



## wwPDB EM Validation Summary Report ⓘ

Jan 20, 2024 – 06:51 am GMT

PDB ID : 8OPH  
EMDB ID : EMD-17053  
Title : Head-to-tail double ring assembly from truncated PVY coat protein  
Authors : Kavcic, L.; Kezar, A.; Podobnik, M.  
Deposited on : 2023-04-07  
Resolution : 2.93 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.dev70  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

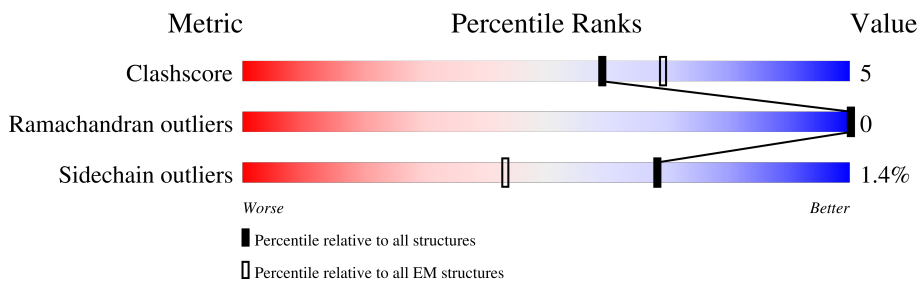
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.93 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.



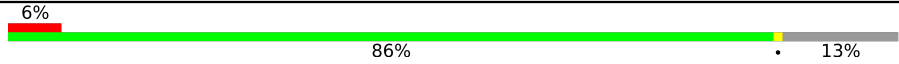
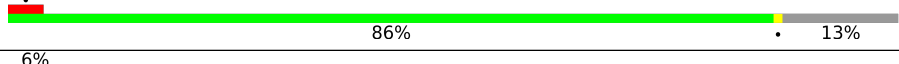
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	Aa	194	
1	Ab	194	
1	Ac	194	
1	Ad	194	
1	Ae	194	
1	Af	194	
1	Ag	194	
1	Ah	194	

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Mol	Chain	Length	Quality of chain
1	Ai	194	 6% 86% 13%
1	Aj	194	 5% 86% 13%
1	Ak	194	 8% 86% 13%
1	Al	194	 6% 86% 13%
1	Am	194	 5% 86% 13%
1	An	194	 1% 86% 13%
1	Ao	194	 6% 86% 13%
1	Ap	194	 5% 86% 13%

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 21824 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 Genome polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	Aa	169	1364	861	235	256	12	0	0
1	Ab	169	1364	861	235	256	12	0	0
1	Ac	169	1364	861	235	256	12	0	0
1	Ad	169	1364	861	235	256	12	0	0
1	Ae	169	1364	861	235	256	12	0	0
1	Af	169	1364	861	235	256	12	0	0
1	Ag	169	1364	861	235	256	12	0	0
1	Ah	169	1364	861	235	256	12	0	0
1	Ai	169	1364	861	235	256	12	0	0
1	Aj	169	1364	861	235	256	12	0	0
1	Ak	169	1364	861	235	256	12	0	0
1	Al	169	1364	861	235	256	12	0	0
1	Am	169	1364	861	235	256	12	0	0
1	An	169	1364	861	235	256	12	0	0
1	Ao	169	1364	861	235	256	12	0	0
1	Ap	169	1364	861	235	256	12	0	0

There are 256 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Aa	49	GLY	-	expression tag	UNP A0A0A7DIZ4
Aa	228	GLU	-	expression tag	UNP A0A0A7DIZ4
Aa	229	ASN	-	expression tag	UNP A0A0A7DIZ4
Aa	230	LEU	-	expression tag	UNP A0A0A7DIZ4
Aa	231	TYR	-	expression tag	UNP A0A0A7DIZ4
Aa	232	PHE	-	expression tag	UNP A0A0A7DIZ4
Aa	233	GLN	-	expression tag	UNP A0A0A7DIZ4
Aa	234	GLY	-	expression tag	UNP A0A0A7DIZ4
Aa	235	LEU	-	expression tag	UNP A0A0A7DIZ4
Aa	236	GLU	-	expression tag	UNP A0A0A7DIZ4
Aa	237	HIS	-	expression tag	UNP A0A0A7DIZ4
Aa	238	HIS	-	expression tag	UNP A0A0A7DIZ4
Aa	239	HIS	-	expression tag	UNP A0A0A7DIZ4
Aa	240	HIS	-	expression tag	UNP A0A0A7DIZ4
Aa	241	HIS	-	expression tag	UNP A0A0A7DIZ4
Aa	242	HIS	-	expression tag	UNP A0A0A7DIZ4
Ab	49	GLY	-	expression tag	UNP A0A0A7DIZ4
Ab	228	GLU	-	expression tag	UNP A0A0A7DIZ4
Ab	229	ASN	-	expression tag	UNP A0A0A7DIZ4
Ab	230	LEU	-	expression tag	UNP A0A0A7DIZ4
Ab	231	TYR	-	expression tag	UNP A0A0A7DIZ4
Ab	232	PHE	-	expression tag	UNP A0A0A7DIZ4
Ab	233	GLN	-	expression tag	UNP A0A0A7DIZ4
Ab	234	GLY	-	expression tag	UNP A0A0A7DIZ4
Ab	235	LEU	-	expression tag	UNP A0A0A7DIZ4
Ab	236	GLU	-	expression tag	UNP A0A0A7DIZ4
Ab	237	HIS	-	expression tag	UNP A0A0A7DIZ4
Ab	238	HIS	-	expression tag	UNP A0A0A7DIZ4
Ab	239	HIS	-	expression tag	UNP A0A0A7DIZ4
Ab	240	HIS	-	expression tag	UNP A0A0A7DIZ4
Ab	241	HIS	-	expression tag	UNP A0A0A7DIZ4
Ab	242	HIS	-	expression tag	UNP A0A0A7DIZ4
Ac	49	GLY	-	expression tag	UNP A0A0A7DIZ4
Ac	228	GLU	-	expression tag	UNP A0A0A7DIZ4
Ac	229	ASN	-	expression tag	UNP A0A0A7DIZ4
Ac	230	LEU	-	expression tag	UNP A0A0A7DIZ4
Ac	231	TYR	-	expression tag	UNP A0A0A7DIZ4
Ac	232	PHE	-	expression tag	UNP A0A0A7DIZ4
Ac	233	GLN	-	expression tag	UNP A0A0A7DIZ4
Ac	234	GLY	-	expression tag	UNP A0A0A7DIZ4
Ac	235	LEU	-	expression tag	UNP A0A0A7DIZ4
Ac	236	GLU	-	expression tag	UNP A0A0A7DIZ4
Ac	237	HIS	-	expression tag	UNP A0A0A7DIZ4

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Chain	Residue	Modelled	Actual	Comment	Reference
Ac	238	HIS	-	expression tag	UNP A0A0A7DIZ4
Ac	239	HIS	-	expression tag	UNP A0A0A7DIZ4
Ac	240	HIS	-	expression tag	UNP A0A0A7DIZ4
Ac	241	HIS	-	expression tag	UNP A0A0A7DIZ4
Ac	242	HIS	-	expression tag	UNP A0A0A7DIZ4
Ad	49	GLY	-	expression tag	UNP A0A0A7DIZ4
Ad	228	GLU	-	expression tag	UNP A0A0A7DIZ4
Ad	229	ASN	-	expression tag	UNP A0A0A7DIZ4
Ad	230	LEU	-	expression tag	UNP A0A0A7DIZ4
Ad	231	TYR	-	expression tag	UNP A0A0A7DIZ4
Ad	232	PHE	-	expression tag	UNP A0A0A7DIZ4
Ad	233	GLN	-	expression tag	UNP A0A0A7DIZ4
Ad	234	GLY	-	expression tag	UNP A0A0A7DIZ4
Ad	235	LEU	-	expression tag	UNP A0A0A7DIZ4
Ad	236	GLU	-	expression tag	UNP A0A0A7DIZ4
Ad	237	HIS	-	expression tag	UNP A0A0A7DIZ4
Ad	238	HIS	-	expression tag	UNP A0A0A7DIZ4
Ad	239	HIS	-	expression tag	UNP A0A0A7DIZ4
Ad	240	HIS	-	expression tag	UNP A0A0A7DIZ4
Ad	241	HIS	-	expression tag	UNP A0A0A7DIZ4
Ad	242	HIS	-	expression tag	UNP A0A0A7DIZ4
Ae	49	GLY	-	expression tag	UNP A0A0A7DIZ4
Ae	228	GLU	-	expression tag	UNP A0A0A7DIZ4
Ae	229	ASN	-	expression tag	UNP A0A0A7DIZ4
Ae	230	LEU	-	expression tag	UNP A0A0A7DIZ4
Ae	231	TYR	-	expression tag	UNP A0A0A7DIZ4
Ae	232	PHE	-	expression tag	UNP A0A0A7DIZ4
Ae	233	GLN	-	expression tag	UNP A0A0A7DIZ4
Ae	234	GLY	-	expression tag	UNP A0A0A7DIZ4
Ae	235	LEU	-	expression tag	UNP A0A0A7DIZ4
Ae	236	GLU	-	expression tag	UNP A0A0A7DIZ4
Ae	237	HIS	-	expression tag	UNP A0A0A7DIZ4
Ae	238	HIS	-	expression tag	UNP A0A0A7DIZ4
Ae	239	HIS	-	expression tag	UNP A0A0A7DIZ4
Ae	240	HIS	-	expression tag	UNP A0A0A7DIZ4
Ae	241	HIS	-	expression tag	UNP A0A0A7DIZ4
Ae	242	HIS	-	expression tag	UNP A0A0A7DIZ4
Af	49	GLY	-	expression tag	UNP A0A0A7DIZ4
Af	228	GLU	-	expression tag	UNP A0A0A7DIZ4
Af	229	ASN	-	expression tag	UNP A0A0A7DIZ4
Af	230	LEU	-	expression tag	UNP A0A0A7DIZ4
Af	231	TYR	-	expression tag	UNP A0A0A7DIZ4

