



## wwPDB EM Validation Summary Report ⓘ

Sep 2, 2025 – 02:26 PM EDT

PDB ID : 9OCJ / pdb\_00009ocj  
EMDB ID : EMD-70317  
Title : Transporter associated with antigen processing (TAP) bound to the viral protein CPXV012 in the outward-facing open state  
Authors : Lee, J.; Manon, V.; Chen, J.  
Deposited on : 2025-04-24  
Resolution : 3.00 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

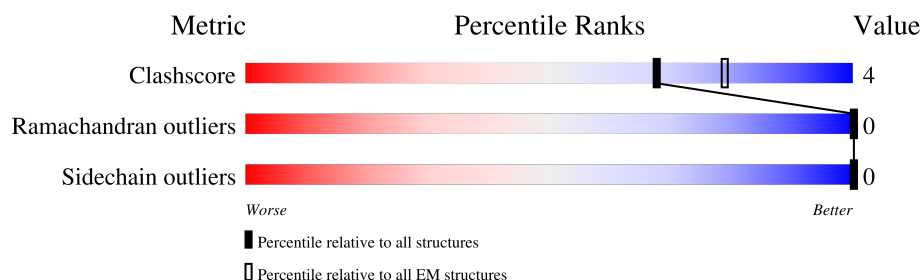
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 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	B	686	
2	D	123	
3	A	907	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9006 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 Antigen peptide transporter 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	550	Total	C	N	O	S	0	0
			4305	2734	758	790	23		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	632	GLN	GLU	engineered mutation	UNP Q03519

- Molecule 2 is a protein called TAP transporter inhibitor CPXV012.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	29	Total	C	N	O	S	0	0
			273	183	49	39	2		

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-53	GLY	-	expression tag	UNP Q8QN49
D	-52	PRO	-	expression tag	UNP Q8QN49
D	-51	THR	-	expression tag	UNP Q8QN49
D	-50	ALA	-	expression tag	UNP Q8QN49
D	-49	ALA	-	expression tag	UNP Q8QN49
D	-48	ALA	-	expression tag	UNP Q8QN49
D	-47	ALA	-	expression tag	UNP Q8QN49
D	-46	MET	-	expression tag	UNP Q8QN49
D	-45	GLY	-	expression tag	UNP Q8QN49
D	-44	ARG	-	expression tag	UNP Q8QN49
D	-43	GLY	-	expression tag	UNP Q8QN49
D	-42	VAL	-	expression tag	UNP Q8QN49
D	-41	PRO	-	expression tag	UNP Q8QN49
D	-40	HIS	-	expression tag	UNP Q8QN49
D	-39	ILE	-	expression tag	UNP Q8QN49
D	-38	VAL	-	expression tag	UNP Q8QN49

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-37	MET	-	expression tag	UNP Q8QN49
D	-36	VAL	-	expression tag	UNP Q8QN49
D	-35	ASP	-	expression tag	UNP Q8QN49
D	-34	ALA	-	expression tag	UNP Q8QN49
D	-33	TYR	-	expression tag	UNP Q8QN49
D	-32	LYS	-	expression tag	UNP Q8QN49
D	-31	ARG	-	expression tag	UNP Q8QN49
D	-30	TYR	-	expression tag	UNP Q8QN49
D	-29	LYS	-	expression tag	UNP Q8QN49
D	-28	GLY	-	expression tag	UNP Q8QN49
D	-27	GLY	-	expression tag	UNP Q8QN49
D	-26	GLY	-	expression tag	UNP Q8QN49
D	-25	SER	-	expression tag	UNP Q8QN49
D	-24	GLY	-	expression tag	UNP Q8QN49
D	-23	GLY	-	expression tag	UNP Q8QN49
D	-22	SER	-	expression tag	UNP Q8QN49
D	-21	GLY	-	expression tag	UNP Q8QN49
D	-20	GLY	-	expression tag	UNP Q8QN49
D	-19	GLY	-	expression tag	UNP Q8QN49
D	-18	GLU	-	expression tag	UNP Q8QN49
D	-17	ASN	-	expression tag	UNP Q8QN49
D	-16	LEU	-	expression tag	UNP Q8QN49
D	-15	TYR	-	expression tag	UNP Q8QN49
D	-14	PHE	-	expression tag	UNP Q8QN49
D	-13	GLN	-	expression tag	UNP Q8QN49
D	-12	GLY	-	expression tag	UNP Q8QN49
D	-11	SER	-	expression tag	UNP Q8QN49
D	-10	GLY	-	expression tag	UNP Q8QN49
D	-9	SER	-	expression tag	UNP Q8QN49
D	-8	SER	-	expression tag	UNP Q8QN49
D	-7	GLY	-	expression tag	UNP Q8QN49
D	-6	GLY	-	expression tag	UNP Q8QN49
D	-5	GLY	-	expression tag	UNP Q8QN49
D	-4	SER	-	expression tag	UNP Q8QN49
D	-3	SER	-	expression tag	UNP Q8QN49
D	-2	GLY	-	expression tag	UNP Q8QN49
D	-1	SER	-	expression tag	UNP Q8QN49
D	0	GLY	-	expression tag	UNP Q8QN49
D	1	GLY	-	expression tag	UNP Q8QN49

- Molecule 3 is a protein called Antigen peptide transporter 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	564	Total	C	N	O	S	0	0
			4364	2787	742	818	17		

There are 159 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	749	GLY	-	expression tag	UNP Q03518
A	750	GLY	-	expression tag	UNP Q03518
A	751	GLY	-	expression tag	UNP Q03518
A	752	SER	-	expression tag	UNP Q03518
A	753	GLY	-	expression tag	UNP Q03518
A	754	GLY	-	expression tag	UNP Q03518
A	755	SER	-	expression tag	UNP Q03518
A	756	GLY	-	expression tag	UNP Q03518
A	757	GLY	-	expression tag	UNP Q03518
A	758	GLY	-	expression tag	UNP Q03518
A	759	GLU	-	expression tag	UNP Q03518
A	760	ASN	-	expression tag	UNP Q03518
A	761	LEU	-	expression tag	UNP Q03518
A	762	TYR	-	expression tag	UNP Q03518
A	763	PHE	-	expression tag	UNP Q03518
A	764	GLN	-	expression tag	UNP Q03518
A	765	GLY	-	expression tag	UNP Q03518
A	766	SER	-	expression tag	UNP Q03518
A	767	GLY	-	expression tag	UNP Q03518
A	768	SER	-	expression tag	UNP Q03518
A	769	SER	-	expression tag	UNP Q03518
A	770	GLY	-	expression tag	UNP Q03518
A	771	GLY	-	expression tag	UNP Q03518
A	772	GLY	-	expression tag	UNP Q03518
A	773	SER	-	expression tag	UNP Q03518
A	774	SER	-	expression tag	UNP Q03518
A	775	GLY	-	expression tag	UNP Q03518
A	776	SER	-	expression tag	UNP Q03518
A	777	GLY	-	expression tag	UNP Q03518
A	778	GLY	-	expression tag	UNP Q03518
A	779	ALA	-	expression tag	UNP Q03518
A	780	MET	-	expression tag	UNP Q03518
A	781	VAL	-	expression tag	UNP Q03518
A	782	THR	-	expression tag	UNP Q03518
A	783	THR	-	expression tag	UNP Q03518
A	784	LEU	-	expression tag	UNP Q03518
A	785	SER	-	expression tag	UNP Q03518

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Chain	Residue	Modelled	Actual	Comment	Reference
A	786	GLY	-	expression tag	UNP Q03518
A	787	LEU	-	expression tag	UNP Q03518
A	788	SER	-	expression tag	UNP Q03518
A	789	GLY	-	expression tag	UNP Q03518
A	790	GLU	-	expression tag	UNP Q03518
A	791	GLN	-	expression tag	UNP Q03518
A	792	GLY	-	expression tag	UNP Q03518
A	793	PRO	-	expression tag	UNP Q03518
A	794	SER	-	expression tag	UNP Q03518
A	795	GLY	-	expression tag	UNP Q03518
A	796	ASP	-	expression tag	UNP Q03518
A	797	MET	-	expression tag	UNP Q03518
A	798	THR	-	expression tag	UNP Q03518
A	799	THR	-	expression tag	UNP Q03518
A	800	GLU	-	expression tag	UNP Q03518
A	801	GLU	-	expression tag	UNP Q03518
A	802	ASP	-	expression tag	UNP Q03518
A	803	SER	-	expression tag	UNP Q03518
A	804	ALA	-	expression tag	UNP Q03518
A	805	THR	-	expression tag	UNP Q03518
A	806	HIS	-	expression tag	UNP Q03518
A	807	ILE	-	expression tag	UNP Q03518
A	808	LYS	-	expression tag	UNP Q03518
A	809	PHE	-	expression tag	UNP Q03518
A	810	SER	-	expression tag	UNP Q03518
A	811	LYS	-	expression tag	UNP Q03518
A	812	ARG	-	expression tag	UNP Q03518
A	813	ASP	-	expression tag	UNP Q03518
A	814	GLU	-	expression tag	UNP Q03518
A	815	ASP	-	expression tag	UNP Q03518
A	816	GLY	-	expression tag	UNP Q03518
A	817	ARG	-	expression tag	UNP Q03518
A	818	GLU	-	expression tag	UNP Q03518
A	819	LEU	-	expression tag	UNP Q03518
A	820	ALA	-	expression tag	UNP Q03518
A	821	GLY	-	expression tag	UNP Q03518
A	822	ALA	-	expression tag	UNP Q03518
A	823	THR	-	expression tag	UNP Q03518
A	824	MET	-	expression tag	UNP Q03518
A	825	GLU	-	expression tag	UNP Q03518
A	826	LEU	-	expression tag	UNP Q03518
A	827	ARG	-	expression tag	UNP Q03518

