



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 04:04 AM UTC

PDB ID : 8OPK / pdb_00008opk
EMDB ID : EMD-17063
Title : Local refinement of cubic assembly from truncated PVY coat protein with K176C mutation
Authors : Kavcic, L.; Kezar, A.; Podobnik, M.
Deposited on : 2023-04-07
Resolution : 3.16 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

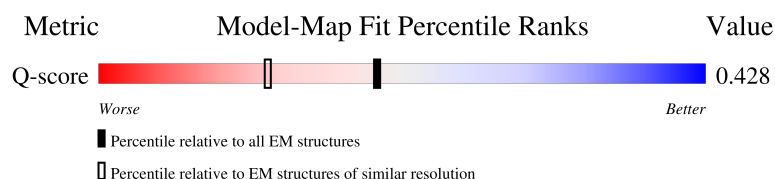
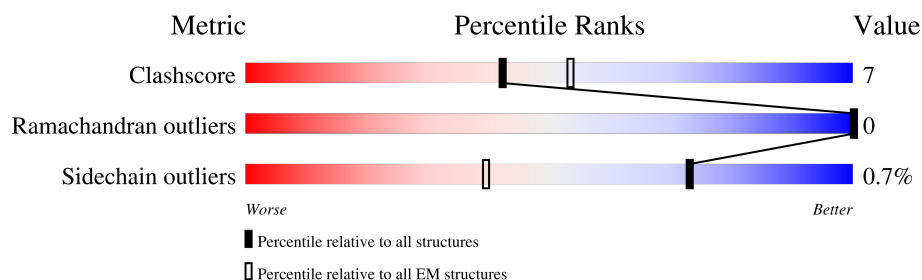
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.16 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14474 (2.66 - 3.66)

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

Mol	Chain	Length	Quality of chain
1	Aa	194	 5% 73% 13% • 13%
1	Ab	194	 1% 73% 14% • 12%
1	Ac	194	 1% 73% 13% • 13%
1	Ad	194	 1% 74% 13% • 12%

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Mol	Chain	Length	Quality of chain
1	Ae	194	
1	Af	194	
1	Ag	194	
1	Ah	194	
1	Ai	194	
1	Aj	194	
1	Ak	194	
1	Al	194	
1	Am	194	
1	An	194	
1	Ao	194	
1	Ap	194	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 21784 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 polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Aa	168	Total	C	N	O	S	0	0
			1353	853	233	255	12		
1	Ab	170	Total	C	N	O	S	0	0
			1370	864	236	257	13		
1	Ac	168	Total	C	N	O	S	0	0
			1353	853	233	255	12		
1	Ad	170	Total	C	N	O	S	0	0
			1370	864	236	257	13		
1	Ae	168	Total	C	N	O	S	0	0
			1353	853	233	255	12		
1	Af	170	Total	C	N	O	S	0	0
			1370	864	236	257	13		
1	Ag	168	Total	C	N	O	S	0	0
			1353	853	233	255	12		
1	Ah	170	Total	C	N	O	S	0	0
			1370	864	236	257	13		
1	Ai	168	Total	C	N	O	S	0	0
			1353	853	233	255	12		
1	Aj	170	Total	C	N	O	S	0	0
			1370	864	236	257	13		
1	Ak	168	Total	C	N	O	S	0	0
			1353	853	233	255	12		
1	Al	170	Total	C	N	O	S	0	0
			1370	864	236	257	13		
1	Am	168	Total	C	N	O	S	0	0
			1353	853	233	255	12		
1	An	170	Total	C	N	O	S	0	0
			1370	864	236	257	13		
1	Ao	168	Total	C	N	O	S	0	0
			1353	853	233	255	12		
1	Ap	170	Total	C	N	O	S	0	0
			1370	864	236	257	13		

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Aa	49	GLY	-	expression tag	UNP A0A0A7DIW7
Aa	176	CYS	LYS	engineered mutation	UNP A0A0A7DIW7
Aa	228	GLU	ALA	conflict	UNP A0A0A7DIW7
Aa	229	ASN	GLN	conflict	UNP A0A0A7DIW7
Aa	230	LEU	SER	conflict	UNP A0A0A7DIW7
Aa	231	TYR	ARG	conflict	UNP A0A0A7DIW7
Aa	232	PHE	LEU	conflict	UNP A0A0A7DIW7
Aa	233	GLN	PHE	conflict	UNP A0A0A7DIW7
Aa	236	GLU	ASP	conflict	UNP A0A0A7DIW7
Aa	237	HIS	-	expression tag	UNP A0A0A7DIW7
Aa	238	HIS	-	expression tag	UNP A0A0A7DIW7
Aa	239	HIS	-	expression tag	UNP A0A0A7DIW7
Aa	240	HIS	-	expression tag	UNP A0A0A7DIW7
Aa	241	HIS	-	expression tag	UNP A0A0A7DIW7
Aa	242	HIS	-	expression tag	UNP A0A0A7DIW7
Ab	49	GLY	-	expression tag	UNP A0A0A7DIW7
Ab	176	CYS	LYS	engineered mutation	UNP A0A0A7DIW7
Ab	228	GLU	ALA	conflict	UNP A0A0A7DIW7
Ab	229	ASN	GLN	conflict	UNP A0A0A7DIW7
Ab	230	LEU	SER	conflict	UNP A0A0A7DIW7
Ab	231	TYR	ARG	conflict	UNP A0A0A7DIW7
Ab	232	PHE	LEU	conflict	UNP A0A0A7DIW7
Ab	233	GLN	PHE	conflict	UNP A0A0A7DIW7
Ab	236	GLU	ASP	conflict	UNP A0A0A7DIW7
Ab	237	HIS	-	expression tag	UNP A0A0A7DIW7
Ab	238	HIS	-	expression tag	UNP A0A0A7DIW7
Ab	239	HIS	-	expression tag	UNP A0A0A7DIW7
Ab	240	HIS	-	expression tag	UNP A0A0A7DIW7
Ab	241	HIS	-	expression tag	UNP A0A0A7DIW7
Ab	242	HIS	-	expression tag	UNP A0A0A7DIW7
Ac	49	GLY	-	expression tag	UNP A0A0A7DIW7
Ac	176	CYS	LYS	engineered mutation	UNP A0A0A7DIW7
Ac	228	GLU	ALA	conflict	UNP A0A0A7DIW7
Ac	229	ASN	GLN	conflict	UNP A0A0A7DIW7
Ac	230	LEU	SER	conflict	UNP A0A0A7DIW7
Ac	231	TYR	ARG	conflict	UNP A0A0A7DIW7
Ac	232	PHE	LEU	conflict	UNP A0A0A7DIW7
Ac	233	GLN	PHE	conflict	UNP A0A0A7DIW7
Ac	236	GLU	ASP	conflict	UNP A0A0A7DIW7
Ac	237	HIS	-	expression tag	UNP A0A0A7DIW7
Ac	238	HIS	-	expression tag	UNP A0A0A7DIW7
Ac	239	HIS	-	expression tag	UNP A0A0A7DIW7
Ac	240	HIS	-	expression tag	UNP A0A0A7DIW7

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Chain	Residue	Modelled	Actual	Comment	Reference
Ac	241	HIS	-	expression tag	UNP A0A0A7DIW7
Ac	242	HIS	-	expression tag	UNP A0A0A7DIW7
Ad	49	GLY	-	expression tag	UNP A0A0A7DIW7
Ad	176	CYS	LYS	engineered mutation	UNP A0A0A7DIW7
Ad	228	GLU	ALA	conflict	UNP A0A0A7DIW7
Ad	229	ASN	GLN	conflict	UNP A0A0A7DIW7
Ad	230	LEU	SER	conflict	UNP A0A0A7DIW7
Ad	231	TYR	ARG	conflict	UNP A0A0A7DIW7
Ad	232	PHE	LEU	conflict	UNP A0A0A7DIW7
Ad	233	GLN	PHE	conflict	UNP A0A0A7DIW7
Ad	236	GLU	ASP	conflict	UNP A0A0A7DIW7
Ad	237	HIS	-	expression tag	UNP A0A0A7DIW7
Ad	238	HIS	-	expression tag	UNP A0A0A7DIW7
Ad	239	HIS	-	expression tag	UNP A0A0A7DIW7
Ad	240	HIS	-	expression tag	UNP A0A0A7DIW7
Ad	241	HIS	-	expression tag	UNP A0A0A7DIW7
Ad	242	HIS	-	expression tag	UNP A0A0A7DIW7
Ae	49	GLY	-	expression tag	UNP A0A0A7DIW7
Ae	176	CYS	LYS	engineered mutation	UNP A0A0A7DIW7
Ae	228	GLU	ALA	conflict	UNP A0A0A7DIW7
Ae	229	ASN	GLN	conflict	UNP A0A0A7DIW7
Ae	230	LEU	SER	conflict	UNP A0A0A7DIW7
Ae	231	TYR	ARG	conflict	UNP A0A0A7DIW7
Ae	232	PHE	LEU	conflict	UNP A0A0A7DIW7
Ae	233	GLN	PHE	conflict	UNP A0A0A7DIW7
Ae	236	GLU	ASP	conflict	UNP A0A0A7DIW7
Ae	237	HIS	-	expression tag	UNP A0A0A7DIW7
Ae	238	HIS	-	expression tag	UNP A0A0A7DIW7
Ae	239	HIS	-	expression tag	UNP A0A0A7DIW7
Ae	240	HIS	-	expression tag	UNP A0A0A7DIW7
Ae	241	HIS	-	expression tag	UNP A0A0A7DIW7
Ae	242	HIS	-	expression tag	UNP A0A0A7DIW7
Af	49	GLY	-	expression tag	UNP A0A0A7DIW7
Af	176	CYS	LYS	engineered mutation	UNP A0A0A7DIW7
Af	228	GLU	ALA	conflict	UNP A0A0A7DIW7
Af	229	ASN	GLN	conflict	UNP A0A0A7DIW7
Af	230	LEU	SER	conflict	UNP A0A0A7DIW7
Af	231	TYR	ARG	conflict	UNP A0A0A7DIW7
Af	232	PHE	LEU	conflict	UNP A0A0A7DIW7
Af	233	GLN	PHE	conflict	UNP A0A0A7DIW7
Af	236	GLU	ASP	conflict	UNP A0A0A7DIW7
Af	237	HIS	-	expression tag	UNP A0A0A7DIW7