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Chain	Residue	Modelled	Actual	Comment	Reference
Af	232	PHE	-	expression tag	UNP A0A0A7DIZ4
Af	233	GLN	-	expression tag	UNP A0A0A7DIZ4
Af	234	GLY	-	expression tag	UNP A0A0A7DIZ4
Af	235	LEU	-	expression tag	UNP A0A0A7DIZ4
Af	236	GLU	-	expression tag	UNP A0A0A7DIZ4
Af	237	HIS	-	expression tag	UNP A0A0A7DIZ4
Af	238	HIS	-	expression tag	UNP A0A0A7DIZ4
Af	239	HIS	-	expression tag	UNP A0A0A7DIZ4
Af	240	HIS	-	expression tag	UNP A0A0A7DIZ4
Af	241	HIS	-	expression tag	UNP A0A0A7DIZ4
Af	242	HIS	-	expression tag	UNP A0A0A7DIZ4
Ag	49	GLY	-	expression tag	UNP A0A0A7DIZ4
Ag	228	GLU	-	expression tag	UNP A0A0A7DIZ4
Ag	229	ASN	-	expression tag	UNP A0A0A7DIZ4
Ag	230	LEU	-	expression tag	UNP A0A0A7DIZ4
Ag	231	TYR	-	expression tag	UNP A0A0A7DIZ4
Ag	232	PHE	-	expression tag	UNP A0A0A7DIZ4
Ag	233	GLN	-	expression tag	UNP A0A0A7DIZ4
Ag	234	GLY	-	expression tag	UNP A0A0A7DIZ4
Ag	235	LEU	-	expression tag	UNP A0A0A7DIZ4
Ag	236	GLU	-	expression tag	UNP A0A0A7DIZ4
Ag	237	HIS	-	expression tag	UNP A0A0A7DIZ4
Ag	238	HIS	-	expression tag	UNP A0A0A7DIZ4
Ag	239	HIS	-	expression tag	UNP A0A0A7DIZ4
Ag	240	HIS	-	expression tag	UNP A0A0A7DIZ4
Ag	241	HIS	-	expression tag	UNP A0A0A7DIZ4
Ag	242	HIS	-	expression tag	UNP A0A0A7DIZ4
Ah	49	GLY	-	expression tag	UNP A0A0A7DIZ4
Ah	228	GLU	-	expression tag	UNP A0A0A7DIZ4
Ah	229	ASN	-	expression tag	UNP A0A0A7DIZ4
Ah	230	LEU	-	expression tag	UNP A0A0A7DIZ4
Ah	231	TYR	-	expression tag	UNP A0A0A7DIZ4
Ah	232	PHE	-	expression tag	UNP A0A0A7DIZ4
Ah	233	GLN	-	expression tag	UNP A0A0A7DIZ4
Ah	234	GLY	-	expression tag	UNP A0A0A7DIZ4
Ah	235	LEU	-	expression tag	UNP A0A0A7DIZ4
Ah	236	GLU	-	expression tag	UNP A0A0A7DIZ4
Ah	237	HIS	-	expression tag	UNP A0A0A7DIZ4
Ah	238	HIS	-	expression tag	UNP A0A0A7DIZ4
Ah	239	HIS	-	expression tag	UNP A0A0A7DIZ4
Ah	240	HIS	-	expression tag	UNP A0A0A7DIZ4
Ah	241	HIS	-	expression tag	UNP A0A0A7DIZ4

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Chain	Residue	Modelled	Actual	Comment	Reference
Ah	242	HIS	-	expression tag	UNP A0A0A7DIZ4
Ai	49	GLY	-	expression tag	UNP A0A0A7DIZ4
Ai	228	GLU	-	expression tag	UNP A0A0A7DIZ4
Ai	229	ASN	-	expression tag	UNP A0A0A7DIZ4
Ai	230	LEU	-	expression tag	UNP A0A0A7DIZ4
Ai	231	TYR	-	expression tag	UNP A0A0A7DIZ4
Ai	232	PHE	-	expression tag	UNP A0A0A7DIZ4
Ai	233	GLN	-	expression tag	UNP A0A0A7DIZ4
Ai	234	GLY	-	expression tag	UNP A0A0A7DIZ4
Ai	235	LEU	-	expression tag	UNP A0A0A7DIZ4
Ai	236	GLU	-	expression tag	UNP A0A0A7DIZ4
Ai	237	HIS	-	expression tag	UNP A0A0A7DIZ4
Ai	238	HIS	-	expression tag	UNP A0A0A7DIZ4
Ai	239	HIS	-	expression tag	UNP A0A0A7DIZ4
Ai	240	HIS	-	expression tag	UNP A0A0A7DIZ4
Ai	241	HIS	-	expression tag	UNP A0A0A7DIZ4
Ai	242	HIS	-	expression tag	UNP A0A0A7DIZ4
Aj	49	GLY	-	expression tag	UNP A0A0A7DIZ4
Aj	228	GLU	-	expression tag	UNP A0A0A7DIZ4
Aj	229	ASN	-	expression tag	UNP A0A0A7DIZ4
Aj	230	LEU	-	expression tag	UNP A0A0A7DIZ4
Aj	231	TYR	-	expression tag	UNP A0A0A7DIZ4
Aj	232	PHE	-	expression tag	UNP A0A0A7DIZ4
Aj	233	GLN	-	expression tag	UNP A0A0A7DIZ4
Aj	234	GLY	-	expression tag	UNP A0A0A7DIZ4
Aj	235	LEU	-	expression tag	UNP A0A0A7DIZ4
Aj	236	GLU	-	expression tag	UNP A0A0A7DIZ4
Aj	237	HIS	-	expression tag	UNP A0A0A7DIZ4
Aj	238	HIS	-	expression tag	UNP A0A0A7DIZ4
Aj	239	HIS	-	expression tag	UNP A0A0A7DIZ4
Aj	240	HIS	-	expression tag	UNP A0A0A7DIZ4
Aj	241	HIS	-	expression tag	UNP A0A0A7DIZ4
Aj	242	HIS	-	expression tag	UNP A0A0A7DIZ4
Ak	49	GLY	-	expression tag	UNP A0A0A7DIZ4
Ak	228	GLU	-	expression tag	UNP A0A0A7DIZ4
Ak	229	ASN	-	expression tag	UNP A0A0A7DIZ4
Ak	230	LEU	-	expression tag	UNP A0A0A7DIZ4
Ak	231	TYR	-	expression tag	UNP A0A0A7DIZ4
Ak	232	PHE	-	expression tag	UNP A0A0A7DIZ4
Ak	233	GLN	-	expression tag	UNP A0A0A7DIZ4
Ak	234	GLY	-	expression tag	UNP A0A0A7DIZ4
Ak	235	LEU	-	expression tag	UNP A0A0A7DIZ4

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Chain	Residue	Modelled	Actual	Comment	Reference
Ak	236	GLU	-	expression tag	UNP A0A0A7DIZ4
Ak	237	HIS	-	expression tag	UNP A0A0A7DIZ4
Ak	238	HIS	-	expression tag	UNP A0A0A7DIZ4
Ak	239	HIS	-	expression tag	UNP A0A0A7DIZ4
Ak	240	HIS	-	expression tag	UNP A0A0A7DIZ4
Ak	241	HIS	-	expression tag	UNP A0A0A7DIZ4
Ak	242	HIS	-	expression tag	UNP A0A0A7DIZ4
Al	49	GLY	-	expression tag	UNP A0A0A7DIZ4
Al	228	GLU	-	expression tag	UNP A0A0A7DIZ4
Al	229	ASN	-	expression tag	UNP A0A0A7DIZ4
Al	230	LEU	-	expression tag	UNP A0A0A7DIZ4
Al	231	TYR	-	expression tag	UNP A0A0A7DIZ4
Al	232	PHE	-	expression tag	UNP A0A0A7DIZ4
Al	233	GLN	-	expression tag	UNP A0A0A7DIZ4
Al	234	GLY	-	expression tag	UNP A0A0A7DIZ4
Al	235	LEU	-	expression tag	UNP A0A0A7DIZ4
Al	236	GLU	-	expression tag	UNP A0A0A7DIZ4
Al	237	HIS	-	expression tag	UNP A0A0A7DIZ4
Al	238	HIS	-	expression tag	UNP A0A0A7DIZ4
Al	239	HIS	-	expression tag	UNP A0A0A7DIZ4
Al	240	HIS	-	expression tag	UNP A0A0A7DIZ4
Al	241	HIS	-	expression tag	UNP A0A0A7DIZ4
Al	242	HIS	-	expression tag	UNP A0A0A7DIZ4
Am	49	GLY	-	expression tag	UNP A0A0A7DIZ4
Am	228	GLU	-	expression tag	UNP A0A0A7DIZ4
Am	229	ASN	-	expression tag	UNP A0A0A7DIZ4
Am	230	LEU	-	expression tag	UNP A0A0A7DIZ4
Am	231	TYR	-	expression tag	UNP A0A0A7DIZ4
Am	232	PHE	-	expression tag	UNP A0A0A7DIZ4
Am	233	GLN	-	expression tag	UNP A0A0A7DIZ4
Am	234	GLY	-	expression tag	UNP A0A0A7DIZ4
Am	235	LEU	-	expression tag	UNP A0A0A7DIZ4
Am	236	GLU	-	expression tag	UNP A0A0A7DIZ4
Am	237	HIS	-	expression tag	UNP A0A0A7DIZ4
Am	238	HIS	-	expression tag	UNP A0A0A7DIZ4
Am	239	HIS	-	expression tag	UNP A0A0A7DIZ4
Am	240	HIS	-	expression tag	UNP A0A0A7DIZ4
Am	241	HIS	-	expression tag	UNP A0A0A7DIZ4
Am	242	HIS	-	expression tag	UNP A0A0A7DIZ4
An	49	GLY	-	expression tag	UNP A0A0A7DIZ4
An	228	GLU	-	expression tag	UNP A0A0A7DIZ4
An	229	ASN	-	expression tag	UNP A0A0A7DIZ4

