



## wwPDB EM Validation Summary Report ⓘ

Oct 14, 2024 – 12:28 PM EDT

PDB ID : 8UT4  
EMDB ID : EMD-42529  
Title : CryoEM structure of A/Michigan/45/2015 H1 in complex with flu HA central stem VH1-18 antibody 09-1B12  
Authors : Huang, J.; Han, J.; Ward, A.B.  
Deposited on : 2023-10-30  
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
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) : 2.39

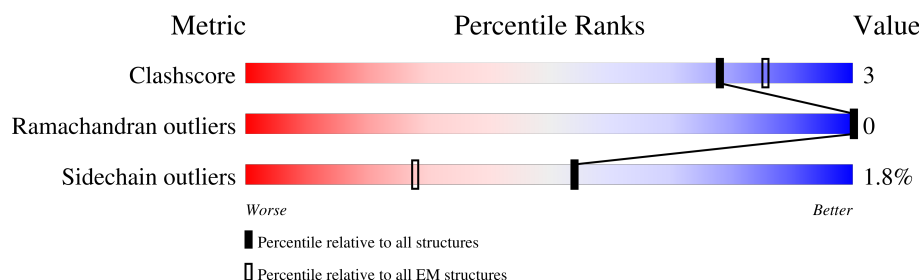
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 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	324	
1	C	324	
1	E	324	
2	B	250	
2	D	250	
2	F	250	
3	I	127	
4	H	109	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13663 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	323	Total	C	N	O	S	0	0
			2528	1594	437	486	11		
1	C	323	Total	C	N	O	S	0	0
			2528	1594	437	486	11		
1	E	323	Total	C	N	O	S	0	0
			2528	1594	437	486	11		

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	164	Total	C	N	O	S	0	0
			1339	838	230	265	6		
2	D	164	Total	C	N	O	S	0	0
			1339	838	230	265	6		
2	F	164	Total	C	N	O	S	0	0
			1339	838	230	265	6		

There are 207 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	178	GLY	-	expression tag	UNP A0A6G7M316
B	179	ALA	-	expression tag	UNP A0A6G7M316
B	180	LEU	-	expression tag	UNP A0A6G7M316
B	181	GLU	-	expression tag	UNP A0A6G7M316
B	182	VAL	-	expression tag	UNP A0A6G7M316
B	183	LEU	-	expression tag	UNP A0A6G7M316
B	184	PHE	-	expression tag	UNP A0A6G7M316
B	185	GLN	-	expression tag	UNP A0A6G7M316
B	186	GLY	-	expression tag	UNP A0A6G7M316
B	187	PRO	-	expression tag	UNP A0A6G7M316
B	188	GLY	-	expression tag	UNP A0A6G7M316
B	189	SER	-	expression tag	UNP A0A6G7M316
B	190	HIS	-	expression tag	UNP A0A6G7M316