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Chain	Residue	Modelled	Actual	Comment	Reference
Af	238	HIS	-	expression tag	UNP A0A0A7DIW7
Af	239	HIS	-	expression tag	UNP A0A0A7DIW7
Af	240	HIS	-	expression tag	UNP A0A0A7DIW7
Af	241	HIS	-	expression tag	UNP A0A0A7DIW7
Af	242	HIS	-	expression tag	UNP A0A0A7DIW7
Ag	49	GLY	-	expression tag	UNP A0A0A7DIW7
Ag	176	CYS	LYS	engineered mutation	UNP A0A0A7DIW7
Ag	228	GLU	ALA	conflict	UNP A0A0A7DIW7
Ag	229	ASN	GLN	conflict	UNP A0A0A7DIW7
Ag	230	LEU	SER	conflict	UNP A0A0A7DIW7
Ag	231	TYR	ARG	conflict	UNP A0A0A7DIW7
Ag	232	PHE	LEU	conflict	UNP A0A0A7DIW7
Ag	233	GLN	PHE	conflict	UNP A0A0A7DIW7
Ag	236	GLU	ASP	conflict	UNP A0A0A7DIW7
Ag	237	HIS	-	expression tag	UNP A0A0A7DIW7
Ag	238	HIS	-	expression tag	UNP A0A0A7DIW7
Ag	239	HIS	-	expression tag	UNP A0A0A7DIW7
Ag	240	HIS	-	expression tag	UNP A0A0A7DIW7
Ag	241	HIS	-	expression tag	UNP A0A0A7DIW7
Ag	242	HIS	-	expression tag	UNP A0A0A7DIW7
Ah	49	GLY	-	expression tag	UNP A0A0A7DIW7
Ah	176	CYS	LYS	engineered mutation	UNP A0A0A7DIW7
Ah	228	GLU	ALA	conflict	UNP A0A0A7DIW7
Ah	229	ASN	GLN	conflict	UNP A0A0A7DIW7
Ah	230	LEU	SER	conflict	UNP A0A0A7DIW7
Ah	231	TYR	ARG	conflict	UNP A0A0A7DIW7
Ah	232	PHE	LEU	conflict	UNP A0A0A7DIW7
Ah	233	GLN	PHE	conflict	UNP A0A0A7DIW7
Ah	236	GLU	ASP	conflict	UNP A0A0A7DIW7
Ah	237	HIS	-	expression tag	UNP A0A0A7DIW7
Ah	238	HIS	-	expression tag	UNP A0A0A7DIW7
Ah	239	HIS	-	expression tag	UNP A0A0A7DIW7
Ah	240	HIS	-	expression tag	UNP A0A0A7DIW7
Ah	241	HIS	-	expression tag	UNP A0A0A7DIW7
Ah	242	HIS	-	expression tag	UNP A0A0A7DIW7
Ai	49	GLY	-	expression tag	UNP A0A0A7DIW7
Ai	176	CYS	LYS	engineered mutation	UNP A0A0A7DIW7
Ai	228	GLU	ALA	conflict	UNP A0A0A7DIW7
Ai	229	ASN	GLN	conflict	UNP A0A0A7DIW7
Ai	230	LEU	SER	conflict	UNP A0A0A7DIW7
Ai	231	TYR	ARG	conflict	UNP A0A0A7DIW7
Ai	232	PHE	LEU	conflict	UNP A0A0A7DIW7

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Chain	Residue	Modelled	Actual	Comment	Reference
Ai	233	GLN	PHE	conflict	UNP A0A0A7DIW7
Ai	236	GLU	ASP	conflict	UNP A0A0A7DIW7
Ai	237	HIS	-	expression tag	UNP A0A0A7DIW7
Ai	238	HIS	-	expression tag	UNP A0A0A7DIW7
Ai	239	HIS	-	expression tag	UNP A0A0A7DIW7
Ai	240	HIS	-	expression tag	UNP A0A0A7DIW7
Ai	241	HIS	-	expression tag	UNP A0A0A7DIW7
Ai	242	HIS	-	expression tag	UNP A0A0A7DIW7
Aj	49	GLY	-	expression tag	UNP A0A0A7DIW7
Aj	176	CYS	LYS	engineered mutation	UNP A0A0A7DIW7
Aj	228	GLU	ALA	conflict	UNP A0A0A7DIW7
Aj	229	ASN	GLN	conflict	UNP A0A0A7DIW7
Aj	230	LEU	SER	conflict	UNP A0A0A7DIW7
Aj	231	TYR	ARG	conflict	UNP A0A0A7DIW7
Aj	232	PHE	LEU	conflict	UNP A0A0A7DIW7
Aj	233	GLN	PHE	conflict	UNP A0A0A7DIW7
Aj	236	GLU	ASP	conflict	UNP A0A0A7DIW7
Aj	237	HIS	-	expression tag	UNP A0A0A7DIW7
Aj	238	HIS	-	expression tag	UNP A0A0A7DIW7
Aj	239	HIS	-	expression tag	UNP A0A0A7DIW7
Aj	240	HIS	-	expression tag	UNP A0A0A7DIW7
Aj	241	HIS	-	expression tag	UNP A0A0A7DIW7
Aj	242	HIS	-	expression tag	UNP A0A0A7DIW7
Ak	49	GLY	-	expression tag	UNP A0A0A7DIW7
Ak	176	CYS	LYS	engineered mutation	UNP A0A0A7DIW7
Ak	228	GLU	ALA	conflict	UNP A0A0A7DIW7
Ak	229	ASN	GLN	conflict	UNP A0A0A7DIW7
Ak	230	LEU	SER	conflict	UNP A0A0A7DIW7
Ak	231	TYR	ARG	conflict	UNP A0A0A7DIW7
Ak	232	PHE	LEU	conflict	UNP A0A0A7DIW7
Ak	233	GLN	PHE	conflict	UNP A0A0A7DIW7
Ak	236	GLU	ASP	conflict	UNP A0A0A7DIW7
Ak	237	HIS	-	expression tag	UNP A0A0A7DIW7
Ak	238	HIS	-	expression tag	UNP A0A0A7DIW7
Ak	239	HIS	-	expression tag	UNP A0A0A7DIW7
Ak	240	HIS	-	expression tag	UNP A0A0A7DIW7
Ak	241	HIS	-	expression tag	UNP A0A0A7DIW7
Ak	242	HIS	-	expression tag	UNP A0A0A7DIW7
Al	49	GLY	-	expression tag	UNP A0A0A7DIW7
Al	176	CYS	LYS	engineered mutation	UNP A0A0A7DIW7
Al	228	GLU	ALA	conflict	UNP A0A0A7DIW7
Al	229	ASN	GLN	conflict	UNP A0A0A7DIW7

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Chain	Residue	Modelled	Actual	Comment	Reference
Al	230	LEU	SER	conflict	UNP A0A0A7DIW7
Al	231	TYR	ARG	conflict	UNP A0A0A7DIW7
Al	232	PHE	LEU	conflict	UNP A0A0A7DIW7
Al	233	GLN	PHE	conflict	UNP A0A0A7DIW7
Al	236	GLU	ASP	conflict	UNP A0A0A7DIW7
Al	237	HIS	-	expression tag	UNP A0A0A7DIW7
Al	238	HIS	-	expression tag	UNP A0A0A7DIW7
Al	239	HIS	-	expression tag	UNP A0A0A7DIW7
Al	240	HIS	-	expression tag	UNP A0A0A7DIW7
Al	241	HIS	-	expression tag	UNP A0A0A7DIW7
Al	242	HIS	-	expression tag	UNP A0A0A7DIW7
Am	49	GLY	-	expression tag	UNP A0A0A7DIW7
Am	176	CYS	LYS	engineered mutation	UNP A0A0A7DIW7
Am	228	GLU	ALA	conflict	UNP A0A0A7DIW7
Am	229	ASN	GLN	conflict	UNP A0A0A7DIW7
Am	230	LEU	SER	conflict	UNP A0A0A7DIW7
Am	231	TYR	ARG	conflict	UNP A0A0A7DIW7
Am	232	PHE	LEU	conflict	UNP A0A0A7DIW7
Am	233	GLN	PHE	conflict	UNP A0A0A7DIW7
Am	236	GLU	ASP	conflict	UNP A0A0A7DIW7
Am	237	HIS	-	expression tag	UNP A0A0A7DIW7
Am	238	HIS	-	expression tag	UNP A0A0A7DIW7
Am	239	HIS	-	expression tag	UNP A0A0A7DIW7
Am	240	HIS	-	expression tag	UNP A0A0A7DIW7
Am	241	HIS	-	expression tag	UNP A0A0A7DIW7
Am	242	HIS	-	expression tag	UNP A0A0A7DIW7
An	49	GLY	-	expression tag	UNP A0A0A7DIW7
An	176	CYS	LYS	engineered mutation	UNP A0A0A7DIW7
An	228	GLU	ALA	conflict	UNP A0A0A7DIW7
An	229	ASN	GLN	conflict	UNP A0A0A7DIW7
An	230	LEU	SER	conflict	UNP A0A0A7DIW7
An	231	TYR	ARG	conflict	UNP A0A0A7DIW7
An	232	PHE	LEU	conflict	UNP A0A0A7DIW7
An	233	GLN	PHE	conflict	UNP A0A0A7DIW7
An	236	GLU	ASP	conflict	UNP A0A0A7DIW7
An	237	HIS	-	expression tag	UNP A0A0A7DIW7
An	238	HIS	-	expression tag	UNP A0A0A7DIW7
An	239	HIS	-	expression tag	UNP A0A0A7DIW7
An	240	HIS	-	expression tag	UNP A0A0A7DIW7
An	241	HIS	-	expression tag	UNP A0A0A7DIW7
An	242	HIS	-	expression tag	UNP A0A0A7DIW7
Ao	49	GLY	-	expression tag	UNP A0A0A7DIW7

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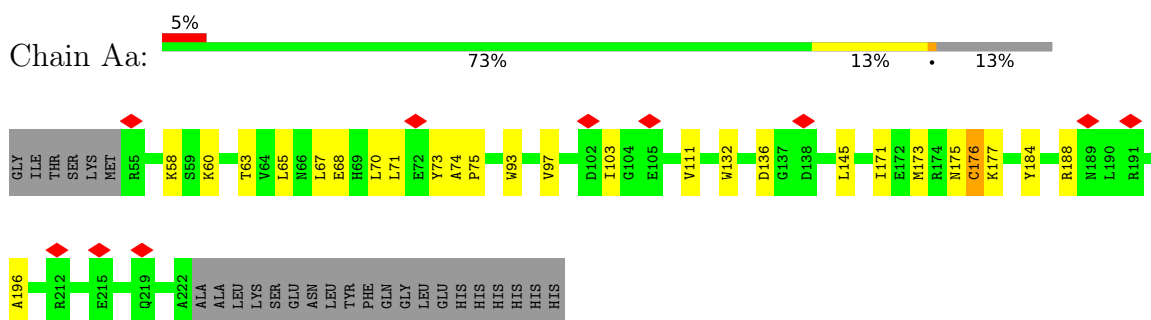
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Chain	Residue	Modelled	Actual	Comment	Reference
Ao	176	CYS	LYS	engineered mutation	UNP A0A0A7DIW7
Ao	228	GLU	ALA	conflict	UNP A0A0A7DIW7
Ao	229	ASN	GLN	conflict	UNP A0A0A7DIW7
Ao	230	LEU	SER	conflict	UNP A0A0A7DIW7
Ao	231	TYR	ARG	conflict	UNP A0A0A7DIW7
Ao	232	PHE	LEU	conflict	UNP A0A0A7DIW7
Ao	233	GLN	PHE	conflict	UNP A0A0A7DIW7
Ao	236	GLU	ASP	conflict	UNP A0A0A7DIW7
Ao	237	HIS	-	expression tag	UNP A0A0A7DIW7
Ao	238	HIS	-	expression tag	UNP A0A0A7DIW7
Ao	239	HIS	-	expression tag	UNP A0A0A7DIW7
Ao	240	HIS	-	expression tag	UNP A0A0A7DIW7
Ao	241	HIS	-	expression tag	UNP A0A0A7DIW7
Ao	242	HIS	-	expression tag	UNP A0A0A7DIW7
Ap	49	GLY	-	expression tag	UNP A0A0A7DIW7
Ap	176	CYS	LYS	engineered mutation	UNP A0A0A7DIW7
Ap	228	GLU	ALA	conflict	UNP A0A0A7DIW7
Ap	229	ASN	GLN	conflict	UNP A0A0A7DIW7
Ap	230	LEU	SER	conflict	UNP A0A0A7DIW7
Ap	231	TYR	ARG	conflict	UNP A0A0A7DIW7
Ap	232	PHE	LEU	conflict	UNP A0A0A7DIW7
Ap	233	GLN	PHE	conflict	UNP A0A0A7DIW7
Ap	236	GLU	ASP	conflict	UNP A0A0A7DIW7
Ap	237	HIS	-	expression tag	UNP A0A0A7DIW7
Ap	238	HIS	-	expression tag	UNP A0A0A7DIW7
Ap	239	HIS	-	expression tag	UNP A0A0A7DIW7
Ap	240	HIS	-	expression tag	UNP A0A0A7DIW7
Ap	241	HIS	-	expression tag	UNP A0A0A7DIW7
Ap	242	HIS	-	expression tag	UNP A0A0A7DIW7

