



## Full wwPDB EM Validation Report ⓘ

Jul 29, 2025 – 12:13 PM EDT

PDB ID : 9CXU / pdb\_00009cxu  
EMDB ID : EMD-45998  
Title : Endo H-treated hemagglutinin A/Hong Kong/1/68  
Authors : Torrents de la Pena, A.; de Paiva Froes Rocha, R.; Ward, A.B.  
Deposited on : 2024-07-31  
Resolution : 2.30 Å(reported)  
Based on initial model : 4ZCJ

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev126  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

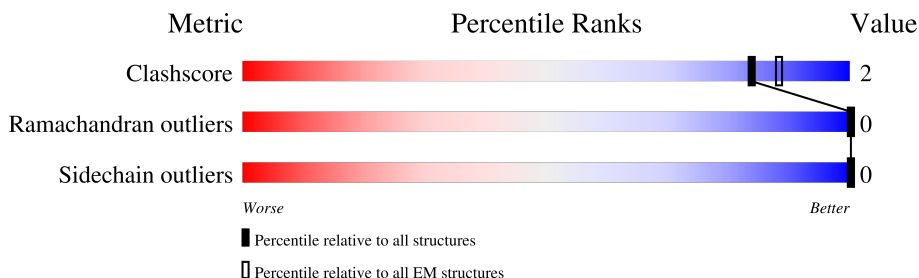
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.30 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	352	
1	C	352	
1	E	352	
2	B	494	
2	D	494	
2	F	494	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11529 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	317	Total	C	N	O	S	0	0
			2445	1532	430	470	13		
1	C	317	Total	C	N	O	S	0	0
			2445	1532	430	470	13		
1	E	317	Total	C	N	O	S	0	0
			2445	1532	430	470	13		

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	UNP Q91MA7
A	-22	PRO	-	expression tag	UNP Q91MA7
A	-21	MET	-	expression tag	UNP Q91MA7
A	-20	GLY	-	expression tag	UNP Q91MA7
A	-19	SER	-	expression tag	UNP Q91MA7
A	-18	LEU	-	expression tag	UNP Q91MA7
A	-17	GLN	-	expression tag	UNP Q91MA7
A	-16	PRO	-	expression tag	UNP Q91MA7
A	-15	LEU	-	expression tag	UNP Q91MA7
A	-14	ALA	-	expression tag	UNP Q91MA7
A	-13	THR	-	expression tag	UNP Q91MA7
A	-12	LEU	-	expression tag	UNP Q91MA7
A	-11	TYR	-	expression tag	UNP Q91MA7
A	-10	LEU	-	expression tag	UNP Q91MA7
A	-9	LEU	-	expression tag	UNP Q91MA7
A	-8	GLY	-	expression tag	UNP Q91MA7
A	-7	MET	-	expression tag	UNP Q91MA7
A	-6	LEU	-	expression tag	UNP Q91MA7
A	-5	VAL	-	expression tag	UNP Q91MA7
A	-4	ALA	-	expression tag	UNP Q91MA7
A	-3	SER	-	expression tag	UNP Q91MA7
A	-2	VAL	-	expression tag	UNP Q91MA7
A	-1	LEU	-	expression tag	UNP Q91MA7
A	0	ALA	-	expression tag	UNP Q91MA7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-23	MET	-	initiating methionine	UNP Q91MA7
C	-22	PRO	-	expression tag	UNP Q91MA7
C	-21	MET	-	expression tag	UNP Q91MA7
C	-20	GLY	-	expression tag	UNP Q91MA7
C	-19	SER	-	expression tag	UNP Q91MA7
C	-18	LEU	-	expression tag	UNP Q91MA7
C	-17	GLN	-	expression tag	UNP Q91MA7
C	-16	PRO	-	expression tag	UNP Q91MA7
C	-15	LEU	-	expression tag	UNP Q91MA7
C	-14	ALA	-	expression tag	UNP Q91MA7
C	-13	THR	-	expression tag	UNP Q91MA7
C	-12	LEU	-	expression tag	UNP Q91MA7
C	-11	TYR	-	expression tag	UNP Q91MA7
C	-10	LEU	-	expression tag	UNP Q91MA7
C	-9	LEU	-	expression tag	UNP Q91MA7
C	-8	GLY	-	expression tag	UNP Q91MA7
C	-7	MET	-	expression tag	UNP Q91MA7
C	-6	LEU	-	expression tag	UNP Q91MA7
C	-5	VAL	-	expression tag	UNP Q91MA7
C	-4	ALA	-	expression tag	UNP Q91MA7
C	-3	SER	-	expression tag	UNP Q91MA7
C	-2	VAL	-	expression tag	UNP Q91MA7
C	-1	LEU	-	expression tag	UNP Q91MA7
C	0	ALA	-	expression tag	UNP Q91MA7
E	-23	MET	-	initiating methionine	UNP Q91MA7
E	-22	PRO	-	expression tag	UNP Q91MA7
E	-21	MET	-	expression tag	UNP Q91MA7
E	-20	GLY	-	expression tag	UNP Q91MA7
E	-19	SER	-	expression tag	UNP Q91MA7
E	-18	LEU	-	expression tag	UNP Q91MA7
E	-17	GLN	-	expression tag	UNP Q91MA7
E	-16	PRO	-	expression tag	UNP Q91MA7
E	-15	LEU	-	expression tag	UNP Q91MA7
E	-14	ALA	-	expression tag	UNP Q91MA7
E	-13	THR	-	expression tag	UNP Q91MA7
E	-12	LEU	-	expression tag	UNP Q91MA7
E	-11	TYR	-	expression tag	UNP Q91MA7
E	-10	LEU	-	expression tag	UNP Q91MA7
E	-9	LEU	-	expression tag	UNP Q91MA7
E	-8	GLY	-	expression tag	UNP Q91MA7
E	-7	MET	-	expression tag	UNP Q91MA7
E	-6	LEU	-	expression tag	UNP Q91MA7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	VAL	-	expression tag	UNP Q91MA7
E	-4	ALA	-	expression tag	UNP Q91MA7
E	-3	SER	-	expression tag	UNP Q91MA7
E	-2	VAL	-	expression tag	UNP Q91MA7
E	-1	LEU	-	expression tag	UNP Q91MA7
E	0	ALA	-	expression tag	UNP Q91MA7

- Molecule 2 is a protein called Hemagglutinin HA2 chain, Green fluorescent protein fusion.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	165	Total	C	N	O	S	0	0
			1342	830	235	271	6		
2	D	165	Total	C	N	O	S	0	0
			1342	830	235	271	6		
2	F	165	Total	C	N	O	S	0	0
			1342	830	235	271	6		