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Chain	Residue	Modelled	Actual	Comment	Reference
B	191	HIS	-	expression tag	UNP A0A6G7M316
B	192	HIS	-	expression tag	UNP A0A6G7M316
B	193	HIS	-	expression tag	UNP A0A6G7M316
B	194	HIS	-	expression tag	UNP A0A6G7M316
B	195	HIS	-	expression tag	UNP A0A6G7M316
B	196	HIS	-	expression tag	UNP A0A6G7M316
B	197	HIS	-	expression tag	UNP A0A6G7M316
B	198	LEU	-	expression tag	UNP A0A6G7M316
B	199	GLY	-	expression tag	UNP A0A6G7M316
B	200	GLY	-	expression tag	UNP A0A6G7M316
B	201	SER	-	expression tag	UNP A0A6G7M316
B	202	GLY	-	expression tag	UNP A0A6G7M316
B	203	TYR	-	expression tag	UNP A0A6G7M316
B	204	ILE	-	expression tag	UNP A0A6G7M316
B	205	PRO	-	expression tag	UNP A0A6G7M316
B	206	GLU	-	expression tag	UNP A0A6G7M316
B	207	ALA	-	expression tag	UNP A0A6G7M316
B	208	PRO	-	expression tag	UNP A0A6G7M316
B	209	ARG	-	expression tag	UNP A0A6G7M316
B	210	ASP	-	expression tag	UNP A0A6G7M316
B	211	GLY	-	expression tag	UNP A0A6G7M316
B	212	GLN	-	expression tag	UNP A0A6G7M316
B	213	ALA	-	expression tag	UNP A0A6G7M316
B	214	TYR	-	expression tag	UNP A0A6G7M316
B	215	VAL	-	expression tag	UNP A0A6G7M316
B	216	ARG	-	expression tag	UNP A0A6G7M316
B	217	LYS	-	expression tag	UNP A0A6G7M316
B	218	ASP	-	expression tag	UNP A0A6G7M316
B	219	GLY	-	expression tag	UNP A0A6G7M316
B	220	GLU	-	expression tag	UNP A0A6G7M316
B	221	TRP	-	expression tag	UNP A0A6G7M316
B	222	VAL	-	expression tag	UNP A0A6G7M316
B	223	LEU	-	expression tag	UNP A0A6G7M316
B	224	LEU	-	expression tag	UNP A0A6G7M316
B	225	SER	-	expression tag	UNP A0A6G7M316
B	226	THR	-	expression tag	UNP A0A6G7M316
B	227	PHE	-	expression tag	UNP A0A6G7M316
B	228	LEU	-	expression tag	UNP A0A6G7M316
B	229	GLY	-	expression tag	UNP A0A6G7M316
B	230	SER	-	expression tag	UNP A0A6G7M316
B	231	GLY	-	expression tag	UNP A0A6G7M316
B	232	GLY	-	expression tag	UNP A0A6G7M316

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Chain	Residue	Modelled	Actual	Comment	Reference
B	233	GLY	-	expression tag	UNP A0A6G7M316
B	234	LEU	-	expression tag	UNP A0A6G7M316
B	235	ASN	-	expression tag	UNP A0A6G7M316
B	236	ASP	-	expression tag	UNP A0A6G7M316
B	237	ILE	-	expression tag	UNP A0A6G7M316
B	238	PHE	-	expression tag	UNP A0A6G7M316
B	239	GLU	-	expression tag	UNP A0A6G7M316
B	240	ALA	-	expression tag	UNP A0A6G7M316
B	241	GLN	-	expression tag	UNP A0A6G7M316
B	242	LYS	-	expression tag	UNP A0A6G7M316
B	243	ILE	-	expression tag	UNP A0A6G7M316
B	244	GLU	-	expression tag	UNP A0A6G7M316
B	245	TRP	-	expression tag	UNP A0A6G7M316
B	246	HIS	-	expression tag	UNP A0A6G7M316
D	178	GLY	-	expression tag	UNP A0A6G7M316
D	179	ALA	-	expression tag	UNP A0A6G7M316
D	180	LEU	-	expression tag	UNP A0A6G7M316
D	181	GLU	-	expression tag	UNP A0A6G7M316
D	182	VAL	-	expression tag	UNP A0A6G7M316
D	183	LEU	-	expression tag	UNP A0A6G7M316
D	184	PHE	-	expression tag	UNP A0A6G7M316
D	185	GLN	-	expression tag	UNP A0A6G7M316
D	186	GLY	-	expression tag	UNP A0A6G7M316
D	187	PRO	-	expression tag	UNP A0A6G7M316
D	188	GLY	-	expression tag	UNP A0A6G7M316
D	189	SER	-	expression tag	UNP A0A6G7M316
D	190	HIS	-	expression tag	UNP A0A6G7M316
D	191	HIS	-	expression tag	UNP A0A6G7M316
D	192	HIS	-	expression tag	UNP A0A6G7M316
D	193	HIS	-	expression tag	UNP A0A6G7M316
D	194	HIS	-	expression tag	UNP A0A6G7M316
D	195	HIS	-	expression tag	UNP A0A6G7M316
D	196	HIS	-	expression tag	UNP A0A6G7M316
D	197	HIS	-	expression tag	UNP A0A6G7M316
D	198	LEU	-	expression tag	UNP A0A6G7M316
D	199	GLY	-	expression tag	UNP A0A6G7M316
D	200	GLY	-	expression tag	UNP A0A6G7M316
D	201	SER	-	expression tag	UNP A0A6G7M316
D	202	GLY	-	expression tag	UNP A0A6G7M316
D	203	TYR	-	expression tag	UNP A0A6G7M316
D	204	ILE	-	expression tag	UNP A0A6G7M316
D	205	PRO	-	expression tag	UNP A0A6G7M316

