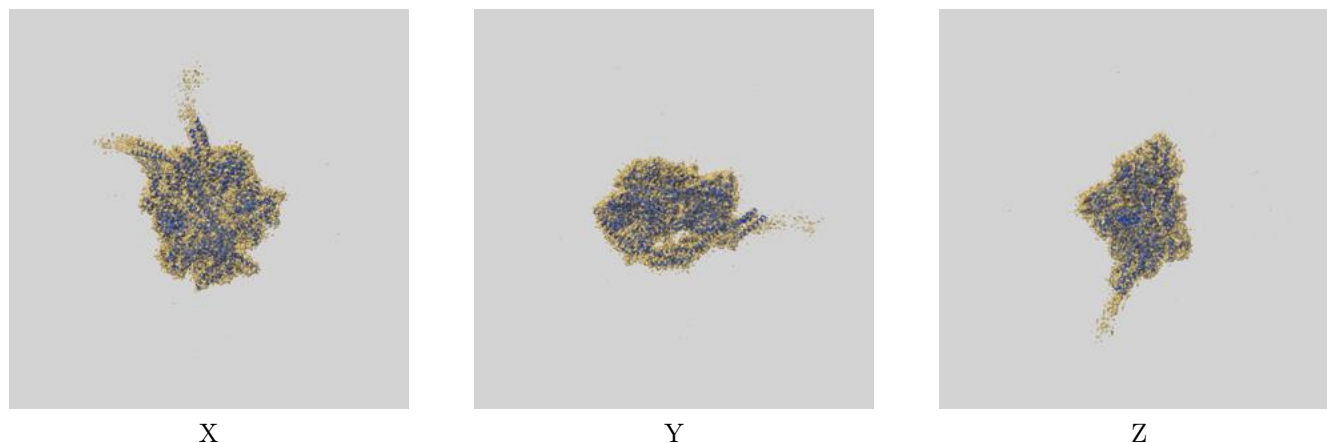
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.43	3.86	3.49
Unmasked-calculated*	4.26	6.87	4.32

\*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 4.26 differs from the reported value 3.5 by more than 10 %

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

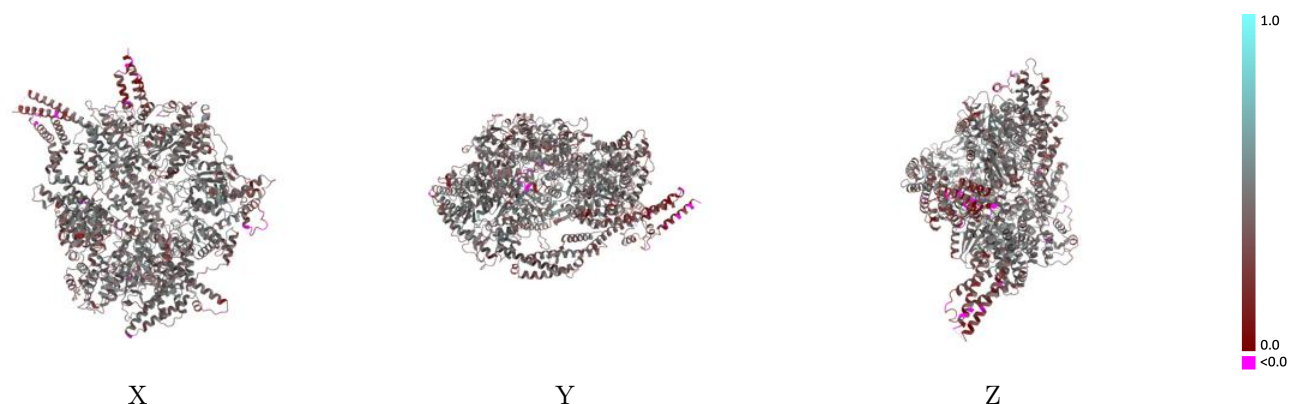
This section contains information regarding the fit between EMDB map EMD-46843 and PDB model 9DGP. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

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



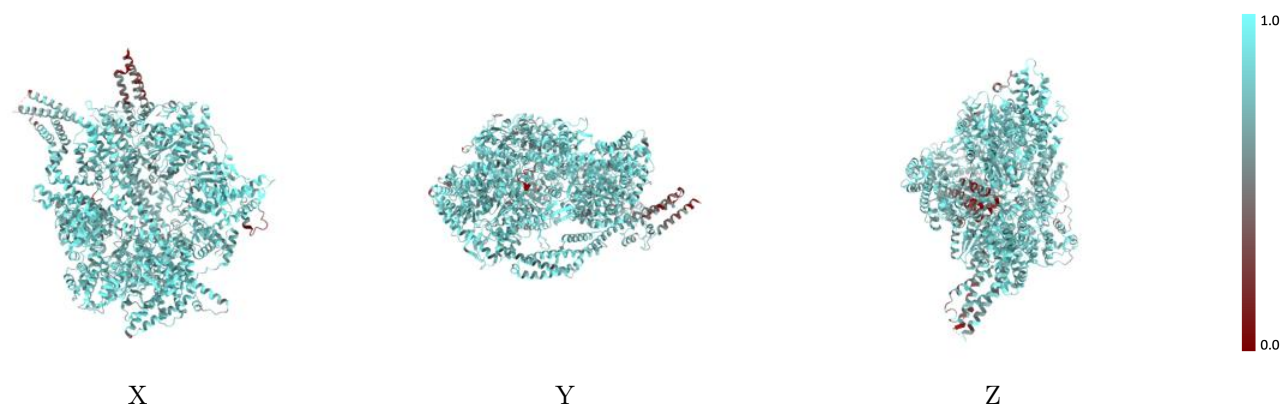
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