There are 282 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	123	GLY	ARG	conflict	UNP Q91MA7
B	180	LEU	-	linker	UNP Q91MA7
B	181	GLU	-	linker	UNP Q91MA7
B	182	LEU	-	linker	UNP Q91MA7
B	183	ILE	-	linker	UNP Q91MA7
B	184	LYS	-	linker	UNP Q91MA7
B	185	ARG	-	linker	UNP Q91MA7
B	186	MET	-	linker	UNP Q91MA7
B	187	LYS	-	linker	UNP Q91MA7
B	188	GLN	-	linker	UNP Q91MA7
B	189	ILE	-	linker	UNP Q91MA7
B	190	GLU	-	linker	UNP Q91MA7
B	191	ASP	-	linker	UNP Q91MA7
B	192	LYS	-	linker	UNP Q91MA7
B	193	ILE	-	linker	UNP Q91MA7
B	194	GLU	-	linker	UNP Q91MA7
B	195	GLU	-	linker	UNP Q91MA7
B	196	ILE	-	linker	UNP Q91MA7
B	197	GLU	-	linker	UNP Q91MA7
B	198	SER	-	linker	UNP Q91MA7
B	199	LYS	-	linker	UNP Q91MA7
B	200	GLN	-	linker	UNP Q91MA7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	201	LYS	-	linker	UNP Q91MA7
B	202	LYS	-	linker	UNP Q91MA7
B	203	ILE	-	linker	UNP Q91MA7
B	204	GLU	-	linker	UNP Q91MA7
B	205	ASN	-	linker	UNP Q91MA7
B	206	GLU	-	linker	UNP Q91MA7
B	207	ILE	-	linker	UNP Q91MA7
B	208	ALA	-	linker	UNP Q91MA7
B	209	ARG	-	linker	UNP Q91MA7
B	210	ILE	-	linker	UNP Q91MA7
B	211	LYS	-	linker	UNP Q91MA7
B	212	LYS	-	linker	UNP Q91MA7
B	213	ILE	-	linker	UNP Q91MA7
B	214	LYS	-	linker	UNP Q91MA7
B	215	LEU	-	linker	UNP Q91MA7
B	216	VAL	-	linker	UNP Q91MA7
B	217	PRO	-	linker	UNP Q91MA7
B	218	ARG	-	linker	UNP Q91MA7
B	219	GLY	-	linker	UNP Q91MA7
B	220	SER	-	linker	UNP Q91MA7
B	221	VAL	-	linker	UNP Q91MA7
B	222	ASP	-	linker	UNP Q91MA7
B	223	GLU	-	linker	UNP Q91MA7
B	224	ASN	-	linker	UNP Q91MA7
B	225	LEU	-	linker	UNP Q91MA7
B	226	TYR	-	linker	UNP Q91MA7
B	227	PHE	-	linker	UNP Q91MA7
B	228	GLN	-	linker	UNP Q91MA7
B	229	ALA	-	linker	UNP Q91MA7
B	259	ARG	SER	conflict	UNP P42212
B	268	ASN	TYR	conflict	UNP P42212
B	293	LEU	PHE	conflict	UNP P42212
B	294	THR	SER	conflict	UNP P42212
B	309	ARG	GLN	conflict	UNP P42212
B	328	SER	PHE	conflict	UNP P42212
B	334	THR	ASN	conflict	UNP P42212
B	374	PHE	TYR	conflict	UNP P42212
B	382	THR	MET	conflict	UNP P42212
B	392	ALA	VAL	conflict	UNP P42212
B	400	VAL	ILE	conflict	UNP P42212
B	435	VAL	ALA	conflict	UNP P42212
B	463	SER	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
B	464	SER	-	expression tag	UNP P42212
B	465	ALA	-	expression tag	UNP P42212
B	466	TRP	-	expression tag	UNP P42212
B	467	SER	-	expression tag	UNP P42212
B	468	HIS	-	expression tag	UNP P42212
B	469	PRO	-	expression tag	UNP P42212
B	470	GLN	-	expression tag	UNP P42212
B	471	PHE	-	expression tag	UNP P42212
B	472	GLU	-	expression tag	UNP P42212
B	473	LYS	-	expression tag	UNP P42212
B	474	GLY	-	expression tag	UNP P42212
B	475	GLY	-	expression tag	UNP P42212
B	476	GLY	-	expression tag	UNP P42212
B	477	SER	-	expression tag	UNP P42212
B	478	GLY	-	expression tag	UNP P42212
B	479	GLY	-	expression tag	UNP P42212
B	480	GLY	-	expression tag	UNP P42212
B	481	SER	-	expression tag	UNP P42212
B	482	GLY	-	expression tag	UNP P42212
B	483	GLY	-	expression tag	UNP P42212
B	484	SER	-	expression tag	UNP P42212
B	485	ALA	-	expression tag	UNP P42212
B	486	TRP	-	expression tag	UNP P42212
B	487	SER	-	expression tag	UNP P42212
B	488	HIS	-	expression tag	UNP P42212
B	489	PRO	-	expression tag	UNP P42212
B	490	GLN	-	expression tag	UNP P42212
B	491	PHE	-	expression tag	UNP P42212
B	492	GLU	-	expression tag	UNP P42212
B	493	LYS	-	expression tag	UNP P42212
D	123	GLY	ARG	conflict	UNP Q91MA7
D	180	LEU	-	linker	UNP Q91MA7
D	181	GLU	-	linker	UNP Q91MA7
D	182	LEU	-	linker	UNP Q91MA7
D	183	ILE	-	linker	UNP Q91MA7
D	184	LYS	-	linker	UNP Q91MA7
D	185	ARG	-	linker	UNP Q91MA7
D	186	MET	-	linker	UNP Q91MA7
D	187	LYS	-	linker	UNP Q91MA7
D	188	GLN	-	linker	UNP Q91MA7
D	189	ILE	-	linker	UNP Q91MA7
D	190	GLU	-	linker	UNP Q91MA7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	191	ASP	-	linker	UNP Q91MA7
D	192	LYS	-	linker	UNP Q91MA7
D	193	ILE	-	linker	UNP Q91MA7
D	194	GLU	-	linker	UNP Q91MA7
D	195	GLU	-	linker	UNP Q91MA7
D	196	ILE	-	linker	UNP Q91MA7
D	197	GLU	-	linker	UNP Q91MA7
D	198	SER	-	linker	UNP Q91MA7
D	199	LYS	-	linker	UNP Q91MA7
D	200	GLN	-	linker	UNP Q91MA7
D	201	LYS	-	linker	UNP Q91MA7
D	202	LYS	-	linker	UNP Q91MA7
D	203	ILE	-	linker	UNP Q91MA7
D	204	GLU	-	linker	UNP Q91MA7
D	205	ASN	-	linker	UNP Q91MA7
D	206	GLU	-	linker	UNP Q91MA7
D	207	ILE	-	linker	UNP Q91MA7
D	208	ALA	-	linker	UNP Q91MA7
D	209	ARG	-	linker	UNP Q91MA7
D	210	ILE	-	linker	UNP Q91MA7
D	211	LYS	-	linker	UNP Q91MA7
D	212	LYS	-	linker	UNP Q91MA7
D	213	ILE	-	linker	UNP Q91MA7
D	214	LYS	-	linker	UNP Q91MA7
D	215	LEU	-	linker	UNP Q91MA7
D	216	VAL	-	linker	UNP Q91MA7
D	217	PRO	-	linker	UNP Q91MA7
D	218	ARG	-	linker	UNP Q91MA7
D	219	GLY	-	linker	UNP Q91MA7
D	220	SER	-	linker	UNP Q91MA7
D	221	VAL	-	linker	UNP Q91MA7
D	222	ASP	-	linker	UNP Q91MA7
D	223	GLU	-	linker	UNP Q91MA7
D	224	ASN	-	linker	UNP Q91MA7
D	225	LEU	-	linker	UNP Q91MA7
D	226	TYR	-	linker	UNP Q91MA7
D	227	PHE	-	linker	UNP Q91MA7
D	228	GLN	-	linker	UNP Q91MA7
D	229	ALA	-	linker	UNP Q91MA7
D	259	ARG	SER	conflict	UNP P42212
D	268	ASN	TYR	conflict	UNP P42212
D	293	LEU	PHE	conflict	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
D	294	THR	SER	conflict	UNP P42212
D	309	ARG	GLN	conflict	UNP P42212
D	328	SER	PHE	conflict	UNP P42212
D	334	THR	ASN	conflict	UNP P42212
D	374	PHE	TYR	conflict	UNP P42212
D	382	THR	MET	conflict	UNP P42212
D	392	ALA	VAL	conflict	UNP P42212
D	400	VAL	ILE	conflict	UNP P42212
D	435	VAL	ALA	conflict	UNP P42212
D	463	SER	-	expression tag	UNP P42212
D	464	SER	-	expression tag	UNP P42212
D	465	ALA	-	expression tag	UNP P42212
D	466	TRP	-	expression tag	UNP P42212
D	467	SER	-	expression tag	UNP P42212
D	468	HIS	-	expression tag	UNP P42212
D	469	PRO	-	expression tag	UNP P42212
D	470	GLN	-	expression tag	UNP P42212
D	471	PHE	-	expression tag	UNP P42212
D	472	GLU	-	expression tag	UNP P42212
D	473	LYS	-	expression tag	UNP P42212
D	474	GLY	-	expression tag	UNP P42212
D	475	GLY	-	expression tag	UNP P42212
D	476	GLY	-	expression tag	UNP P42212
D	477	SER	-	expression tag	UNP P42212
D	478	GLY	-	expression tag	UNP P42212
D	479	GLY	-	expression tag	UNP P42212
D	480	GLY	-	expression tag	UNP P42212
D	481	SER	-	expression tag	UNP P42212
D	482	GLY	-	expression tag	UNP P42212
D	483	GLY	-	expression tag	UNP P42212
D	484	SER	-	expression tag	UNP P42212
D	485	ALA	-	expression tag	UNP P42212
D	486	TRP	-	expression tag	UNP P42212
D	487	SER	-	expression tag	UNP P42212
D	488	HIS	-	expression tag	UNP P42212
D	489	PRO	-	expression tag	UNP P42212
D	490	GLN	-	expression tag	UNP P42212
D	491	PHE	-	expression tag	UNP P42212
D	492	GLU	-	expression tag	UNP P42212
D	493	LYS	-	expression tag	UNP P42212
F	123	GLY	ARG	conflict	UNP Q91MA7
F	180	LEU	-	linker	UNP Q91MA7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	181	GLU	-	linker	UNP Q91MA7
F	182	LEU	-	linker	UNP Q91MA7
F	183	ILE	-	linker	UNP Q91MA7
F	184	LYS	-	linker	UNP Q91MA7
F	185	ARG	-	linker	UNP Q91MA7
F	186	MET	-	linker	UNP Q91MA7
F	187	LYS	-	linker	UNP Q91MA7
F	188	GLN	-	linker	UNP Q91MA7
F	189	ILE	-	linker	UNP Q91MA7
F	190	GLU	-	linker	UNP Q91MA7
F	191	ASP	-	linker	UNP Q91MA7
F	192	LYS	-	linker	UNP Q91MA7
F	193	ILE	-	linker	UNP Q91MA7
F	194	GLU	-	linker	UNP Q91MA7
F	195	GLU	-	linker	UNP Q91MA7
F	196	ILE	-	linker	UNP Q91MA7
F	197	GLU	-	linker	UNP Q91MA7
F	198	SER	-	linker	UNP Q91MA7
F	199	LYS	-	linker	UNP Q91MA7
F	200	GLN	-	linker	UNP Q91MA7
F	201	LYS	-	linker	UNP Q91MA7
F	202	LYS	-	linker	UNP Q91MA7
F	203	ILE	-	linker	UNP Q91MA7
F	204	GLU	-	linker	UNP Q91MA7
F	205	ASN	-	linker	UNP Q91MA7
F	206	GLU	-	linker	UNP Q91MA7
F	207	ILE	-	linker	UNP Q91MA7
F	208	ALA	-	linker	UNP Q91MA7
F	209	ARG	-	linker	UNP Q91MA7
F	210	ILE	-	linker	UNP Q91MA7
F	211	LYS	-	linker	UNP Q91MA7
F	212	LYS	-	linker	UNP Q91MA7
F	213	ILE	-	linker	UNP Q91MA7
F	214	LYS	-	linker	UNP Q91MA7
F	215	LEU	-	linker	UNP Q91MA7
F	216	VAL	-	linker	UNP Q91MA7
F	217	PRO	-	linker	UNP Q91MA7
F	218	ARG	-	linker	UNP Q91MA7
F	219	GLY	-	linker	UNP Q91MA7
F	220	SER	-	linker	UNP Q91MA7
F	221	VAL	-	linker	UNP Q91MA7
F	222	ASP	-	linker	UNP Q91MA7

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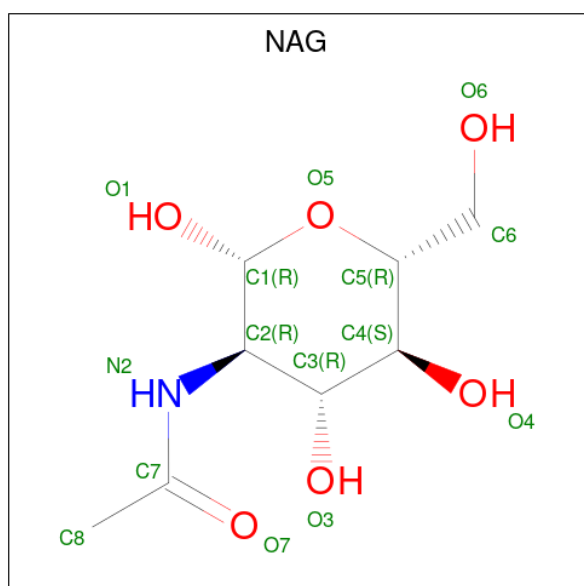
Chain	Residue	Modelled	Actual	Comment	Reference
F	223	GLU	-	linker	UNP Q91MA7
F	224	ASN	-	linker	UNP Q91MA7
F	225	LEU	-	linker	UNP Q91MA7
F	226	TYR	-	linker	UNP Q91MA7
F	227	PHE	-	linker	UNP Q91MA7
F	228	GLN	-	linker	UNP Q91MA7
F	229	ALA	-	linker	UNP Q91MA7
F	259	ARG	SER	conflict	UNP P42212
F	268	ASN	TYR	conflict	UNP P42212
F	293	LEU	PHE	conflict	UNP P42212
F	294	THR	SER	conflict	UNP P42212
F	309	ARG	GLN	conflict	UNP P42212
F	328	SER	PHE	conflict	UNP P42212
F	334	THR	ASN	conflict	UNP P42212
F	374	PHE	TYR	conflict	UNP P42212
F	382	THR	MET	conflict	UNP P42212
F	392	ALA	VAL	conflict	UNP P42212
F	400	VAL	ILE	conflict	UNP P42212
F	435	VAL	ALA	conflict	UNP P42212
F	463	SER	-	expression tag	UNP P42212
F	464	SER	-	expression tag	UNP P42212
F	465	ALA	-	expression tag	UNP P42212
F	466	TRP	-	expression tag	UNP P42212
F	467	SER	-	expression tag	UNP P42212
F	468	HIS	-	expression tag	UNP P42212
F	469	PRO	-	expression tag	UNP P42212
F	470	GLN	-	expression tag	UNP P42212
F	471	PHE	-	expression tag	UNP P42212
F	472	GLU	-	expression tag	UNP P42212
F	473	LYS	-	expression tag	UNP P42212
F	474	GLY	-	expression tag	UNP P42212
F	475	GLY	-	expression tag	UNP P42212
F	476	GLY	-	expression tag	UNP P42212
F	477	SER	-	expression tag	UNP P42212
F	478	GLY	-	expression tag	UNP P42212
F	479	GLY	-	expression tag	UNP P42212
F	480	GLY	-	expression tag	UNP P42212
F	481	SER	-	expression tag	UNP P42212
F	482	GLY	-	expression tag	UNP P42212
F	483	GLY	-	expression tag	UNP P42212
F	484	SER	-	expression tag	UNP P42212
F	485	ALA	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
F	486	TRP	-	expression tag	UNP P42212
F	487	SER	-	expression tag	UNP P42212
F	488	HIS	-	expression tag	UNP P42212
F	489	PRO	-	expression tag	UNP P42212
F	490	GLN	-	expression tag	UNP P42212
F	491	PHE	-	expression tag	UNP P42212
F	492	GLU	-	expression tag	UNP P42212
F	493	LYS	-	expression tag	UNP P42212