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Chain	Residue	Modelled	Actual	Comment	Reference
D	206	GLU	-	expression tag	UNP A0A6G7M316
D	207	ALA	-	expression tag	UNP A0A6G7M316
D	208	PRO	-	expression tag	UNP A0A6G7M316
D	209	ARG	-	expression tag	UNP A0A6G7M316
D	210	ASP	-	expression tag	UNP A0A6G7M316
D	211	GLY	-	expression tag	UNP A0A6G7M316
D	212	GLN	-	expression tag	UNP A0A6G7M316
D	213	ALA	-	expression tag	UNP A0A6G7M316
D	214	TYR	-	expression tag	UNP A0A6G7M316
D	215	VAL	-	expression tag	UNP A0A6G7M316
D	216	ARG	-	expression tag	UNP A0A6G7M316
D	217	LYS	-	expression tag	UNP A0A6G7M316
D	218	ASP	-	expression tag	UNP A0A6G7M316
D	219	GLY	-	expression tag	UNP A0A6G7M316
D	220	GLU	-	expression tag	UNP A0A6G7M316
D	221	TRP	-	expression tag	UNP A0A6G7M316
D	222	VAL	-	expression tag	UNP A0A6G7M316
D	223	LEU	-	expression tag	UNP A0A6G7M316
D	224	LEU	-	expression tag	UNP A0A6G7M316
D	225	SER	-	expression tag	UNP A0A6G7M316
D	226	THR	-	expression tag	UNP A0A6G7M316
D	227	PHE	-	expression tag	UNP A0A6G7M316
D	228	LEU	-	expression tag	UNP A0A6G7M316
D	229	GLY	-	expression tag	UNP A0A6G7M316
D	230	SER	-	expression tag	UNP A0A6G7M316
D	231	GLY	-	expression tag	UNP A0A6G7M316
D	232	GLY	-	expression tag	UNP A0A6G7M316
D	233	GLY	-	expression tag	UNP A0A6G7M316
D	234	LEU	-	expression tag	UNP A0A6G7M316
D	235	ASN	-	expression tag	UNP A0A6G7M316
D	236	ASP	-	expression tag	UNP A0A6G7M316
D	237	ILE	-	expression tag	UNP A0A6G7M316
D	238	PHE	-	expression tag	UNP A0A6G7M316
D	239	GLU	-	expression tag	UNP A0A6G7M316
D	240	ALA	-	expression tag	UNP A0A6G7M316
D	241	GLN	-	expression tag	UNP A0A6G7M316
D	242	LYS	-	expression tag	UNP A0A6G7M316
D	243	ILE	-	expression tag	UNP A0A6G7M316
D	244	GLU	-	expression tag	UNP A0A6G7M316
D	245	TRP	-	expression tag	UNP A0A6G7M316
D	246	HIS	-	expression tag	UNP A0A6G7M316
F	178	GLY	-	expression tag	UNP A0A6G7M316