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Chain	Residue	Modelled	Actual	Comment	Reference
An	230	LEU	-	expression tag	UNP A0A0A7DIZ4
An	231	TYR	-	expression tag	UNP A0A0A7DIZ4
An	232	PHE	-	expression tag	UNP A0A0A7DIZ4
An	233	GLN	-	expression tag	UNP A0A0A7DIZ4
An	234	GLY	-	expression tag	UNP A0A0A7DIZ4
An	235	LEU	-	expression tag	UNP A0A0A7DIZ4
An	236	GLU	-	expression tag	UNP A0A0A7DIZ4
An	237	HIS	-	expression tag	UNP A0A0A7DIZ4
An	238	HIS	-	expression tag	UNP A0A0A7DIZ4
An	239	HIS	-	expression tag	UNP A0A0A7DIZ4
An	240	HIS	-	expression tag	UNP A0A0A7DIZ4
An	241	HIS	-	expression tag	UNP A0A0A7DIZ4
An	242	HIS	-	expression tag	UNP A0A0A7DIZ4
Ao	49	GLY	-	expression tag	UNP A0A0A7DIZ4
Ao	228	GLU	-	expression tag	UNP A0A0A7DIZ4
Ao	229	ASN	-	expression tag	UNP A0A0A7DIZ4
Ao	230	LEU	-	expression tag	UNP A0A0A7DIZ4
Ao	231	TYR	-	expression tag	UNP A0A0A7DIZ4
Ao	232	PHE	-	expression tag	UNP A0A0A7DIZ4
Ao	233	GLN	-	expression tag	UNP A0A0A7DIZ4
Ao	234	GLY	-	expression tag	UNP A0A0A7DIZ4
Ao	235	LEU	-	expression tag	UNP A0A0A7DIZ4
Ao	236	GLU	-	expression tag	UNP A0A0A7DIZ4
Ao	237	HIS	-	expression tag	UNP A0A0A7DIZ4
Ao	238	HIS	-	expression tag	UNP A0A0A7DIZ4
Ao	239	HIS	-	expression tag	UNP A0A0A7DIZ4
Ao	240	HIS	-	expression tag	UNP A0A0A7DIZ4
Ao	241	HIS	-	expression tag	UNP A0A0A7DIZ4
Ao	242	HIS	-	expression tag	UNP A0A0A7DIZ4
Ap	49	GLY	-	expression tag	UNP A0A0A7DIZ4
Ap	228	GLU	-	expression tag	UNP A0A0A7DIZ4
Ap	229	ASN	-	expression tag	UNP A0A0A7DIZ4
Ap	230	LEU	-	expression tag	UNP A0A0A7DIZ4
Ap	231	TYR	-	expression tag	UNP A0A0A7DIZ4
Ap	232	PHE	-	expression tag	UNP A0A0A7DIZ4
Ap	233	GLN	-	expression tag	UNP A0A0A7DIZ4
Ap	234	GLY	-	expression tag	UNP A0A0A7DIZ4
Ap	235	LEU	-	expression tag	UNP A0A0A7DIZ4
Ap	236	GLU	-	expression tag	UNP A0A0A7DIZ4
Ap	237	HIS	-	expression tag	UNP A0A0A7DIZ4
Ap	238	HIS	-	expression tag	UNP A0A0A7DIZ4
Ap	239	HIS	-	expression tag	UNP A0A0A7DIZ4

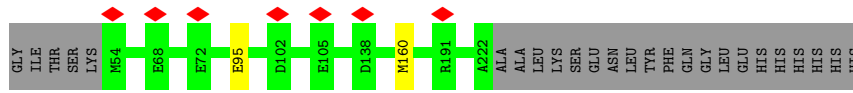
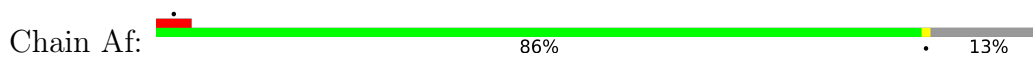
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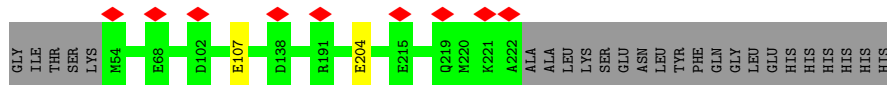
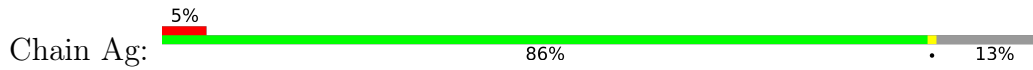
<b>Chain</b>	<b>Residue</b>	<b>Modelled</b>	<b>Actual</b>	<b>Comment</b>	<b>Reference</b>
Ap	240	HIS	-	expression tag	UNP A0A0A7DIZ4
Ap	241	HIS	-	expression tag	UNP A0A0A7DIZ4
Ap	242	HIS	-	expression tag	UNP A0A0A7DIZ4



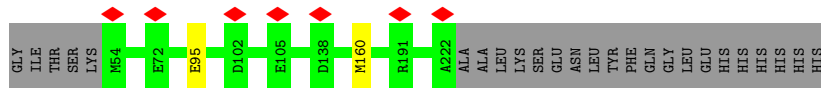
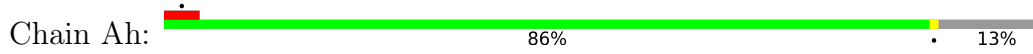
• Molecule 1: Genome polyprotein



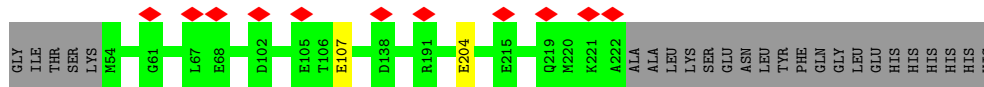
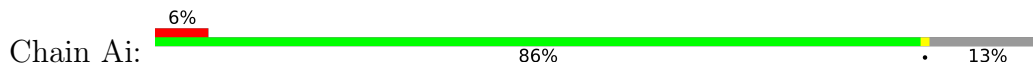
• Molecule 1: Genome polyprotein



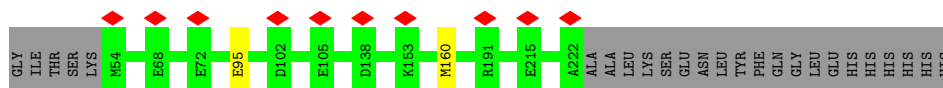
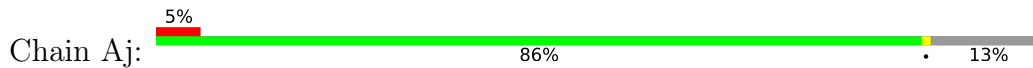
• Molecule 1: Genome polyprotein



• Molecule 1: Genome polyprotein



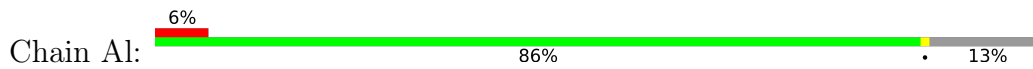
• Molecule 1: Genome polyprotein

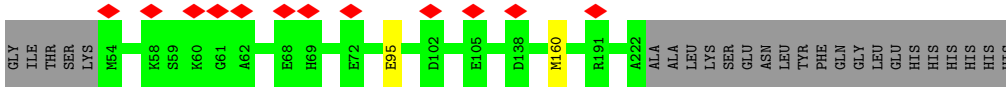


• Molecule 1: Genome polyprotein

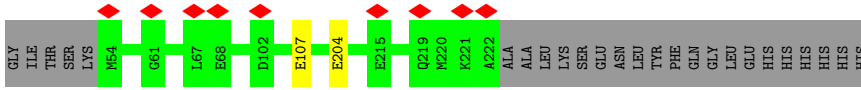
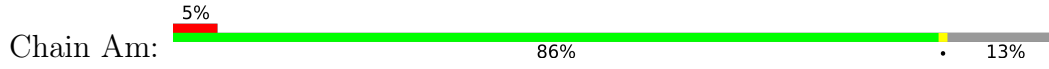


• Molecule 1: Genome polyprotein

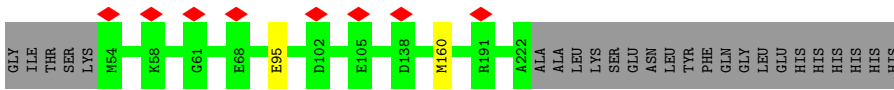
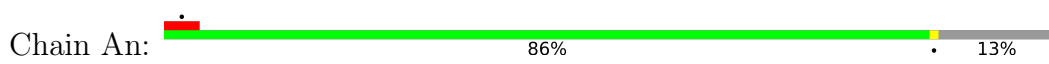




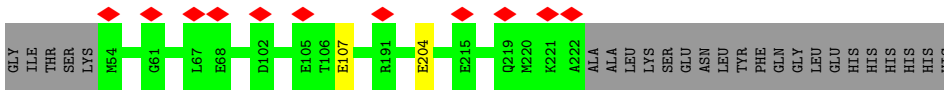
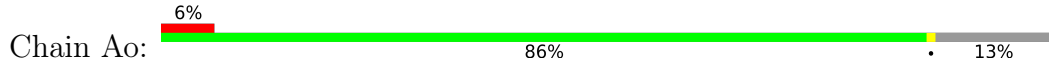
• Molecule 1: Genome polyprotein



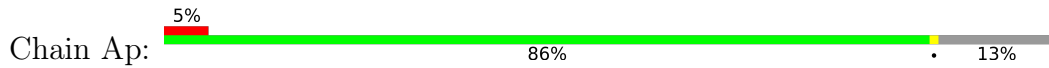
• Molecule 1: Genome polyprotein



• Molecule 1: Genome polyprotein



• Molecule 1: Genome polyprotein



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C8	Depositor
Number of particles used	174238	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; patchCTF correction	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	150000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.983	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.122	Depositor
Map size (Å)	332.5, 332.5, 332.5	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	Depositor

## 5 Model quality [i](#)

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

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	Aa	0.31	0/1395	0.51	0/1891
1	Ab	0.26	0/1395	0.48	0/1891
1	Ac	0.31	0/1395	0.52	0/1891
1	Ad	0.26	0/1395	0.48	0/1891
1	Ae	0.31	0/1395	0.51	0/1891
1	Af	0.26	0/1395	0.49	0/1891
1	Ag	0.31	0/1395	0.52	0/1891
1	Ah	0.26	0/1395	0.49	0/1891
1	Ai	0.31	0/1395	0.52	0/1891
1	Aj	0.26	0/1395	0.48	0/1891
1	Ak	0.31	0/1395	0.52	0/1891
1	Al	0.26	0/1395	0.48	0/1891
1	Am	0.31	0/1395	0.52	0/1891
1	An	0.26	0/1395	0.48	0/1891
1	Ao	0.31	0/1395	0.52	0/1891
1	Ap	0.26	0/1395	0.49	0/1891
All	All	0.29	0/22320	0.50	0/30256

There are no bond length outliers.