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Chain	Residue	Modelled	Actual	Comment	Reference
A	828	ASP	-	expression tag	UNP Q03518
A	829	SER	-	expression tag	UNP Q03518
A	830	SER	-	expression tag	UNP Q03518
A	831	GLY	-	expression tag	UNP Q03518
A	832	LYS	-	expression tag	UNP Q03518
A	833	THR	-	expression tag	UNP Q03518
A	834	ILE	-	expression tag	UNP Q03518
A	835	SER	-	expression tag	UNP Q03518
A	836	THR	-	expression tag	UNP Q03518
A	837	TRP	-	expression tag	UNP Q03518
A	838	ILE	-	expression tag	UNP Q03518
A	839	SER	-	expression tag	UNP Q03518
A	840	ASP	-	expression tag	UNP Q03518
A	841	GLY	-	expression tag	UNP Q03518
A	842	HIS	-	expression tag	UNP Q03518
A	843	VAL	-	expression tag	UNP Q03518
A	844	LYS	-	expression tag	UNP Q03518
A	845	ASP	-	expression tag	UNP Q03518
A	846	PHE	-	expression tag	UNP Q03518
A	847	TYR	-	expression tag	UNP Q03518
A	848	LEU	-	expression tag	UNP Q03518
A	849	TYR	-	expression tag	UNP Q03518
A	850	PRO	-	expression tag	UNP Q03518
A	851	GLY	-	expression tag	UNP Q03518
A	852	LYS	-	expression tag	UNP Q03518
A	853	TYR	-	expression tag	UNP Q03518
A	854	THR	-	expression tag	UNP Q03518
A	855	PHE	-	expression tag	UNP Q03518
A	856	VAL	-	expression tag	UNP Q03518
A	857	GLU	-	expression tag	UNP Q03518
A	858	THR	-	expression tag	UNP Q03518
A	859	ALA	-	expression tag	UNP Q03518
A	860	ALA	-	expression tag	UNP Q03518
A	861	PRO	-	expression tag	UNP Q03518
A	862	ASP	-	expression tag	UNP Q03518
A	863	GLY	-	expression tag	UNP Q03518
A	864	TYR	-	expression tag	UNP Q03518
A	865	GLU	-	expression tag	UNP Q03518
A	866	VAL	-	expression tag	UNP Q03518
A	867	ALA	-	expression tag	UNP Q03518
A	868	THR	-	expression tag	UNP Q03518
A	869	PRO	-	expression tag	UNP Q03518

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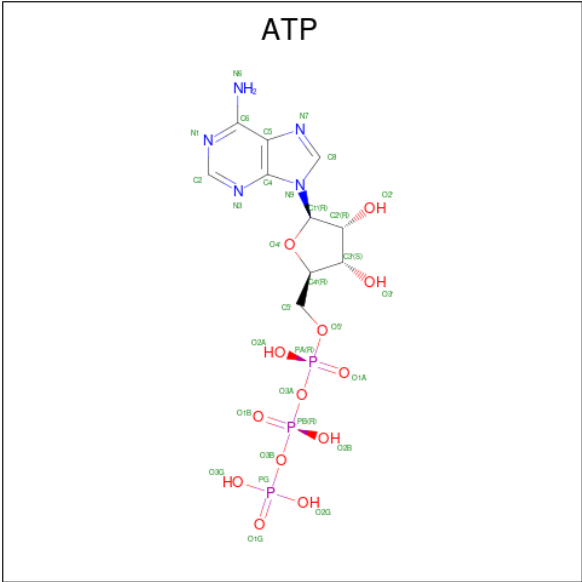


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Chain	Residue	Modelled	Actual	Comment	Reference
A	870	ILE	-	expression tag	UNP Q03518
A	871	GLU	-	expression tag	UNP Q03518
A	872	PHE	-	expression tag	UNP Q03518
A	873	THR	-	expression tag	UNP Q03518
A	874	VAL	-	expression tag	UNP Q03518
A	875	ASN	-	expression tag	UNP Q03518
A	876	GLU	-	expression tag	UNP Q03518
A	877	ASP	-	expression tag	UNP Q03518
A	878	GLY	-	expression tag	UNP Q03518
A	879	GLN	-	expression tag	UNP Q03518
A	880	VAL	-	expression tag	UNP Q03518
A	881	THR	-	expression tag	UNP Q03518
A	882	VAL	-	expression tag	UNP Q03518
A	883	ASP	-	expression tag	UNP Q03518
A	884	GLY	-	expression tag	UNP Q03518
A	885	GLU	-	expression tag	UNP Q03518
A	886	ALA	-	expression tag	UNP Q03518
A	887	THR	-	expression tag	UNP Q03518
A	888	GLU	-	expression tag	UNP Q03518
A	889	GLY	-	expression tag	UNP Q03518
A	890	ASP	-	expression tag	UNP Q03518
A	891	ALA	-	expression tag	UNP Q03518
A	892	HIS	-	expression tag	UNP Q03518
A	893	THR	-	expression tag	UNP Q03518
A	894	SER	-	expression tag	UNP Q03518
A	895	GLY	-	expression tag	UNP Q03518
A	896	GLY	-	expression tag	UNP Q03518
A	897	GLY	-	expression tag	UNP Q03518
A	898	HIS	-	expression tag	UNP Q03518
A	899	HIS	-	expression tag	UNP Q03518
A	900	HIS	-	expression tag	UNP Q03518
A	901	HIS	-	expression tag	UNP Q03518
A	902	HIS	-	expression tag	UNP Q03518
A	903	HIS	-	expression tag	UNP Q03518
A	904	HIS	-	expression tag	UNP Q03518
A	905	HIS	-	expression tag	UNP Q03518
A	906	HIS	-	expression tag	UNP Q03518
A	907	HIS	-	expression tag	UNP Q03518

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



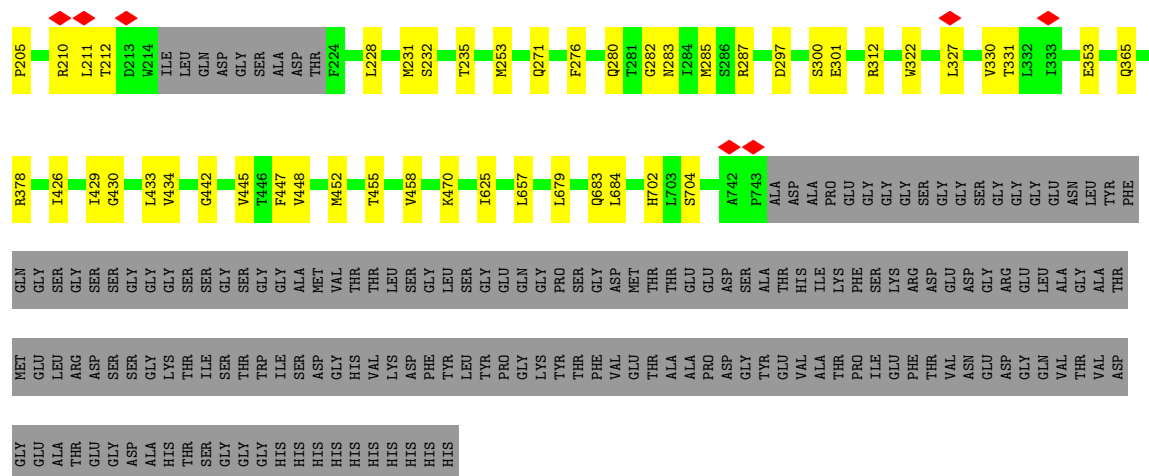


Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Mg	0
			1	1	
5	A	1	Total	Mg	0
			1	1	





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34592	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.134	Depositor
Minimum map value	-0.380	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.18	Depositor
Map size ( $\text{\AA}$ )	385.28, 385.28, 385.28	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.86, 0.86, 0.86	Depositor

## 5 Model quality [i](#)

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

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

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	B	0.15	0/4385	0.30	0/5939
2	D	0.43	1/284 (0.4%)	1.00	4/379 (1.1%)
3	A	0.15	0/4445	0.34	1/6034 (0.0%)
All	All	0.17	1/9114 (0.0%)	0.36	5/12352 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	42	PHE	CA-C	6.13	1.61	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	43	LYS	N-CA-C	9.77	123.64	110.35
2	D	42	PHE	CA-C-O	6.02	127.13	120.63
2	D	42	PHE	N-CA-C	5.70	118.22	111.33
2	D	49	TRP	N-CA-C	5.54	117.31	111.28
3	A	625	ILE	N-CA-C	-5.15	105.69	110.53

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	B	4305	0	4351	38	0
2	D	273	0	271	8	0
3	A	4364	0	4433	37	0
4	A	31	0	12	0	0
4	B	31	0	12	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	9006	0	9079	65	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 4.