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Chain	Residue	Modelled	Actual	Comment	Reference
F	179	ALA	-	expression tag	UNP A0A6G7M316
F	180	LEU	-	expression tag	UNP A0A6G7M316
F	181	GLU	-	expression tag	UNP A0A6G7M316
F	182	VAL	-	expression tag	UNP A0A6G7M316
F	183	LEU	-	expression tag	UNP A0A6G7M316
F	184	PHE	-	expression tag	UNP A0A6G7M316
F	185	GLN	-	expression tag	UNP A0A6G7M316
F	186	GLY	-	expression tag	UNP A0A6G7M316
F	187	PRO	-	expression tag	UNP A0A6G7M316
F	188	GLY	-	expression tag	UNP A0A6G7M316
F	189	SER	-	expression tag	UNP A0A6G7M316
F	190	HIS	-	expression tag	UNP A0A6G7M316
F	191	HIS	-	expression tag	UNP A0A6G7M316
F	192	HIS	-	expression tag	UNP A0A6G7M316
F	193	HIS	-	expression tag	UNP A0A6G7M316
F	194	HIS	-	expression tag	UNP A0A6G7M316
F	195	HIS	-	expression tag	UNP A0A6G7M316
F	196	HIS	-	expression tag	UNP A0A6G7M316
F	197	HIS	-	expression tag	UNP A0A6G7M316
F	198	LEU	-	expression tag	UNP A0A6G7M316
F	199	GLY	-	expression tag	UNP A0A6G7M316
F	200	GLY	-	expression tag	UNP A0A6G7M316
F	201	SER	-	expression tag	UNP A0A6G7M316
F	202	GLY	-	expression tag	UNP A0A6G7M316
F	203	TYR	-	expression tag	UNP A0A6G7M316
F	204	ILE	-	expression tag	UNP A0A6G7M316
F	205	PRO	-	expression tag	UNP A0A6G7M316
F	206	GLU	-	expression tag	UNP A0A6G7M316
F	207	ALA	-	expression tag	UNP A0A6G7M316
F	208	PRO	-	expression tag	UNP A0A6G7M316
F	209	ARG	-	expression tag	UNP A0A6G7M316
F	210	ASP	-	expression tag	UNP A0A6G7M316
F	211	GLY	-	expression tag	UNP A0A6G7M316
F	212	GLN	-	expression tag	UNP A0A6G7M316
F	213	ALA	-	expression tag	UNP A0A6G7M316
F	214	TYR	-	expression tag	UNP A0A6G7M316
F	215	VAL	-	expression tag	UNP A0A6G7M316
F	216	ARG	-	expression tag	UNP A0A6G7M316
F	217	LYS	-	expression tag	UNP A0A6G7M316
F	218	ASP	-	expression tag	UNP A0A6G7M316
F	219	GLY	-	expression tag	UNP A0A6G7M316
F	220	GLU	-	expression tag	UNP A0A6G7M316

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Chain	Residue	Modelled	Actual	Comment	Reference
F	221	TRP	-	expression tag	UNP A0A6G7M316
F	222	VAL	-	expression tag	UNP A0A6G7M316
F	223	LEU	-	expression tag	UNP A0A6G7M316
F	224	LEU	-	expression tag	UNP A0A6G7M316
F	225	SER	-	expression tag	UNP A0A6G7M316
F	226	THR	-	expression tag	UNP A0A6G7M316
F	227	PHE	-	expression tag	UNP A0A6G7M316
F	228	LEU	-	expression tag	UNP A0A6G7M316
F	229	GLY	-	expression tag	UNP A0A6G7M316
F	230	SER	-	expression tag	UNP A0A6G7M316
F	231	GLY	-	expression tag	UNP A0A6G7M316
F	232	GLY	-	expression tag	UNP A0A6G7M316
F	233	GLY	-	expression tag	UNP A0A6G7M316
F	234	LEU	-	expression tag	UNP A0A6G7M316
F	235	ASN	-	expression tag	UNP A0A6G7M316
F	236	ASP	-	expression tag	UNP A0A6G7M316
F	237	ILE	-	expression tag	UNP A0A6G7M316
F	238	PHE	-	expression tag	UNP A0A6G7M316
F	239	GLU	-	expression tag	UNP A0A6G7M316
F	240	ALA	-	expression tag	UNP A0A6G7M316
F	241	GLN	-	expression tag	UNP A0A6G7M316
F	242	LYS	-	expression tag	UNP A0A6G7M316
F	243	ILE	-	expression tag	UNP A0A6G7M316
F	244	GLU	-	expression tag	UNP A0A6G7M316
F	245	TRP	-	expression tag	UNP A0A6G7M316
F	246	HIS	-	expression tag	UNP A0A6G7M316

- Molecule 3 is a protein called 09-1B12 HC Fv.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	126	Total	C	N	O	S	0	0
			974	617	167	186	4		

- Molecule 4 is a protein called 09-1B12 LC Fv.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	107	Total	C	N	O	S	0	0
			836	526	148	160	2		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).