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	
3	F	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	

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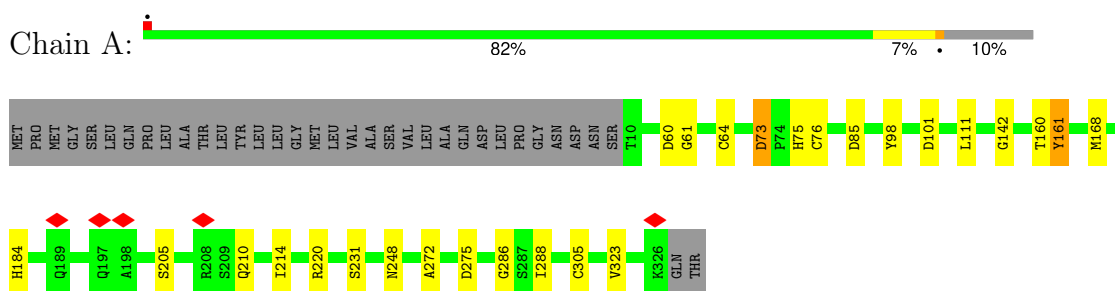
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Mol	Chain	Residues	Atoms				AltConf
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	E	1	Total	C	N	O	0
			14	8	1	5	
3	E	1	Total	C	N	O	0
			14	8	1	5	
3	E	1	Total	C	N	O	0
			14	8	1	5	

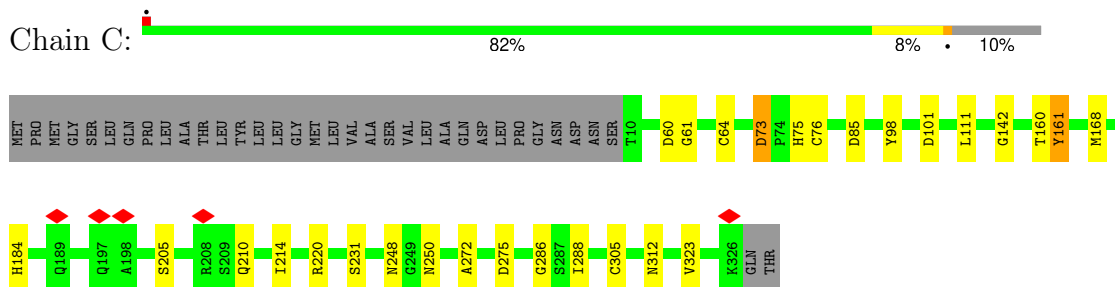
### 3 Residue-property plots [i](#)

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.

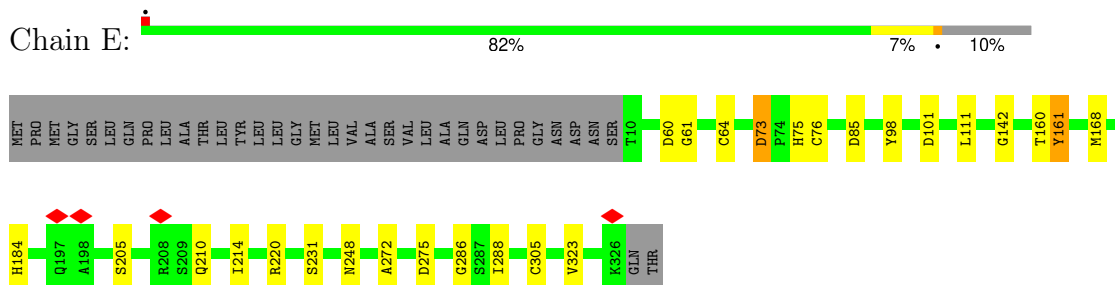
- Molecule 1: Hemagglutinin HA1 chain



- Molecule 1: Hemagglutinin HA1 chain



- Molecule 1: Hemagglutinin HA1 chain



- Molecule 2: Hemagglutinin HA2 chain, Green fluorescent protein fusion





VAL	ASP
TYR	PRO
ILE	ASN
THR	GLU
ALA	LYS
ASP	ARG
LYS	ASP
GLN	HIS
LYS	MET
ASN	VAL
GLY	LEU
ILE	LEU
LYS	GLI
ALA	PHE
ASN	VAL
PHE	THR
LYS	ALA
ILE	ALA
ARG	GLY
HIS	ILE
ASN	THR
VAL	HIS
GLU	GLY
ASP	MET
GLY	SER
SER	SER
VAL	ALA
GLN	TRP
LEU	SER
ALA	HIS
ASP	PRO
HIS	GLN
TYR	PHE
GLN	GLU
GLN	LYS
ASN	GLY
THR	GLY
PRO	GLY
ILE	SER
GLY	GLY
ASP	GLY
GLY	GLY
PRO	SER
VAL	GLY
LEU	GLY
LEU	SER
PRO	ALA
ASP	TRP
ASN	SER
HIS	SER
TYR	HIS
LEU	PRO
SER	GLN
THR	PHE
GLN	GLU
SER	LYS
VAL	
LEU	
SER	
SER	
LYS	



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	332294	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.580	Depositor
Minimum map value	-2.006	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	368.0, 368.0, 368.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	Depositor

## 5 Model quality [i](#)

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

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.05	0/2501	1.31	29/3407 (0.9%)
1	C	1.05	1/2501 (0.0%)	1.31	29/3407 (0.9%)
1	E	1.05	0/2501	1.31	29/3407 (0.9%)
2	B	1.17	0/1365	1.13	9/1835 (0.5%)
2	D	1.17	0/1365	1.13	9/1835 (0.5%)
2	F	1.17	0/1365	1.13	9/1835 (0.5%)
All	All	1.09	1/11598 (0.0%)	1.25	114/15726 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	250	ASN	CB-CG	-5.01	1.39	1.52

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	10	ILE	N-CA-C	-10.51	103.39	111.90
2	F	10	ILE	N-CA-C	-10.44	103.45	111.90
2	D	10	ILE	N-CA-C	-10.40	103.47	111.90
1	A	214	ILE	CA-C-N	8.16	128.18	119.78
1	A	214	ILE	C-N-CA	8.16	128.18	119.78
1	C	214	ILE	CA-C-N	8.12	128.15	119.78
1	C	214	ILE	C-N-CA	8.12	128.15	119.78
1	E	214	ILE	CA-C-N	8.09	128.11	119.78
1	E	214	ILE	C-N-CA	8.09	128.11	119.78
1	E	305	CYS	CA-C-N	7.34	127.78	119.92
1	E	305	CYS	C-N-CA	7.34	127.78	119.92
1	A	305	CYS	CA-C-N	7.34	127.77	119.92
1	A	305	CYS	C-N-CA	7.34	127.77	119.92
1	C	305	CYS	CA-C-N	7.33	127.76	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	305	CYS	C-N-CA	7.33	127.76	119.92
1	A	85	ASP	N-CA-C	-7.32	104.48	113.41
1	E	85	ASP	N-CA-C	-7.32	104.49	113.41
1	C	184	HIS	CA-C-N	7.07	127.06	119.78
1	C	184	HIS	C-N-CA	7.07	127.06	119.78
1	A	184	HIS	CA-C-N	7.05	127.04	119.78
1	A	184	HIS	C-N-CA	7.05	127.04	119.78
1	E	184	HIS	CA-C-N	7.04	127.03	119.78
1	E	184	HIS	C-N-CA	7.04	127.03	119.78
1	C	85	ASP	N-CA-C	-6.89	104.50	113.12
2	D	76	ARG	N-CA-C	6.84	118.73	111.28
2	F	76	ARG	N-CA-C	6.77	118.66	111.28
2	B	76	ARG	N-CA-C	6.73	118.61	111.28
2	B	127	ARG	CB-CA-C	-6.68	108.15	117.23
1	E	60	ASP	CA-CB-CG	6.68	119.28	112.60
1	A	60	ASP	CA-CB-CG	6.65	119.25	112.60
2	F	127	ARG	CB-CA-C	-6.64	108.19	117.23
1	C	60	ASP	CA-CB-CG	6.64	119.24	112.60
2	D	127	ARG	CB-CA-C	-6.62	108.23	117.23
1	A	323	VAL	CA-C-N	6.49	126.46	119.78
1	A	323	VAL	C-N-CA	6.49	126.46	119.78
1	E	323	VAL	CA-C-N	6.48	126.45	119.78
1	E	323	VAL	C-N-CA	6.48	126.45	119.78
1	C	323	VAL	CA-C-N	6.48	126.45	119.78
1	C	323	VAL	C-N-CA	6.48	126.45	119.78
1	C	168	MET	CA-C-N	6.44	126.35	119.85
1	C	168	MET	C-N-CA	6.44	126.35	119.85
1	E	168	MET	CA-C-N	6.43	126.34	119.85
1	E	168	MET	C-N-CA	6.43	126.34	119.85
1	A	168	MET	CA-C-N	6.41	126.32	119.85
1	A	168	MET	C-N-CA	6.41	126.32	119.85
1	E	161	TYR	CA-C-N	6.25	126.44	120.31
1	E	161	TYR	C-N-CA	6.25	126.44	120.31
1	A	161	TYR	CA-C-N	6.17	126.35	120.31
1	A	161	TYR	C-N-CA	6.17	126.35	120.31
1	C	161	TYR	CA-C-N	6.15	126.34	120.31
1	C	161	TYR	C-N-CA	6.15	126.34	120.31
1	C	288	ILE	CA-C-N	6.14	126.11	119.78
1	C	288	ILE	C-N-CA	6.14	126.11	119.78
1	A	288	ILE	CA-C-N	6.12	126.08	119.78
1	A	288	ILE	C-N-CA	6.12	126.08	119.78
1	E	288	ILE	CA-C-N	6.10	126.06	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	288	ILE	C-N-CA	6.10	126.06	119.78
2	F	125	GLN	N-CA-C	-6.03	104.07	112.45
2	B	125	GLN	N-CA-C	-6.03	104.08	112.45
2	D	125	GLN	N-CA-C	-6.00	104.11	112.45
1	A	272	ALA	CA-C-N	5.96	125.93	120.03
1	A	272	ALA	C-N-CA	5.96	125.93	120.03
1	E	272	ALA	CA-C-N	5.94	125.91	120.03
1	E	272	ALA	C-N-CA	5.94	125.91	120.03
1	A	73	ASP	CA-C-N	5.93	126.35	119.47
1	A	73	ASP	C-N-CA	5.93	126.35	119.47
1	E	73	ASP	CA-C-N	5.91	126.32	119.47
1	E	73	ASP	C-N-CA	5.91	126.32	119.47
1	C	272	ALA	CA-C-N	5.88	125.86	120.03
1	C	272	ALA	C-N-CA	5.88	125.86	120.03
1	C	73	ASP	CA-C-N	5.88	126.29	119.47
1	C	73	ASP	C-N-CA	5.88	126.29	119.47
2	F	90	ASP	CA-CB-CG	5.71	118.31	112.60
2	B	90	ASP	CA-CB-CG	5.71	118.31	112.60
2	D	90	ASP	CA-CB-CG	5.65	118.25	112.60
2	D	76	ARG	CB-CA-C	-5.62	101.46	110.79
1	C	98	TYR	CA-C-N	5.61	125.62	119.90
1	C	98	TYR	C-N-CA	5.61	125.62	119.90
1	E	98	TYR	CA-C-N	5.60	125.61	119.90
1	E	98	TYR	C-N-CA	5.60	125.61	119.90
2	B	76	ARG	CB-CA-C	-5.59	101.51	110.79
1	A	98	TYR	CA-C-N	5.57	125.58	119.90
1	A	98	TYR	C-N-CA	5.57	125.58	119.90
2	F	76	ARG	CB-CA-C	-5.57	101.55	110.79
1	E	61	GLY	N-CA-C	-5.50	100.16	113.18
1	A	61	GLY	N-CA-C	-5.49	100.17	113.18
1	C	61	GLY	N-CA-C	-5.48	100.19	113.18
1	C	111	LEU	CB-CA-C	-5.44	101.75	110.79
1	A	111	LEU	CB-CA-C	-5.44	101.76	110.79
1	E	111	LEU	CB-CA-C	-5.43	101.77	110.79
1	C	286	GLY	CA-C-O	-5.21	118.70	122.45
1	C	275	ASP	N-CA-C	5.17	116.53	109.18
1	E	275	ASP	N-CA-C	5.16	116.50	109.18
1	A	275	ASP	N-CA-C	5.15	116.49	109.18
2	F	9	PHE	CA-CB-CG	5.11	118.91	113.80
1	E	205	SER	N-CA-C	5.10	116.94	109.24
1	C	142	GLY	CA-C-N	5.10	124.71	119.56
1	C	142	GLY	C-N-CA	5.10	124.71	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	GLY	CA-C-N	5.09	124.70	119.56
1	A	142	GLY	C-N-CA	5.09	124.70	119.56
1	C	205	SER	N-CA-C	5.08	116.91	109.24
1	A	205	SER	N-CA-C	5.08	116.91	109.24
2	D	9	PHE	CA-CB-CG	5.07	118.87	113.80
1	A	286	GLY	CA-C-O	-5.07	118.80	122.45
2	F	147	ALA	CA-C-N	5.04	126.99	120.44
2	F	147	ALA	C-N-CA	5.04	126.99	120.44
1	E	286	GLY	CA-C-O	-5.03	118.83	122.45
1	E	142	GLY	CA-C-N	5.02	124.63	119.56
1	E	142	GLY	C-N-CA	5.02	124.63	119.56
2	B	9	PHE	CA-CB-CG	5.02	118.82	113.80
2	D	147	ALA	CA-C-N	5.01	126.96	120.44
2	D	147	ALA	C-N-CA	5.01	126.96	120.44
2	B	147	ALA	CA-C-N	5.00	126.94	120.44
2	B	147	ALA	C-N-CA	5.00	126.94	120.44