The worst 5 of 65 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:B:343:ARG:NH2	3:A:271:GLN:O	2.22	0.70
3:A:353:GLU:HG3	3:A:470:LYS:HG3	1.76	0.68
1:B:236:GLN:O	3:A:378:ARG:NH2	2.28	0.67
1:B:333:ARG:HD3	3:A:285:MET:HE1	1.78	0.66
1:B:414:ILE:HG23	2:D:50:TYR:CD2	2.31	0.65

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	B	548/686 (80%)	531 (97%)	17 (3%)	0	100	100
2	D	27/123 (22%)	27 (100%)	0	0	100	100
3	A	560/907 (62%)	558 (100%)	2 (0%)	0	100	100
All	All	1135/1716 (66%)	1116 (98%)	19 (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	B	468/573 (82%)	468 (100%)	0	100	100
2	D	29/97 (30%)	29 (100%)	0	100	100
3	A	479/728 (66%)	479 (100%)	0	100	100
All	All	976/1398 (70%)	976 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	521	GLN
1	B	539	HIS
3	A	556	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

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	ATP	B	701	5	28,33,33	0.70	0	34,52,52	0.60	1 (2%)
4	ATP	A	1001	5	28,33,33	0.79	0	34,52,52	0.60	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	ATP	B	701	5	-	4/18/38/38	0/3/3/3
4	ATP	A	1001	5	-	7/18/38/38	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	ATP	C5-C6-N6	2.32	123.84	120.31
4	B	701	ATP	C5-C6-N6	2.29	123.80	120.31

There are no chirality outliers.

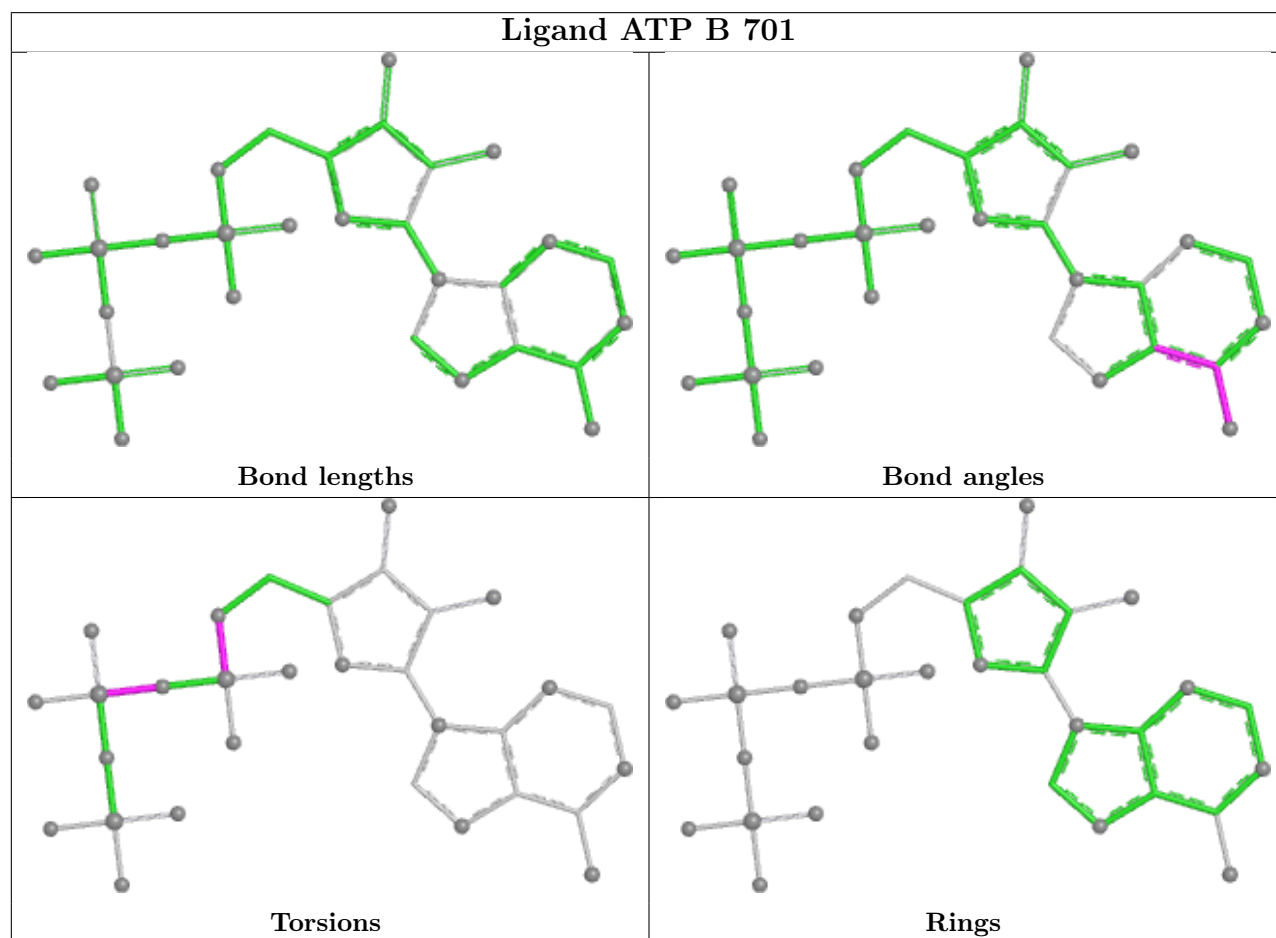
5 of 11 torsion outliers are listed below:

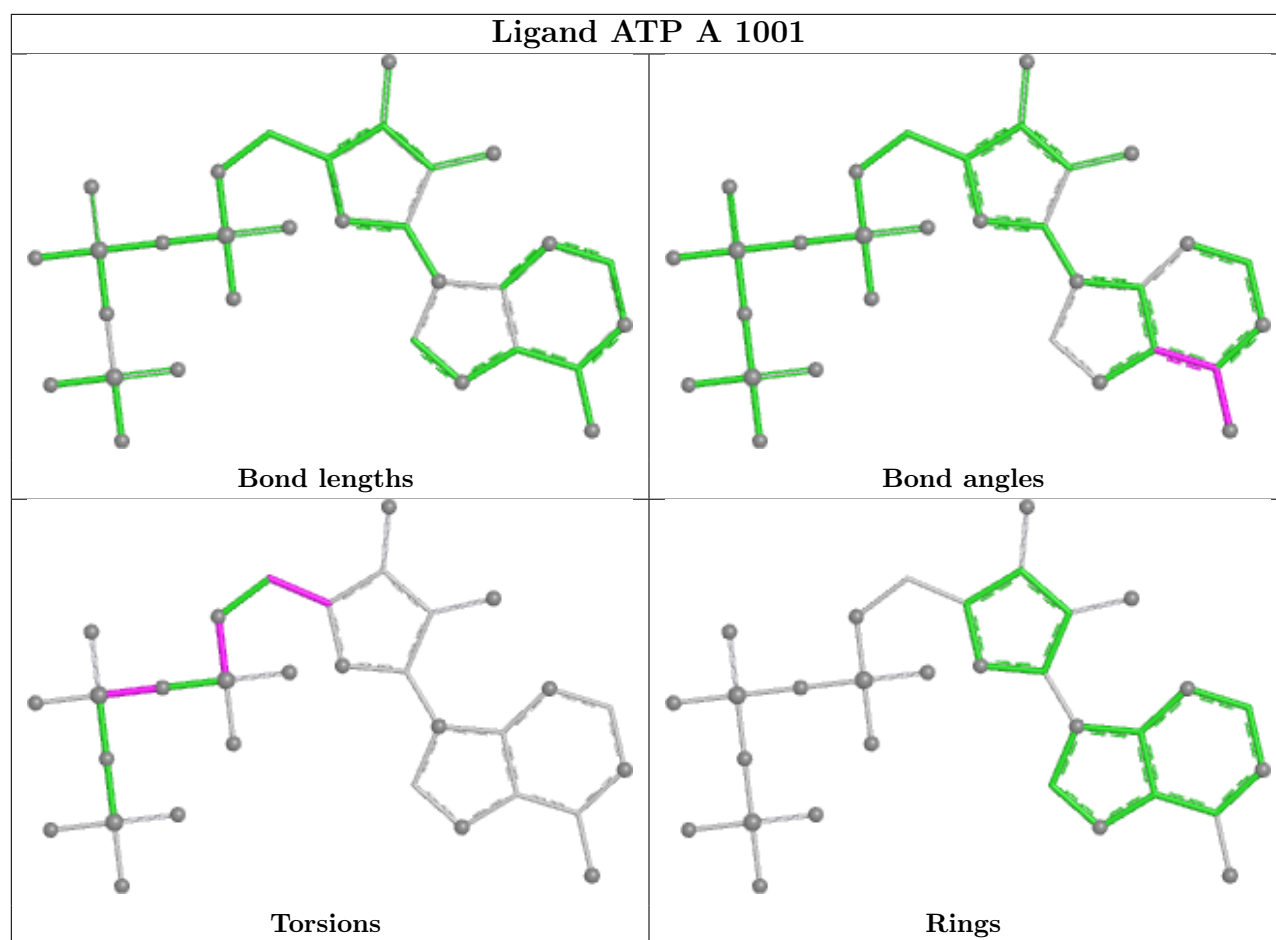
Mol	Chain	Res	Type	Atoms
4	B	701	ATP	C5'-O5'-PA-O2A
4	A	1001	ATP	C5'-O5'-PA-O2A
4	A	1001	ATP	C5'-O5'-PA-O3A
4	A	1001	ATP	O4'-C4'-C5'-O5'
4	A	1001	ATP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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.