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

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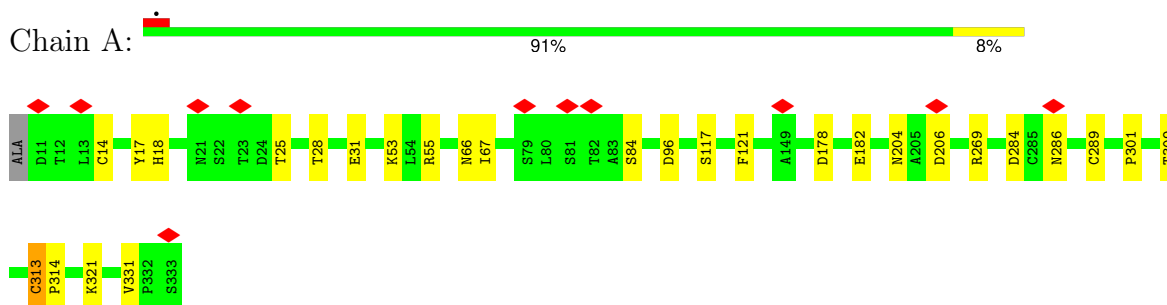
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Mol	Chain	Residues	Atoms				AltConf
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	

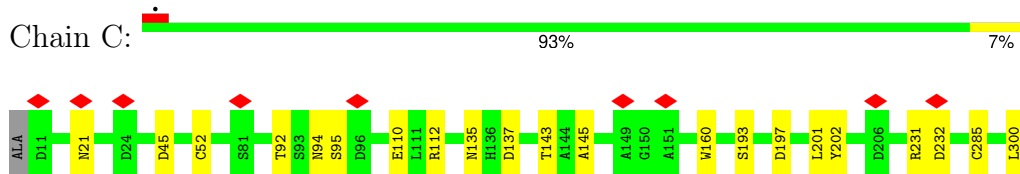
### 3 Residue-property plots [i](#)

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.