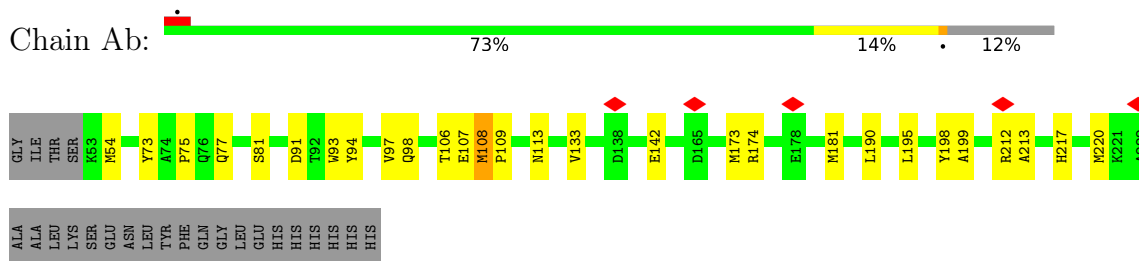
3 Residue-property plots

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.

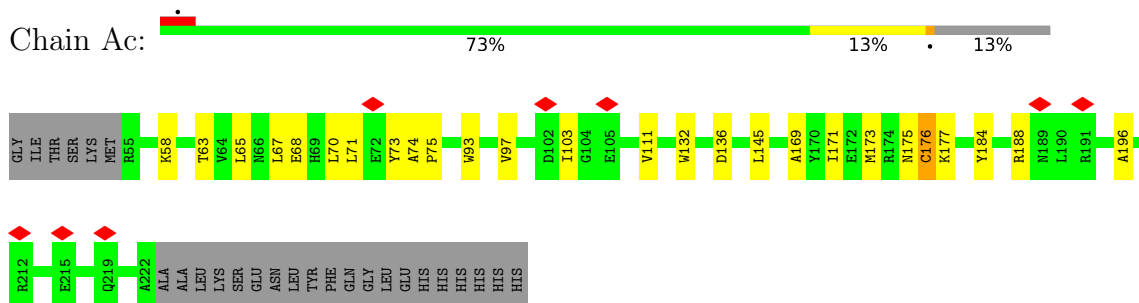
- Molecule 1: Genome polyprotein



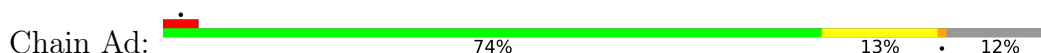
- Molecule 1: Genome polyprotein

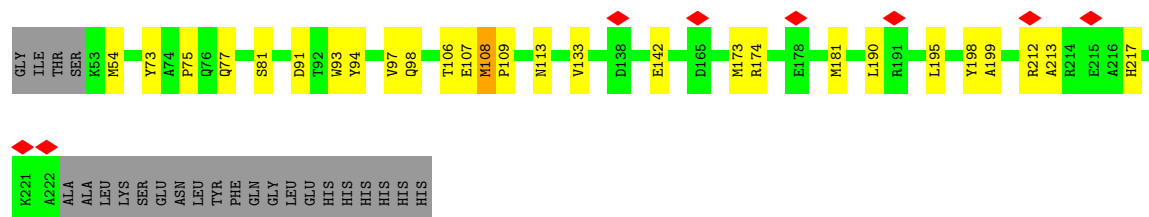


- Molecule 1: Genome polyprotein

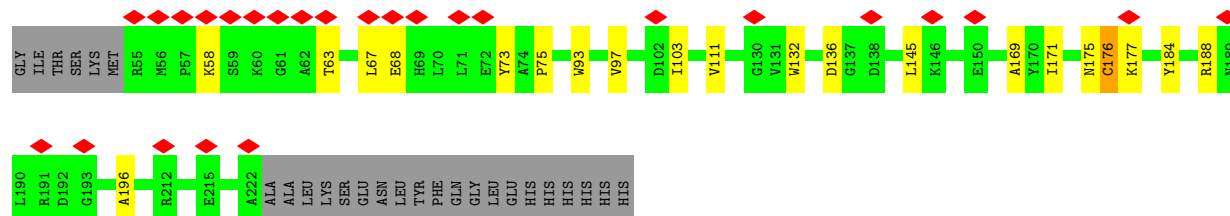
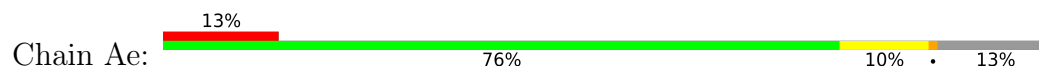


- Molecule 1: Genome polyprotein

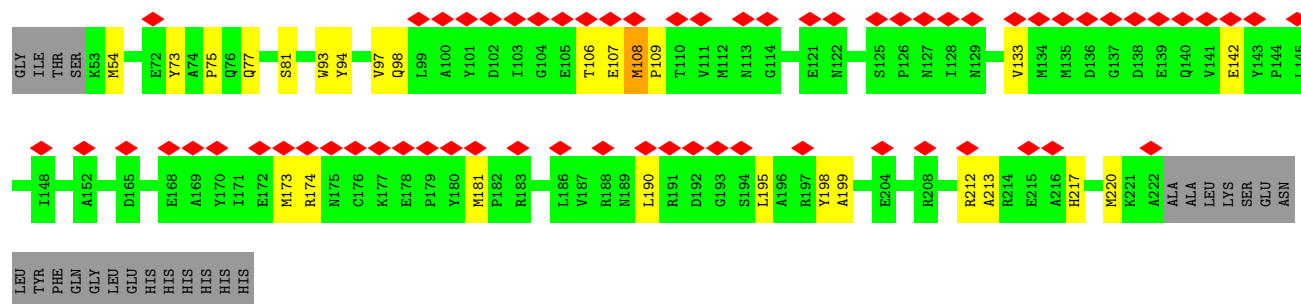
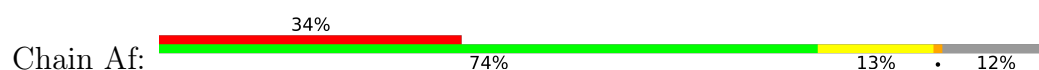




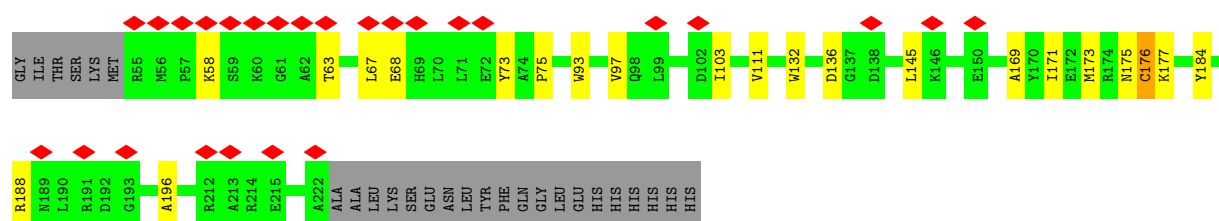
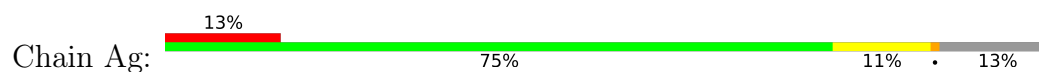
• Molecule 1: Genome polyprotein



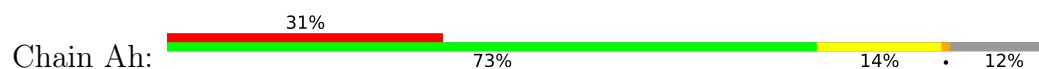
• Molecule 1: Genome polyprotein

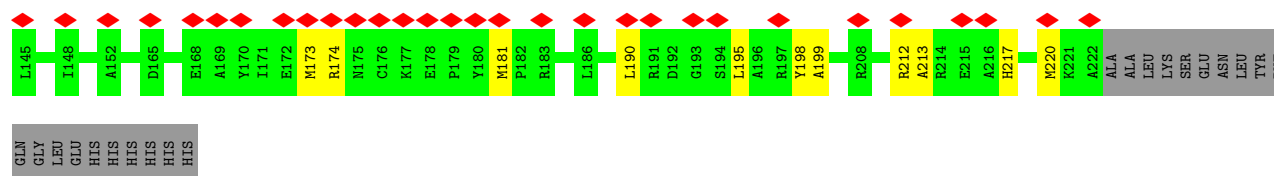


• Molecule 1: Genome polyprotein

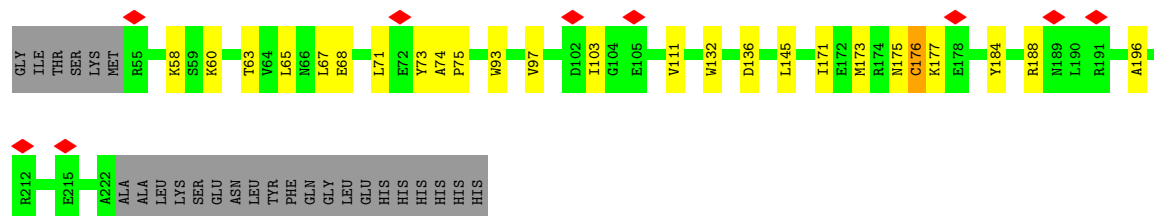
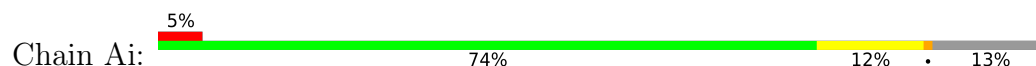