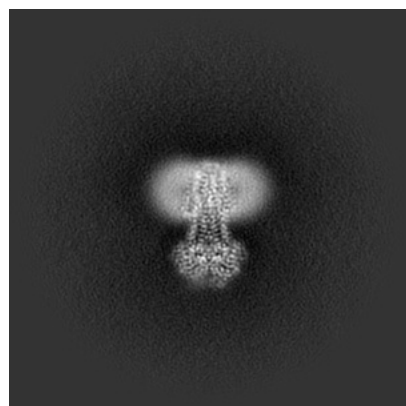
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70317. These allow visual inspection of the internal detail of the map and identification of artifacts.

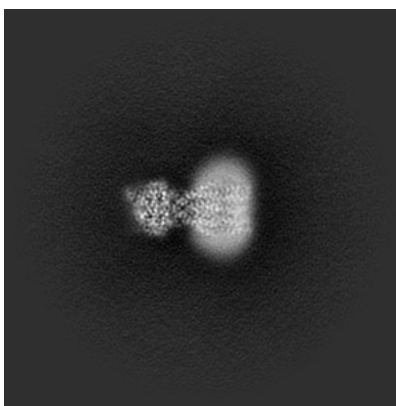
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

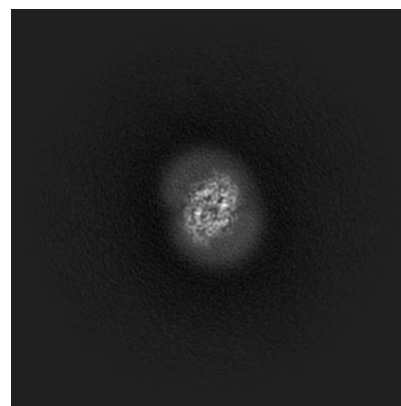
#### 6.1.1 Primary map



X

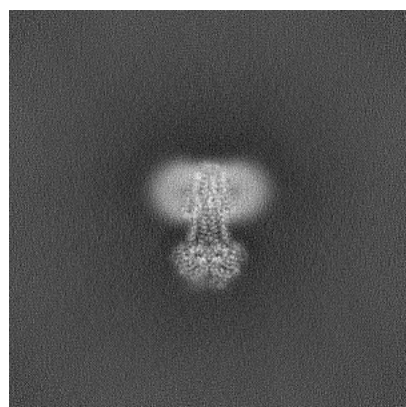


Y

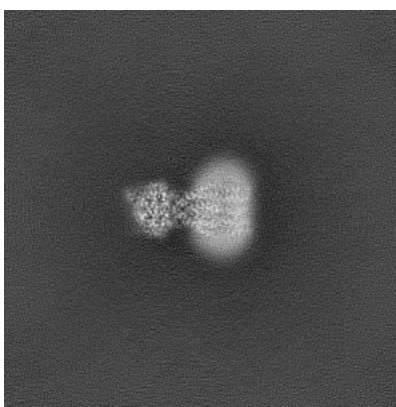


Z

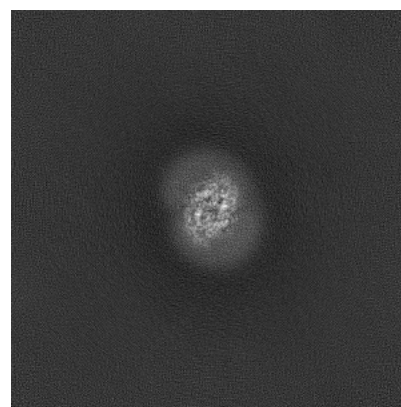
#### 6.1.2 Raw map



X



Y

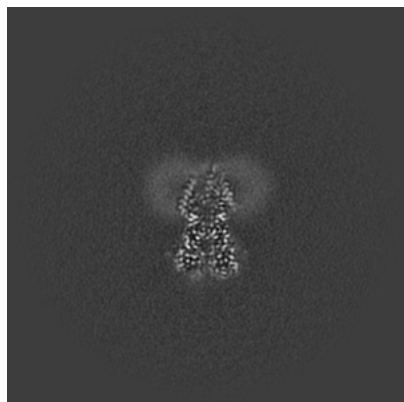


Z

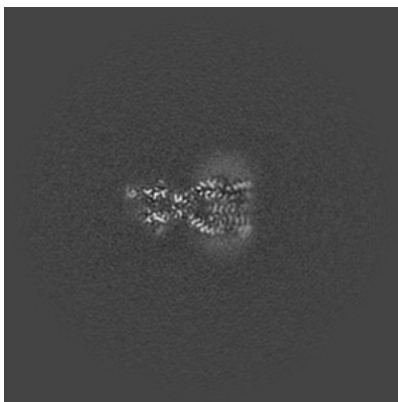
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

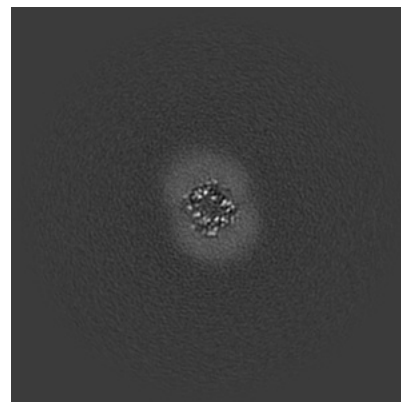
### 6.2.1 Primary map



X Index: 224

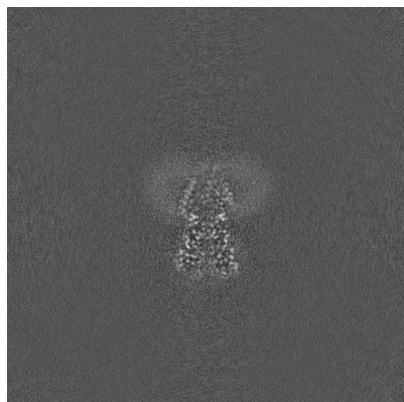


Y Index: 224

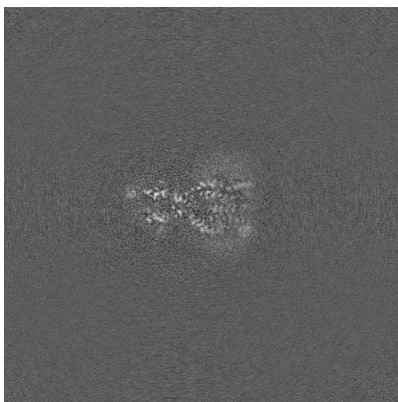


Z Index: 224

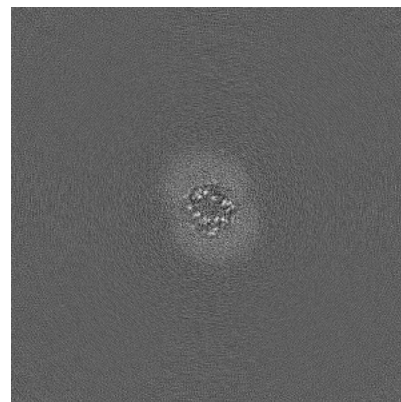
### 6.2.2 Raw map



X Index: 224



Y Index: 224

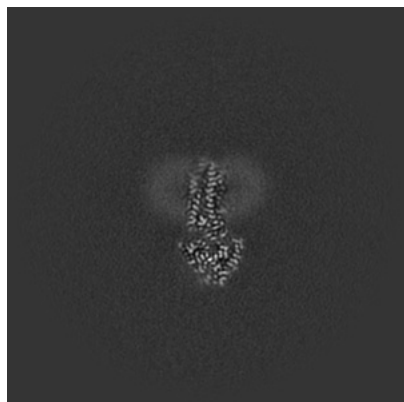


Z Index: 224

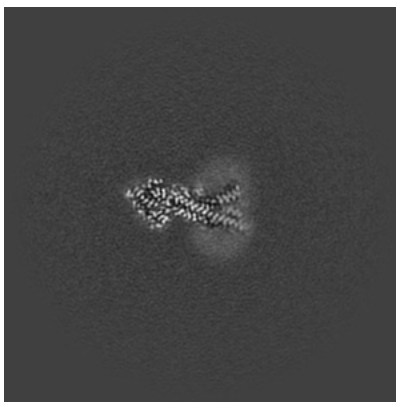
The images above show central slices of the map in three orthogonal directions.