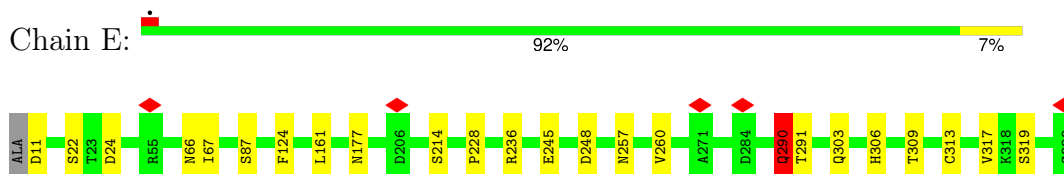
- Molecule 1: Hemagglutinin HA1 chain



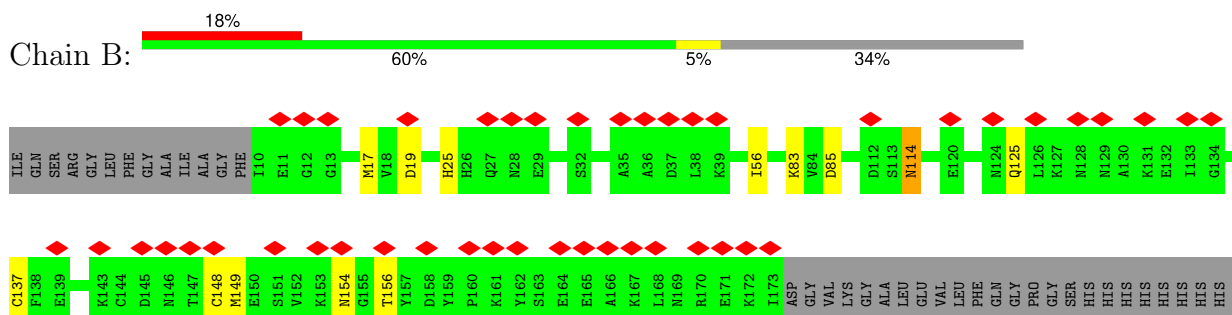
- Molecule 1: Hemagglutinin HA1 chain



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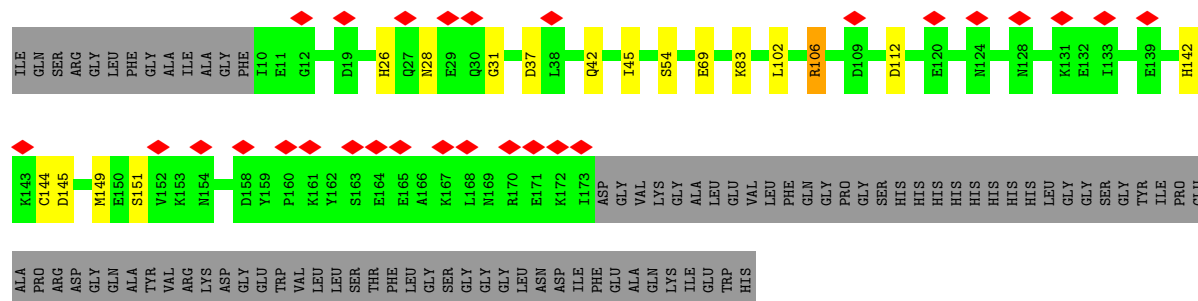
- Molecule 2: Hemagglutinin HA2 chain