There are no bond angle outliers.

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	Aa	1364	0	1336	0	0
1	Ab	1364	0	1336	0	0
1	Ac	1364	0	1336	0	0
1	Ad	1364	0	1336	0	0
1	Ae	1364	0	1336	0	0
1	Af	1364	0	1336	0	0
1	Ag	1364	0	1336	0	0
1	Ah	1364	0	1336	0	0
1	Ai	1364	0	1336	0	0
1	Aj	1364	0	1336	0	0
1	Ak	1364	0	1336	0	0
1	Al	1364	0	1336	0	0
1	Am	1364	0	1336	0	0
1	An	1364	0	1336	0	0
1	Ao	1364	0	1336	0	0
1	Ap	1364	0	1336	0	0
All	All	21824	0	21376	0	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 5.

There are no clashes within the asymmetric unit.

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	Aa	167/194 (86%)	159 (95%)	8 (5%)	0	100	100
1	Ab	167/194 (86%)	158 (95%)	9 (5%)	0	100	100
1	Ac	167/194 (86%)	159 (95%)	8 (5%)	0	100	100
1	Ad	167/194 (86%)	158 (95%)	9 (5%)	0	100	100
1	Ae	167/194 (86%)	158 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Af	167/194 (86%)	158 (95%)	9 (5%)	0	100	100
1	Ag	167/194 (86%)	159 (95%)	8 (5%)	0	100	100
1	Ah	167/194 (86%)	158 (95%)	9 (5%)	0	100	100
1	Ai	167/194 (86%)	159 (95%)	8 (5%)	0	100	100
1	Aj	167/194 (86%)	158 (95%)	9 (5%)	0	100	100
1	Ak	167/194 (86%)	159 (95%)	8 (5%)	0	100	100
1	Al	167/194 (86%)	158 (95%)	9 (5%)	0	100	100
1	Am	167/194 (86%)	159 (95%)	8 (5%)	0	100	100
1	An	167/194 (86%)	158 (95%)	9 (5%)	0	100	100
1	Ao	167/194 (86%)	159 (95%)	8 (5%)	0	100	100
1	Ap	167/194 (86%)	158 (95%)	9 (5%)	0	100	100
All	All	2672/3104 (86%)	2535 (95%)	137 (5%)	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	Aa	147/168 (88%)	145 (99%)	2 (1%)	67	86
1	Ab	147/168 (88%)	145 (99%)	2 (1%)	67	86
1	Ac	147/168 (88%)	145 (99%)	2 (1%)	67	86
1	Ad	147/168 (88%)	145 (99%)	2 (1%)	67	86
1	Ae	147/168 (88%)	145 (99%)	2 (1%)	67	86
1	Af	147/168 (88%)	145 (99%)	2 (1%)	67	86
1	Ag	147/168 (88%)	145 (99%)	2 (1%)	67	86
1	Ah	147/168 (88%)	145 (99%)	2 (1%)	67	86
1	Ai	147/168 (88%)	145 (99%)	2 (1%)	67	86
1	Aj	147/168 (88%)	145 (99%)	2 (1%)	67	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ak	147/168 (88%)	145 (99%)	2 (1%)	67	86
1	Al	147/168 (88%)	145 (99%)	2 (1%)	67	86
1	Am	147/168 (88%)	145 (99%)	2 (1%)	67	86
1	An	147/168 (88%)	145 (99%)	2 (1%)	67	86
1	Ao	147/168 (88%)	145 (99%)	2 (1%)	67	86
1	Ap	147/168 (88%)	145 (99%)	2 (1%)	67	86
All	All	2352/2688 (88%)	2320 (99%)	32 (1%)	68	86

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Ao	107	GLU
1	Ao	204	GLU
1	Ag	107	GLU
1	Af	160	MET
1	Ap	95	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	Ap	69	HIS
1	An	69	HIS
1	Aj	69	HIS
1	Ah	69	HIS
1	Al	69	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.

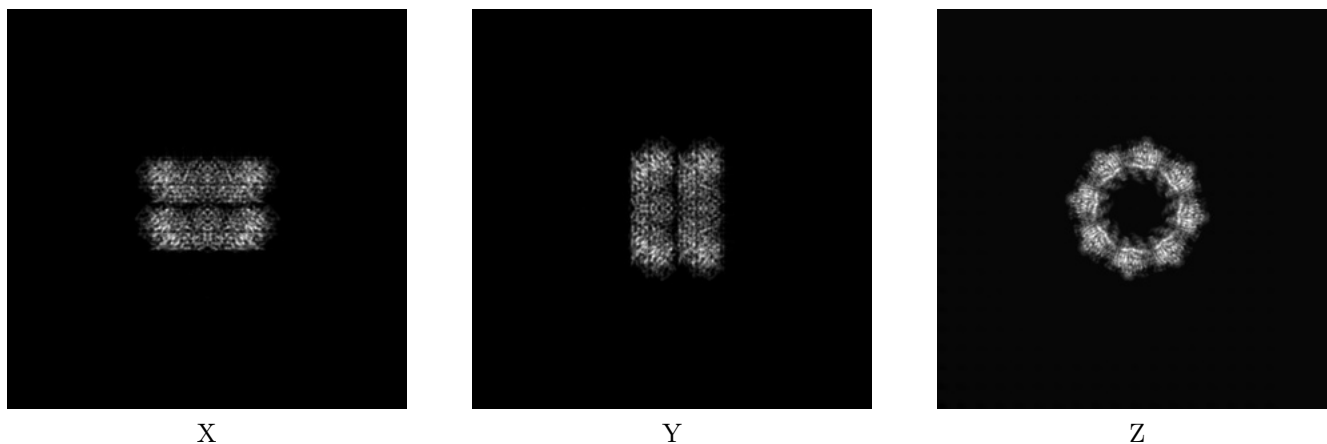
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17053. These allow visual inspection of the internal detail of the map and identification of artifacts.

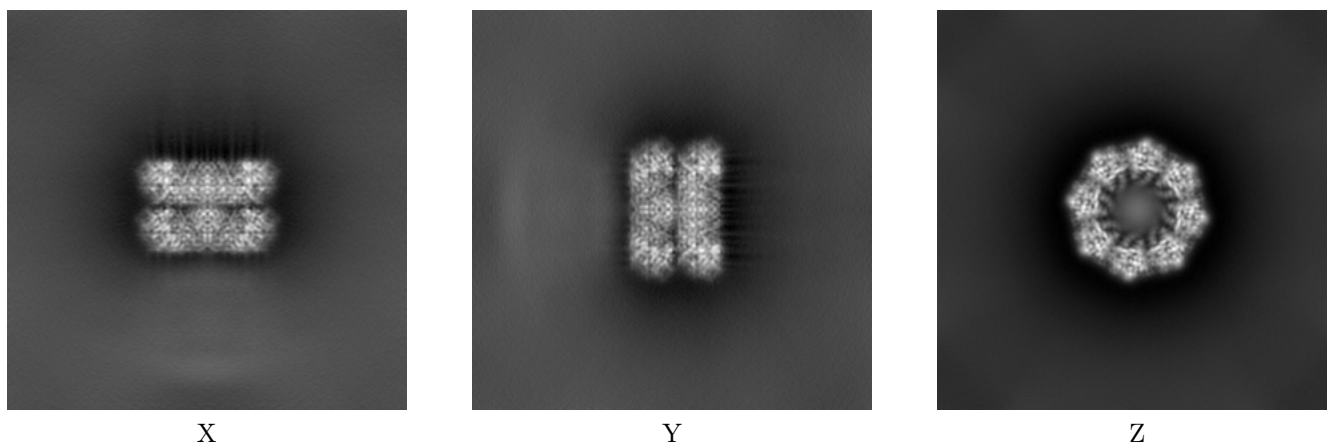
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



#### 6.1.2 Raw map



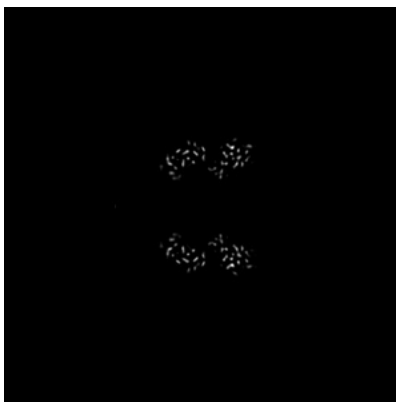
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

