



Full wwPDB EM Validation Report ⓘ

Dec 31, 2024 – 07:43 PM EST

PDB ID : 8OPJ
EMDB ID : EMD-17062
Title : Global 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 : 2.99 Å(reported)

This is a Full wwPDB EM Validation 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.dev113
MolProbity : 4.02b-467
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) : 2.40

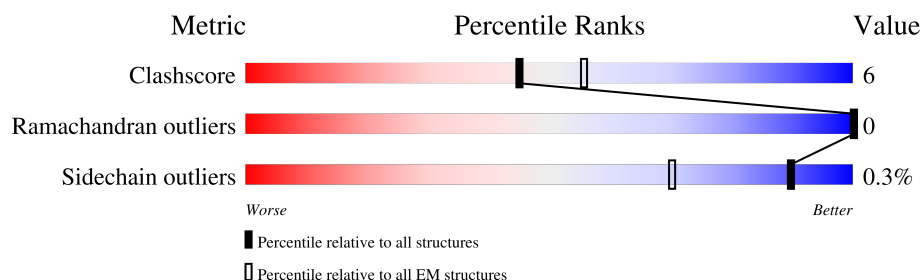
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.99 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.









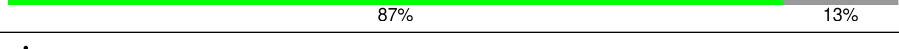
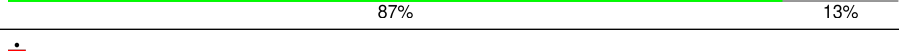
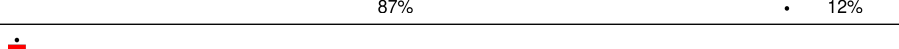
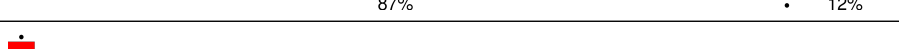
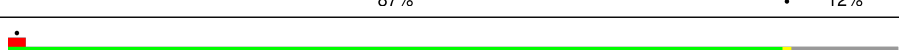

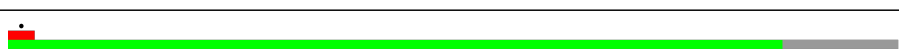

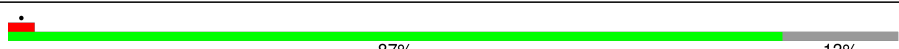





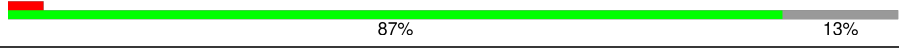
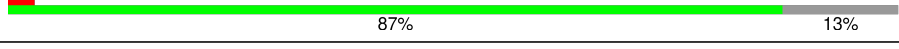



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 ≥ 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	
1	Aj	194	
1	Ak	194	
1	Al	194	
1	Am	194	
1	An	194	
1	Ao	194	
1	Ap	194	
1	Aq	194	
1	Ar	194	
1	As	194	
1	At	194	
1	Au	194	
1	Av	194	
1	Aw	194	
1	Ax	194	
1	Ay	194	
1	Az	194	
1	Ba	194	
1	Bb	194	
1	Bc	194	
1	Bd	194	
1	Be	194	
1	Bf	194	
1	Bg	194	

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Mol	Chain	Length	Quality of chain
1	Bh	194	
1	Bi	194	
1	Bj	194	
1	Bk	194	
1	Bl	194	
1	Bm	194	
1	Bn	194	
1	Bo	194	
1	Bp	194	
1	Bq	194	
1	Br	194	
1	Bs	194	
1	Bt	194	
1	Bu	194	
1	Bv	194	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 65352 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 (Fragment).

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ar	170	Total	C	N	O	S	0	0
			1370	864	236	257	13		
1	As	170	Total	C	N	O	S	0	0
			1370	864	236	257	13		
1	At	170	Total	C	N	O	S	0	0
			1370	864	236	257	13		
1	Au	168	Total	C	N	O	S	0	0
			1353	853	233	255	12		
1	Av	168	Total	C	N	O	S	0	0
			1353	853	233	255	12		
1	Aw	168	Total	C	N	O	S	0	0
			1353	853	233	255	12		
1	Ax	168	Total	C	N	O	S	0	0
			1353	853	233	255	12		
1	Ay	170	Total	C	N	O	S	0	0
			1370	864	236	257	13		
1	Az	170	Total	C	N	O	S	0	0
			1370	864	236	257	13		
1	Ba	170	Total	C	N	O	S	0	0
			1370	864	236	257	13		
1	Bb	170	Total	C	N	O	S	0	0
			1370	864	236	257	13		
1	Bc	168	Total	C	N	O	S	0	0
			1353	853	233	255	12		
1	Bd	168	Total	C	N	O	S	0	0
			1353	853	233	255	12		
1	Be	168	Total	C	N	O	S	0	0
			1353	853	233	255	12		
1	Bf	168	Total	C	N	O	S	0	0
			1353	853	233	255	12		
1	Bg	170	Total	C	N	O	S	0	0
			1370	864	236	257	13		
1	Bh	170	Total	C	N	O	S	0	0
			1370	864	236	257	13		
1	Bi	170	Total	C	N	O	S	0	0
			1370	864	236	257	13		
1	Bj	170	Total	C	N	O	S	0	0
			1370	864	236	257	13		
1	Bk	168	Total	C	N	O	S	0	0
			1353	853	233	255	12		
1	Bl	168	Total	C	N	O	S	0	0
			1353	853	233	255	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Bm	168	Total	C	N	O	S	0	0
			1353	853	233	255	12		
1	Bn	168	Total	C	N	O	S	0	0
			1353	853	233	255	12		
1	Bo	170	Total	C	N	O	S	0	0
			1370	864	236	257	13		
1	Bp	170	Total	C	N	O	S	0	0
			1370	864	236	257	13		
1	Bq	170	Total	C	N	O	S	0	0
			1370	864	236	257	13		
1	Br	170	Total	C	N	O	S	0	0
			1370	864	236	257	13		
1	Bs	168	Total	C	N	O	S	0	0
			1353	853	233	255	12		
1	Bt	168	Total	C	N	O	S	0	0
			1353	853	233	255	12		
1	Bu	168	Total	C	N	O	S	0	0
			1353	853	233	255	12		
1	Bv	168	Total	C	N	O	S	0	0
			1353	853	233	255	12		

There are 720 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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

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

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

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

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

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

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
B1	238	HIS	-	expression tag	UNP A0A0A7DIW7
B1	239	HIS	-	expression tag	UNP A0A0A7DIW7
B1	240	HIS	-	expression tag	UNP A0A0A7DIW7
B1	241	HIS	-	expression tag	UNP A0A0A7DIW7
B1	242	HIS	-	expression tag	UNP A0A0A7DIW7
Bm	49	GLY	-	expression tag	UNP A0A0A7DIW7
Bm	176	CYS	LYS	engineered mutation	UNP A0A0A7DIW7
Bm	228	GLU	ALA	conflict	UNP A0A0A7DIW7
Bm	229	ASN	GLN	conflict	UNP A0A0A7DIW7
Bm	230	LEU	SER	conflict	UNP A0A0A7DIW7
Bm	231	TYR	ARG	conflict	UNP A0A0A7DIW7
Bm	232	PHE	LEU	conflict	UNP A0A0A7DIW7
Bm	233	GLN	PHE	conflict	UNP A0A0A7DIW7
Bm	236	GLU	ASP	conflict	UNP A0A0A7DIW7
Bm	237	HIS	-	expression tag	UNP A0A0A7DIW7
Bm	238	HIS	-	expression tag	UNP A0A0A7DIW7
Bm	239	HIS	-	expression tag	UNP A0A0A7DIW7
Bm	240	HIS	-	expression tag	UNP A0A0A7DIW7
Bm	241	HIS	-	expression tag	UNP A0A0A7DIW7
Bm	242	HIS	-	expression tag	UNP A0A0A7DIW7
Bn	49	GLY	-	expression tag	UNP A0A0A7DIW7
Bn	176	CYS	LYS	engineered mutation	UNP A0A0A7DIW7
Bn	228	GLU	ALA	conflict	UNP A0A0A7DIW7
Bn	229	ASN	GLN	conflict	UNP A0A0A7DIW7
Bn	230	LEU	SER	conflict	UNP A0A0A7DIW7
Bn	231	TYR	ARG	conflict	UNP A0A0A7DIW7
Bn	232	PHE	LEU	conflict	UNP A0A0A7DIW7
Bn	233	GLN	PHE	conflict	UNP A0A0A7DIW7
Bn	236	GLU	ASP	conflict	UNP A0A0A7DIW7
Bn	237	HIS	-	expression tag	UNP A0A0A7DIW7
Bn	238	HIS	-	expression tag	UNP A0A0A7DIW7
Bn	239	HIS	-	expression tag	UNP A0A0A7DIW7
Bn	240	HIS	-	expression tag	UNP A0A0A7DIW7
Bn	241	HIS	-	expression tag	UNP A0A0A7DIW7
Bn	242	HIS	-	expression tag	UNP A0A0A7DIW7
Bo	49	GLY	-	expression tag	UNP A0A0A7DIW7
Bo	176	CYS	LYS	engineered mutation	UNP A0A0A7DIW7
Bo	228	GLU	ALA	conflict	UNP A0A0A7DIW7
Bo	229	ASN	GLN	conflict	UNP A0A0A7DIW7
Bo	230	LEU	SER	conflict	UNP A0A0A7DIW7
Bo	231	TYR	ARG	conflict	UNP A0A0A7DIW7
Bo	232	PHE	LEU	conflict	UNP A0A0A7DIW7

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

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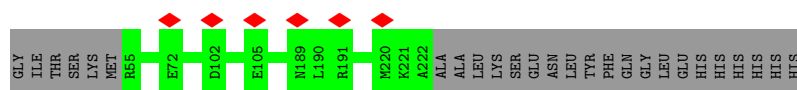
Chain	Residue	Modelled	Actual	Comment	Reference
Br	230	LEU	SER	conflict	UNP A0A0A7DIW7
Br	231	TYR	ARG	conflict	UNP A0A0A7DIW7
Br	232	PHE	LEU	conflict	UNP A0A0A7DIW7
Br	233	GLN	PHE	conflict	UNP A0A0A7DIW7
Br	236	GLU	ASP	conflict	UNP A0A0A7DIW7
Br	237	HIS	-	expression tag	UNP A0A0A7DIW7
Br	238	HIS	-	expression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