• Molecule 1: Genome polyprotein

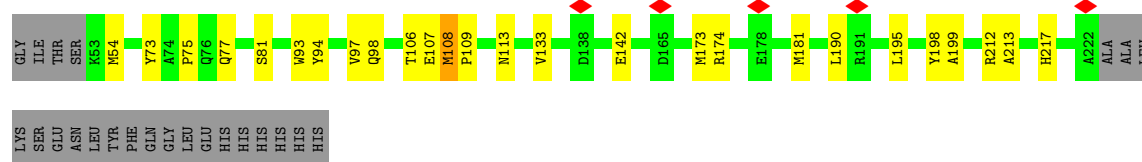
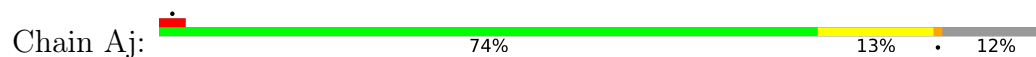




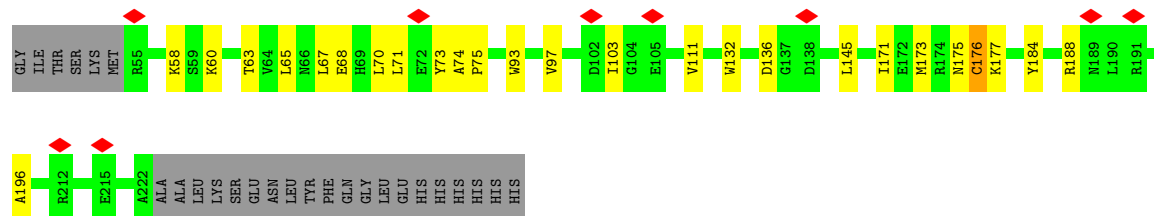
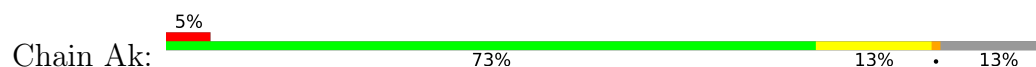
- Molecule 1: Genome polyprotein



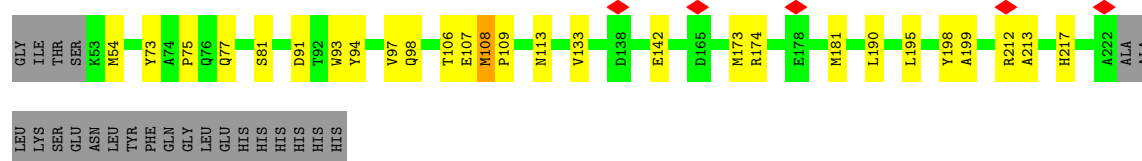
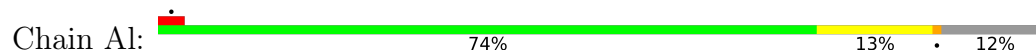
- Molecule 1: Genome polyprotein



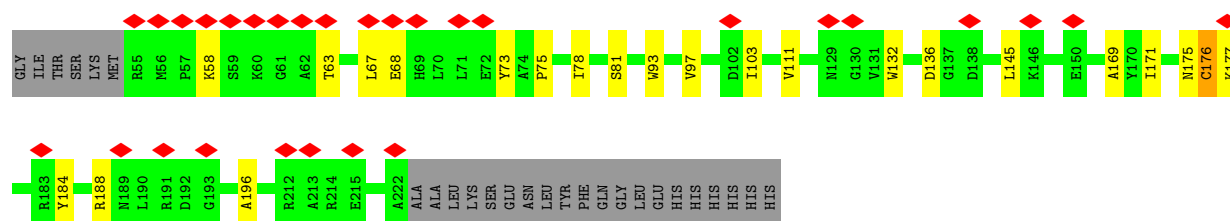
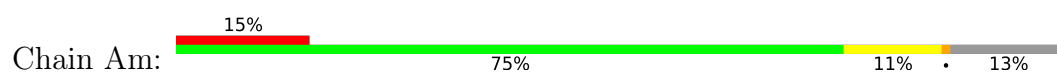
- Molecule 1: Genome polyprotein



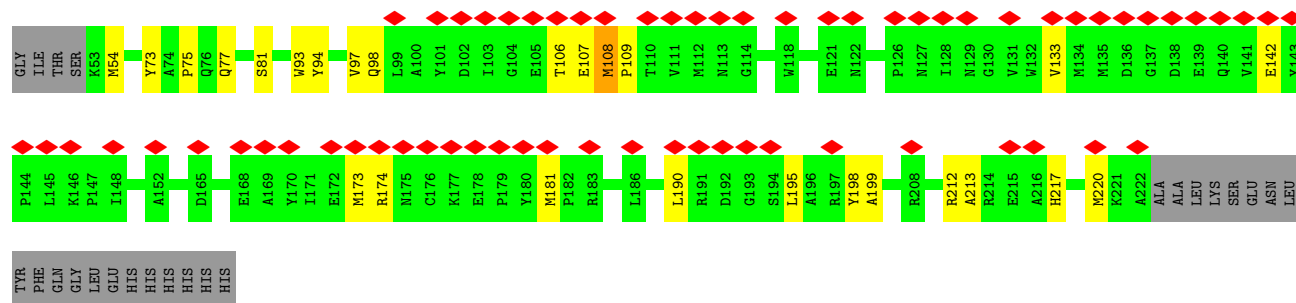
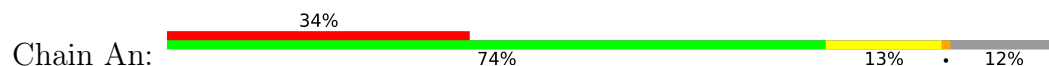
- Molecule 1: Genome polyprotein



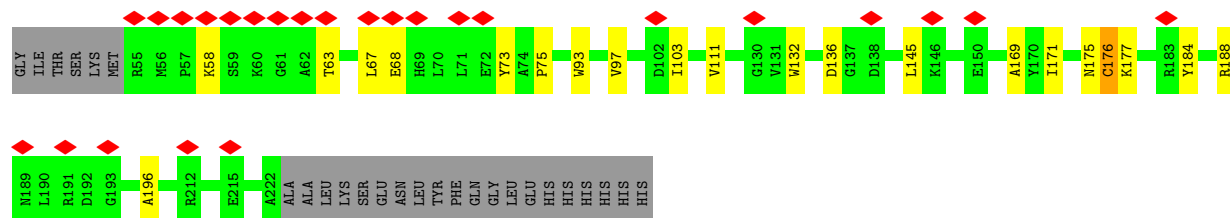
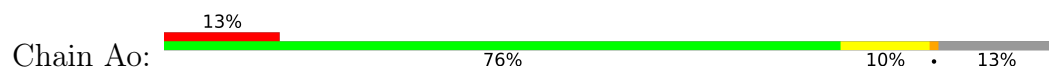
- Molecule 1: Genome polyprotein



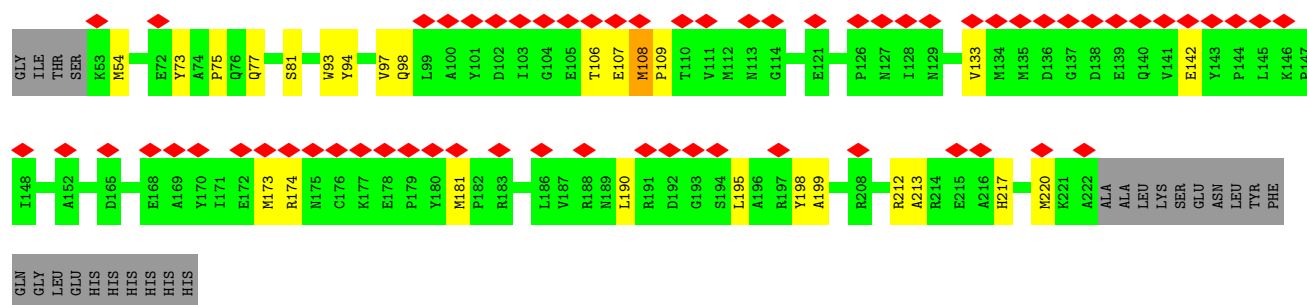
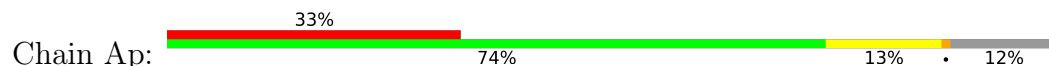
• Molecule 1: Genome polyprotein



• Molecule 1: Genome polyprotein



• Molecule 1: Genome polyprotein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	843116	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; patchCTF correction	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.915	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.104	Depositor
Map size (Å)	493.2, 493.2, 493.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	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	0.57	0/1384	0.57	3/1878 (0.2%)
1	Ab	0.37	0/1401	0.50	2/1899 (0.1%)
1	Ac	0.57	0/1384	0.57	3/1878 (0.2%)
1	Ad	0.37	0/1401	0.50	2/1899 (0.1%)
1	Ae	0.57	0/1384	0.57	3/1878 (0.2%)
1	Af	0.37	0/1401	0.50	2/1899 (0.1%)
1	Ag	0.57	0/1384	0.57	3/1878 (0.2%)
1	Ah	0.37	0/1401	0.50	2/1899 (0.1%)
1	Ai	0.57	0/1384	0.57	3/1878 (0.2%)
1	Aj	0.37	0/1401	0.50	2/1899 (0.1%)
1	Ak	0.57	0/1384	0.57	3/1878 (0.2%)
1	Al	0.37	0/1401	0.50	2/1899 (0.1%)
1	Am	0.57	0/1384	0.57	3/1878 (0.2%)
1	An	0.37	0/1401	0.50	2/1899 (0.1%)
1	Ao	0.57	0/1384	0.57	3/1878 (0.2%)
1	Ap	0.37	0/1401	0.50	2/1899 (0.1%)
All	All	0.48	0/22280	0.54	40/30216 (0.1%)

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	Ai	175	ASN	N-CA-C	-6.99	104.89	113.41
1	Ao	175	ASN	N-CA-C	-6.97	104.91	113.41
1	Ac	175	ASN	N-CA-C	-6.95	104.94	113.41
1	Ak	175	ASN	N-CA-C	-6.94	104.95	113.41
1	Aa	175	ASN	N-CA-C	-6.93	104.95	113.41

There are no chirality outliers.

There are no planarity outliers.

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	Aa	1353	0	1319	22	0
1	Ab	1370	0	1341	24	0
1	Ac	1353	0	1319	24	0
1	Ad	1370	0	1341	23	0
1	Ae	1353	0	1319	17	0
1	Af	1370	0	1341	18	0
1	Ag	1353	0	1319	18	0
1	Ah	1370	0	1341	19	0
1	Ai	1353	0	1319	21	0
1	Aj	1370	0	1341	22	0
1	Ak	1353	0	1319	23	0
1	Al	1370	0	1341	22	0
1	Am	1353	0	1319	18	0
1	An	1370	0	1341	18	0
1	Ao	1353	0	1319	16	0
1	Ap	1370	0	1341	18	0
All	All	21784	0	21280	288	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 7.