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

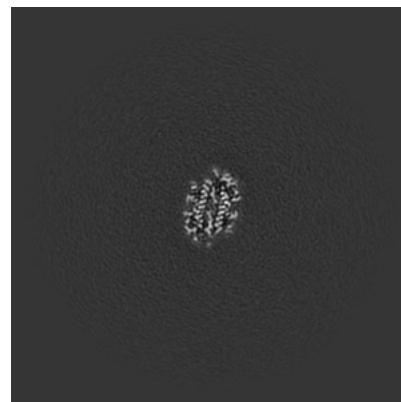
### 6.3.1 Primary map



X Index: 237

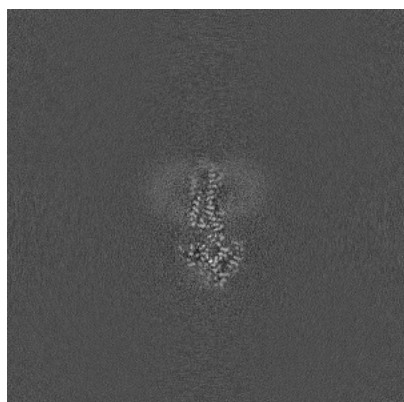


Y Index: 240

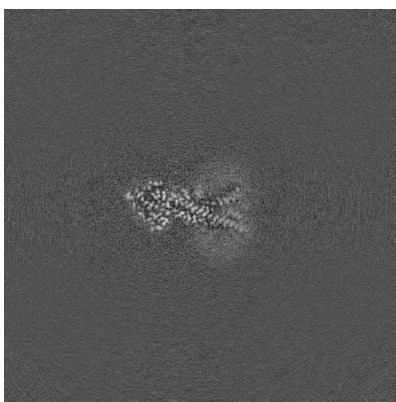


Z Index: 169

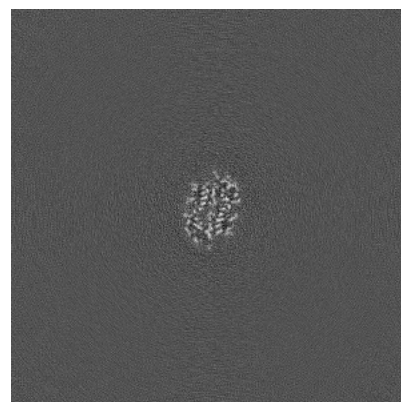
### 6.3.2 Raw map



X Index: 238



Y Index: 240



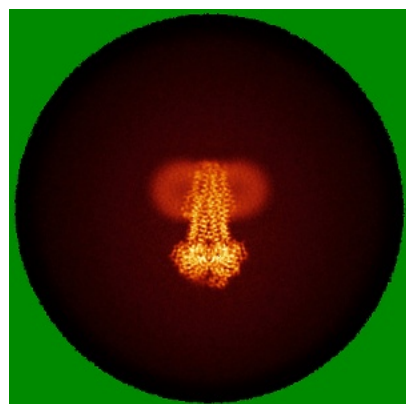
Z Index: 170

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

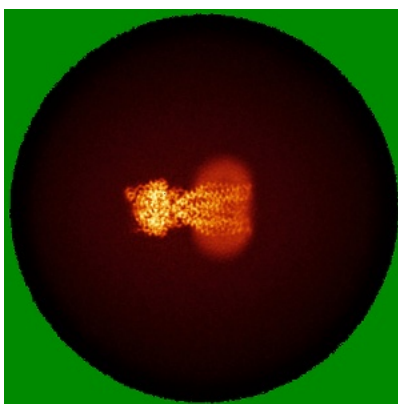


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

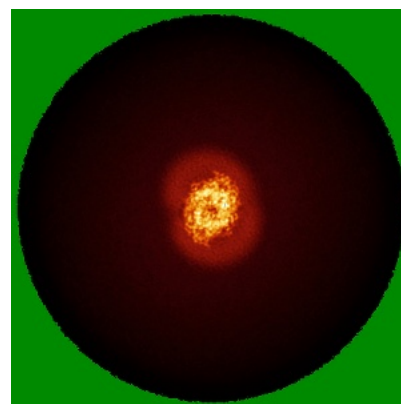
### 6.4.1 Primary map



X

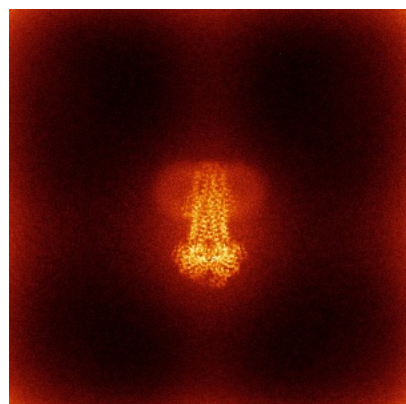


Y

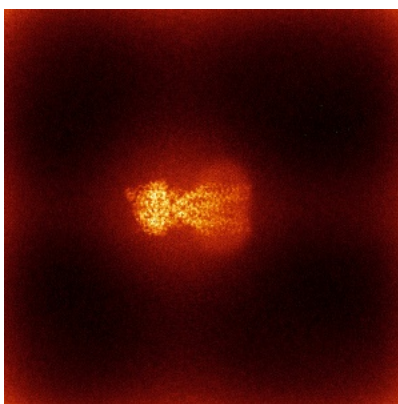


Z

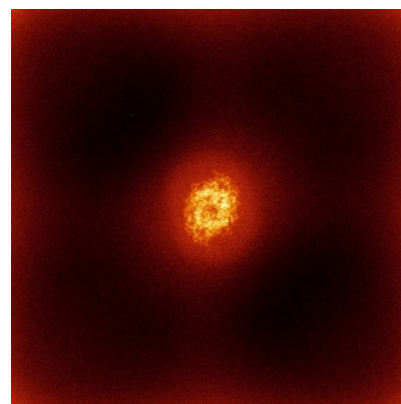
### 6.4.2 Raw map



X



Y



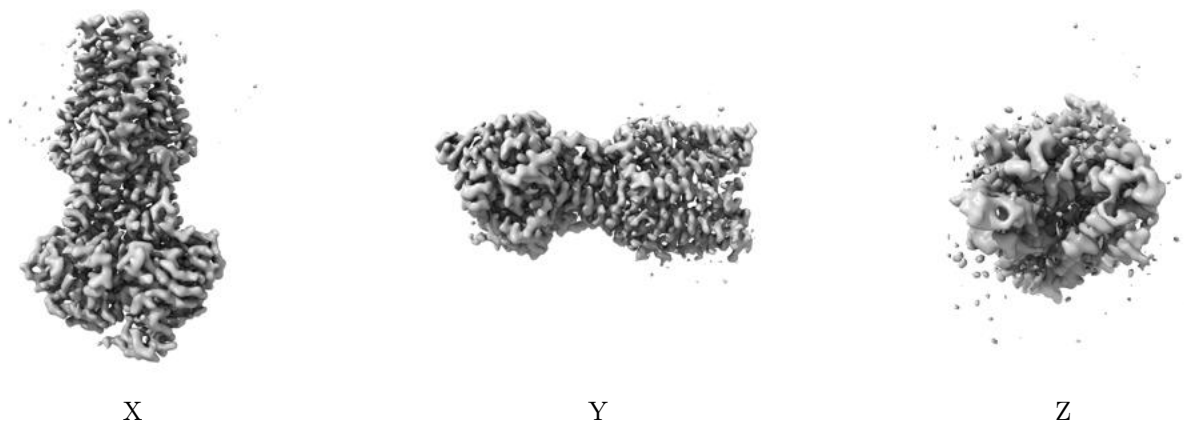
Z

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.