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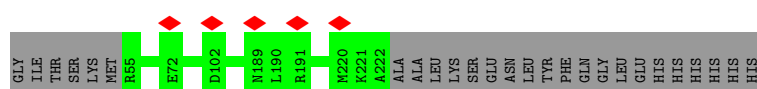
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Chain	Residue	Modelled	Actual	Comment	Reference
Bu	176	CYS	LYS	engineered mutation	UNP A0A0A7DIW7
Bu	228	GLU	ALA	conflict	UNP A0A0A7DIW7
Bu	229	ASN	GLN	conflict	UNP A0A0A7DIW7
Bu	230	LEU	SER	conflict	UNP A0A0A7DIW7
Bu	231	TYR	ARG	conflict	UNP A0A0A7DIW7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


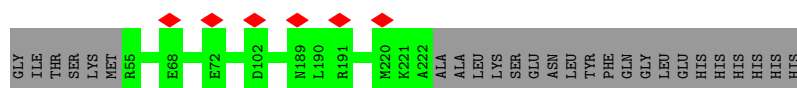
• Molecule 1: Genome polyprotein (Fragment)

Chain Af:  87% 13%


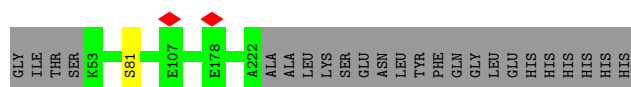
• Molecule 1: Genome polyprotein (Fragment)

Chain Ag:  87% 13%


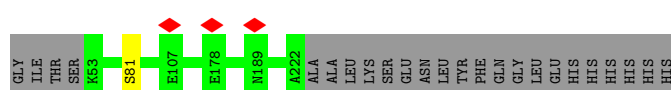
• Molecule 1: Genome polyprotein (Fragment)

Chain Ah:  87% 13%


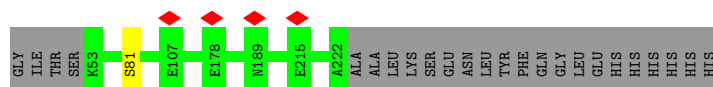
• Molecule 1: Genome polyprotein (Fragment)

Chain Ai:  87% 12%


• Molecule 1: Genome polyprotein (Fragment)

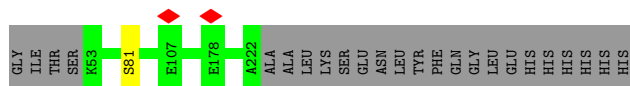
Chain Aj:  87% 12%

• Molecule 1: Genome polyprotein (Fragment)

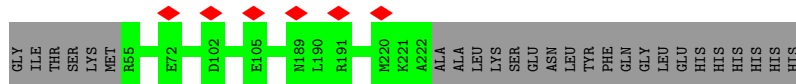
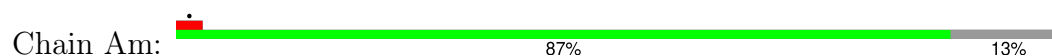
Chain Ak:  87% 12%

• Molecule 1: Genome polyprotein (Fragment)

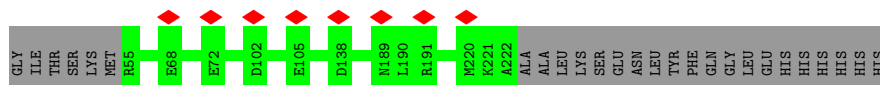
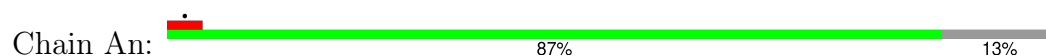
Chain Al:  87% 12%



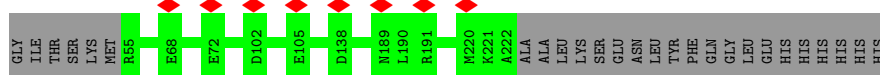
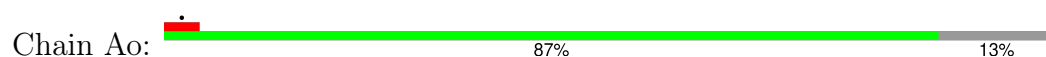
- Molecule 1: Genome polyprotein (Fragment)



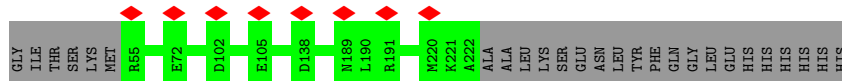
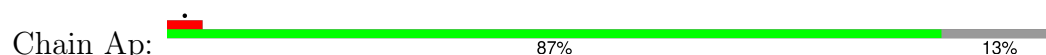
- Molecule 1: Genome polyprotein (Fragment)



- Molecule 1: Genome polyprotein (Fragment)



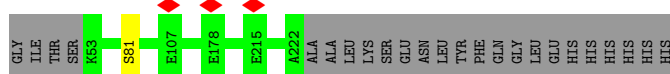
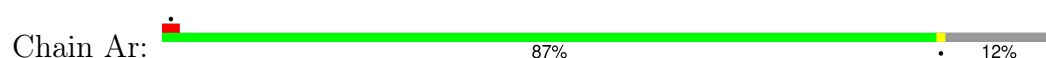
- Molecule 1: Genome polyprotein (Fragment)



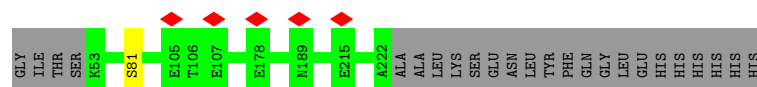
- Molecule 1: Genome polyprotein (Fragment)



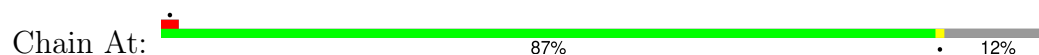
- Molecule 1: Genome polyprotein (Fragment)



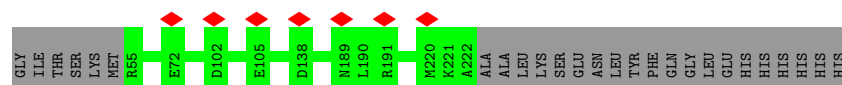
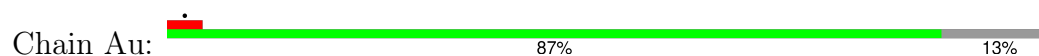
- Molecule 1: Genome polyprotein (Fragment)



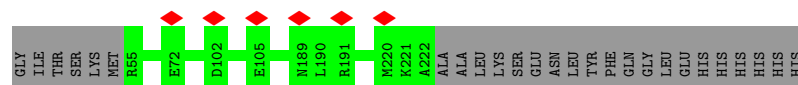
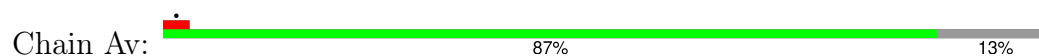
- Molecule 1: Genome polyprotein (Fragment)



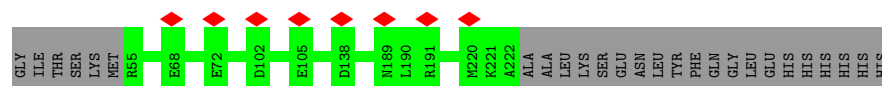
- Molecule 1: Genome polyprotein (Fragment)



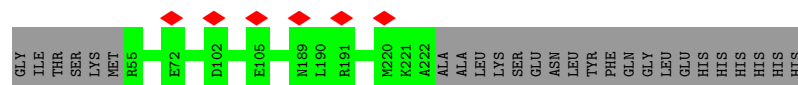
- Molecule 1: Genome polyprotein (Fragment)



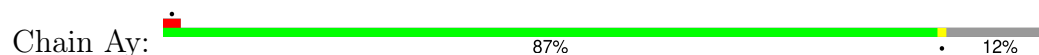
- Molecule 1: Genome polyprotein (Fragment)

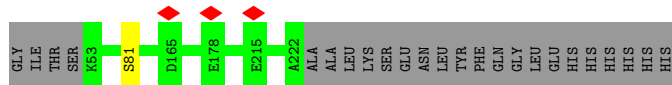


- Molecule 1: Genome polyprotein (Fragment)

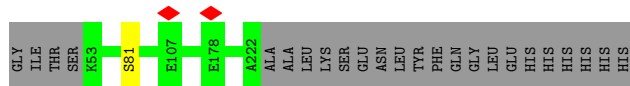
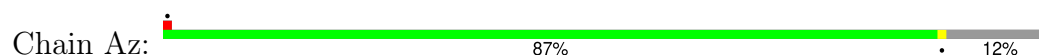


- Molecule 1: Genome polyprotein (Fragment)

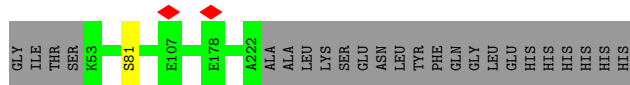
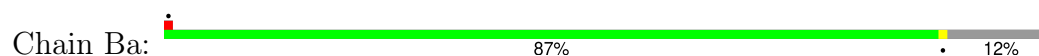




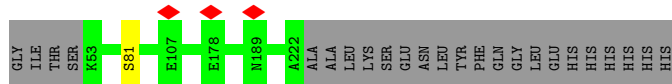
- Molecule 1: Genome polyprotein (Fragment)



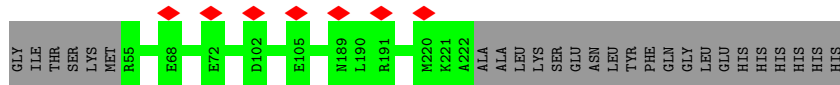
- Molecule 1: Genome polyprotein (Fragment)



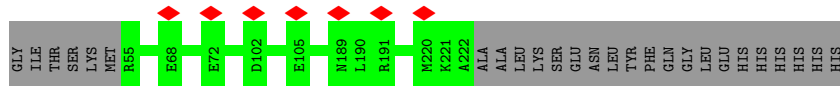
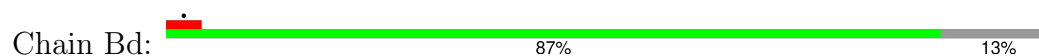
- Molecule 1: Genome polyprotein (Fragment)