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	A	2445	0	2395	24	0
1	C	2445	0	2395	25	0
1	E	2445	0	2395	24	0
2	B	1342	0	1254	0	0
2	D	1342	0	1254	0	0
2	F	1342	0	1254	0	0
3	A	42	0	39	0	0
3	B	14	0	13	0	0
3	C	42	0	39	0	0
3	D	14	0	13	0	0
3	E	42	0	39	0	0
3	F	14	0	13	0	0
All	All	11529	0	11103	49	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 2.

All (49) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ARG:NE	1:C:210:GLN:OE1	1.80	1.15
1:C:220:ARG:NE	1:E:210:GLN:OE1	1.80	1.14
1:A:210:GLN:OE1	1:E:220:ARG:NE	1.80	1.13
1:C:73:ASP:OD1	1:C:75:HIS:ND1	1.85	1.10
1:E:73:ASP:OD1	1:E:75:HIS:ND1	1.85	1.10
1:A:73:ASP:OD1	1:A:75:HIS:ND1	1.85	1.09
1:E:73:ASP:CG	1:E:75:HIS:CE1	2.65	0.74
1:A:73:ASP:CG	1:A:75:HIS:CE1	2.65	0.74
1:C:73:ASP:CG	1:C:75:HIS:CE1	2.65	0.74
1:E:73:ASP:OD1	1:E:75:HIS:CE1	2.44	0.71
1:A:73:ASP:OD1	1:A:75:HIS:CE1	2.44	0.70
1:C:73:ASP:OD1	1:C:75:HIS:CE1	2.44	0.70
1:C:220:ARG:HH21	1:E:210:GLN:CD	2.02	0.68
1:A:220:ARG:CZ	1:C:210:GLN:OE1	2.43	0.67
1:A:210:GLN:CD	1:E:220:ARG:HH21	2.02	0.66
1:A:220:ARG:HH21	1:C:210:GLN:CD	2.02	0.66
1:C:220:ARG:CZ	1:E:210:GLN:OE1	2.43	0.66
1:A:210:GLN:OE1	1:E:220:ARG:CZ	2.43	0.66
1:A:210:GLN:NE2	1:E:220:ARG:HH21	1.96	0.64
1:C:220:ARG:HH21	1:E:210:GLN:NE2	1.96	0.64
1:A:220:ARG:HH21	1:C:210:GLN:NE2	1.96	0.63
1:A:210:GLN:NE2	1:E:220:ARG:NH2	2.47	0.62
1:A:220:ARG:NH2	1:C:210:GLN:NE2	2.47	0.62
1:C:220:ARG:NH2	1:E:210:GLN:NE2	2.47	0.62
1:A:101:ASP:OD1	1:A:231:SER:HA	2.01	0.61
1:C:64:CYS:SG	1:C:75:HIS:CD2	2.94	0.61
1:E:64:CYS:SG	1:E:75:HIS:CD2	2.94	0.61
1:A:64:CYS:SG	1:A:75:HIS:CD2	2.94	0.61
1:E:101:ASP:OD1	1:E:231:SER:HA	2.01	0.60
1:C:101:ASP:OD1	1:C:231:SER:HA	2.01	0.60
1:C:220:ARG:NH2	1:E:210:GLN:HE22	2.03	0.56
1:A:220:ARG:NH2	1:C:210:GLN:HE22	2.03	0.56
1:A:210:GLN:HE22	1:E:220:ARG:NH2	2.03	0.56
1:A:220:ARG:NH2	1:C:210:GLN:CD	2.69	0.50
1:C:220:ARG:NH2	1:E:210:GLN:CD	2.69	0.49
1:A:210:GLN:CD	1:E:220:ARG:NH2	2.69	0.48
1:A:220:ARG:NH2	1:C:210:GLN:OE1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:ARG:NH2	1:E:210:GLN:OE1	2.49	0.46
1:A:160:THR:OG1	1:A:161:TYR:N	2.49	0.45
1:A:210:GLN:OE1	1:E:220:ARG:NH2	2.49	0.45
1:E:160:THR:OG1	1:E:161:TYR:N	2.50	0.44
1:C:160:THR:OG1	1:C:161:TYR:N	2.50	0.43
1:C:75:HIS:CD2	1:C:76:CYS:SG	3.12	0.43
1:A:75:HIS:CD2	1:A:76:CYS:SG	3.12	0.42
1:E:75:HIS:CD2	1:E:76:CYS:SG	3.12	0.42
1:C:248:ASN:OD1	1:C:248:ASN:N	2.51	0.42
1:E:248:ASN:N	1:E:248:ASN:OD1	2.51	0.42
1:A:248:ASN:OD1	1:A:248:ASN:N	2.51	0.41
1:C:312:ASN:OD1	1:C:312:ASN:N	2.54	0.41

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	A	315/352 (90%)	312 (99%)	3 (1%)	0	100	100
1	C	315/352 (90%)	312 (99%)	3 (1%)	0	100	100
1	E	315/352 (90%)	312 (99%)	3 (1%)	0	100	100
2	B	163/494 (33%)	161 (99%)	2 (1%)	0	100	100
2	D	163/494 (33%)	161 (99%)	2 (1%)	0	100	100
2	F	163/494 (33%)	161 (99%)	2 (1%)	0	100	100
All	All	1434/2538 (56%)	1419 (99%)	15 (1%)	0	100	100

There are no Ramachandran outliers to report.

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	278/308 (90%)	278 (100%)	0	100	100
1	C	278/308 (90%)	278 (100%)	0	100	100
1	E	278/308 (90%)	278 (100%)	0	100	100
2	B	142/424 (34%)	142 (100%)	0	100	100
2	D	142/424 (34%)	142 (100%)	0	100	100
2	F	142/424 (34%)	142 (100%)	0	100	100
All	All	1260/2196 (57%)	1260 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	246	ASN
1	C	188	ASN
1	C	246	ASN
1	E	246	ASN
1	E	296	ASN

### 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

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	NAG	E	403	1	14,14,15	0.31	0	17,19,21	0.99	1 (5%)
3	NAG	C	401	1	14,14,15	2.11	6 (42%)	17,19,21	1.12	2 (11%)
3	NAG	F	501	2	14,14,15	2.11	5 (35%)	17,19,21	1.02	1 (5%)
3	NAG	A	403	1	14,14,15	0.31	0	17,19,21	0.99	1 (5%)
3	NAG	C	403	1	14,14,15	0.33	0	17,19,21	0.99	1 (5%)
3	NAG	A	402	1	14,14,15	0.35	0	17,19,21	0.81	0
3	NAG	B	501	2	14,14,15	2.11	5 (35%)	17,19,21	1.03	1 (5%)
3	NAG	E	402	1	14,14,15	0.36	0	17,19,21	0.81	0
3	NAG	D	501	2	14,14,15	2.11	5 (35%)	17,19,21	1.02	1 (5%)
3	NAG	E	401	1	14,14,15	2.13	6 (42%)	17,19,21	1.11	2 (11%)
3	NAG	A	401	1	14,14,15	2.13	6 (42%)	17,19,21	1.11	2 (11%)
3	NAG	C	402	1	14,14,15	0.33	0	17,19,21	0.82	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	403	1	-	5/6/23/26	0/1/1/1
3	NAG	C	401	1	-	1/6/23/26	0/1/1/1
3	NAG	F	501	2	-	0/6/23/26	0/1/1/1
3	NAG	A	403	1	-	5/6/23/26	0/1/1/1
3	NAG	C	403	1	-	5/6/23/26	0/1/1/1
3	NAG	A	402	1	-	5/6/23/26	0/1/1/1
3	NAG	B	501	2	-	0/6/23/26	0/1/1/1
3	NAG	E	402	1	-	5/6/23/26	0/1/1/1
3	NAG	D	501	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	401	1	-	1/6/23/26	0/1/1/1
3	NAG	A	401	1	-	1/6/23/26	0/1/1/1
3	NAG	C	402	1	-	5/6/23/26	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	501	NAG	C1-C2	5.73	1.60	1.52
3	A	401	NAG	C1-C2	5.72	1.60	1.52
3	E	401	NAG	C1-C2	5.71	1.60	1.52
3	B	501	NAG	C1-C2	5.69	1.60	1.52
3	D	501	NAG	C1-C2	5.66	1.60	1.52
3	C	401	NAG	C1-C2	5.59	1.60	1.52
3	D	501	NAG	O5-C5	3.04	1.49	1.43
3	F	501	NAG	O5-C5	2.99	1.49	1.43
3	B	501	NAG	O5-C5	2.95	1.49	1.43
3	E	401	NAG	O5-C5	2.88	1.49	1.43
3	A	401	NAG	O5-C5	2.86	1.49	1.43
3	C	401	NAG	O5-C5	2.80	1.48	1.43
3	B	501	NAG	O5-C1	2.33	1.47	1.43
3	C	401	NAG	O5-C1	2.28	1.47	1.43
3	D	501	NAG	O5-C1	2.28	1.47	1.43
3	E	401	NAG	O5-C1	2.25	1.47	1.43
3	F	501	NAG	O5-C1	2.24	1.47	1.43
3	D	501	NAG	C3-C2	2.24	1.57	1.52
3	B	501	NAG	C3-C2	2.23	1.57	1.52
3	C	401	NAG	C4-C5	2.23	1.57	1.53
3	A	401	NAG	C4-C5	2.19	1.57	1.53
3	F	501	NAG	C3-C2	2.19	1.57	1.52
3	B	501	NAG	C4-C5	2.18	1.57	1.53
3	F	501	NAG	C4-C5	2.18	1.57	1.53
3	A	401	NAG	O5-C1	2.17	1.47	1.43
3	E	401	NAG	C4-C5	2.16	1.57	1.53
3	A	401	NAG	C2-N2	2.15	1.49	1.46
3	C	401	NAG	C2-N2	2.14	1.49	1.46
3	D	501	NAG	C4-C5	2.13	1.57	1.53
3	E	401	NAG	C2-N2	2.10	1.49	1.46
3	E	401	NAG	C3-C2	2.10	1.56	1.52
3	A	401	NAG	C3-C2	2.07	1.56	1.52
3	C	401	NAG	C3-C2	2.07	1.56	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	NAG	C2-N2-C7	2.82	126.68	122.90
3	C	403	NAG	C2-N2-C7	2.81	126.67	122.90
3	E	403	NAG	C2-N2-C7	2.78	126.63	122.90
3	C	401	NAG	C8-C7-N2	2.77	120.71	116.12
3	E	401	NAG	C8-C7-N2	2.74	120.66	116.12
3	A	401	NAG	C8-C7-N2	2.71	120.61	116.12
3	B	501	NAG	C8-C7-N2	2.26	119.87	116.12
3	F	501	NAG	C8-C7-N2	2.23	119.82	116.12
3	D	501	NAG	C8-C7-N2	2.23	119.81	116.12
3	A	401	NAG	O7-C7-C8	-2.18	118.18	122.05
3	E	401	NAG	O7-C7-C8	-2.17	118.19	122.05
3	C	401	NAG	O7-C7-C8	-2.16	118.20	122.05