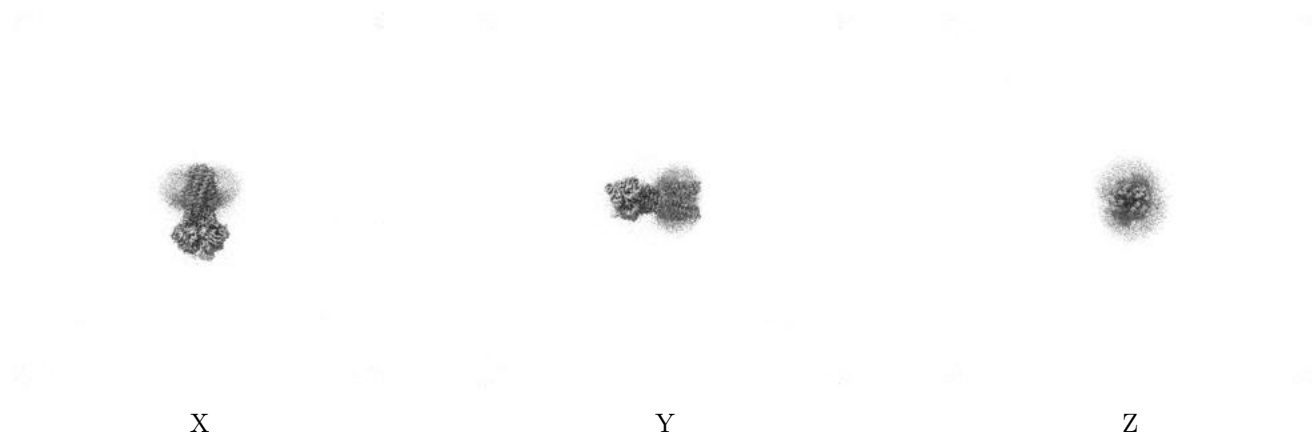
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. 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.

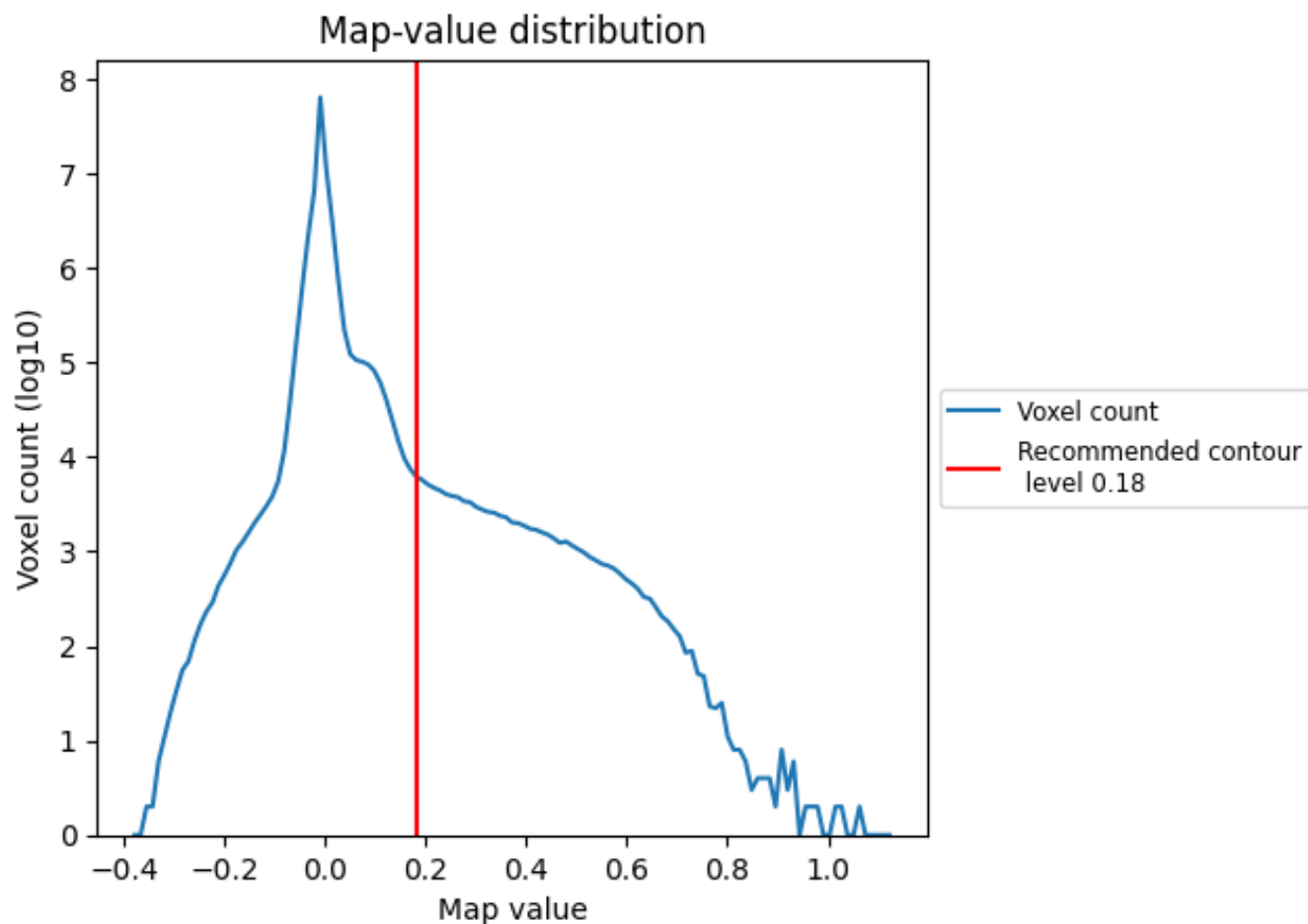
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

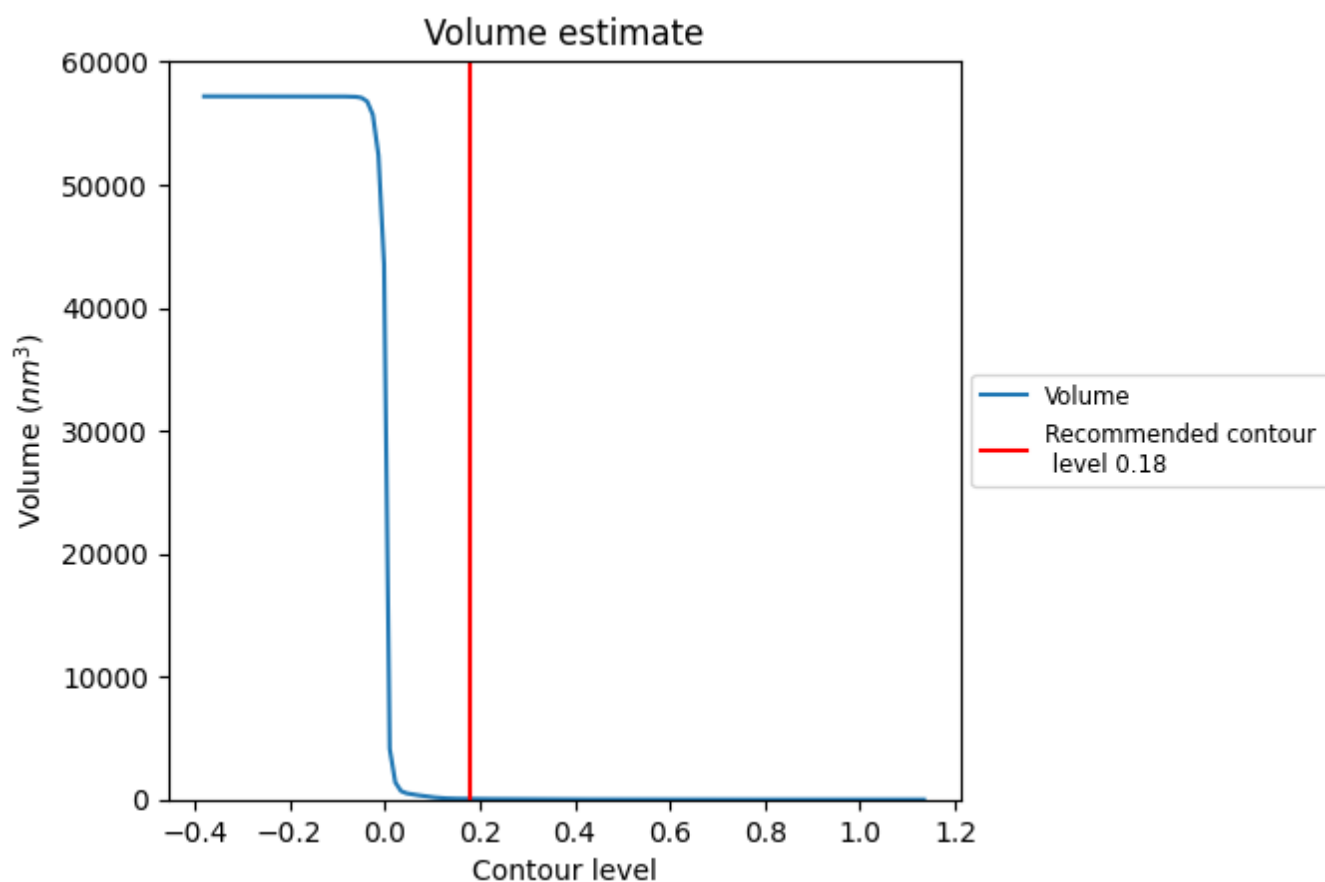
This section contains the results of statistical analysis of the map.