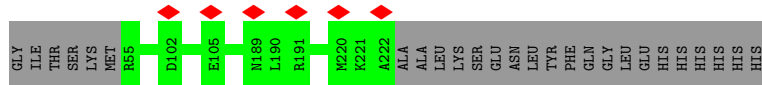
- Molecule 1: Genome polyprotein (Fragment)



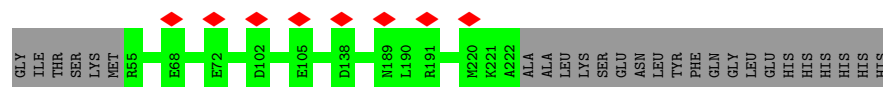
- Molecule 1: Genome polyprotein (Fragment)



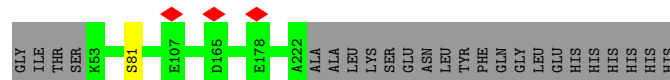
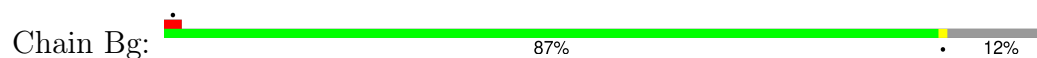
- Molecule 1: Genome polyprotein (Fragment)



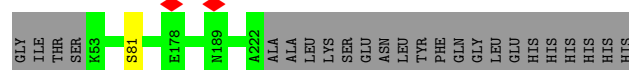
- Molecule 1: Genome polyprotein (Fragment)



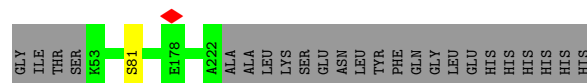
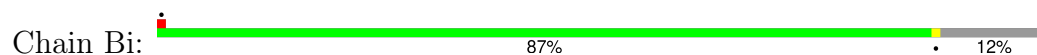
- Molecule 1: Genome polyprotein (Fragment)



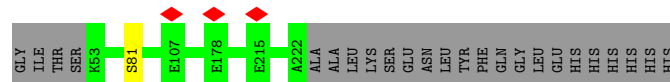
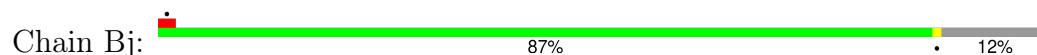
- Molecule 1: Genome polyprotein (Fragment)



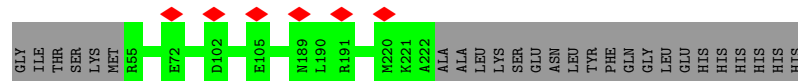
- Molecule 1: Genome polyprotein (Fragment)



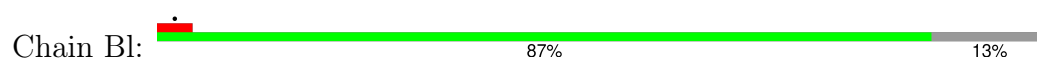
- Molecule 1: Genome polyprotein (Fragment)

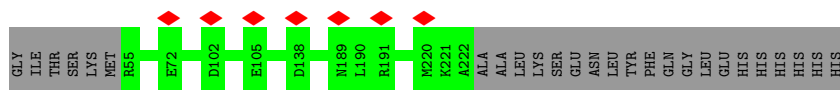


- Molecule 1: Genome polyprotein (Fragment)

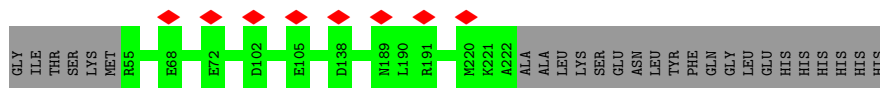
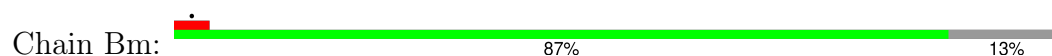


- Molecule 1: Genome polyprotein (Fragment)

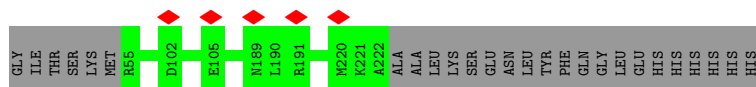
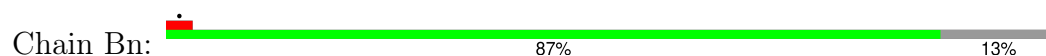




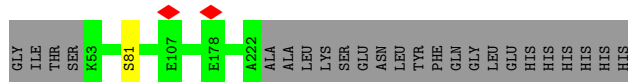
- Molecule 1: Genome polyprotein (Fragment)



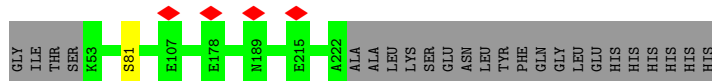
- Molecule 1: Genome polyprotein (Fragment)



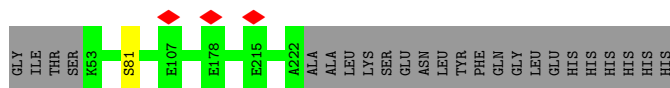
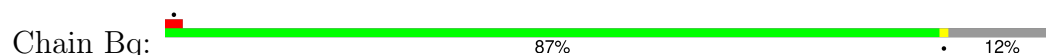
- Molecule 1: Genome polyprotein (Fragment)



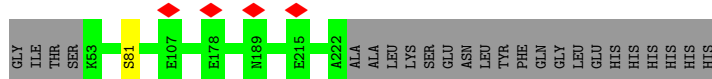
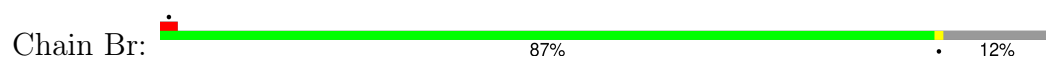
- Molecule 1: Genome polyprotein (Fragment)



- Molecule 1: Genome polyprotein (Fragment)

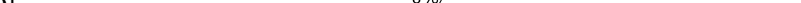


- Molecule 1: Genome polyprotein (Fragment)

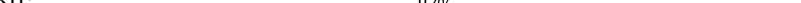


- Molecule 1: Genome polyprotein (Fragment)

GLY
ILE
THR
SER
LYS
MET
R55
E72
D102
E105
D138
M189
L190
R191
K220
K221
A232
ALA
LEU
LYS
SER
GLU
ASN
LEU
TYR
PHE
GLN
GLY
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

- Chain Bt:  87% 13%

GLY
ILE
THR
SER
SER
LYS
LYS
MET
R55
E72
D102
E105
N189
L190
R191
M220
K221
A222
ALA
ALA
LEU
LEU
LYS
SER
GLU
ASN
LEU
TYR
PHE
GLN
GLY
LEU
GLU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

- Chain Bu: 

GLY
ILE
THR
SER
LYS
SER
MET

R55
E68
E72
D102
E105
D138
M189
L190
R191
M220
K221
A222

ALA
LEU
LYS
SER
GLU
ASN
LEU
TYR
PHE
GLN
GLY
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

- Chain Bv: 87% 13%

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, O	Depositor
Number of particles used	210779	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	1.962	Depositor
Minimum map value	-0.031	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.1	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

5.1 Standard geometry

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	0.34	0/1401	0.53	0/1899
1	Ab	0.34	0/1401	0.53	0/1899
1	Ac	0.34	0/1401	0.53	0/1899
1	Ad	0.34	0/1401	0.53	0/1899
1	Ae	0.42	0/1384	0.57	0/1878
1	Af	0.42	0/1384	0.57	0/1878
1	Ag	0.42	0/1384	0.57	0/1878
1	Ah	0.42	0/1384	0.56	0/1878
1	Ai	0.34	0/1401	0.53	0/1899
1	Aj	0.34	0/1401	0.53	0/1899
1	Ak	0.34	0/1401	0.53	0/1899
1	Al	0.34	0/1401	0.53	0/1899
1	Am	0.42	0/1384	0.56	0/1878
1	An	0.42	0/1384	0.57	0/1878
1	Ao	0.42	0/1384	0.57	0/1878
1	Ap	0.42	0/1384	0.57	0/1878
1	Aq	0.34	0/1401	0.54	0/1899
1	Ar	0.34	0/1401	0.53	0/1899
1	As	0.34	0/1401	0.53	0/1899
1	At	0.34	0/1401	0.53	0/1899
1	Au	0.42	0/1384	0.57	0/1878
1	Av	0.42	0/1384	0.57	0/1878
1	Aw	0.42	0/1384	0.56	0/1878
1	Ax	0.42	0/1384	0.56	0/1878
1	Ay	0.34	0/1401	0.53	0/1899
1	Az	0.34	0/1401	0.53	0/1899
1	Ba	0.34	0/1401	0.53	0/1899
1	Bb	0.34	0/1401	0.54	0/1899
1	Bc	0.42	0/1384	0.56	0/1878
1	Bd	0.42	0/1384	0.57	0/1878
1	Be	0.42	0/1384	0.56	0/1878
1	Bf	0.42	0/1384	0.57	0/1878
1	Bg	0.34	0/1401	0.53	0/1899
1	Bh	0.34	0/1401	0.53	0/1899

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Bi	0.34	0/1401	0.53	0/1899
1	Bj	0.34	0/1401	0.53	0/1899
1	Bk	0.42	0/1384	0.56	0/1878
1	Bl	0.42	0/1384	0.56	0/1878
1	Bm	0.42	0/1384	0.57	0/1878
1	Bn	0.42	0/1384	0.57	0/1878
1	Bo	0.34	0/1401	0.53	0/1899
1	Bp	0.34	0/1401	0.53	0/1899
1	Bq	0.34	0/1401	0.53	0/1899
1	Br	0.34	0/1401	0.53	0/1899
1	Bs	0.42	0/1384	0.57	0/1878
1	Bt	0.42	0/1384	0.57	0/1878
1	Bu	0.42	0/1384	0.56	0/1878
1	Bv	0.42	0/1384	0.56	0/1878
All	All	0.38	0/66840	0.55	0/90648