The worst 5 of 288 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:Ac:176:CYS:SG	1:Ah:54:MET:HE3	2.31	0.71
1:Ak:176:CYS:SG	1:Ap:54:MET:HE3	2.32	0.69
1:Aa:176:CYS:SG	1:Af:54:MET:HE3	2.34	0.68
1:Ai:176:CYS:SG	1:An:54:MET:HE3	2.34	0.67
1:Ad:54:MET:HE3	1:Ag:176:CYS:SG	2.41	0.61

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	166/194 (86%)	157 (95%)	9 (5%)	0	100	100
1	Ab	168/194 (87%)	161 (96%)	7 (4%)	0	100	100
1	Ac	166/194 (86%)	157 (95%)	9 (5%)	0	100	100
1	Ad	168/194 (87%)	161 (96%)	7 (4%)	0	100	100
1	Ae	166/194 (86%)	157 (95%)	9 (5%)	0	100	100
1	Af	168/194 (87%)	161 (96%)	7 (4%)	0	100	100
1	Ag	166/194 (86%)	157 (95%)	9 (5%)	0	100	100
1	Ah	168/194 (87%)	161 (96%)	7 (4%)	0	100	100
1	Ai	166/194 (86%)	157 (95%)	9 (5%)	0	100	100
1	Aj	168/194 (87%)	161 (96%)	7 (4%)	0	100	100
1	Ak	166/194 (86%)	157 (95%)	9 (5%)	0	100	100
1	Al	168/194 (87%)	161 (96%)	7 (4%)	0	100	100
1	Am	166/194 (86%)	157 (95%)	9 (5%)	0	100	100
1	An	168/194 (87%)	161 (96%)	7 (4%)	0	100	100
1	Ao	166/194 (86%)	157 (95%)	9 (5%)	0	100	100
1	Ap	168/194 (87%)	161 (96%)	7 (4%)	0	100	100
All	All	2672/3104 (86%)	2544 (95%)	128 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	146/168 (87%)	146 (100%)	0	100	100
1	Ab	148/168 (88%)	146 (99%)	2 (1%)	59	73
1	Ac	146/168 (87%)	146 (100%)	0	100	100
1	Ad	148/168 (88%)	146 (99%)	2 (1%)	59	73
1	Ae	146/168 (87%)	146 (100%)	0	100	100
1	Af	148/168 (88%)	146 (99%)	2 (1%)	59	73
1	Ag	146/168 (87%)	146 (100%)	0	100	100
1	Ah	148/168 (88%)	146 (99%)	2 (1%)	59	73
1	Ai	146/168 (87%)	146 (100%)	0	100	100
1	Aj	148/168 (88%)	146 (99%)	2 (1%)	59	73
1	Ak	146/168 (87%)	146 (100%)	0	100	100
1	Al	148/168 (88%)	146 (99%)	2 (1%)	59	73
1	Am	146/168 (87%)	146 (100%)	0	100	100
1	An	148/168 (88%)	146 (99%)	2 (1%)	59	73
1	Ao	146/168 (87%)	146 (100%)	0	100	100
1	Ap	148/168 (88%)	146 (99%)	2 (1%)	59	73
All	All	2352/2688 (88%)	2336 (99%)	16 (1%)	73	80

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Ap	97	VAL
1	An	98	GLN
1	Aj	97	VAL
1	An	97	VAL
1	Ah	98	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	Al	89	GLN
1	Ao	151	ASN
1	Am	151	ASN
1	An	89	GLN
1	Ap	77	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

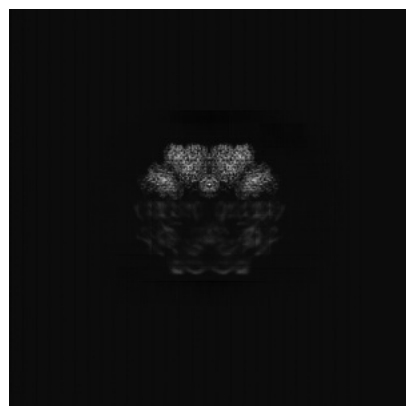
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17063. These allow visual inspection of the internal detail of the map and identification of artifacts.

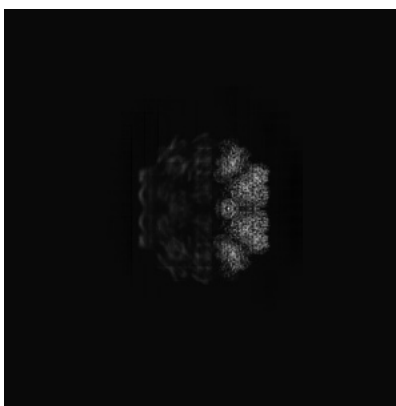
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

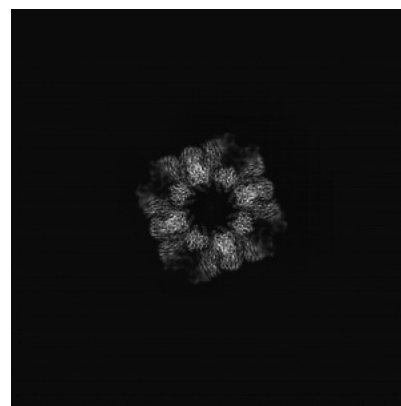
6.1.1 Primary map



X

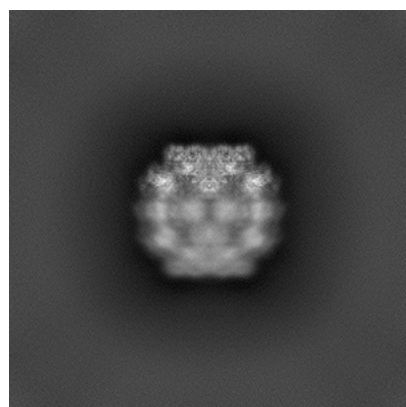


Y

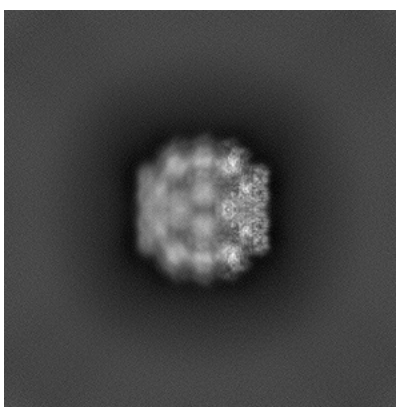


Z

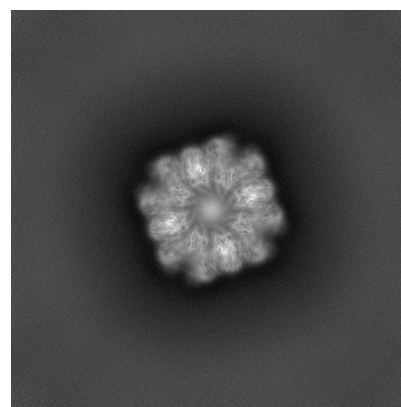
6.1.2 Raw map



X



Y

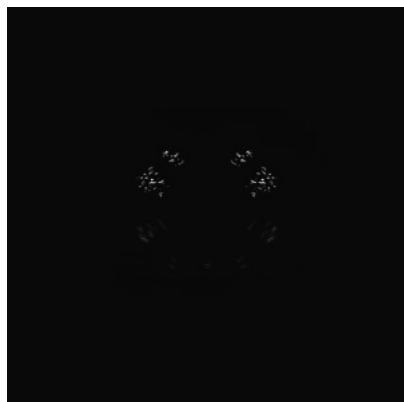


Z

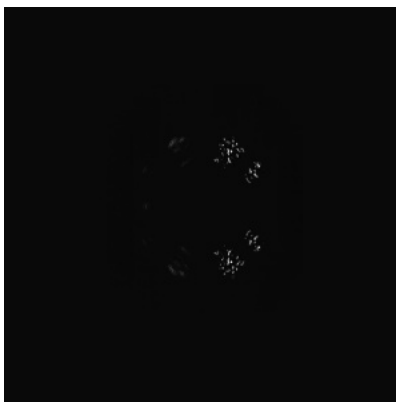
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 300

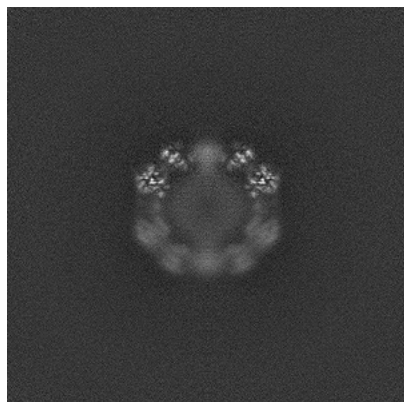


Y Index: 300

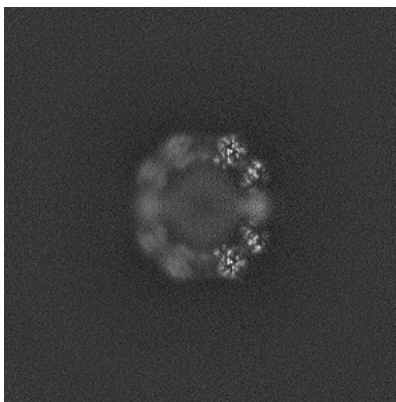


Z Index: 300

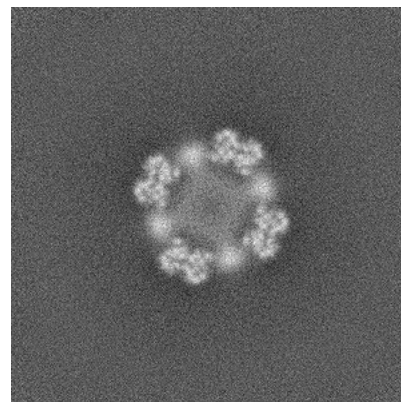
6.2.2 Raw map



X Index: 300



Y Index: 300

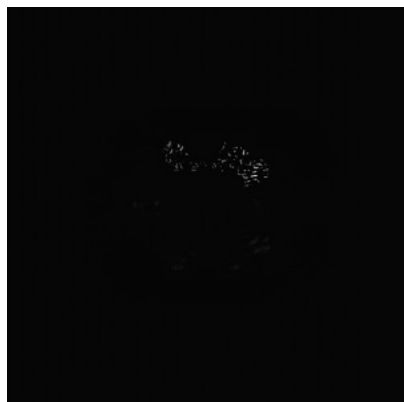


Z Index: 300

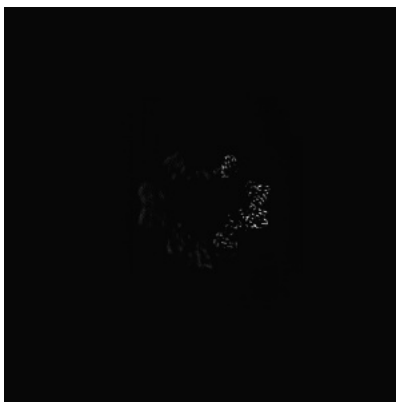
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