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	NAG	O7-C7-N2-C2
3	C	403	NAG	O7-C7-N2-C2
3	E	403	NAG	O7-C7-N2-C2
3	A	402	NAG	C8-C7-N2-C2
3	A	403	NAG	C8-C7-N2-C2
3	C	402	NAG	C8-C7-N2-C2
3	C	403	NAG	C8-C7-N2-C2
3	E	402	NAG	C8-C7-N2-C2
3	E	403	NAG	C8-C7-N2-C2
3	C	402	NAG	O7-C7-N2-C2
3	A	402	NAG	O7-C7-N2-C2
3	E	402	NAG	O7-C7-N2-C2
3	A	402	NAG	C4-C5-C6-O6
3	C	402	NAG	C4-C5-C6-O6
3	E	402	NAG	C4-C5-C6-O6
3	A	401	NAG	O5-C5-C6-O6
3	C	401	NAG	O5-C5-C6-O6
3	E	401	NAG	O5-C5-C6-O6
3	A	403	NAG	C1-C2-N2-C7
3	C	403	NAG	C1-C2-N2-C7
3	E	403	NAG	C1-C2-N2-C7
3	A	403	NAG	C4-C5-C6-O6
3	E	403	NAG	C4-C5-C6-O6
3	C	403	NAG	C4-C5-C6-O6
3	A	403	NAG	C3-C2-N2-C7
3	C	403	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	E	403	NAG	C3-C2-N2-C7
3	E	402	NAG	O5-C5-C6-O6
3	C	402	NAG	O5-C5-C6-O6
3	A	402	NAG	O5-C5-C6-O6
3	A	402	NAG	C1-C2-N2-C7
3	C	402	NAG	C1-C2-N2-C7
3	E	402	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

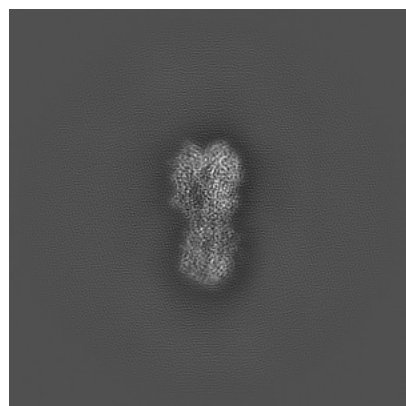
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45998. These allow visual inspection of the internal detail of the map and identification of artifacts.

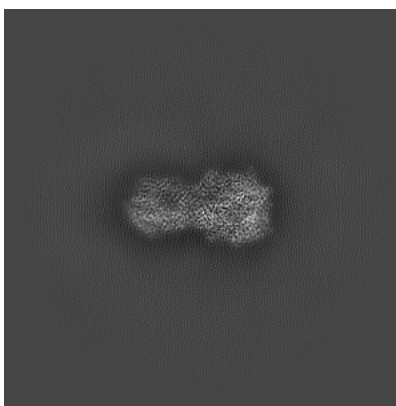
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

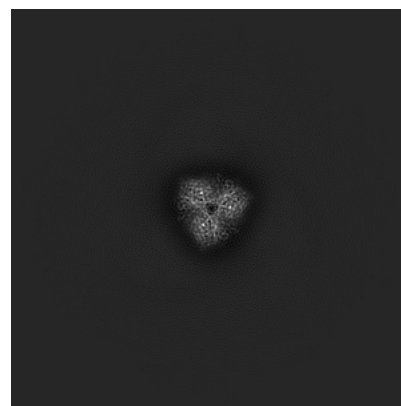
#### 6.1.1 Primary map



X

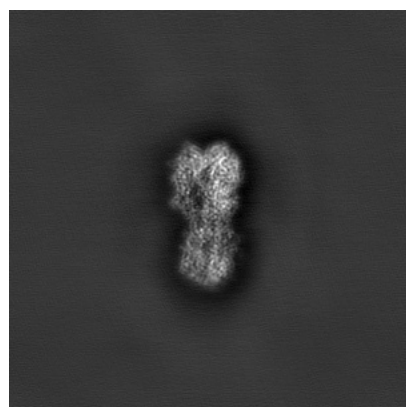


Y

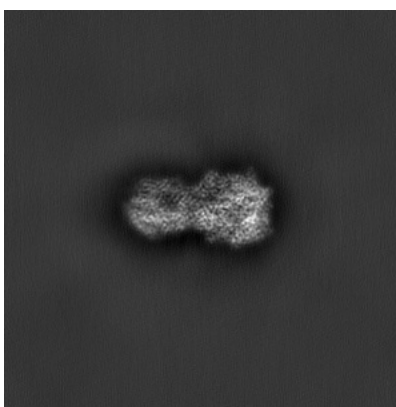


Z

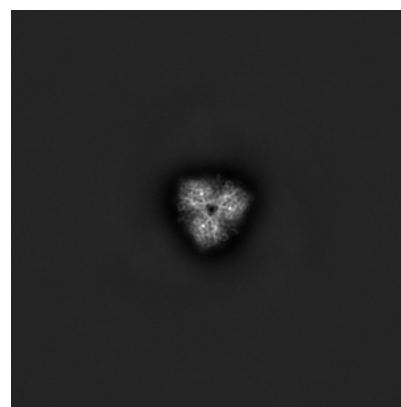
#### 6.1.2 Raw map



X



Y

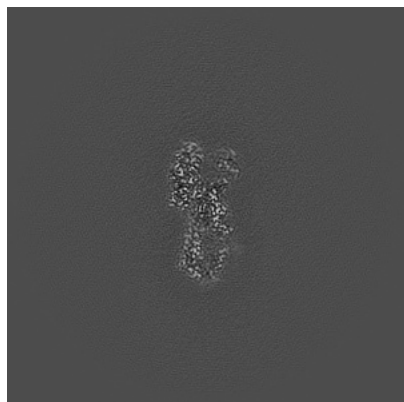


Z

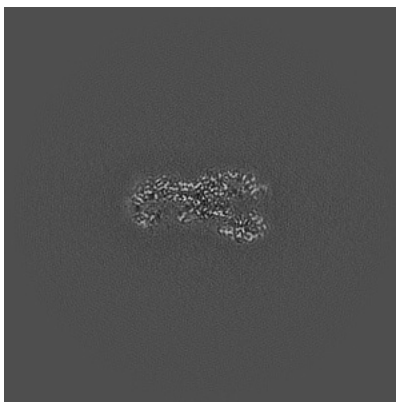
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

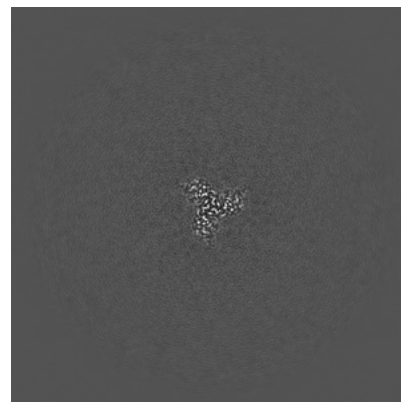
### 6.2.1 Primary map



X Index: 160

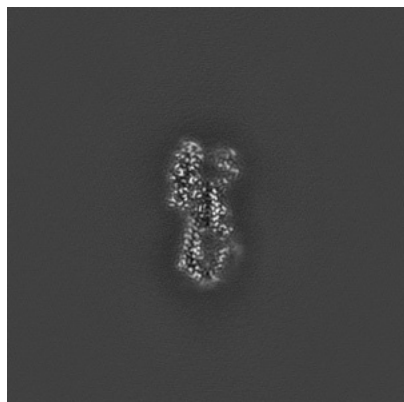


Y Index: 160

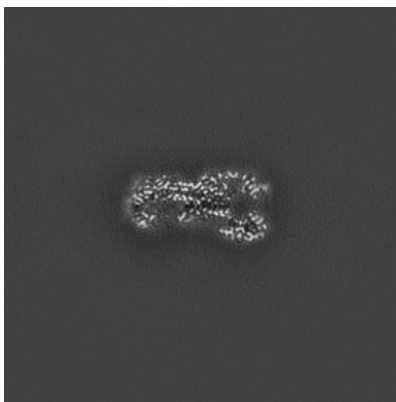


Z Index: 160

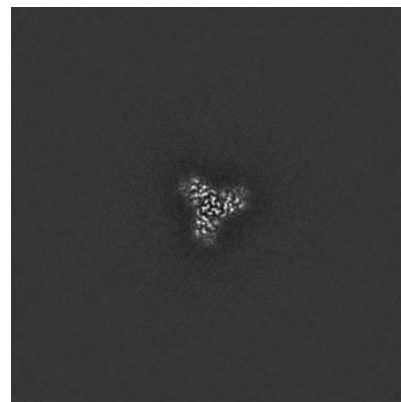
### 6.2.2 Raw map



X Index: 160



Y Index: 160

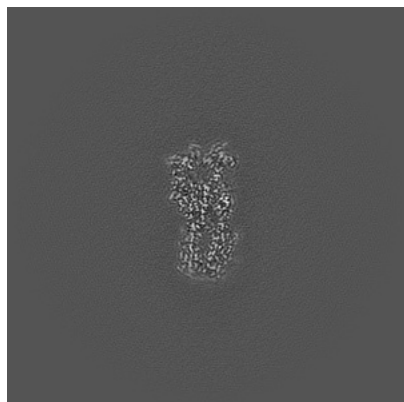


Z Index: 160

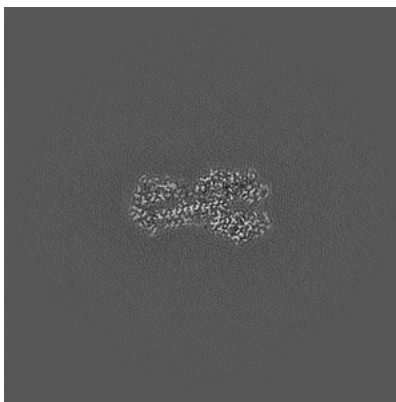
The images above show central slices of the map in three orthogonal directions.