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	1370	0	1341	0	0
1	Ab	1370	0	1341	0	0
1	Ac	1370	0	1341	0	0
1	Ad	1370	0	1341	0	0
1	Ae	1353	0	1319	0	0
1	Af	1353	0	1319	0	0
1	Ag	1353	0	1319	0	0
1	Ah	1353	0	1319	0	0
1	Ai	1370	0	1341	0	0
1	Aj	1370	0	1341	0	0
1	Ak	1370	0	1341	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Al	1370	0	1341	0	0
1	Am	1353	0	1319	0	0
1	An	1353	0	1319	0	0
1	Ao	1353	0	1319	0	0
1	Ap	1353	0	1319	0	0
1	Aq	1370	0	1341	0	0
1	Ar	1370	0	1341	0	0
1	As	1370	0	1341	0	0
1	At	1370	0	1341	0	0
1	Au	1353	0	1319	0	0
1	Av	1353	0	1319	0	0
1	Aw	1353	0	1319	0	0
1	Ax	1353	0	1319	0	0
1	Ay	1370	0	1341	0	0
1	Az	1370	0	1341	0	0
1	Ba	1370	0	1341	0	0
1	Bb	1370	0	1341	0	0
1	Bc	1353	0	1319	0	0
1	Bd	1353	0	1319	0	0
1	Be	1353	0	1319	0	0
1	Bf	1353	0	1319	0	0
1	Bg	1370	0	1341	0	0
1	Bh	1370	0	1341	0	0
1	Bi	1370	0	1341	0	0
1	Bj	1370	0	1341	0	0
1	Bk	1353	0	1319	0	0
1	Bl	1353	0	1319	0	0
1	Bm	1353	0	1319	0	0
1	Bn	1353	0	1319	0	0
1	Bo	1370	0	1341	0	0
1	Bp	1370	0	1341	0	0
1	Bq	1370	0	1341	0	0
1	Br	1370	0	1341	0	0
1	Bs	1353	0	1319	0	0
1	Bt	1353	0	1319	0	0
1	Bu	1353	0	1319	0	0
1	Bv	1353	0	1319	0	0
All	All	65352	0	63840	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 6.

There are no clashes within the asymmetric unit.

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	168/194 (87%)	161 (96%)	7 (4%)	0	100	100
1	Ab	168/194 (87%)	161 (96%)	7 (4%)	0	100	100
1	Ac	168/194 (87%)	161 (96%)	7 (4%)	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	166/194 (86%)	157 (95%)	9 (5%)	0	100	100
1	Ag	166/194 (86%)	157 (95%)	9 (5%)	0	100	100
1	Ah	166/194 (86%)	157 (95%)	9 (5%)	0	100	100
1	Ai	168/194 (87%)	161 (96%)	7 (4%)	0	100	100
1	Aj	168/194 (87%)	161 (96%)	7 (4%)	0	100	100
1	Ak	168/194 (87%)	161 (96%)	7 (4%)	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	166/194 (86%)	157 (95%)	9 (5%)	0	100	100
1	Ao	166/194 (86%)	157 (95%)	9 (5%)	0	100	100
1	Ap	166/194 (86%)	157 (95%)	9 (5%)	0	100	100
1	Aq	168/194 (87%)	161 (96%)	7 (4%)	0	100	100
1	Ar	168/194 (87%)	161 (96%)	7 (4%)	0	100	100
1	As	168/194 (87%)	161 (96%)	7 (4%)	0	100	100
1	At	168/194 (87%)	161 (96%)	7 (4%)	0	100	100
1	Au	166/194 (86%)	157 (95%)	9 (5%)	0	100	100
1	Av	166/194 (86%)	157 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Aw	166/194 (86%)	157 (95%)	9 (5%)	0	100	100
1	Ax	166/194 (86%)	157 (95%)	9 (5%)	0	100	100
1	Ay	168/194 (87%)	161 (96%)	7 (4%)	0	100	100
1	Az	168/194 (87%)	161 (96%)	7 (4%)	0	100	100
1	Ba	168/194 (87%)	161 (96%)	7 (4%)	0	100	100
1	Bb	168/194 (87%)	160 (95%)	8 (5%)	0	100	100
1	Bc	166/194 (86%)	157 (95%)	9 (5%)	0	100	100
1	Bd	166/194 (86%)	157 (95%)	9 (5%)	0	100	100
1	Be	166/194 (86%)	157 (95%)	9 (5%)	0	100	100
1	Bf	166/194 (86%)	157 (95%)	9 (5%)	0	100	100
1	Bg	168/194 (87%)	161 (96%)	7 (4%)	0	100	100
1	Bh	168/194 (87%)	161 (96%)	7 (4%)	0	100	100
1	Bi	168/194 (87%)	161 (96%)	7 (4%)	0	100	100
1	Bj	168/194 (87%)	161 (96%)	7 (4%)	0	100	100
1	Bk	166/194 (86%)	157 (95%)	9 (5%)	0	100	100
1	Bl	166/194 (86%)	157 (95%)	9 (5%)	0	100	100
1	Bm	166/194 (86%)	157 (95%)	9 (5%)	0	100	100
1	Bn	166/194 (86%)	157 (95%)	9 (5%)	0	100	100
1	Bo	168/194 (87%)	162 (96%)	6 (4%)	0	100	100
1	Bp	168/194 (87%)	161 (96%)	7 (4%)	0	100	100
1	Bq	168/194 (87%)	161 (96%)	7 (4%)	0	100	100
1	Br	168/194 (87%)	161 (96%)	7 (4%)	0	100	100
1	Bs	166/194 (86%)	157 (95%)	9 (5%)	0	100	100
1	Bt	166/194 (86%)	157 (95%)	9 (5%)	0	100	100
1	Bu	166/194 (86%)	157 (95%)	9 (5%)	0	100	100
1	Bv	166/194 (86%)	157 (95%)	9 (5%)	0	100	100
All	All	8016/9312 (86%)	7632 (95%)	384 (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	148/168 (88%)	147 (99%)	1 (1%)	81	91
1	Ab	148/168 (88%)	147 (99%)	1 (1%)	81	91
1	Ac	148/168 (88%)	147 (99%)	1 (1%)	81	91
1	Ad	148/168 (88%)	147 (99%)	1 (1%)	81	91
1	Ae	146/168 (87%)	146 (100%)	0	100	100
1	Af	146/168 (87%)	146 (100%)	0	100	100
1	Ag	146/168 (87%)	146 (100%)	0	100	100
1	Ah	146/168 (87%)	146 (100%)	0	100	100
1	Ai	148/168 (88%)	147 (99%)	1 (1%)	81	91
1	Aj	148/168 (88%)	147 (99%)	1 (1%)	81	91
1	Ak	148/168 (88%)	147 (99%)	1 (1%)	81	91
1	Al	148/168 (88%)	147 (99%)	1 (1%)	81	91
1	Am	146/168 (87%)	146 (100%)	0	100	100
1	An	146/168 (87%)	146 (100%)	0	100	100
1	Ao	146/168 (87%)	146 (100%)	0	100	100
1	Ap	146/168 (87%)	146 (100%)	0	100	100
1	Aq	148/168 (88%)	147 (99%)	1 (1%)	81	91
1	Ar	148/168 (88%)	147 (99%)	1 (1%)	81	91
1	As	148/168 (88%)	147 (99%)	1 (1%)	81	91
1	At	148/168 (88%)	147 (99%)	1 (1%)	81	91
1	Au	146/168 (87%)	146 (100%)	0	100	100
1	Av	146/168 (87%)	146 (100%)	0	100	100
1	Aw	146/168 (87%)	146 (100%)	0	100	100
1	Ax	146/168 (87%)	146 (100%)	0	100	100
1	Ay	148/168 (88%)	147 (99%)	1 (1%)	81	91
1	Az	148/168 (88%)	147 (99%)	1 (1%)	81	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ba	148/168 (88%)	147 (99%)	1 (1%)	81	91
1	Bb	148/168 (88%)	147 (99%)	1 (1%)	81	91
1	Bc	146/168 (87%)	146 (100%)	0	100	100
1	Bd	146/168 (87%)	146 (100%)	0	100	100
1	Be	146/168 (87%)	146 (100%)	0	100	100
1	Bf	146/168 (87%)	146 (100%)	0	100	100
1	Bg	148/168 (88%)	147 (99%)	1 (1%)	81	91
1	Bh	148/168 (88%)	147 (99%)	1 (1%)	81	91
1	Bi	148/168 (88%)	147 (99%)	1 (1%)	81	91
1	Bj	148/168 (88%)	147 (99%)	1 (1%)	81	91
1	Bk	146/168 (87%)	146 (100%)	0	100	100
1	Bl	146/168 (87%)	146 (100%)	0	100	100
1	Bm	146/168 (87%)	146 (100%)	0	100	100
1	Bn	146/168 (87%)	146 (100%)	0	100	100
1	Bo	148/168 (88%)	147 (99%)	1 (1%)	81	91
1	Bp	148/168 (88%)	147 (99%)	1 (1%)	81	91
1	Bq	148/168 (88%)	147 (99%)	1 (1%)	81	91
1	Br	148/168 (88%)	147 (99%)	1 (1%)	81	91
1	Bs	146/168 (87%)	146 (100%)	0	100	100
1	Bt	146/168 (87%)	146 (100%)	0	100	100
1	Bu	146/168 (87%)	146 (100%)	0	100	100
1	Bv	146/168 (87%)	146 (100%)	0	100	100
All	All	7056/8064 (88%)	7032 (100%)	24 (0%)	90	96

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Aa	81	SER
1	Ab	81	SER
1	Ac	81	SER
1	Ad	81	SER
1	Ai	81	SER
1	Aj	81	SER
1	Ak	81	SER

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Mol	Chain	Res	Type
1	Al	81	SER
1	Aq	81	SER
1	Ar	81	SER
1	As	81	SER
1	At	81	SER
1	Ay	81	SER
1	Az	81	SER
1	Ba	81	SER
1	Bb	81	SER
1	Bg	81	SER
1	Bh	81	SER
1	Bi	81	SER
1	Bj	81	SER
1	Bo	81	SER
1	Bp	81	SER
1	Bq	81	SER
1	Br	81	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

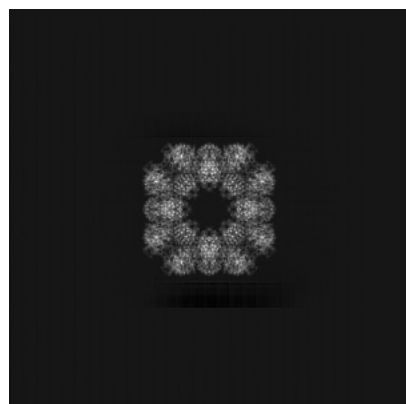
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17062. These allow visual inspection of the internal detail of the map and identification of artifacts.