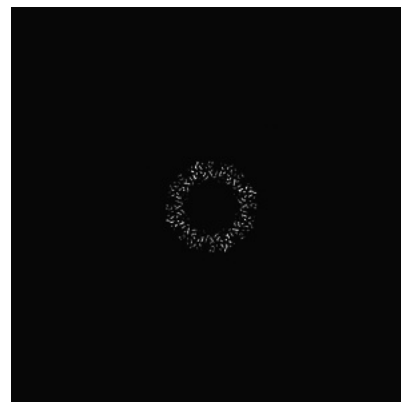
6.3.1 Primary map



X Index: 268

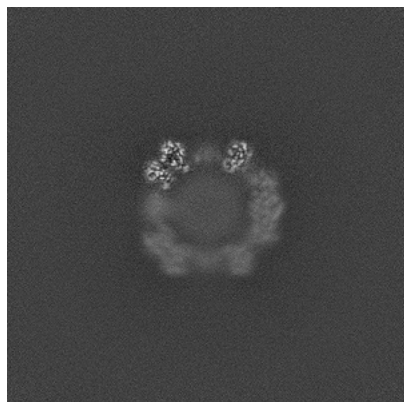


Y Index: 353

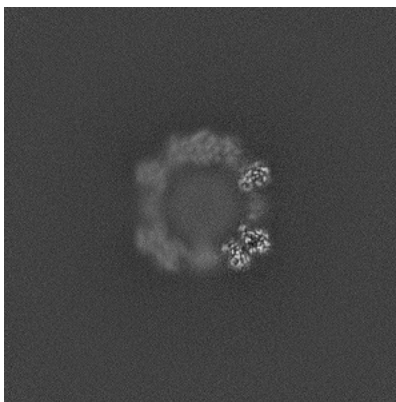


Z Index: 376

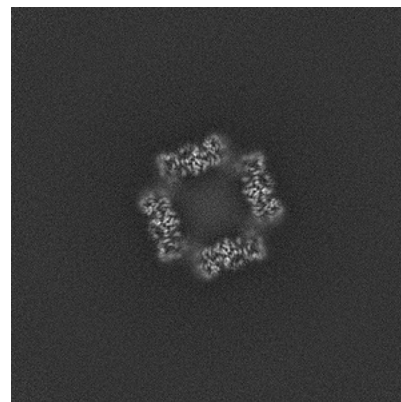
6.3.2 Raw map



X Index: 320



Y Index: 280



Z Index: 342

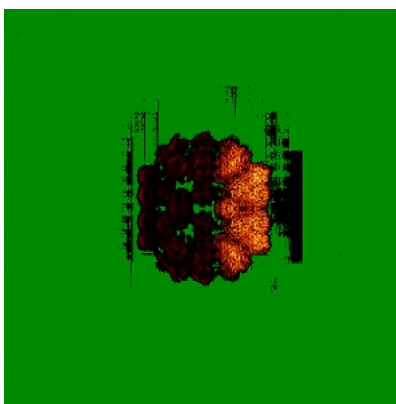
The images above show the largest variance slices of the map in three orthogonal directions.

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

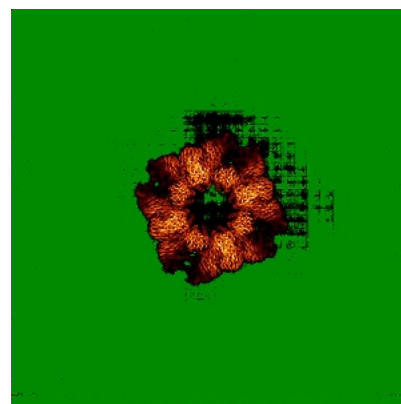
6.4.1 Primary map



X

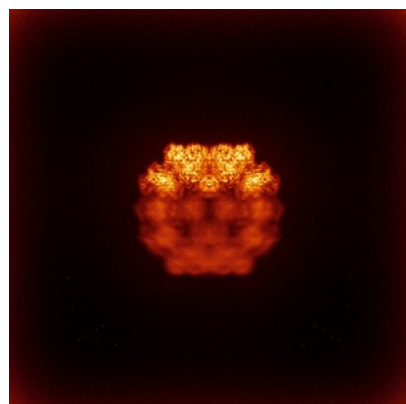


Y

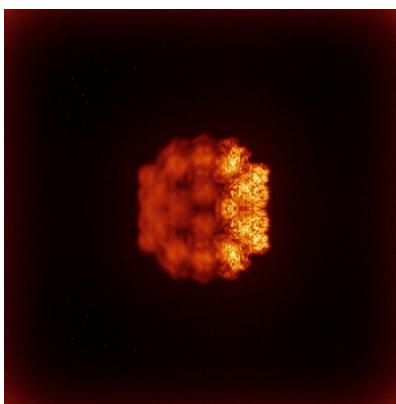


Z

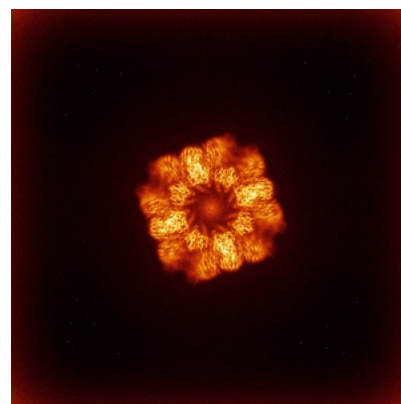
6.4.2 Raw map



X



Y

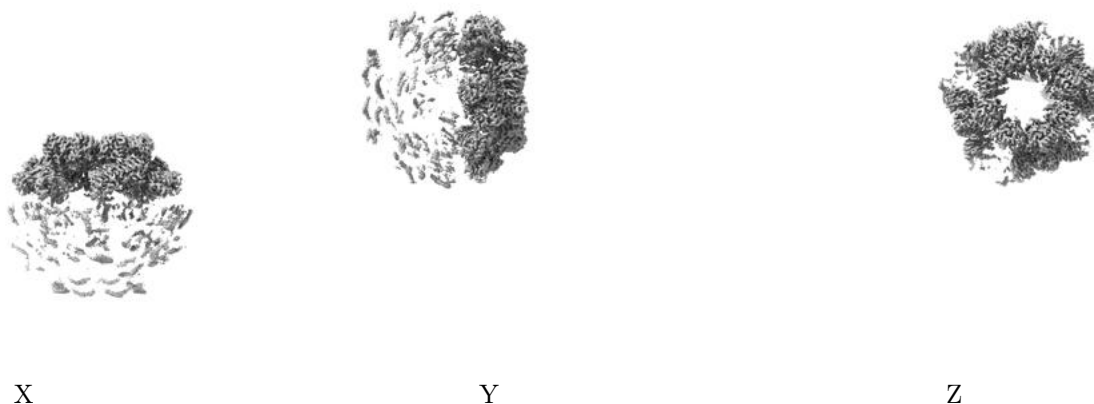


Z

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.

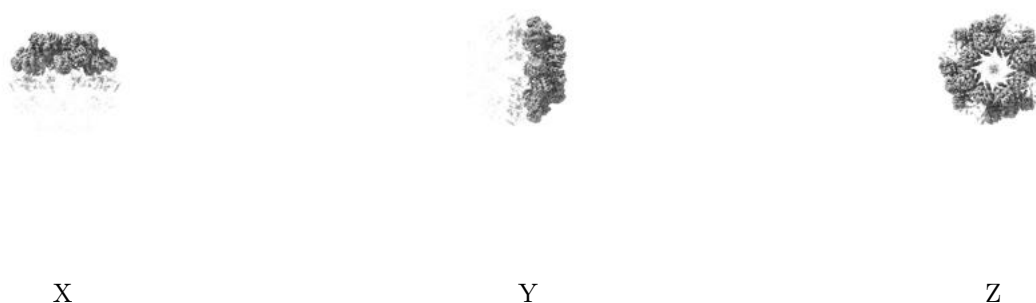
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.104. 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.

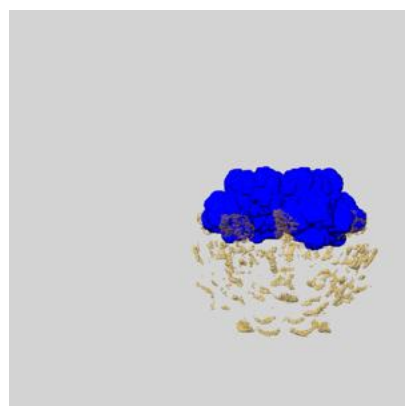
6.6 Mask visualisation [i](#)

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

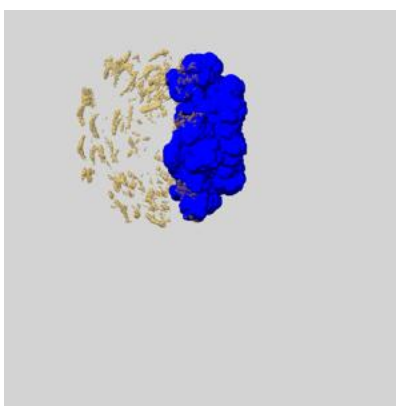
A mask typically either:

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

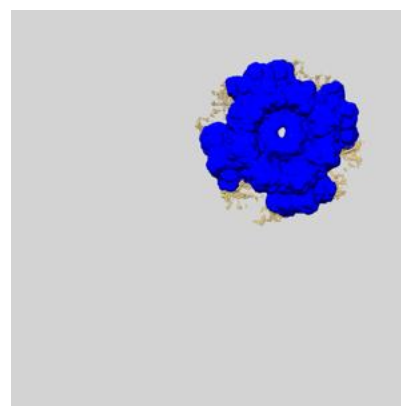
6.6.1 emd_17063_msk_1.map [i](#)