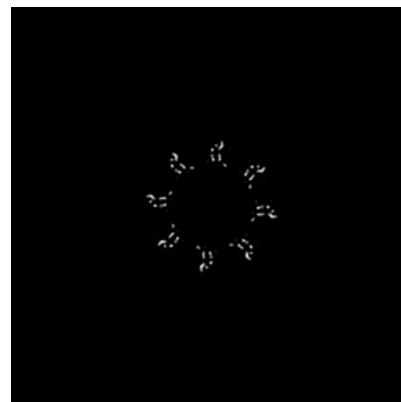
### 6.2.1 Primary map



X Index: 175

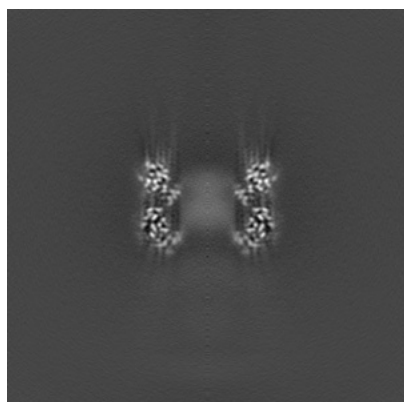


Y Index: 175

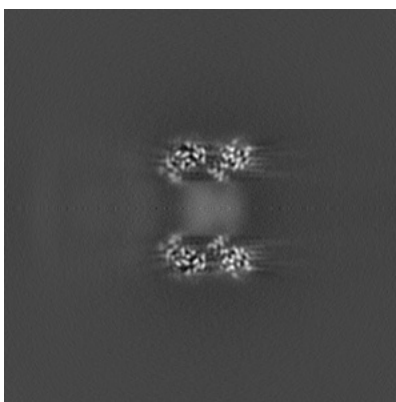


Z Index: 175

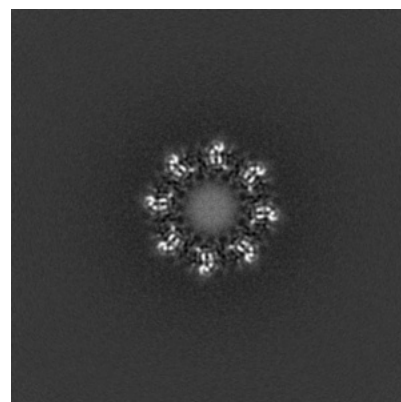
### 6.2.2 Raw map



X Index: 175



Y Index: 175



Z Index: 175

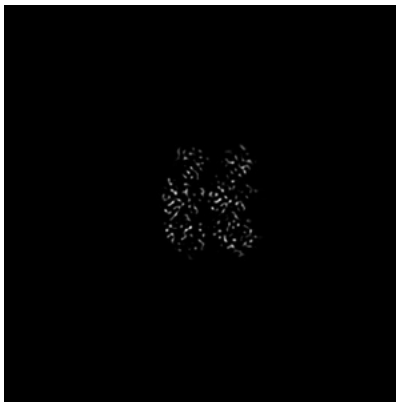
The images above show central slices of the map in three orthogonal directions.

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

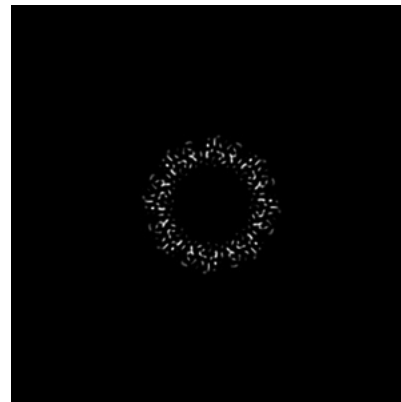
### 6.3.1 Primary map



X Index: 138

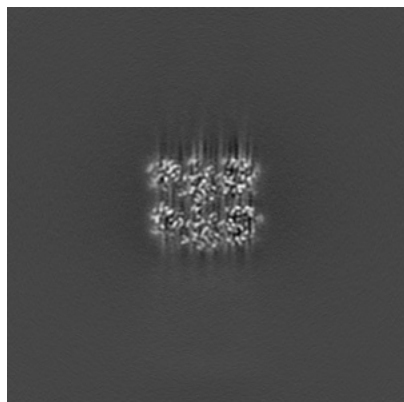


Y Index: 212

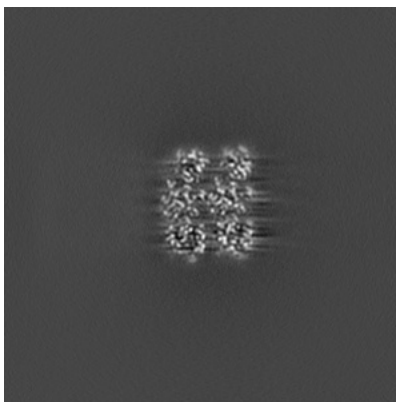


Z Index: 158

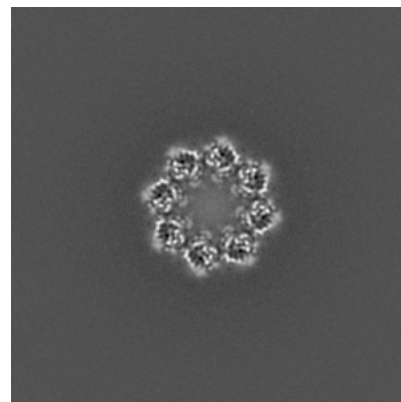
### 6.3.2 Raw map



X Index: 211



Y Index: 211

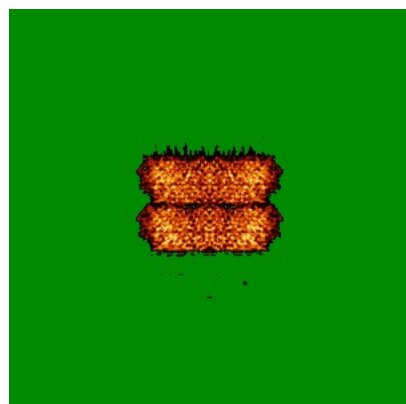


Z Index: 194

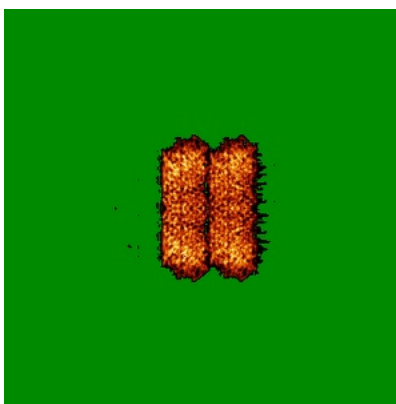
The images above show the largest variance slices of the map in three orthogonal directions.

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

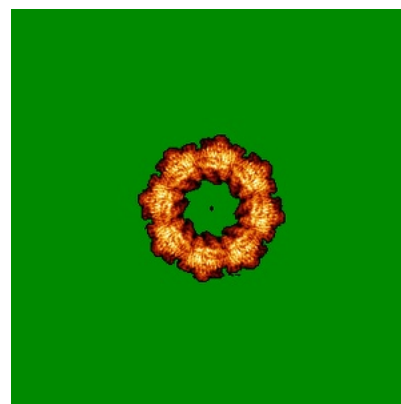
### 6.4.1 Primary map



X

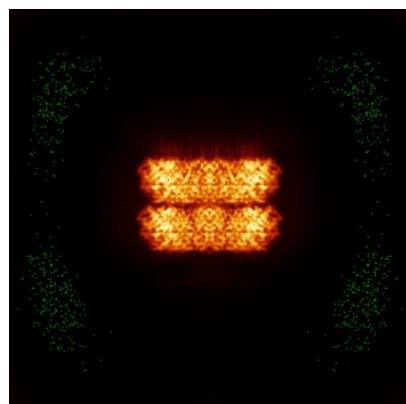


Y

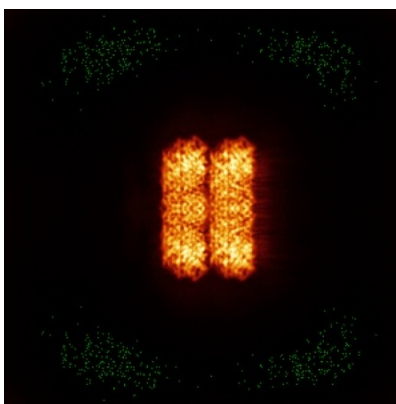


Z

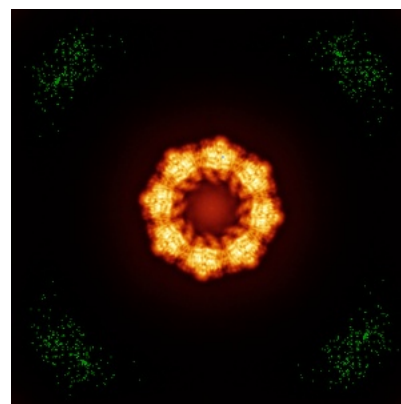
### 6.4.2 Raw map



X



Y



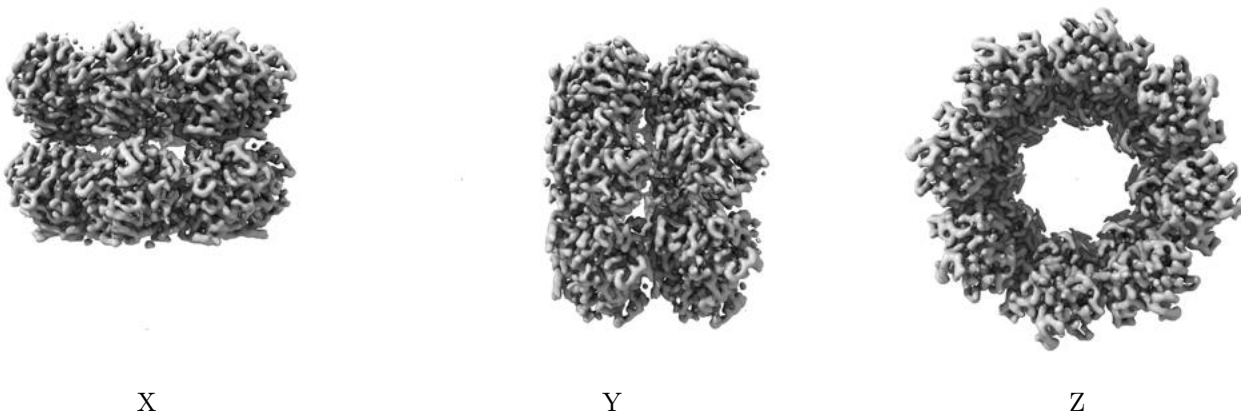
Z

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.