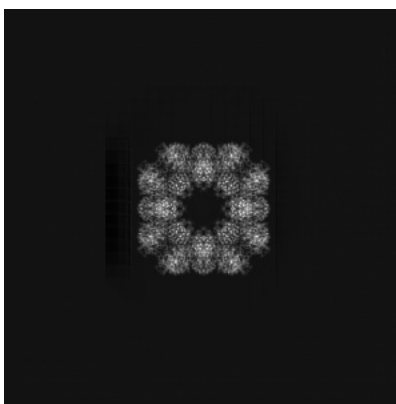
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

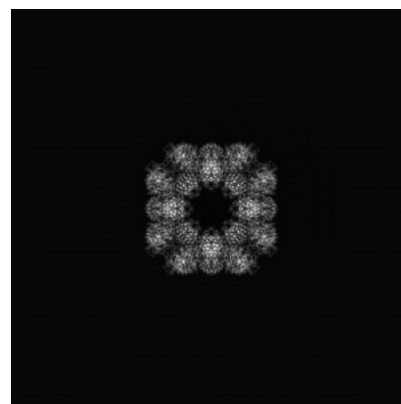
6.1.1 Primary map



X

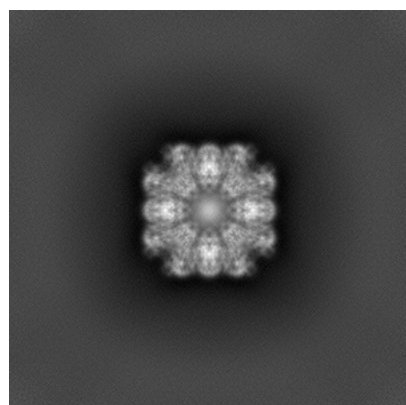


Y

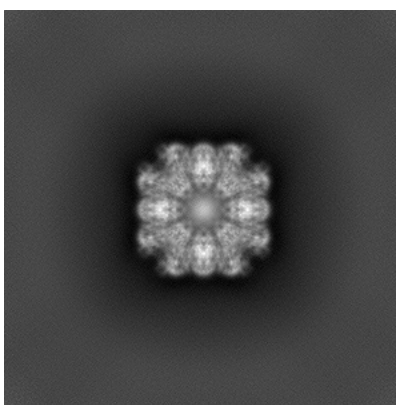


Z

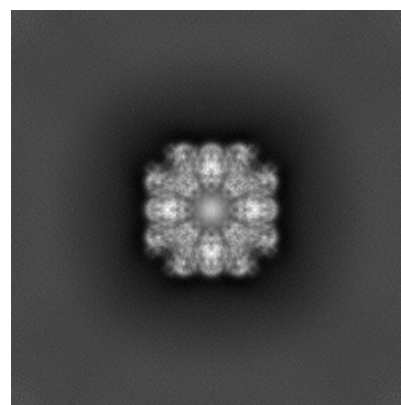
6.1.2 Raw map



X



Y

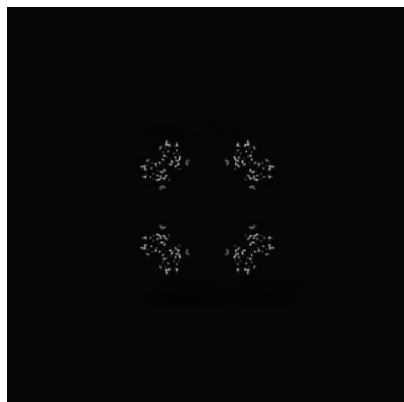


Z

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

6.2 Central slices [i](#)

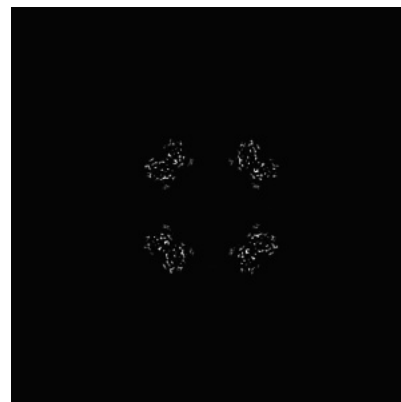
6.2.1 Primary map



X Index: 300

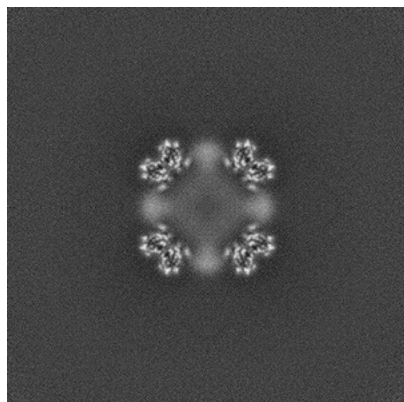


Y Index: 300

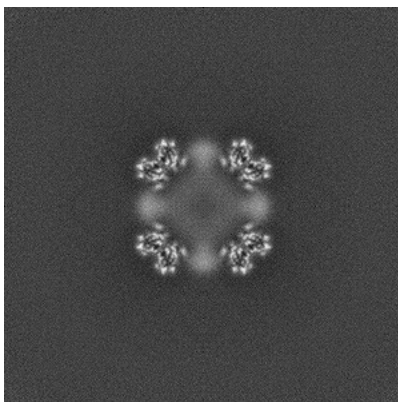


Z Index: 300

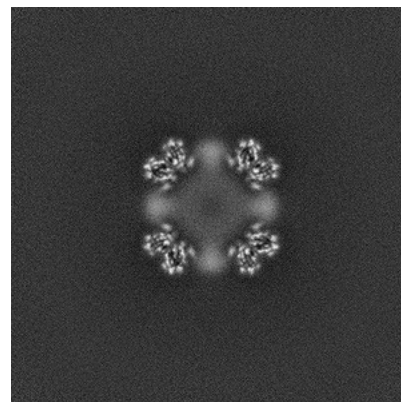
6.2.2 Raw map



X Index: 300



Y Index: 300

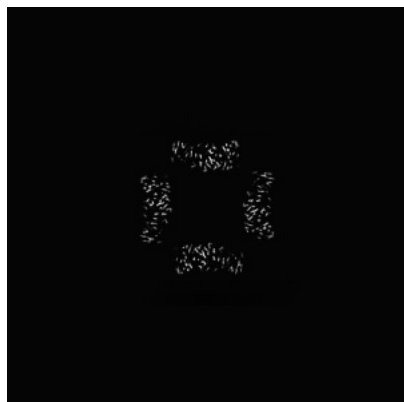


Z Index: 300

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: 344

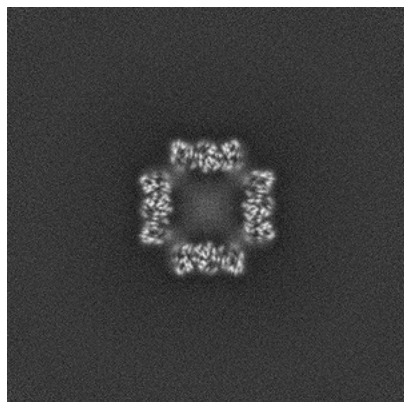


Y Index: 256

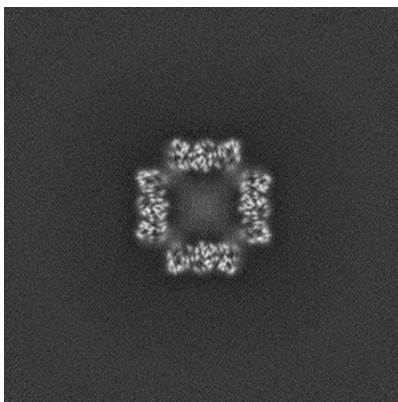


Z Index: 343

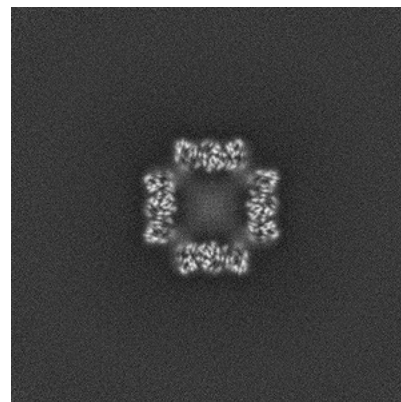
6.3.2 Raw map



X Index: 344



Y Index: 256

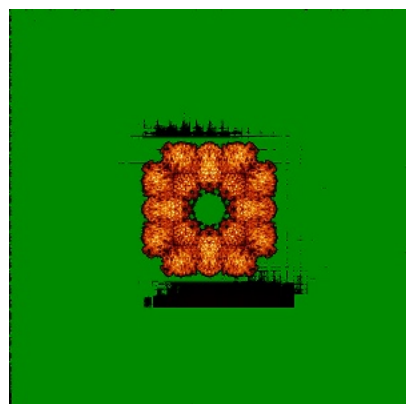


Z Index: 343

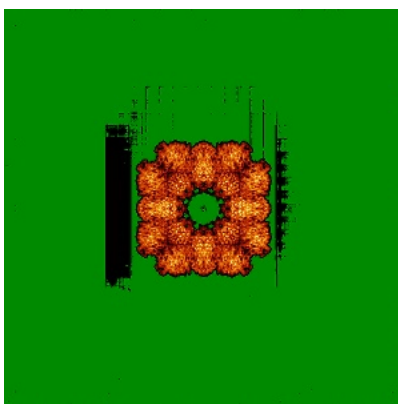
The images above show the largest variance slices of the map in three orthogonal directions.