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

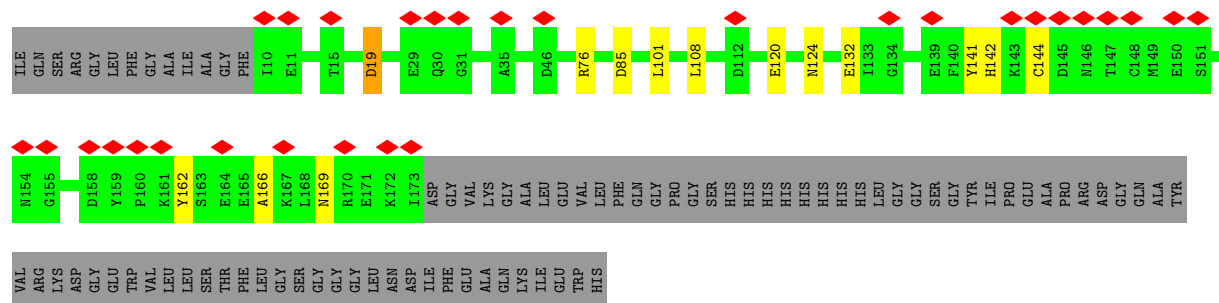
• Molecule 2: Hemagglutinin HA2 chain

Chain D: 11% 59% 6% 34%



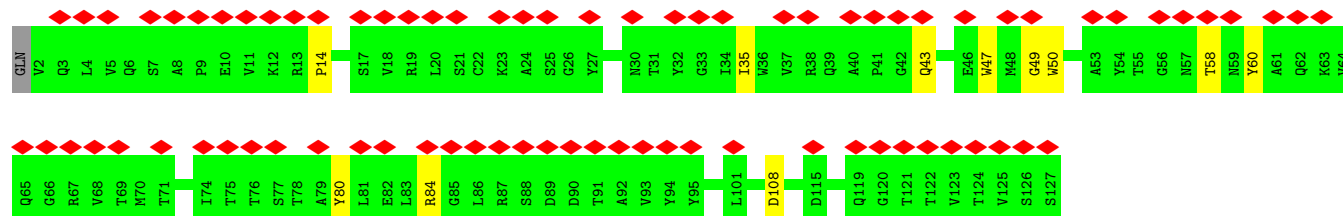
• Molecule 2: Hemagglutinin HA2 chain

Chain F: 12% 60% 5% 34%



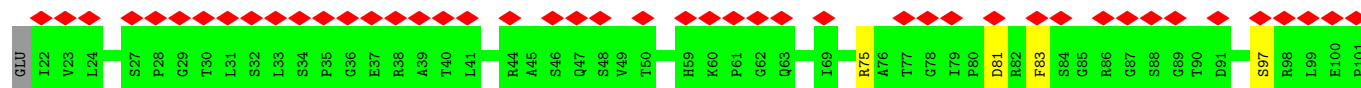
• Molecule 3: 09-1B12 HC Fv

Chain I: 61% 91% 9%



• Molecule 4: 09-1B12 LC Fv

Chain H: 53% 92% 6%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	89540	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.554	Depositor
Minimum map value	-0.336	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	301.6, 301.6, 301.6	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.725, 0.725, 0.725	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	0.35	1/2591 (0.0%)	0.69	2/3525 (0.1%)
1	C	0.33	0/2591	0.69	2/3525 (0.1%)
1	E	0.38	2/2591 (0.1%)	0.67	0/3525
2	B	0.34	0/1365	0.64	0/1838
2	D	0.33	0/1365	0.62	0/1838
2	F	0.34	0/1365	0.71	3/1838 (0.2%)
3	I	0.37	0/996	0.83	1/1358 (0.1%)
4	H	0.33	0/857	0.79	1/1164 (0.1%)
All	All	0.35	3/13721 (0.0%)	0.70	9/18611 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	306	HIS	C-N	7.94	1.49	1.34
1	A	313	CYS	CB-SG	-6.21	1.71	1.82
1	E	290	GLN	C-N	5.76	1.47	1.34

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	ASP	CB-CG-OD1	8.70	126.13	118.30
1	A	206	ASP	CB-CG-OD1	7.76	125.28	118.30
2	F	19	ASP	CB-CG-OD1	7.33	124.90	118.30
1	C	300	LEU	CB-CG-CD1	6.89	122.72	111.00
4	H	81	ASP	CB-CG-OD1	6.59	124.23	118.30

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	2528	0	2462	21	0
1	C	2528	0	2462	16	0
1	E	2528	0	2462	12	0
2	B	1339	0	1274	8	0
2	D	1339	0	1273	7	0
2	F	1339	0	1273	8	0
3	I	974	0	948	5	0
4	H	836	0	812	3	0
5	A	70	0	65	1	0
5	B	14	0	13	0	0
5	C	70	0	65	0	0
5	D	14	0	13	0	0
5	E	70	0	65	0	0
5	F	14	0	13	0	0
All	All	13663	0	13200	71	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 3.

The worst 5 of 71 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:C:52:CYS:SG	1:C:285:CYS:HB2	1.76	1.23
1:C:52:CYS:SG	1:C:285:CYS:CB	2.61	0.88
1:A:14:CYS:HG	2:B:137:CYS:HG	1.11	0.86
1:A:289:CYS:CB	1:A:313:CYS:HB3	2.16	0.75
1:C:52:CYS:HG	1:C:285:CYS:CB	2.01	0.73

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	321/324 (99%)	312 (97%)	9 (3%)	0	100	100
1	C	321/324 (99%)	308 (96%)	13 (4%)	0	100	100
1	E	321/324 (99%)	309 (96%)	12 (4%)	0	100	100
2	B	162/250 (65%)	159 (98%)	3 (2%)	0	100	100
2	D	162/250 (65%)	161 (99%)	1 (1%)	0	100	100
2	F	162/250 (65%)	160 (99%)	2 (1%)	0	100	100
3	I	124/127 (98%)	109 (88%)	15 (12%)	0	100	100
4	H	105/109 (96%)	98 (93%)	7 (7%)	0	100	100
All	All	1678/1958 (86%)	1616 (96%)	62 (4%)	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	A	284/284 (100%)	282 (99%)	2 (1%)	81	88
1	C	284/284 (100%)	279 (98%)	5 (2%)	54	74
1	E	284/284 (100%)	281 (99%)	3 (1%)	70	82
2	B	145/209 (69%)	140 (97%)	5 (3%)	32	59
2	D	145/209 (69%)	139 (96%)	6 (4%)	26	54
2	F	145/209 (69%)	144 (99%)	1 (1%)	81	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	102/103 (99%)	99 (97%)	3 (3%)	37	63
4	H	91/93 (98%)	90 (99%)	1 (1%)	70	82
All	All	1480/1675 (88%)	1454 (98%)	26 (2%)	54	74