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

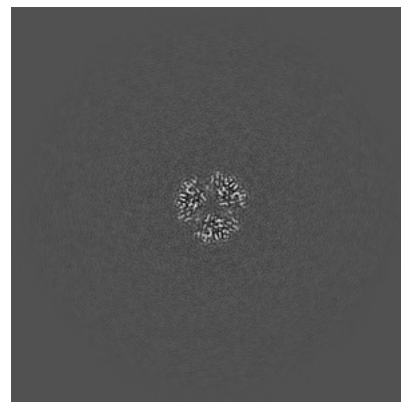
### 6.3.1 Primary map



X Index: 153

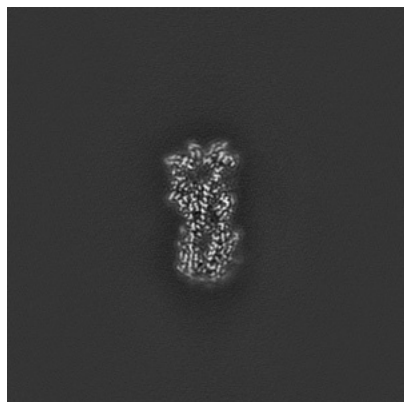


Y Index: 165

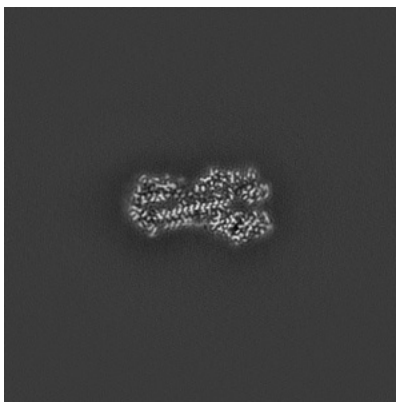


Z Index: 189

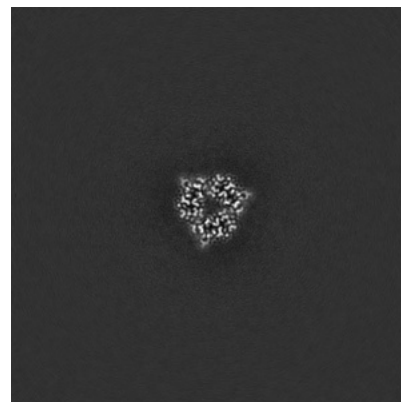
### 6.3.2 Raw map



X Index: 153



Y Index: 165



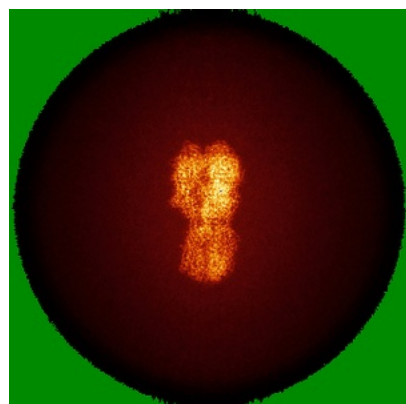
Z Index: 194

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

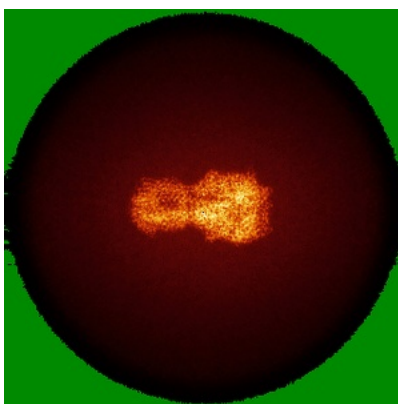


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

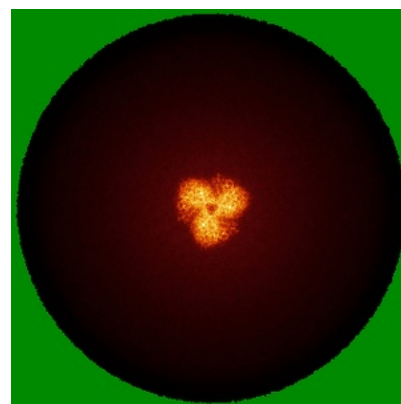
### 6.4.1 Primary map



X

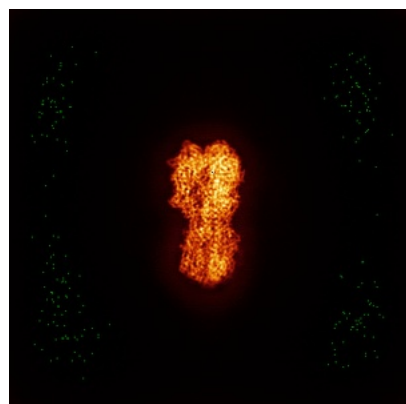


Y

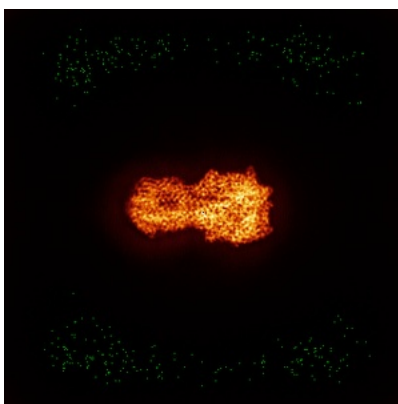


Z

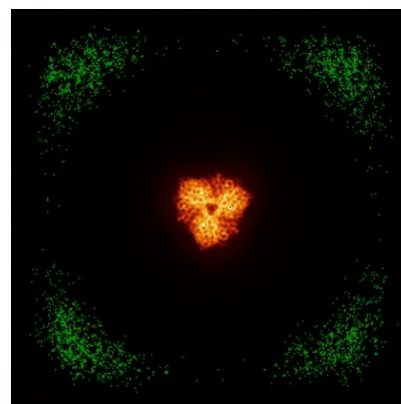
### 6.4.2 Raw map



X



Y



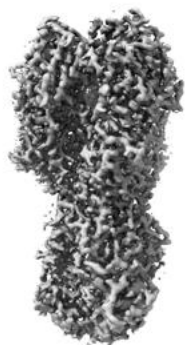
Z

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



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

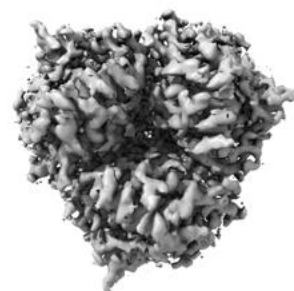
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

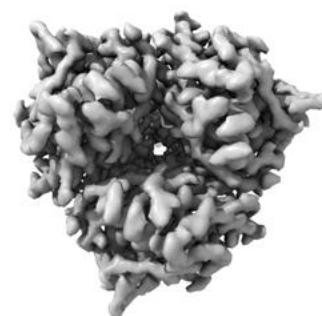
### 6.5.2 Raw map



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.

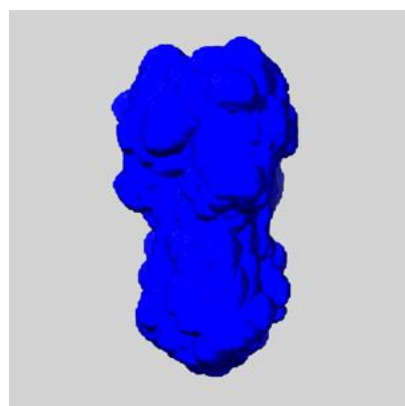
## 6.6 Mask visualisation [i](#)

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

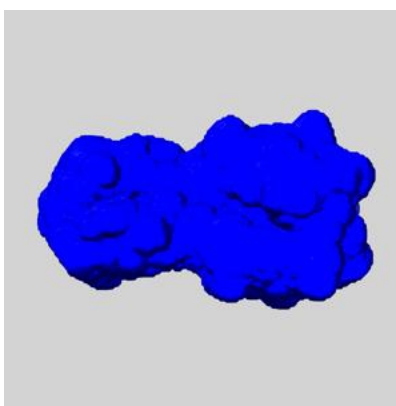
A mask typically either:

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

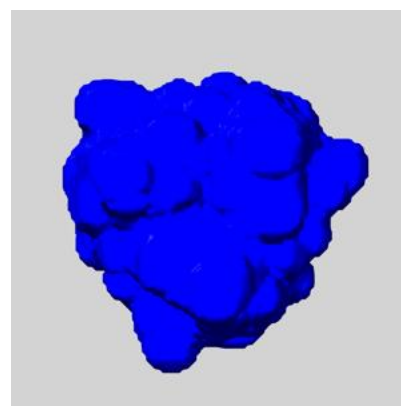
### 6.6.1 emd\_45998\_msk\_1.map [i](#)