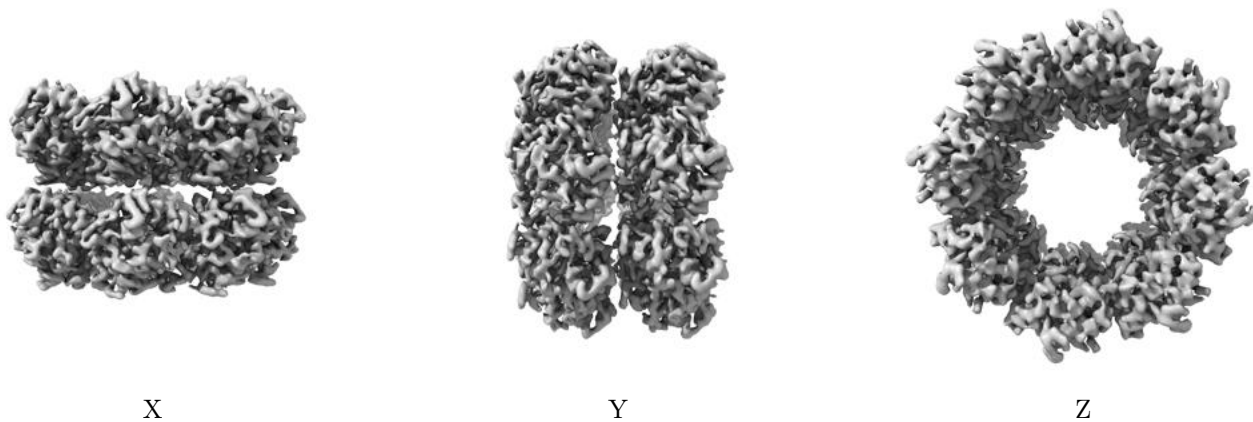
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.122. 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.

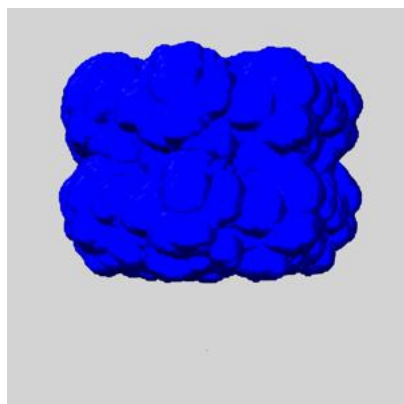
## 6.6 Mask visualisation [i](#)

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

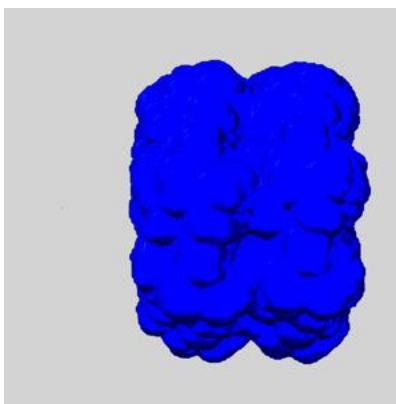
A mask typically either:

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

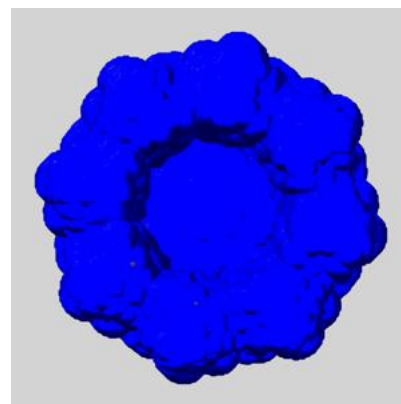
### 6.6.1 emd\_17053\_msk\_1.map [i](#)



X



Y

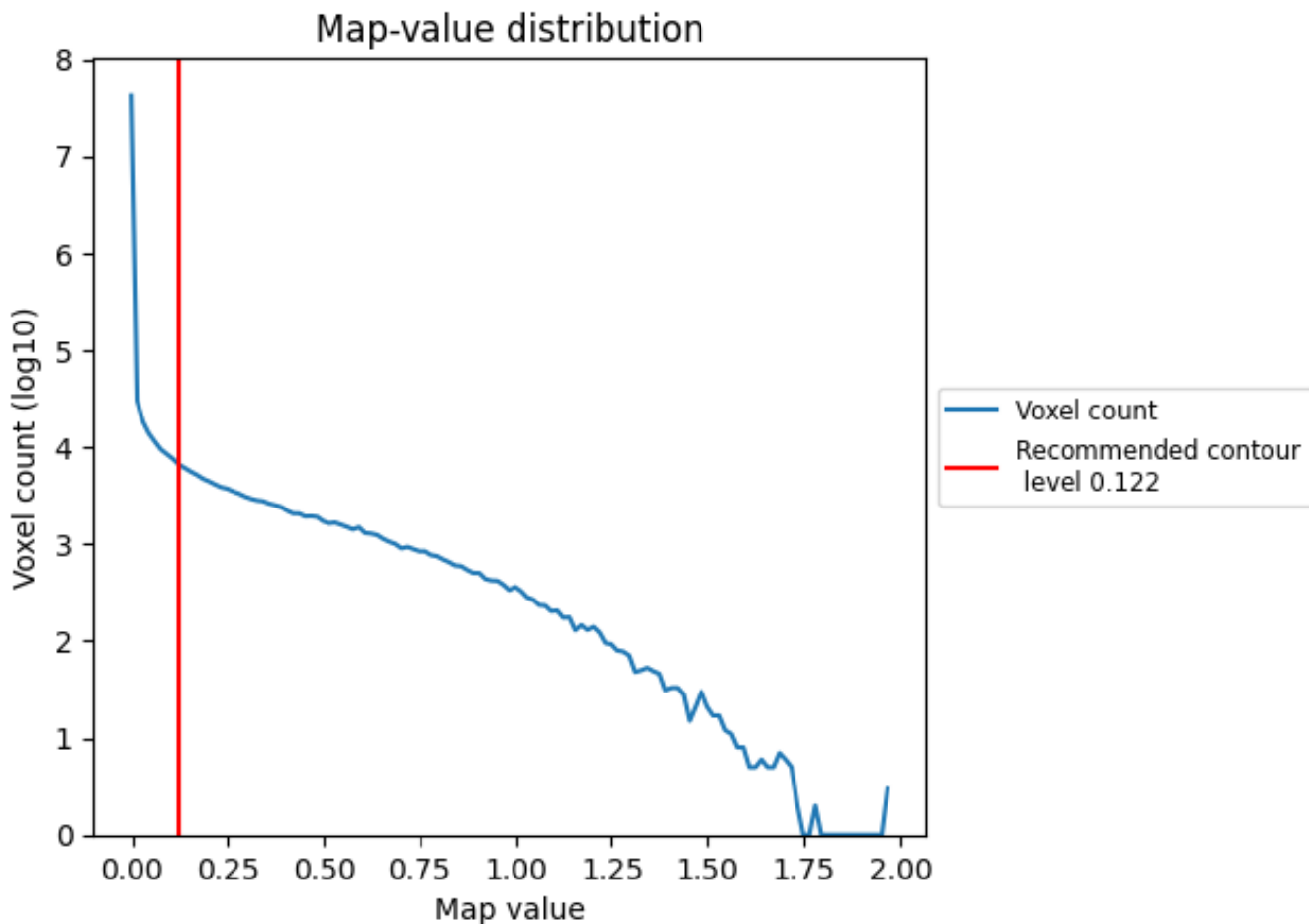


Z

## 7 Map analysis [i](#)

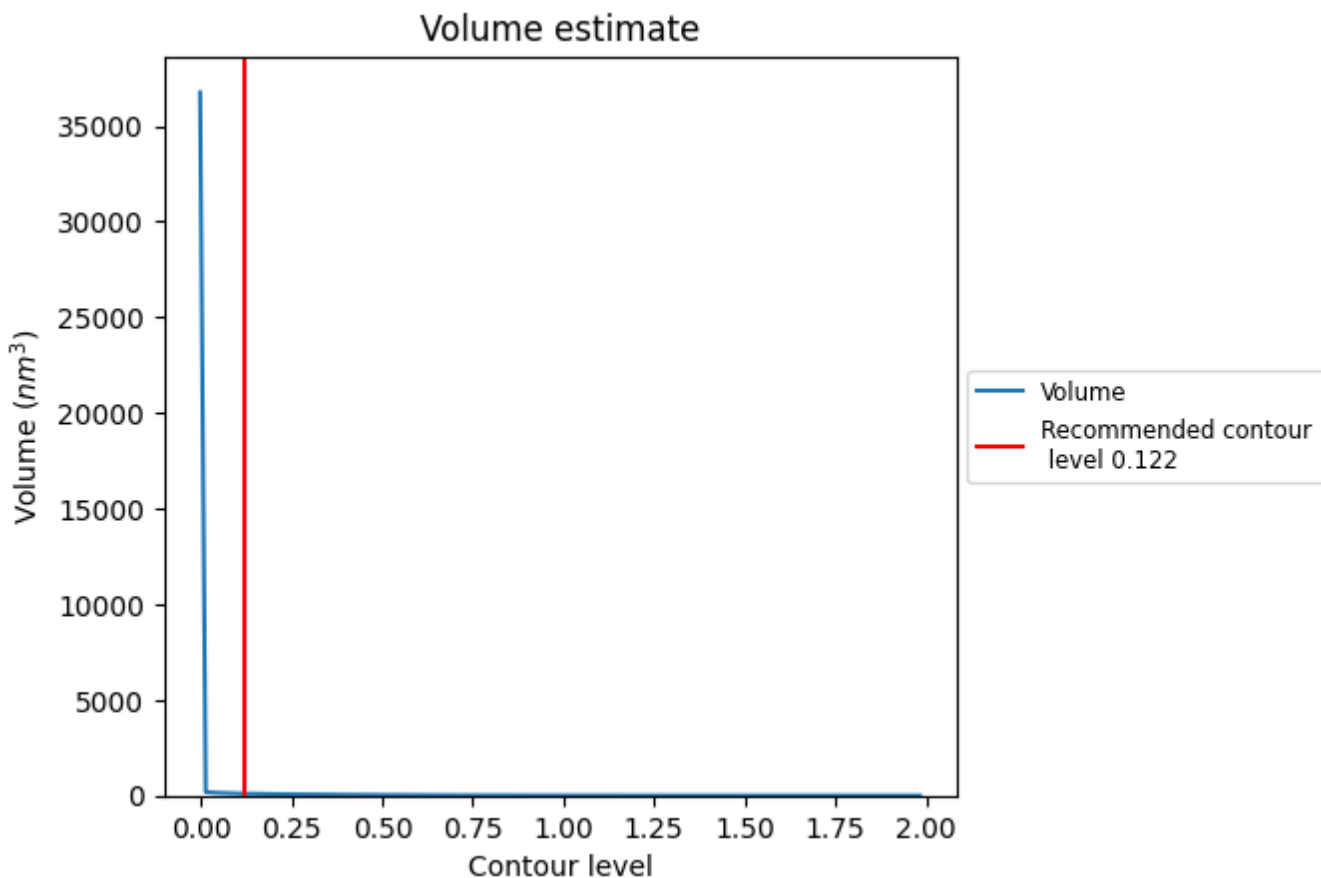
This section contains the results of statistical analysis of the map.