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

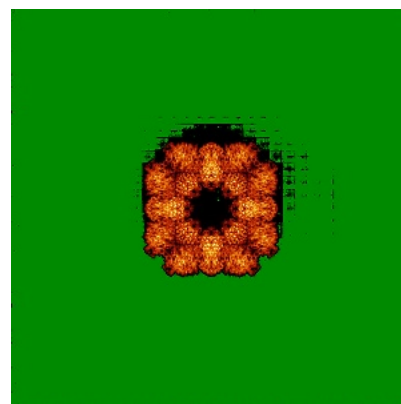
6.4.1 Primary map



X

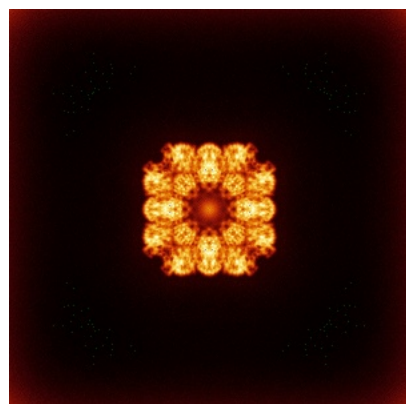


Y

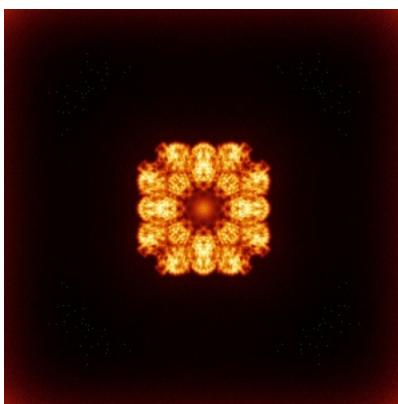


Z

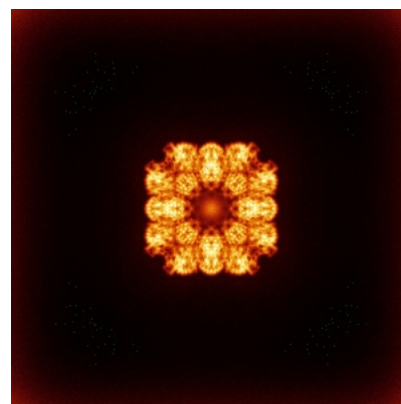
6.4.2 Raw map



X



Y

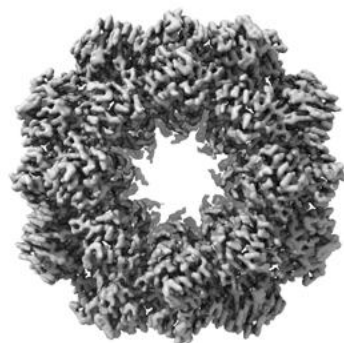


Z

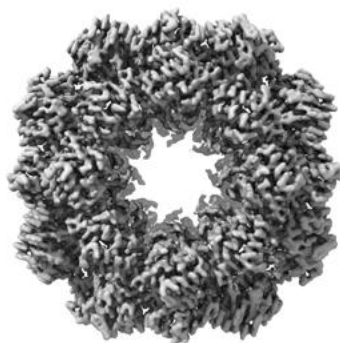
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

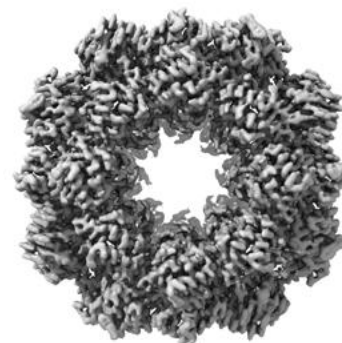
6.5.1 Primary map



X



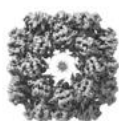
Y



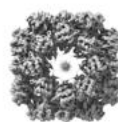
Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. 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



X



Y



Z

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.

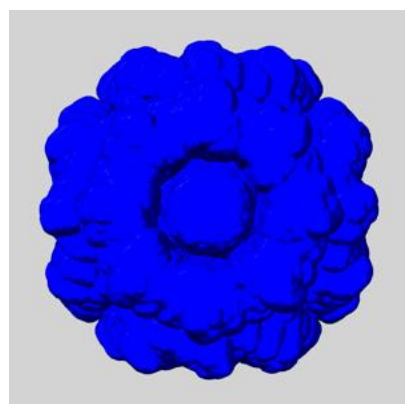
6.6 Mask visualisation [i](#)

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

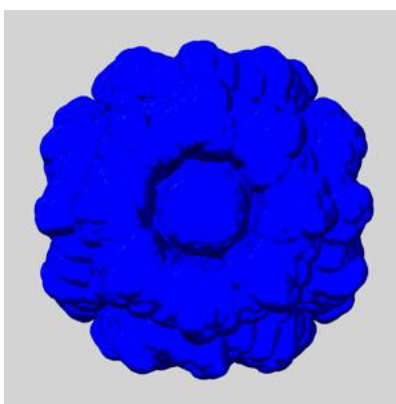
A mask typically either:

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

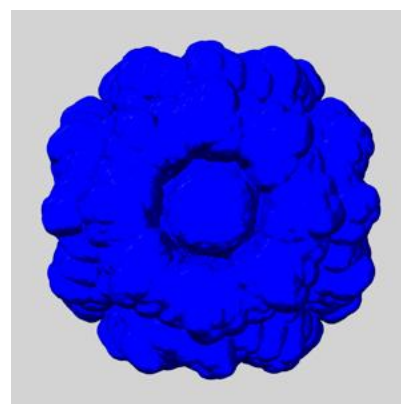
6.6.1 emd_17062_msk_1.map [i](#)



X



Y

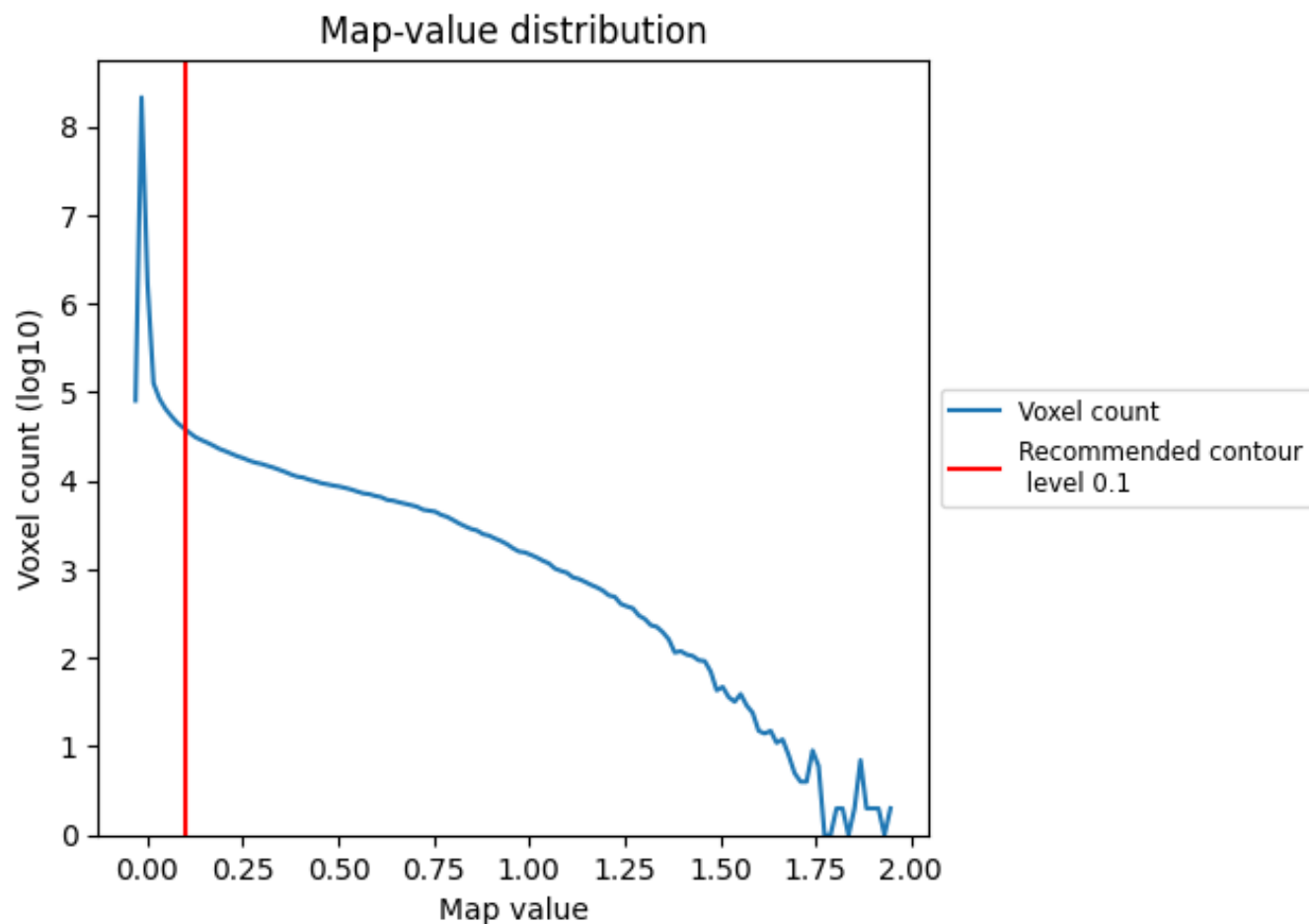


Z

7 Map analysis [i](#)

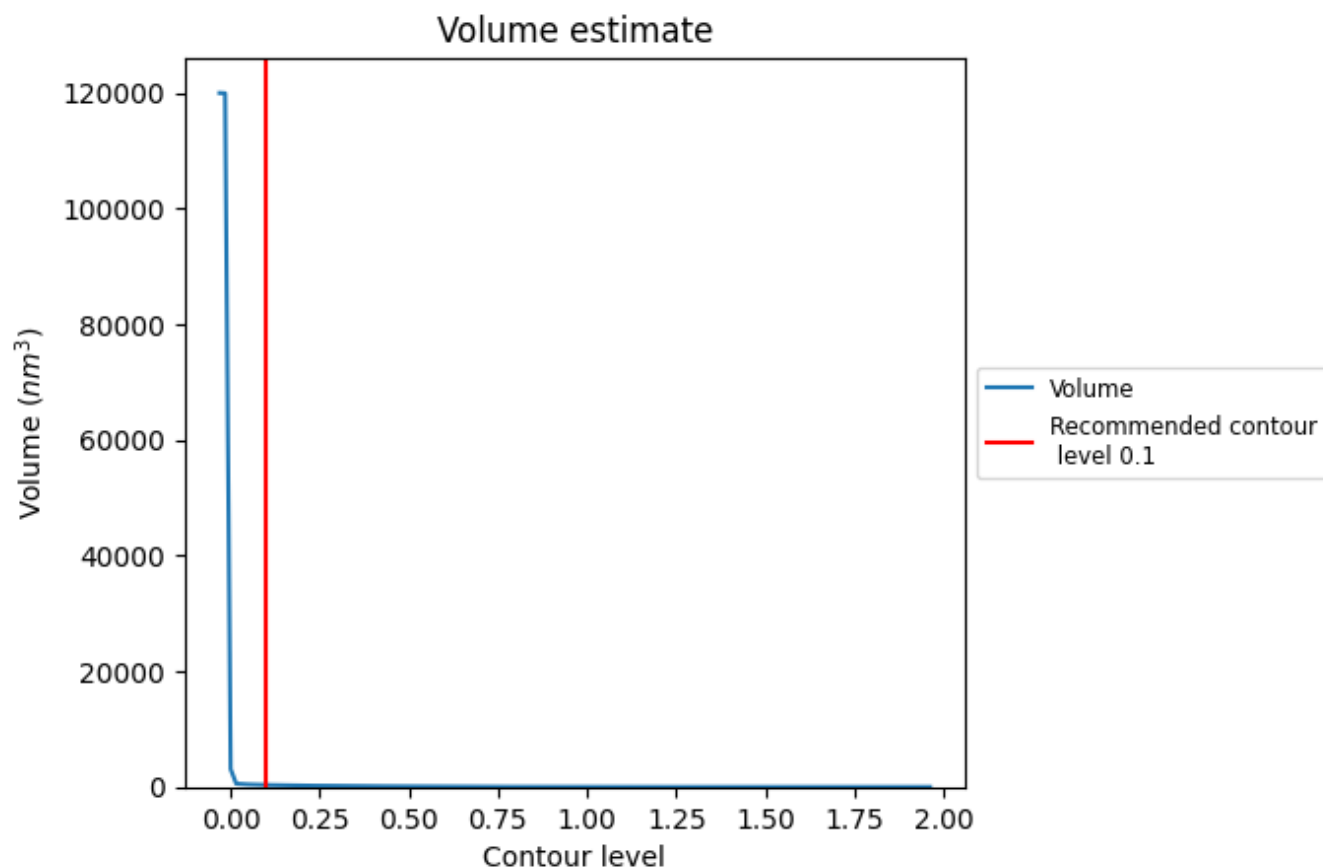
This section contains the results of statistical analysis of the map.