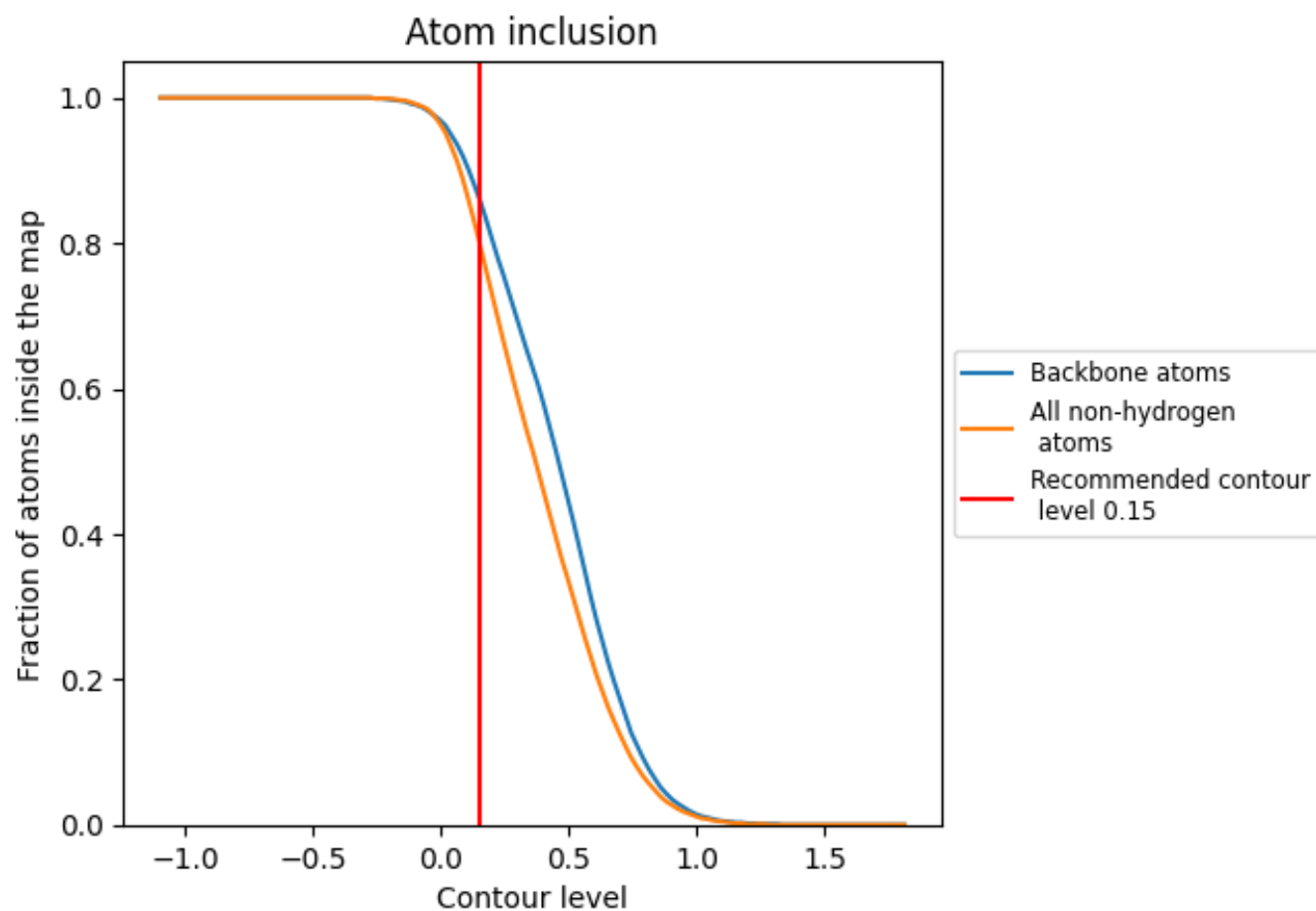
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8050	<div></div> 0.4120
A	<div></div> 0.8050	<div></div> 0.4120