### 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.

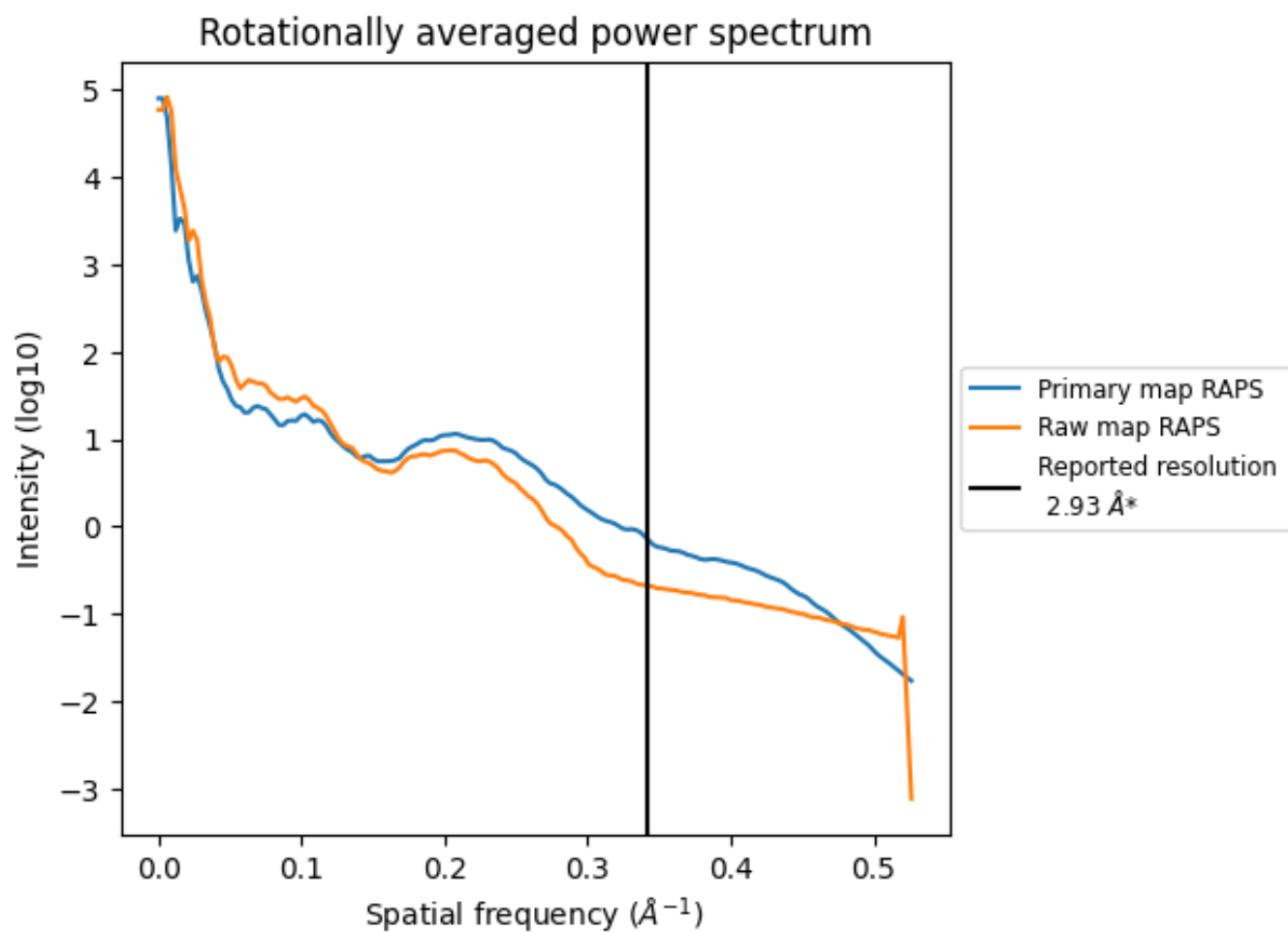
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 101 nm<sup>3</sup>; this corresponds to an approximate mass of 91 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 i