X



Y

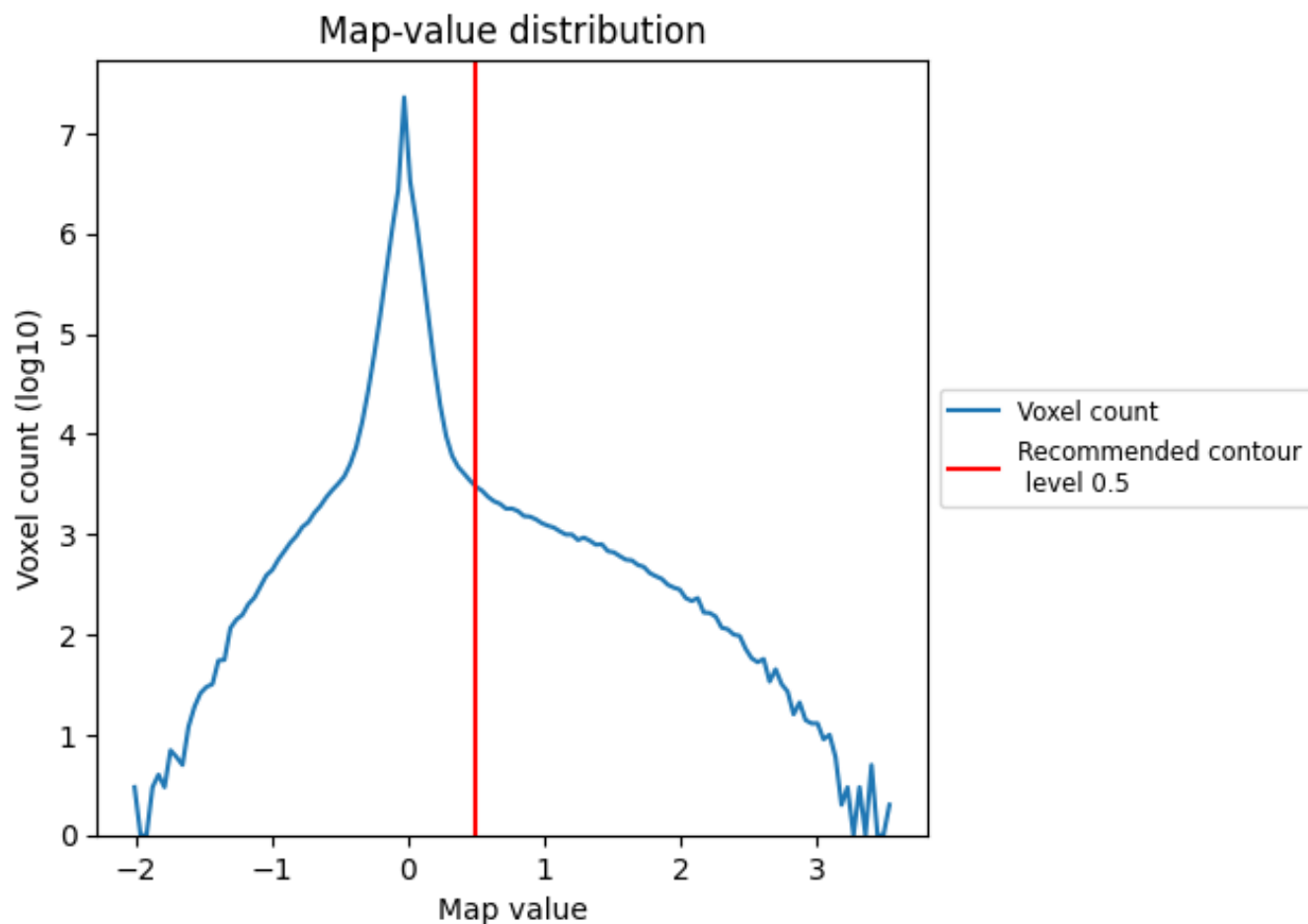


Z

## 7 Map analysis [i](#)

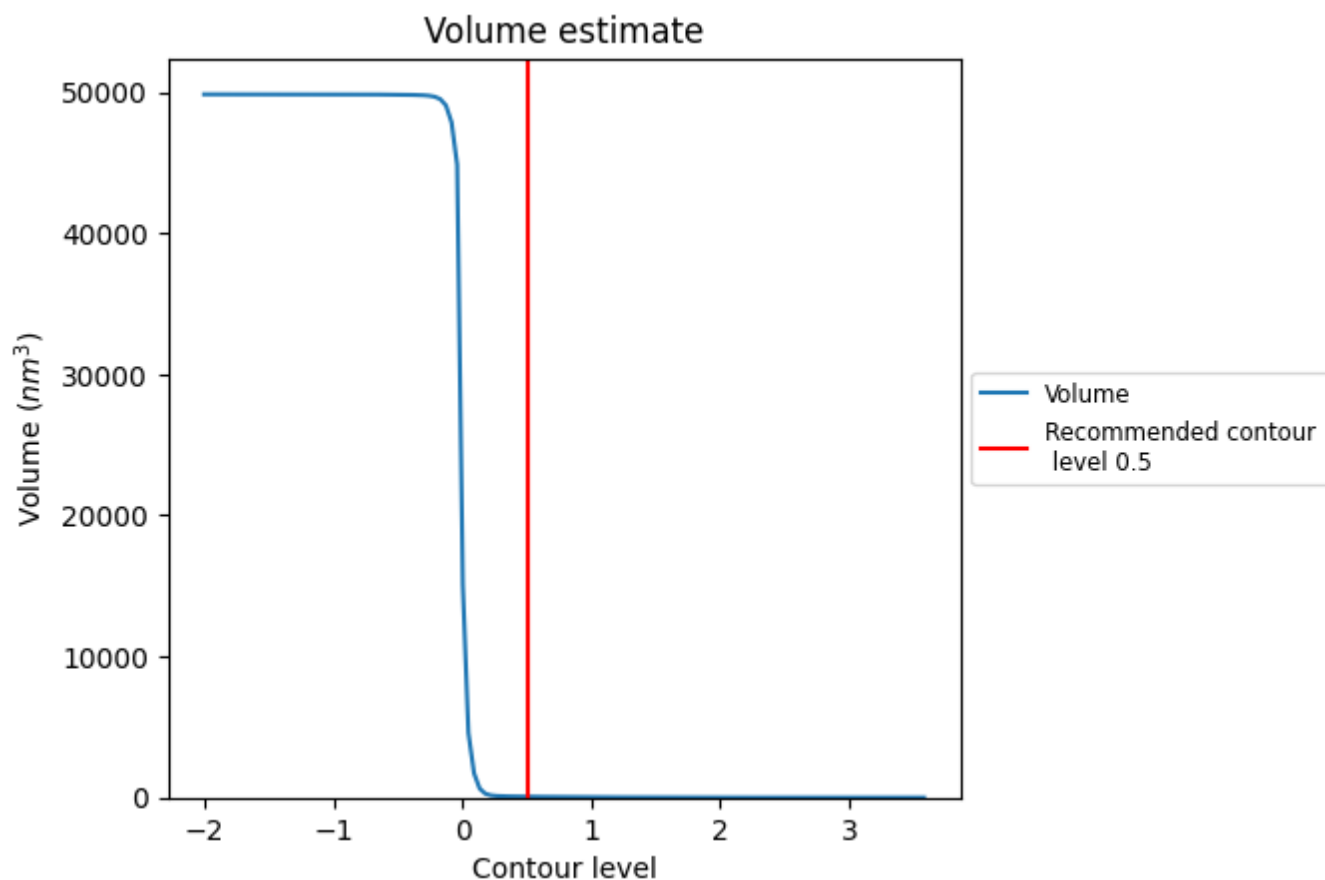
This section contains the results of statistical analysis of the map.

### 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.

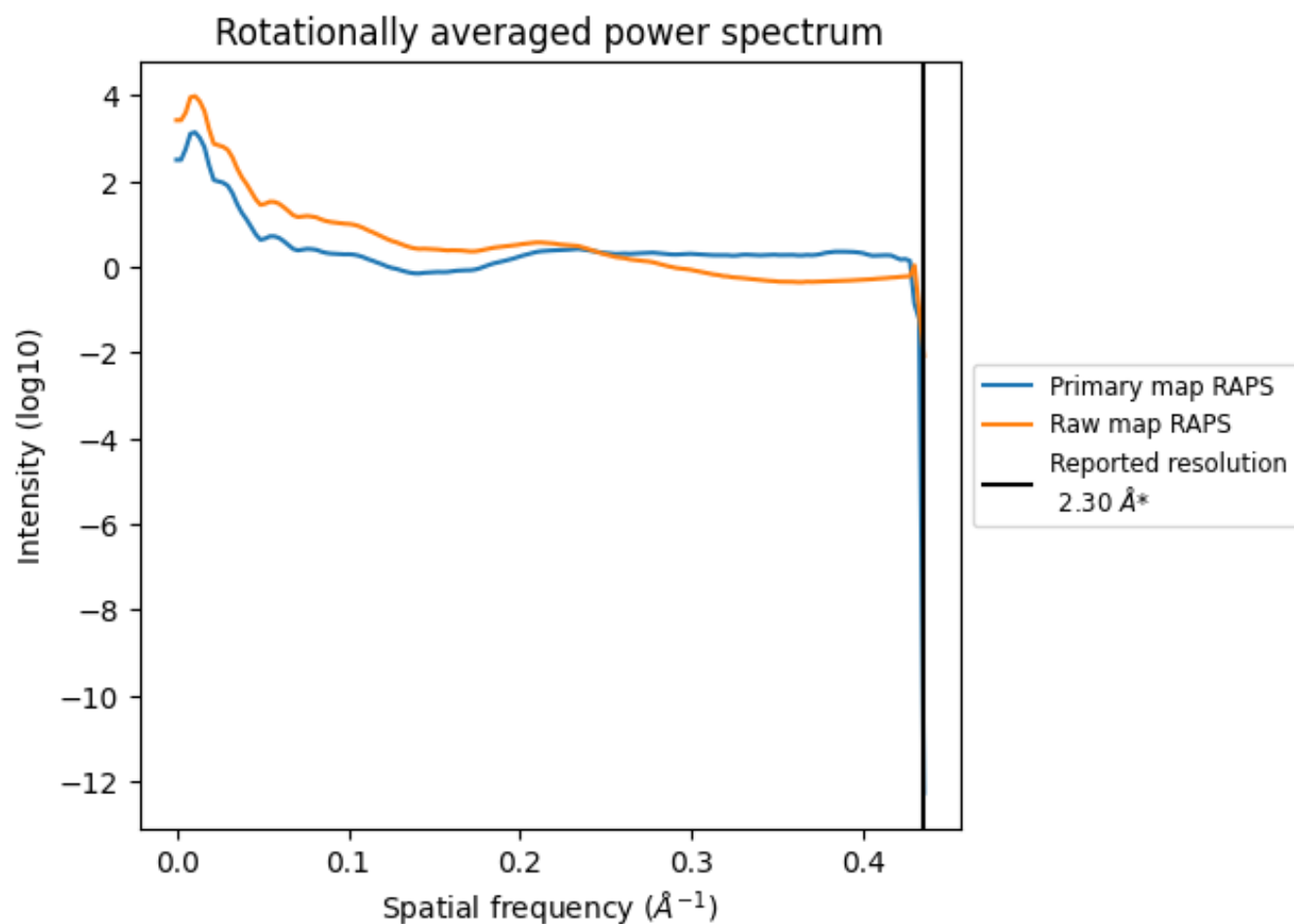
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 63  $\text{nm}^3$ ; this corresponds to an approximate mass of 57 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 ⓘ

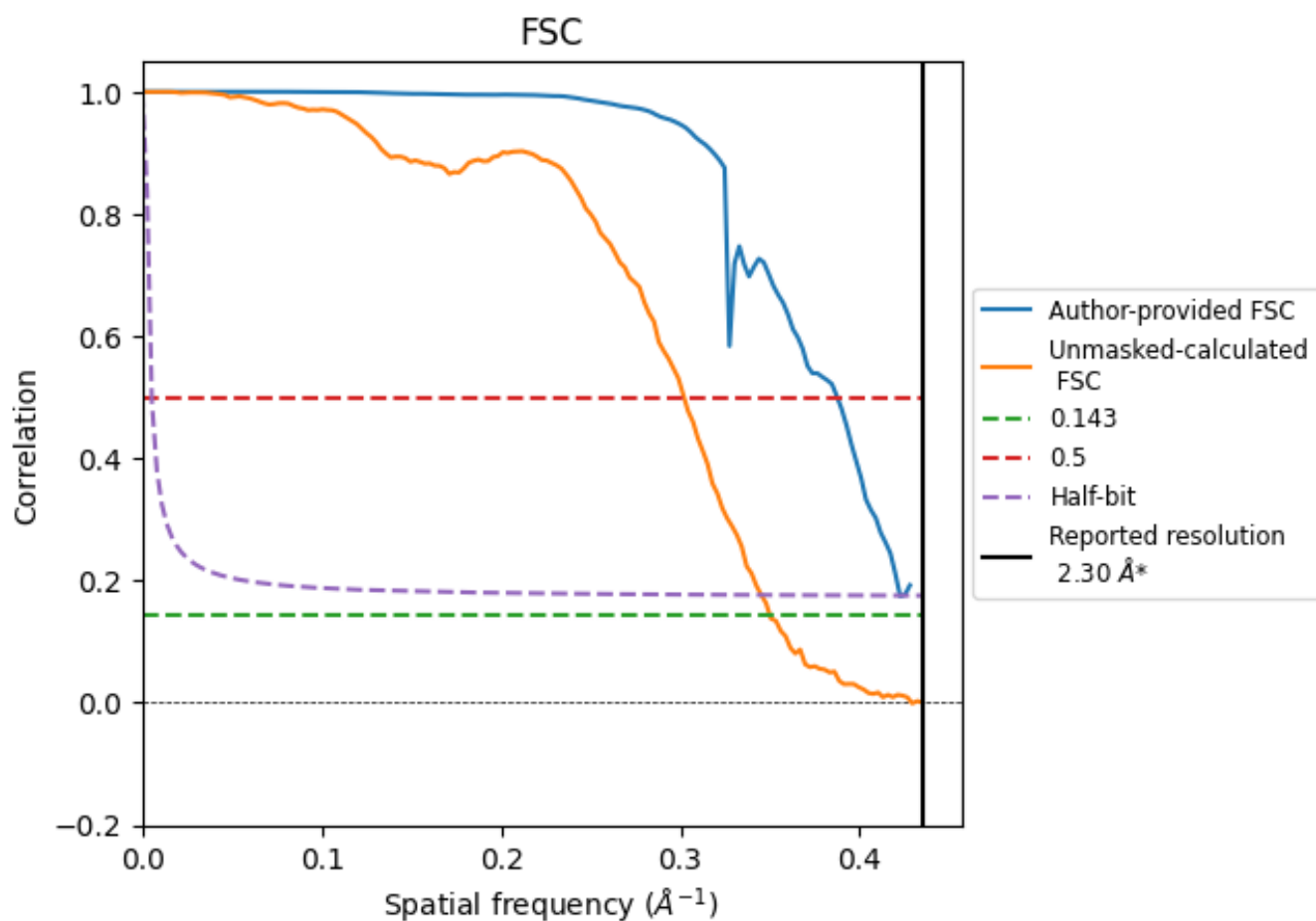


\*Reported resolution corresponds to spatial frequency of 0.435 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.435  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