### 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.

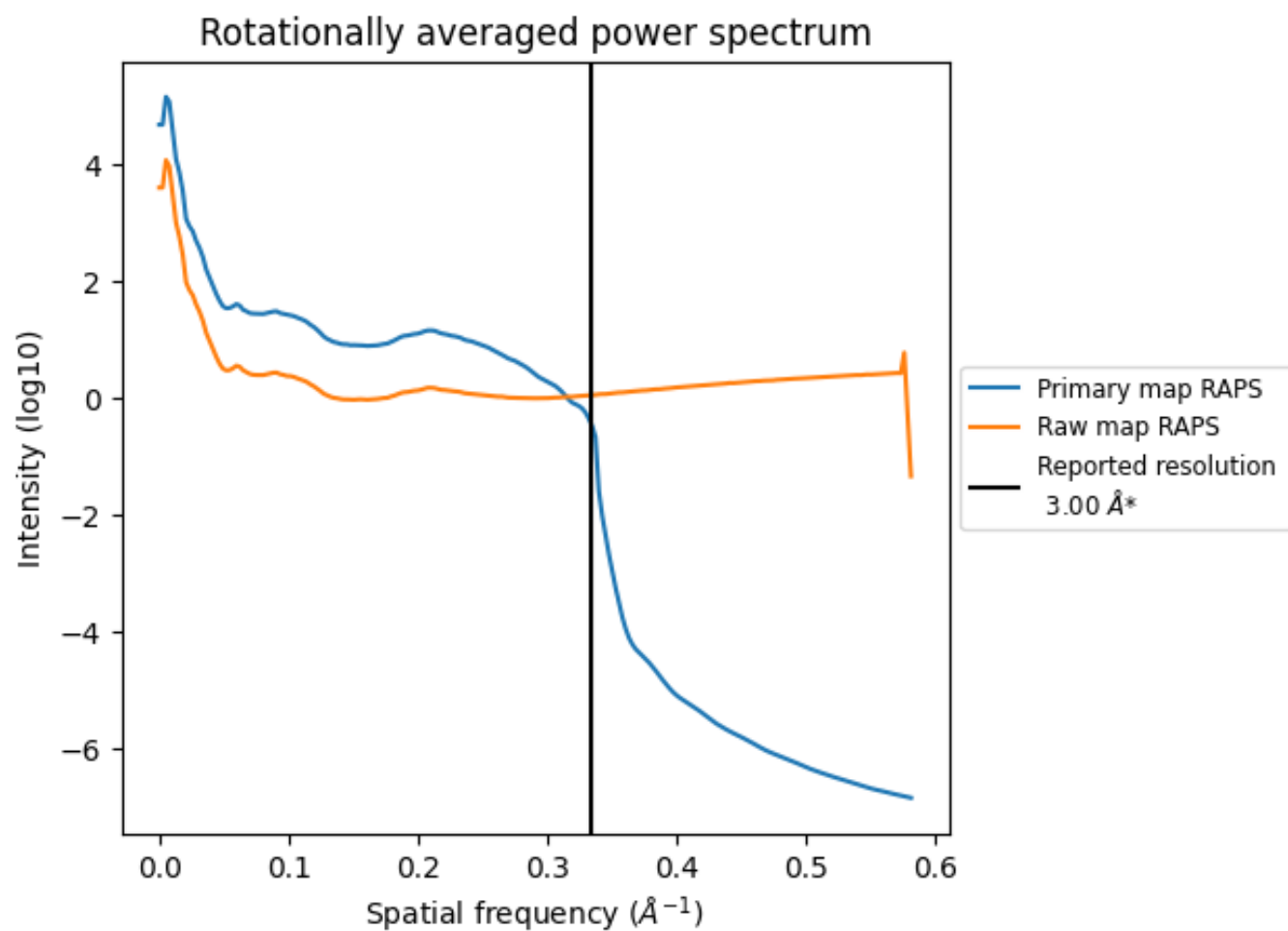
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 56  $\text{nm}^3$ ; this corresponds to an approximate mass of 51 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 ⓘ

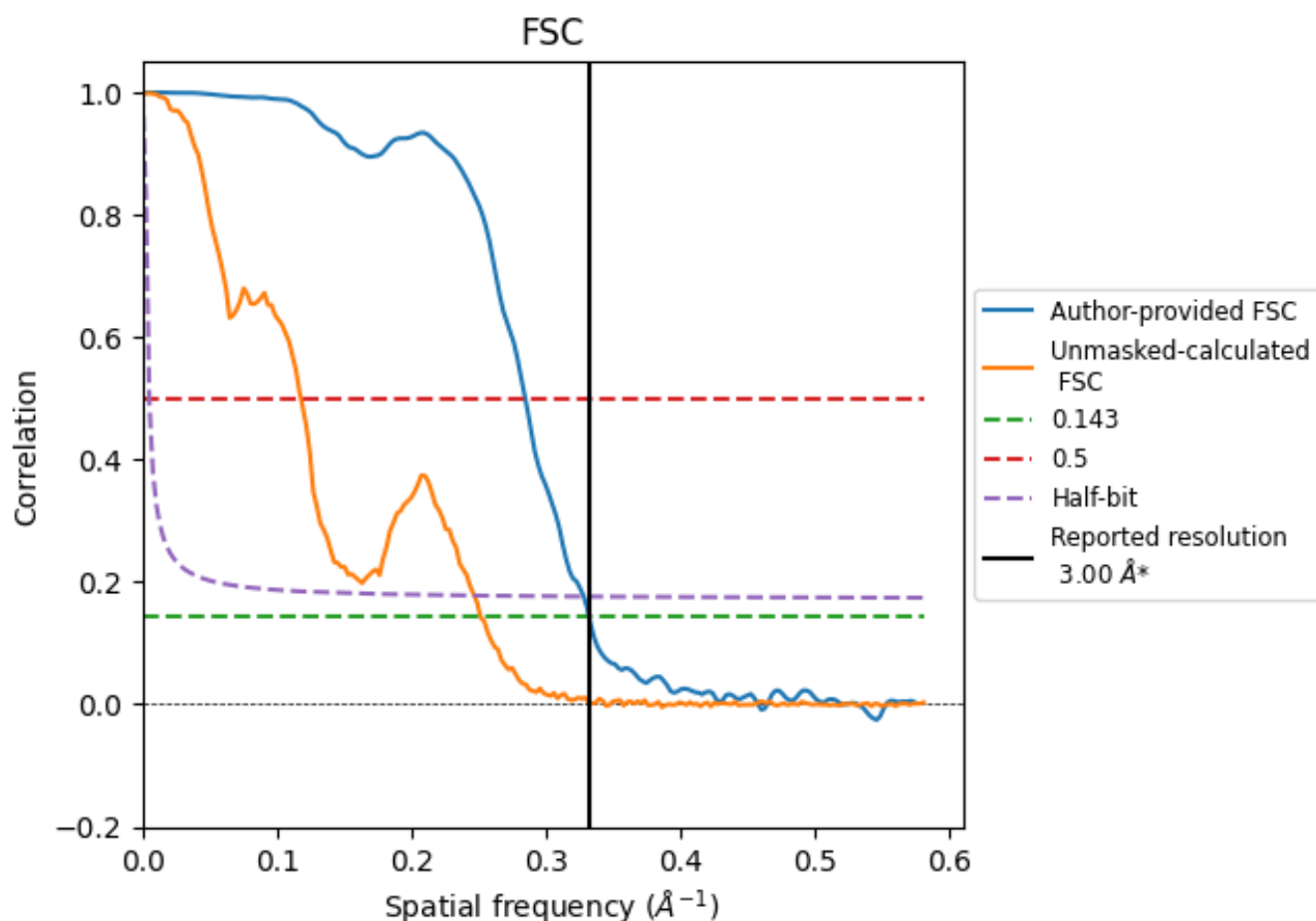


\*Reported resolution corresponds to spatial frequency of 0.333  $\text{\AA}^{-1}$

## 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 0.333 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

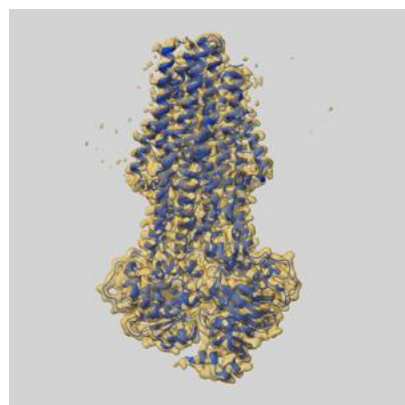
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.01	3.51	3.05
Unmasked-calculated*	3.97	8.48	4.05