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.

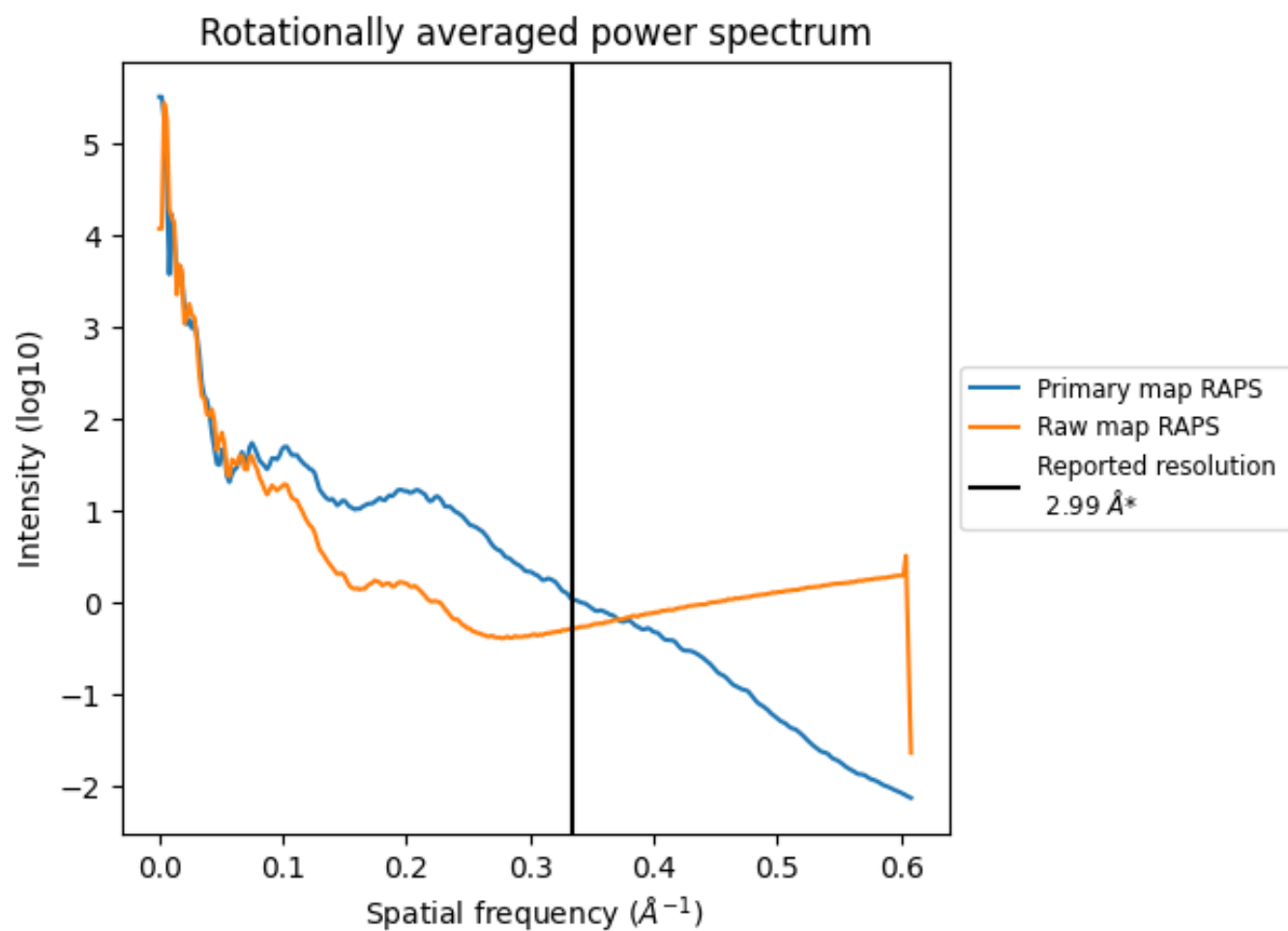
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 346 nm^3 ; this corresponds to an approximate mass of 312 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 ⓘ

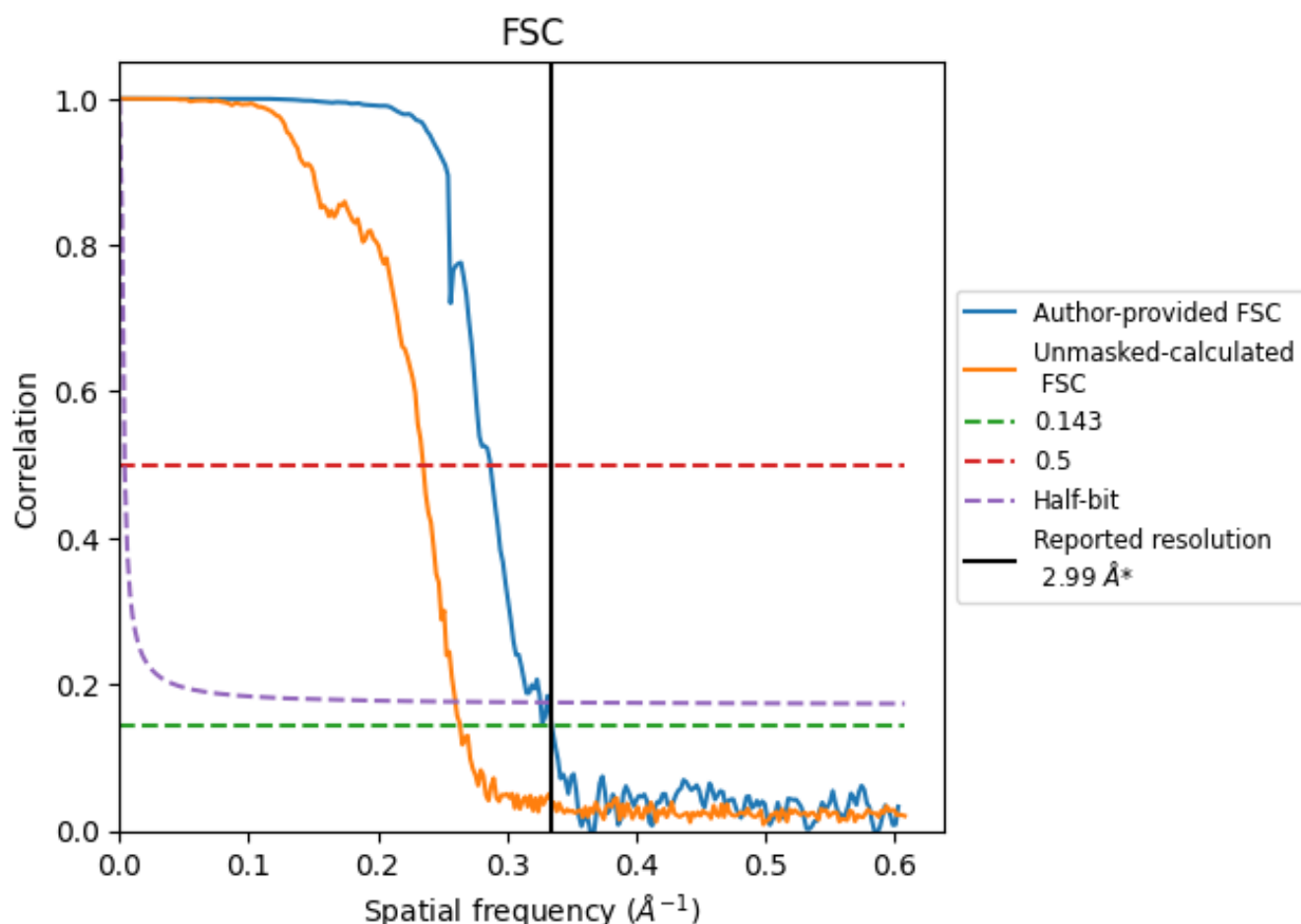


*Reported resolution corresponds to spatial frequency of 0.334 Å⁻¹

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 0.334 \AA^{-1}

8.2 Resolution estimates [i](#)

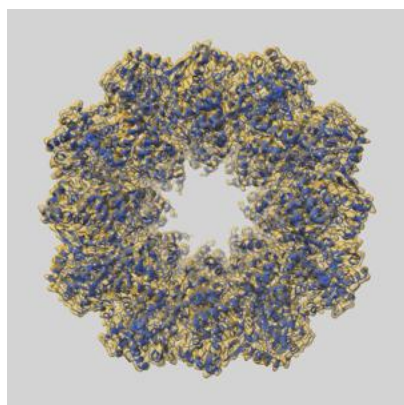
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.99	-	-
Author-provided FSC curve	2.99	3.48	3.07
Unmasked-calculated*	3.79	4.25	3.84

*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 3.79 differs from the reported value 2.99 by more than 10 %

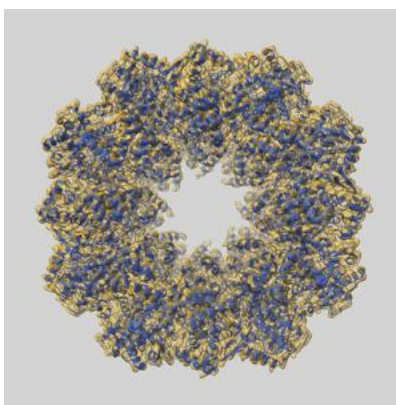
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17062 and PDB model 8OPJ. Per-residue inclusion information can be found in [section 3](#) on [page 25](#).