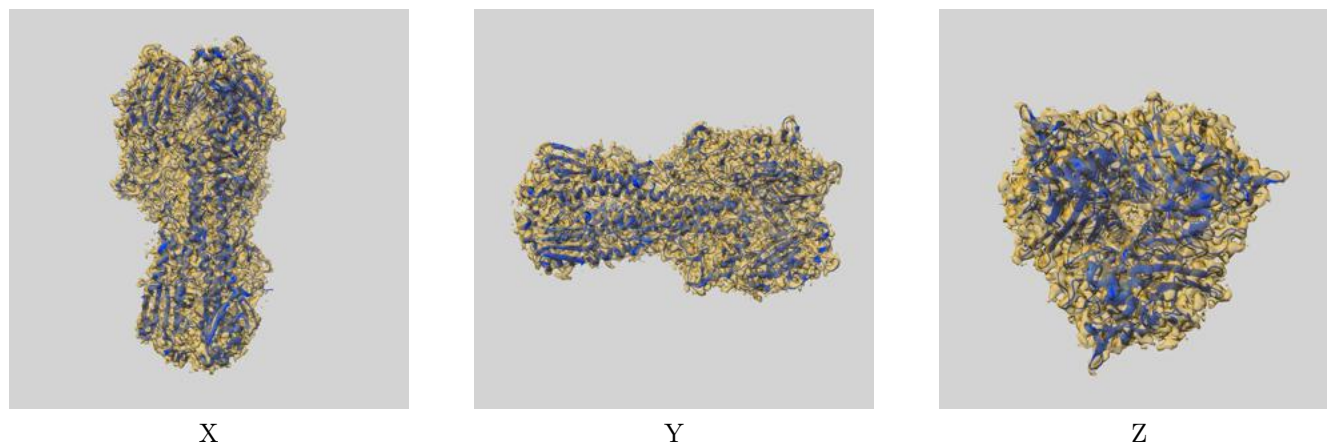
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	-	2.58	2.37
Unmasked-calculated*	2.86	3.31	2.90

\*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 2.86 differs from the reported value 2.3 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-45998 and PDB model 9CXU. Per-residue inclusion information can be found in section [3](#) on page [14](#).

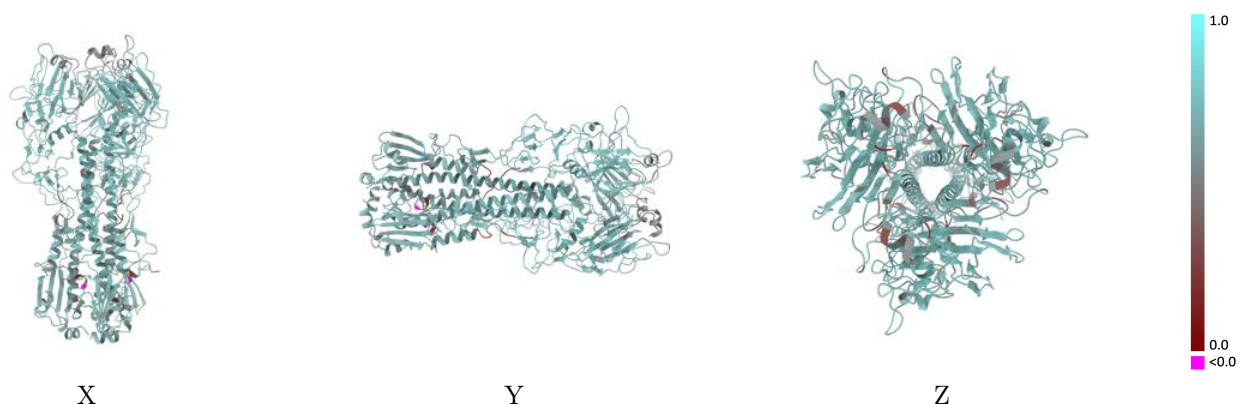
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

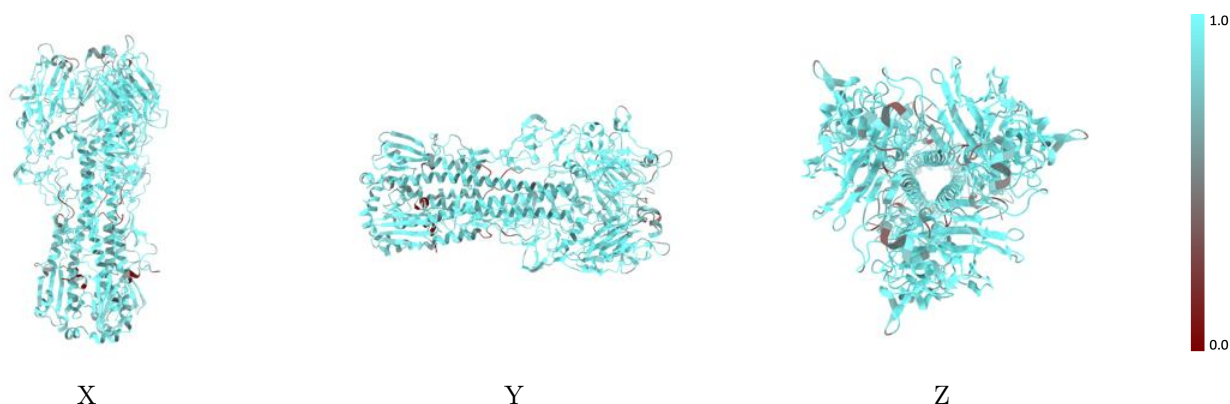


## 9.2 Q-score mapped to coordinate model [i](#)



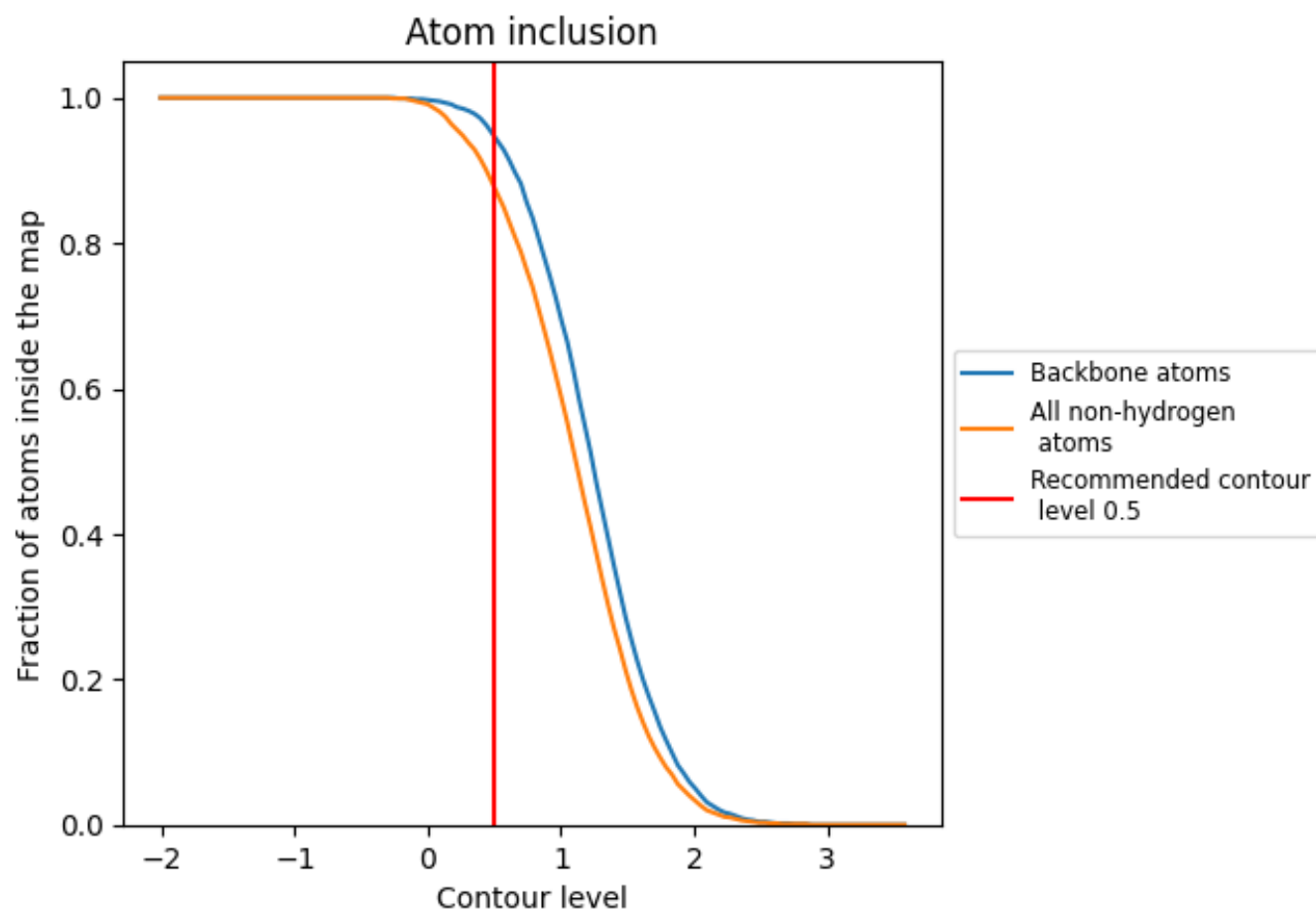
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 88% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8770	<div><div></div></div> 0.6340
A	<div><div></div></div> 0.9020	<div><div></div></div> 0.6480
B	<div><div></div></div> 0.8300	<div><div></div></div> 0.6130
C	<div><div></div></div> 0.9010	<div><div></div></div> 0.6450
D	<div><div></div></div> 0.8320	<div><div></div></div> 0.6140
E	<div><div></div></div> 0.9040	<div><div></div></div> 0.6440
F	<div><div></div></div> 0.8330	<div><div></div></div> 0.6130

1.0

0.0

<0.0