\*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 3.97 differs from the reported value 3.0 by more than 10 %

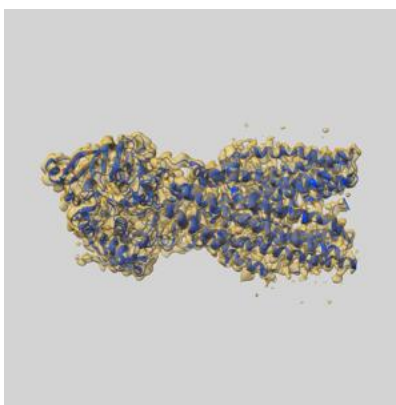
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70317 and PDB model 9OCJ. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

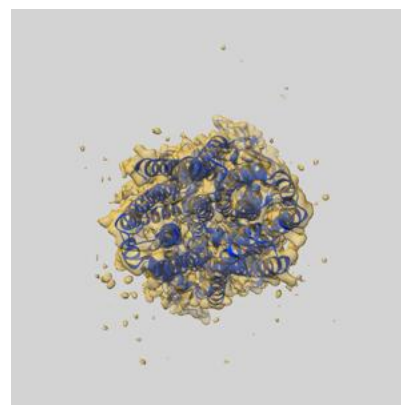
### 9.1 Map-model overlay [i](#)



X



Y

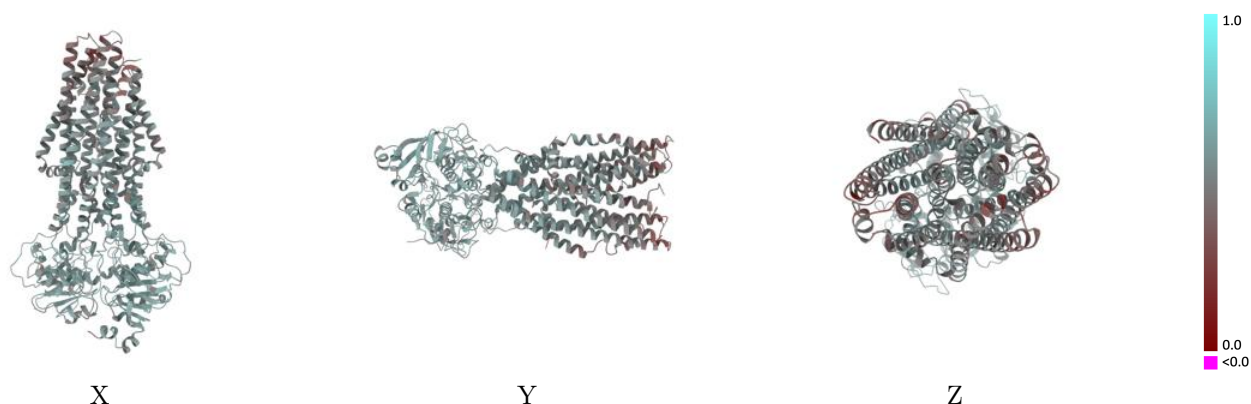


Z

The images above show the 3D surface view of the map at the recommended contour level 0.18 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.

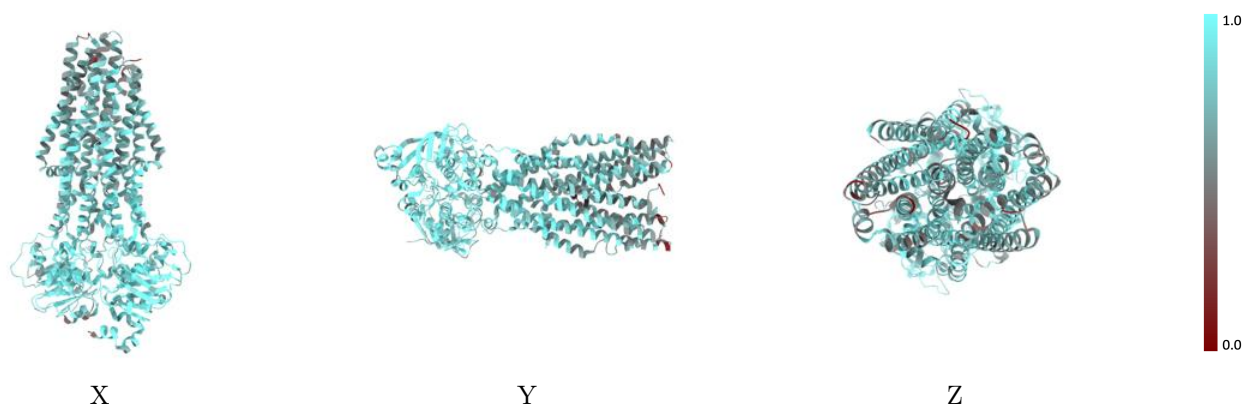


## 9.2 Q-score mapped to coordinate model [i](#)



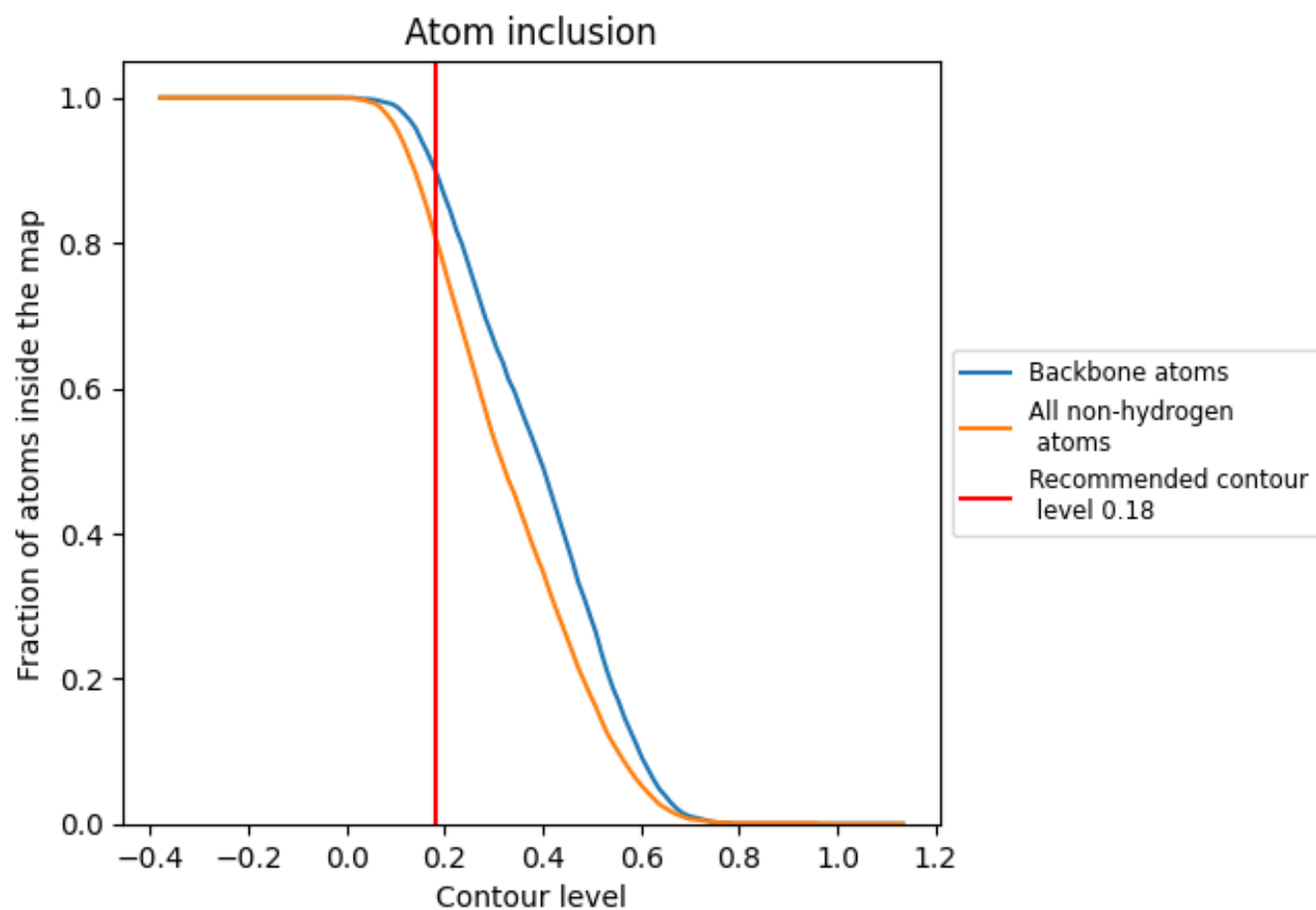
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.18).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 81% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8100	<div></div> 0.5290
A	<div></div> 0.8320	<div></div> 0.5370
B	<div></div> 0.8060	<div></div> 0.5240
D	<div></div> 0.5340	<div></div> 0.4760