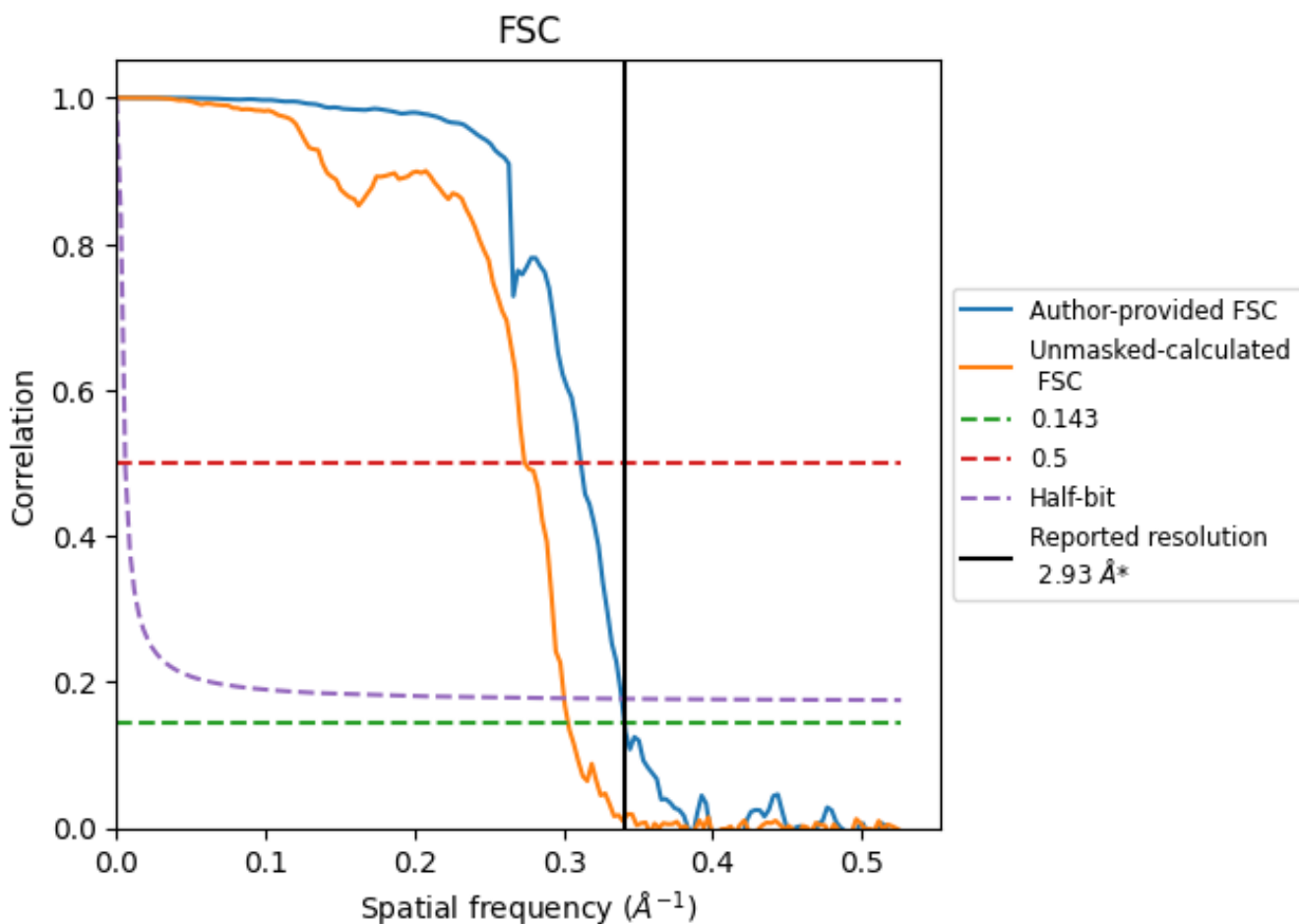


\*Reported resolution corresponds to spatial frequency of 0.341 Å<sup>-1</sup>

## 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 0.341 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

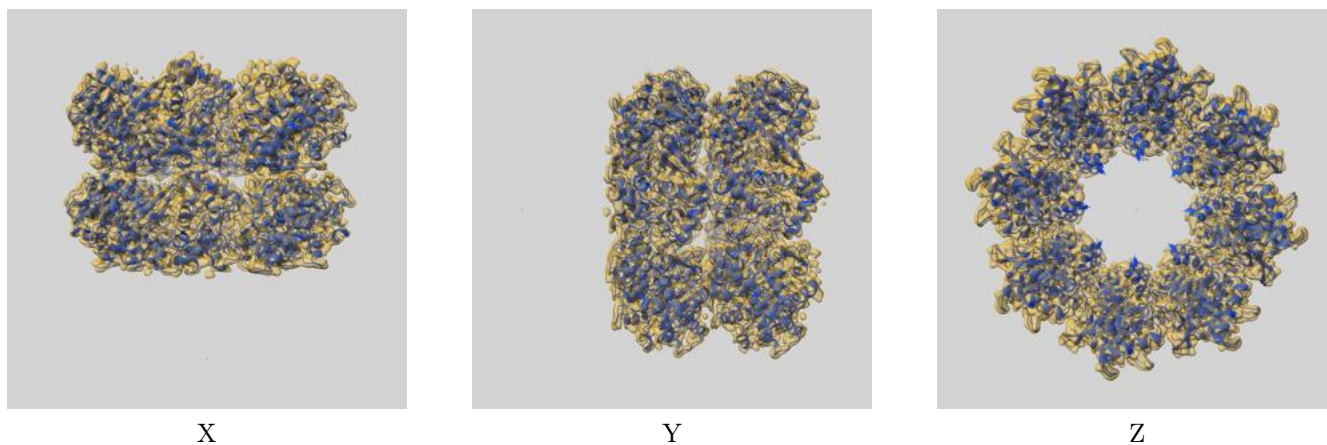
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.93	-	-
Author-provided FSC curve	2.94	3.21	2.95
Unmasked-calculated*	3.30	3.65	3.33

\*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 3.30 differs from the reported value 2.93 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-17053 and PDB model 8OPH. Per-residue inclusion information can be found in section 3 on page 12.

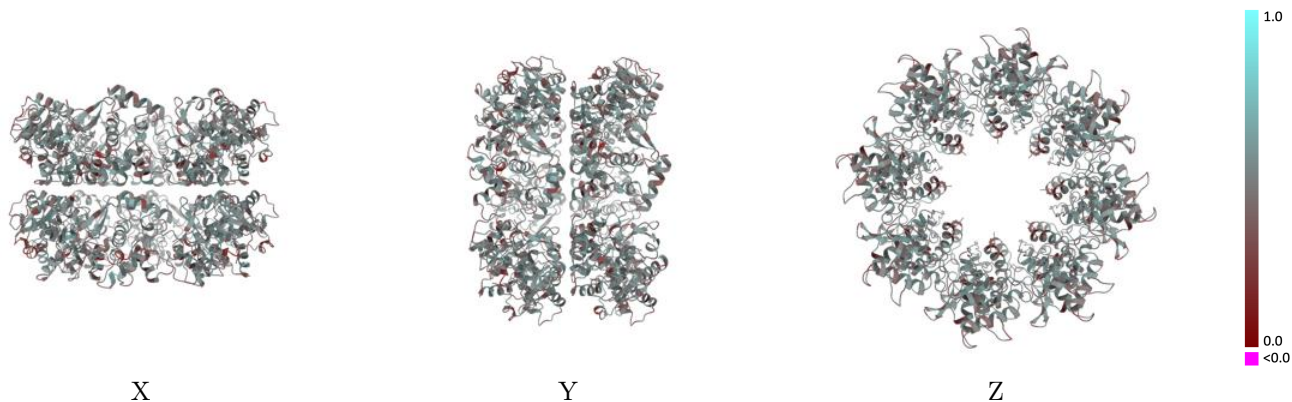
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.122 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.

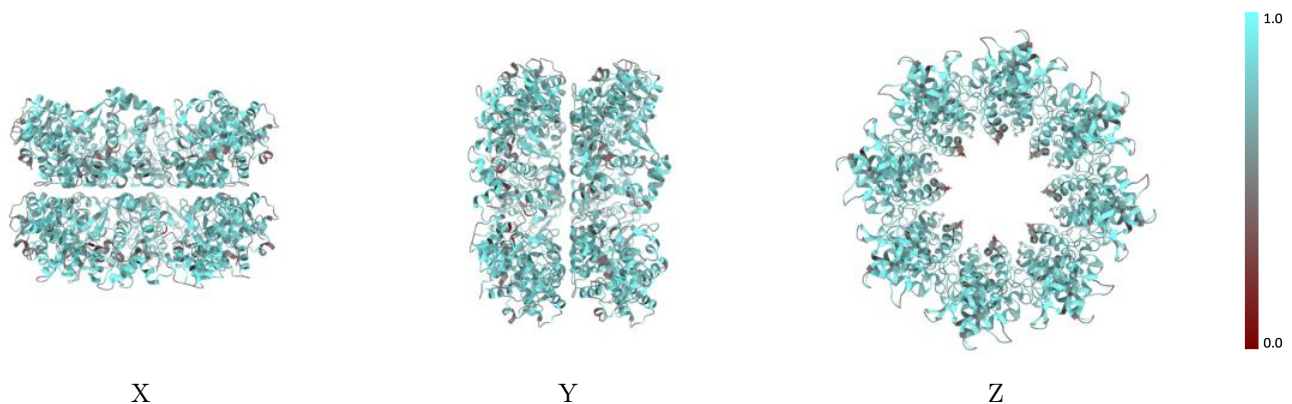


## 9.2 Q-score mapped to coordinate model [\(i\)](#)



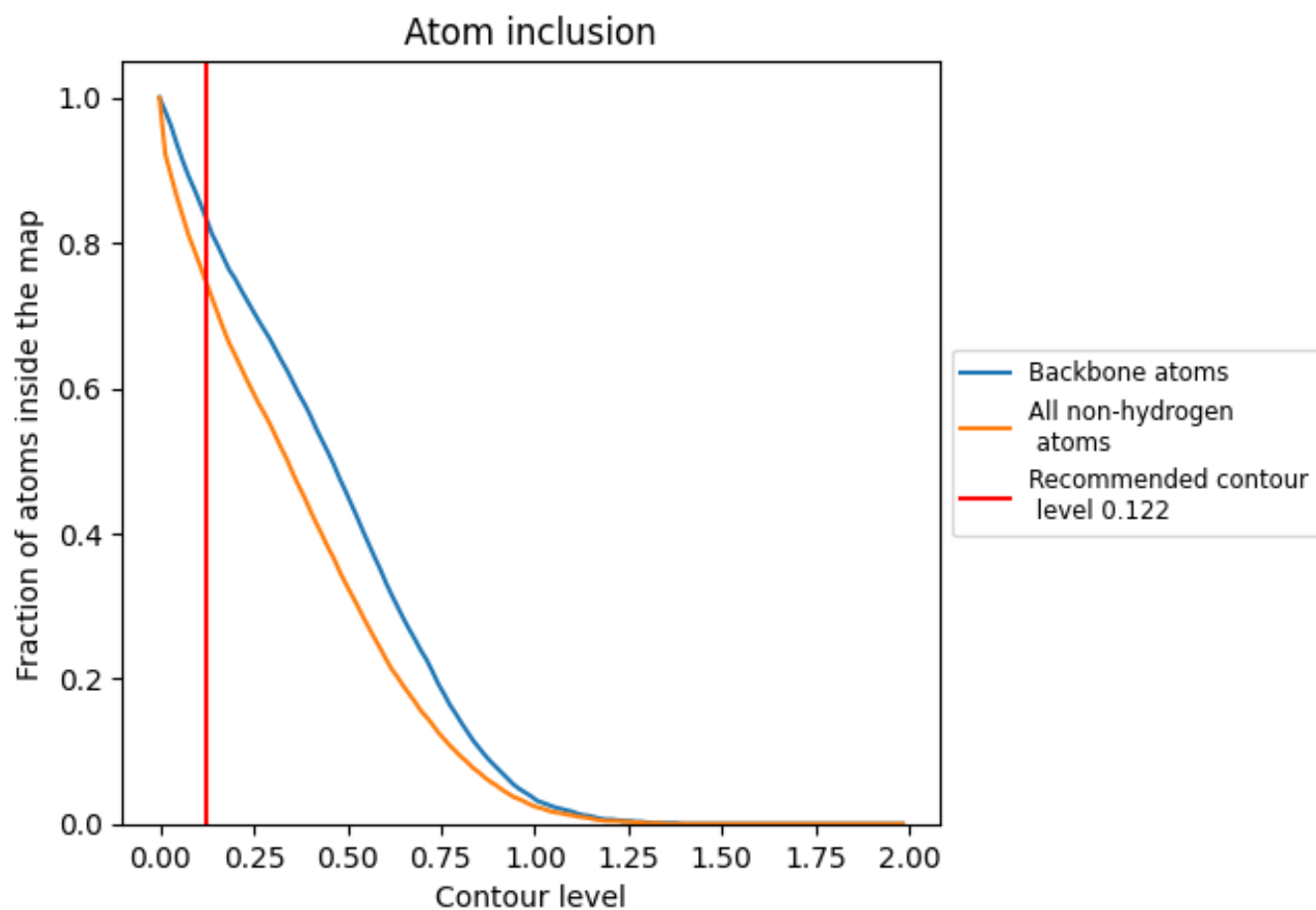
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.122).



































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 75% 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 (0.122) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7470	 0.4740
Aa	 0.7420	 0.4740
Ab	 0.7410	 0.4740
Ac	 0.7450	 0.4720
Ad	 0.7500	 0.4680
Ae	 0.7540	 0.4720
Af	 0.7570	 0.4740
Ag	 0.7410	 0.4740
Ah	 0.7470	 0.4720
Ai	 0.7470	 0.4750
Aj	 0.7440	 0.4800
Ak	 0.7500	 0.4770
Al	 0.7440	 0.4720
Am	 0.7530	 0.4740
An	 0.7500	 0.4780
Ao	 0.7480	 0.4730
Ap	 0.7430	 0.4710