X



Y

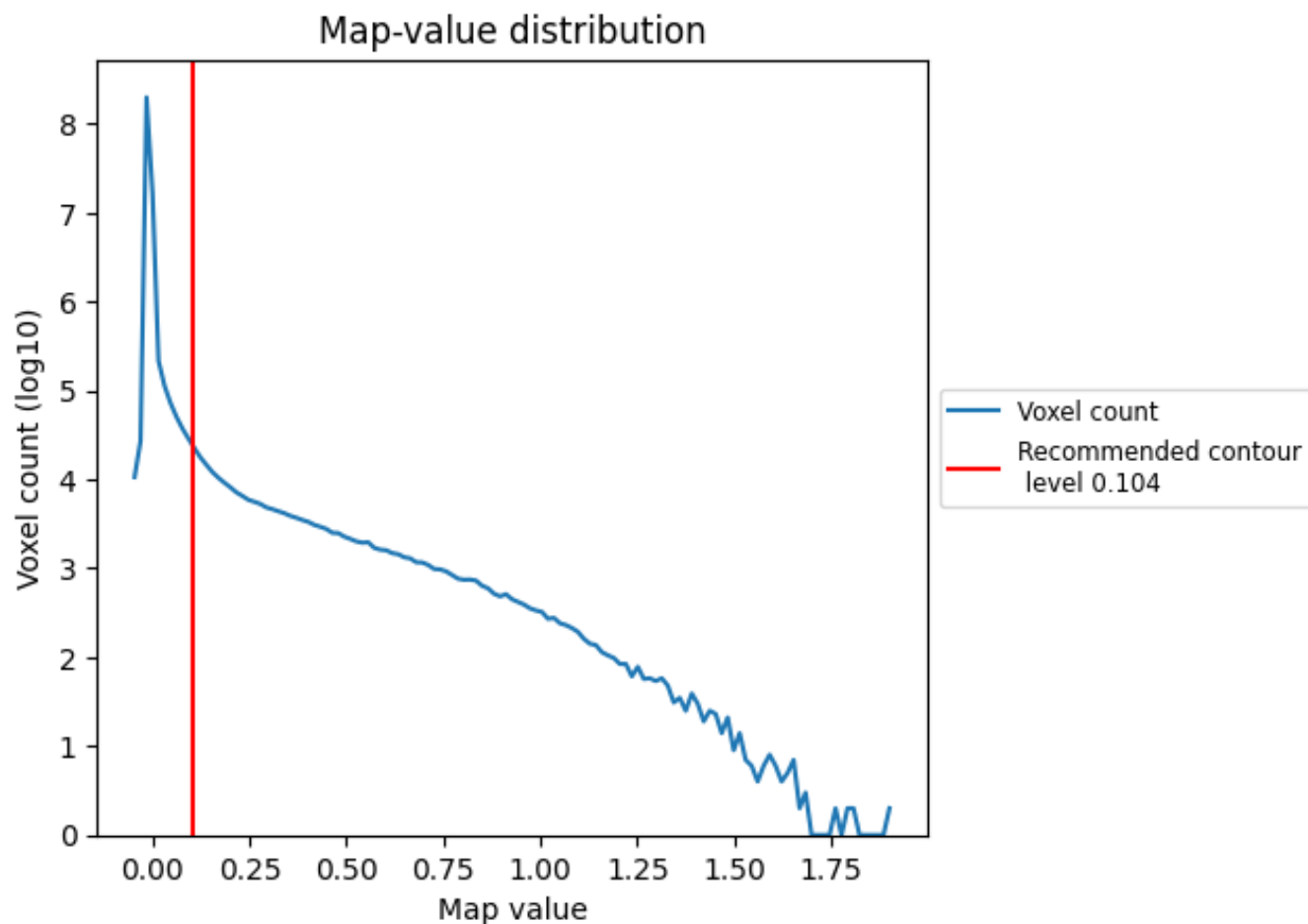


Z

7 Map analysis [i](#)

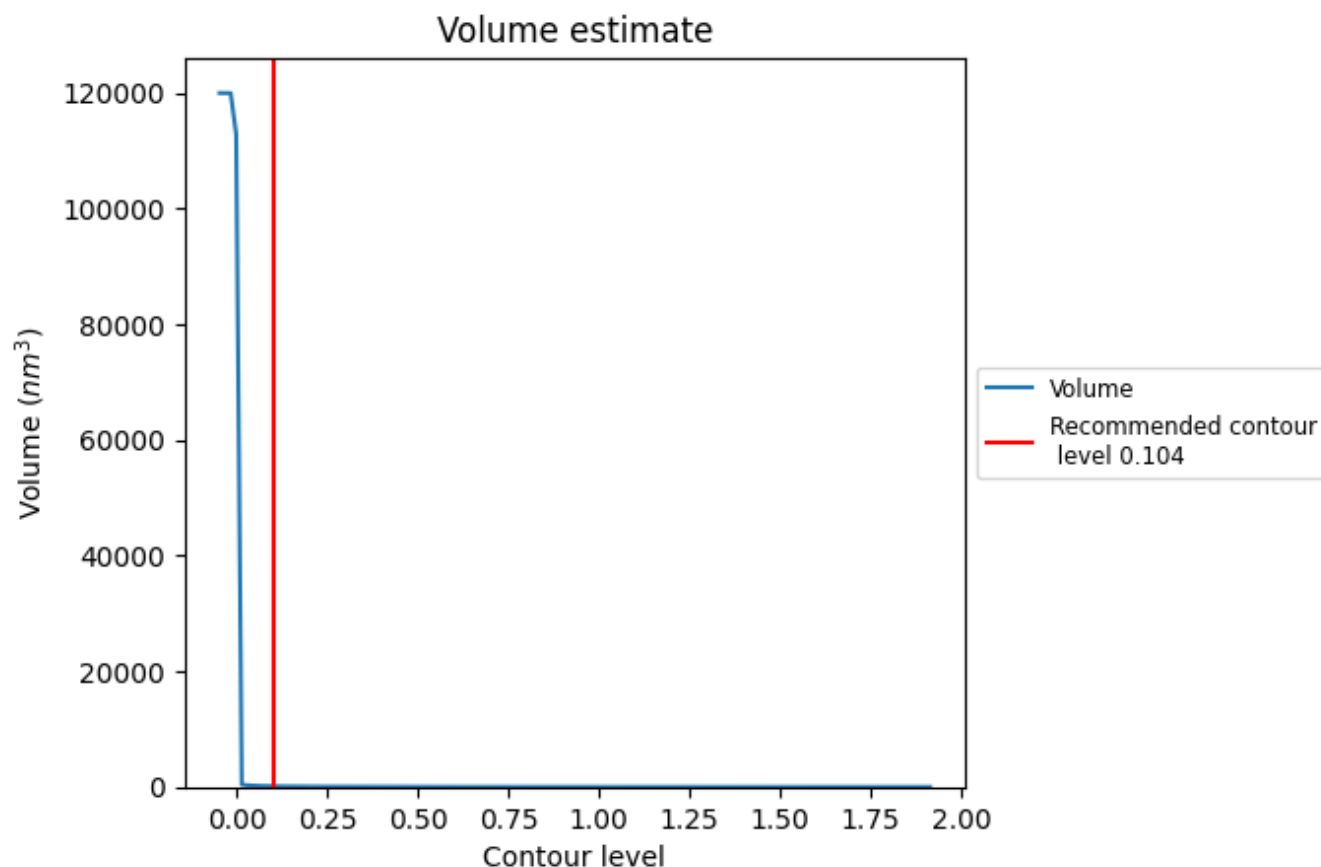
This section contains the results of statistical analysis of the map.

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.

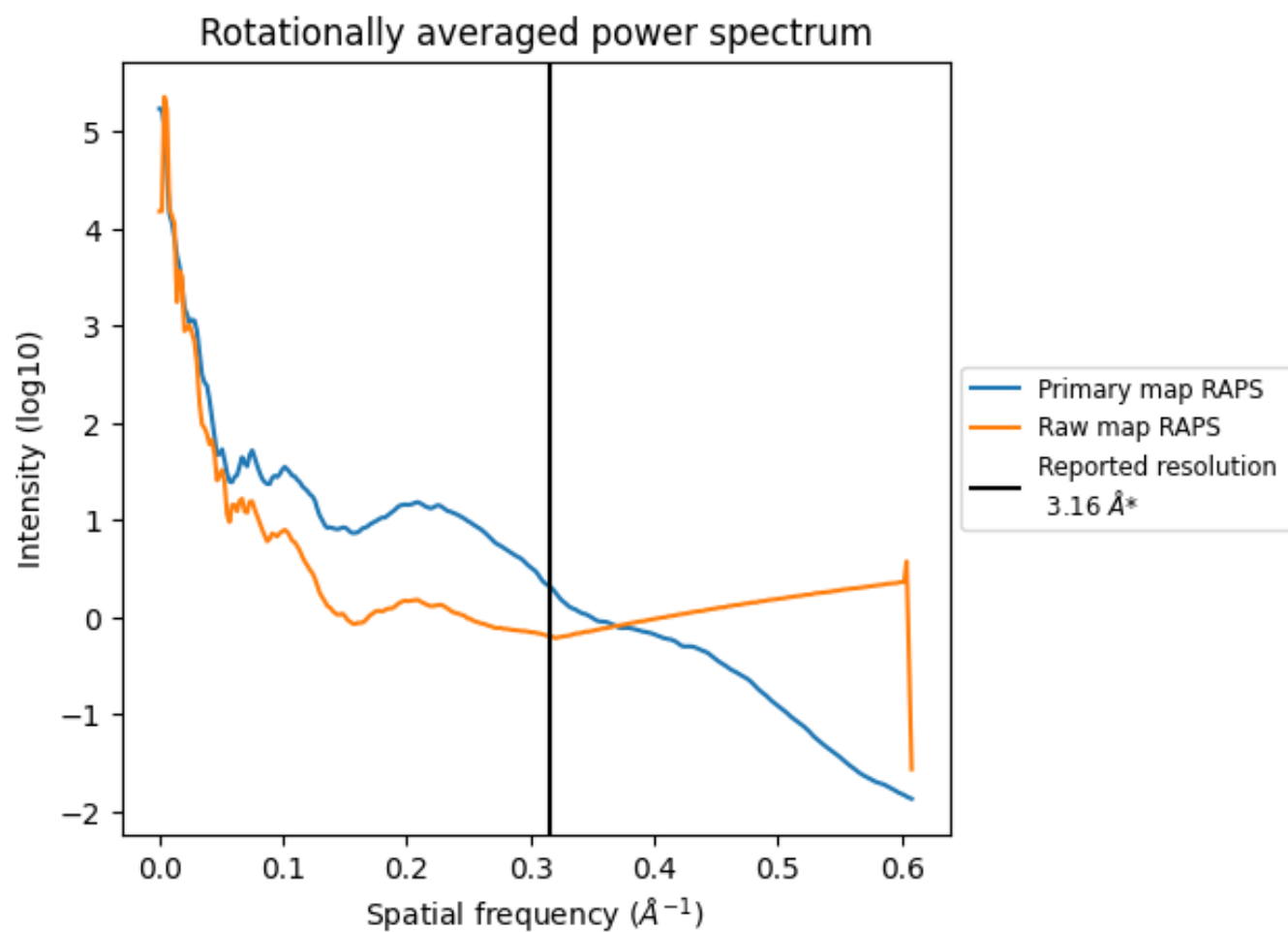
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 121 nm³; this corresponds to an approximate mass of 109 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 ⓘ