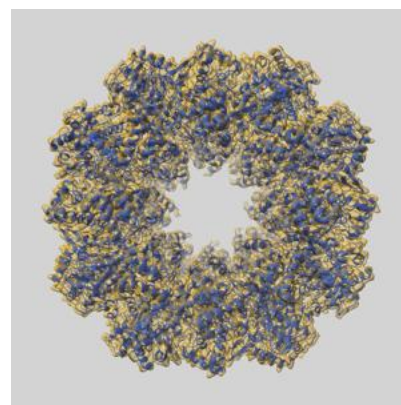
9.1 Map-model overlay [i](#)



X



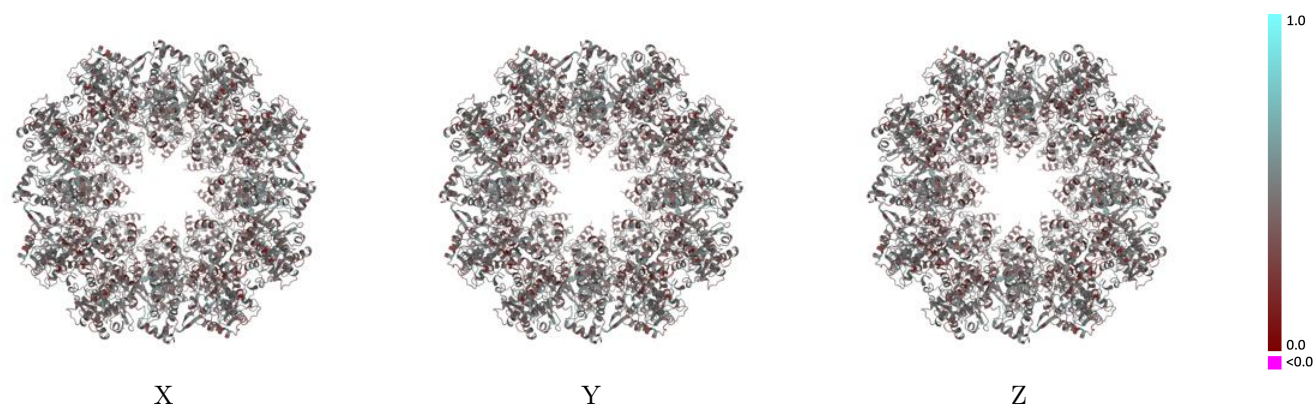
Y



Z

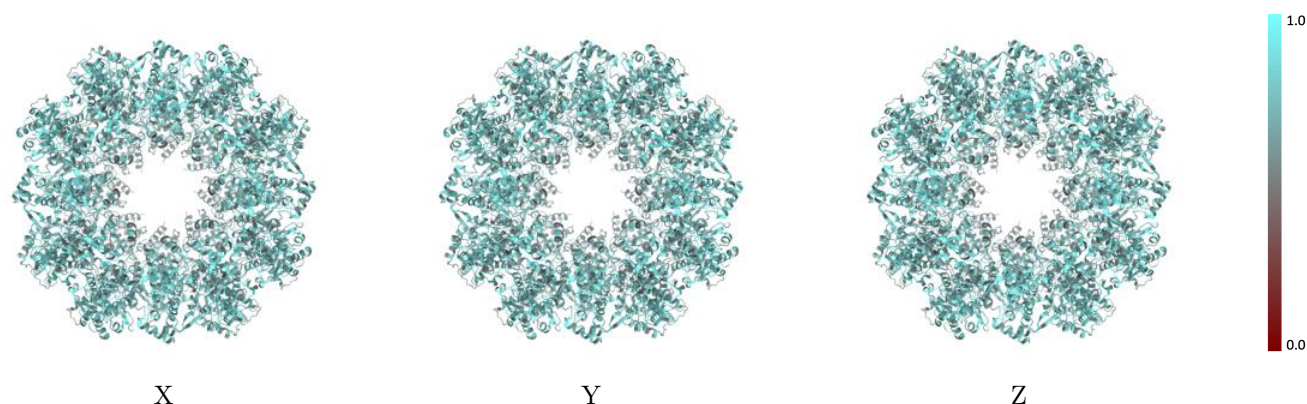
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



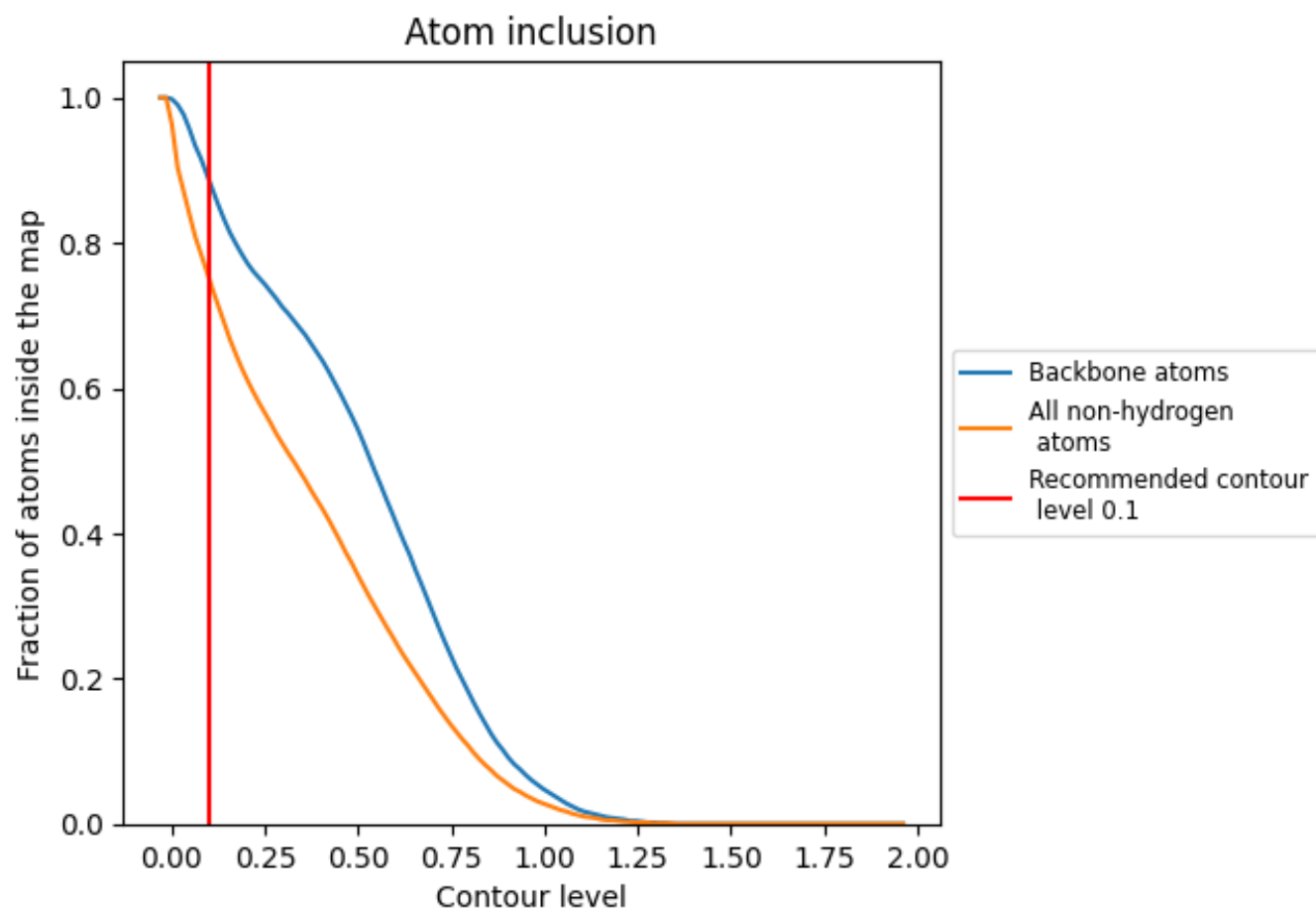
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 89% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7510	 0.4210
Aa	 0.7630	 0.4210
Ab	 0.7620	 0.4240
Ac	 0.7570	 0.4190
Ad	 0.7630	 0.4250
Ae	 0.7630	 0.4220
Af	 0.7540	 0.4180
Ag	 0.7590	 0.4210
Ah	 0.7600	 0.4220
Ai	 0.7510	 0.4230
Aj	 0.7490	 0.4240
Ak	 0.7430	 0.4170
Al	 0.7530	 0.4220
Am	 0.7520	 0.4200
An	 0.7450	 0.4180
Ao	 0.7430	 0.4190
Ap	 0.7430	 0.4200
Aq	 0.7460	 0.4190
Ar	 0.7500	 0.4200
As	 0.7460	 0.4220
At	 0.7530	 0.4250
Au	 0.7470	 0.4190
Av	 0.7510	 0.4220
Aw	 0.7420	 0.4210
Ax	 0.7440	 0.4210
Ay	 0.7540	 0.4210
Az	 0.7500	 0.4270
Ba	 0.7530	 0.4210
Bb	 0.7500	 0.4190
Bc	 0.7520	 0.4210
Bd	 0.7450	 0.4240
Be	 0.7490	 0.4180
Bf	 0.7420	 0.4200
Bg	 0.7540	 0.4260
Bh	 0.7560	 0.4260



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Chain	Atom inclusion	Q-score
Bi	 0.7600	 0.4250
Bj	 0.7570	 0.4200
Bk	 0.7490	 0.4240
Bl	 0.7550	 0.4250
Bm	 0.7540	 0.4230
Bn	 0.7560	 0.4200
Bo	 0.7490	 0.4220
Bp	 0.7430	 0.4180
Bq	 0.7460	 0.4230
Br	 0.7530	 0.4210
Bs	 0.7350	 0.4210
Bt	 0.7470	 0.4190
Bu	 0.7380	 0.4220
Bv	 0.7430	 0.4200