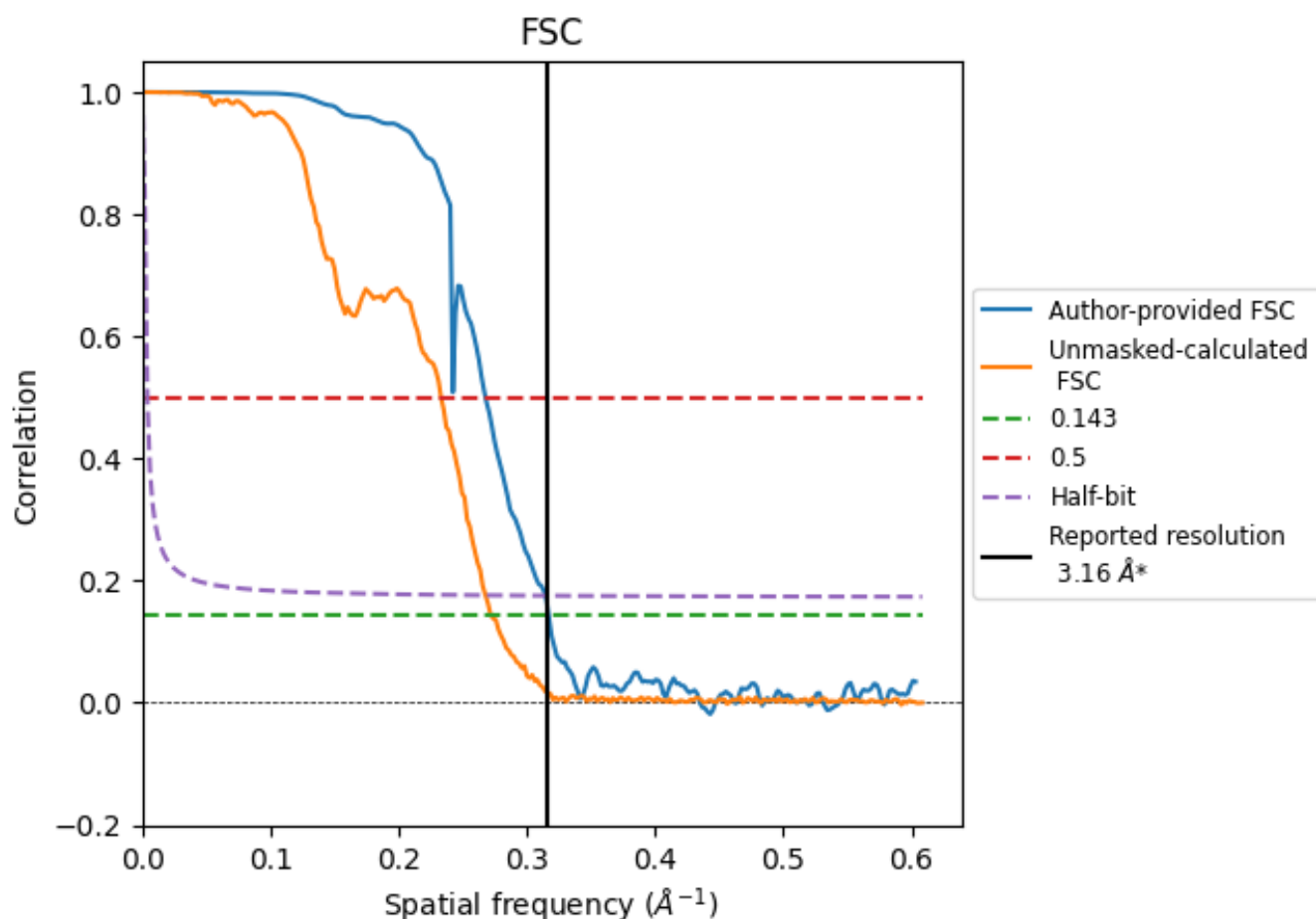


*Reported resolution corresponds to spatial frequency of 0.316 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.316 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	3.15	3.73	3.18
Unmasked-calculated*	3.67	4.29	3.73

*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 3.67 differs from the reported value 3.16 by more than 10 %

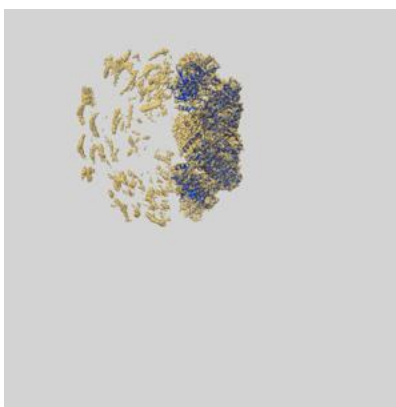
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17063 and PDB model 8OPK. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

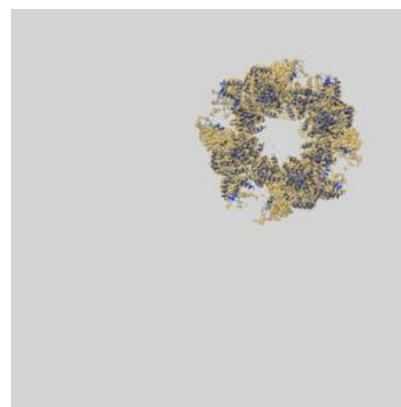
9.1 Map-model overlay [i](#)



X



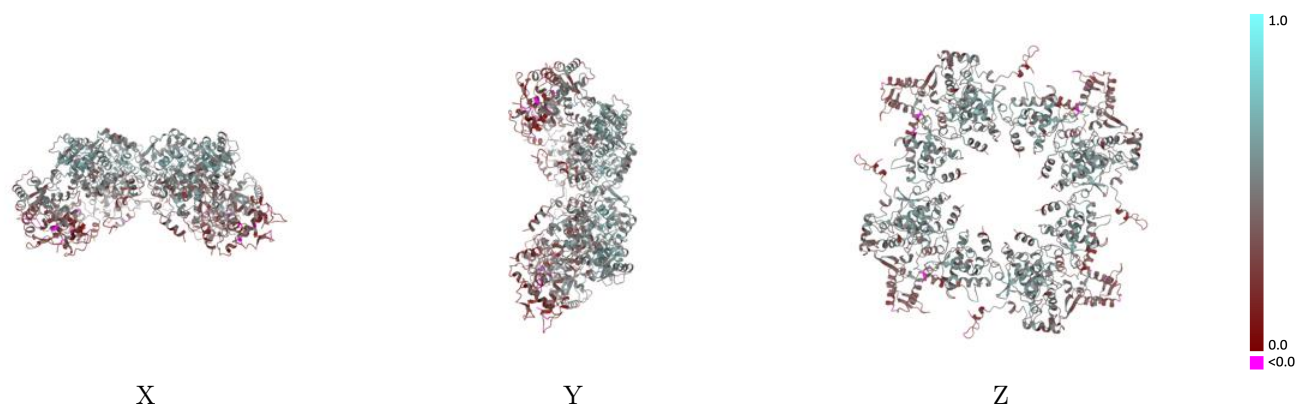
Y



Z

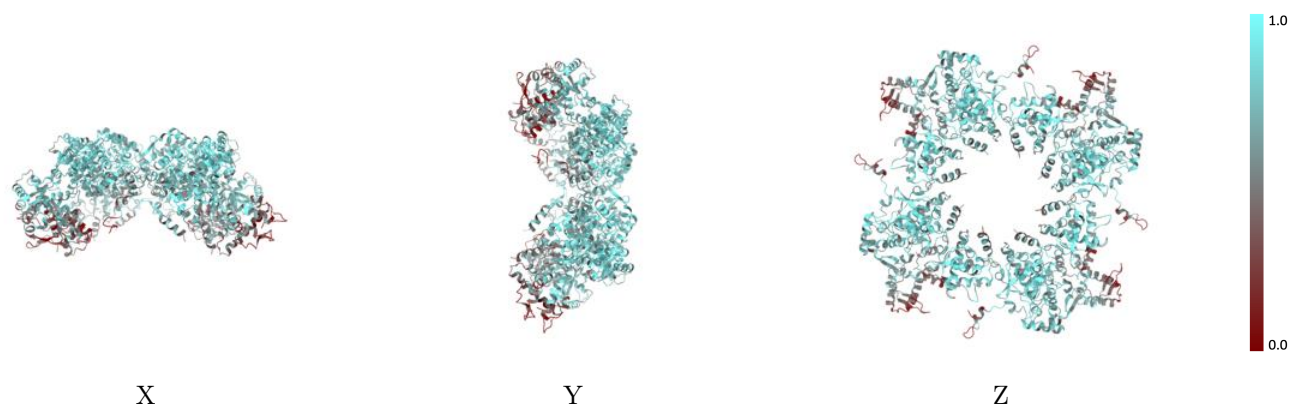
The images above show the 3D surface view of the map at the recommended contour level 0.104 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



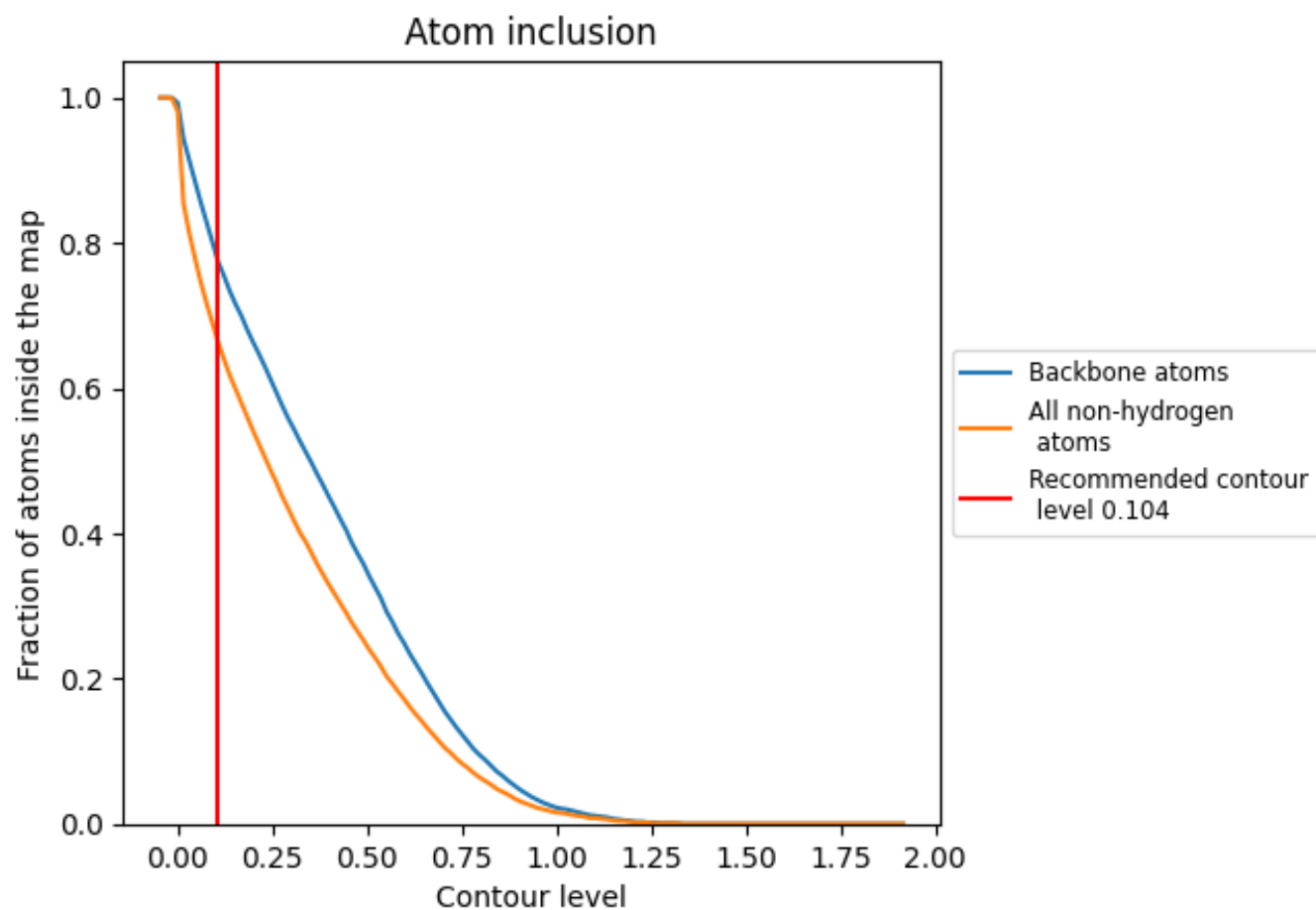
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.104).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 67% 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 (0.104) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6670	0.4280
Aa	0.7550	0.5040
Ab	0.7540	0.4990
Ac	0.7600	0.4990
Ad	0.7440	0.4930
Ae	0.6640	0.3980
Af	0.4950	0.3170
Ag	0.6650	0.4000
Ah	0.5000	0.3190
Ai	0.7600	0.4970
Aj	0.7510	0.4970
Ak	0.7660	0.5030
Al	0.7620	0.5000
Am	0.6560	0.3990
An	0.4810	0.3130
Ao	0.6750	0.4050
Ap	0.4860	0.3120