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	106	ARG
2	D	151	SER
3	I	108	ASP
2	D	145	ASP
1	E	87	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 ⓘ

18 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
5	NAG	B	301	-	14,14,15	0.22	0	17,19,21	0.56	0
5	NAG	E	401	1	14,14,15	0.29	0	17,19,21	0.53	0
5	NAG	D	301	2	14,14,15	0.23	0	17,19,21	0.49	0
5	NAG	E	402	1	14,14,15	0.30	0	17,19,21	0.61	0
5	NAG	A	401	1	14,14,15	0.42	0	17,19,21	0.54	0
5	NAG	E	403	1	14,14,15	0.23	0	17,19,21	0.55	0
5	NAG	E	404	1	14,14,15	0.27	0	17,19,21	0.52	0
5	NAG	E	405	1	14,14,15	0.23	0	17,19,21	0.60	0
5	NAG	F	301	2	14,14,15	0.17	0	17,19,21	0.57	0
5	NAG	C	403	1	14,14,15	0.27	0	17,19,21	0.53	0
5	NAG	C	405	1	14,14,15	2.15	2 (14%)	17,19,21	2.74	2 (11%)
5	NAG	C	401	1	14,14,15	0.22	0	17,19,21	0.49	0
5	NAG	A	404	1	14,14,15	0.29	0	17,19,21	0.53	0
5	NAG	A	403	1	14,14,15	0.32	0	17,19,21	0.56	0
5	NAG	C	404	1	14,14,15	0.36	0	17,19,21	0.54	0
5	NAG	C	402	1	14,14,15	0.27	0	17,19,21	0.53	0
5	NAG	A	402	1	14,14,15	0.27	0	17,19,21	0.55	0
5	NAG	A	405	1	14,14,15	0.21	0	17,19,21	0.46	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
5	NAG	B	301	-	-	0/6/23/26	0/1/1/1
5	NAG	E	401	1	-	2/6/23/26	0/1/1/1
5	NAG	D	301	2	-	1/6/23/26	0/1/1/1
5	NAG	E	402	1	-	2/6/23/26	0/1/1/1
5	NAG	A	401	1	-	2/6/23/26	0/1/1/1
5	NAG	E	403	1	-	0/6/23/26	0/1/1/1
5	NAG	E	404	1	-	1/6/23/26	0/1/1/1
5	NAG	E	405	1	-	1/6/23/26	0/1/1/1
5	NAG	F	301	2	-	2/6/23/26	0/1/1/1
5	NAG	C	403	1	-	2/6/23/26	0/1/1/1
5	NAG	C	405	1	-	4/6/23/26	0/1/1/1
5	NAG	C	401	1	-	0/6/23/26	0/1/1/1
5	NAG	A	404	1	-	0/6/23/26	0/1/1/1
5	NAG	A	403	1	-	0/6/23/26	0/1/1/1
5	NAG	C	404	1	-	1/6/23/26	0/1/1/1
5	NAG	C	402	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	402	1	-	0/6/23/26	0/1/1/1
5	NAG	A	405	1	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	405	NAG	O5-C1	6.25	1.54	1.43
5	C	405	NAG	C1-C2	4.92	1.59	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	405	NAG	C1-O5-C5	10.75	126.59	112.19
5	C	405	NAG	C2-N2-C7	2.65	126.45	122.90

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	405	NAG	C4-C5-C6-O6
5	C	403	NAG	O5-C5-C6-O6
5	E	401	NAG	O5-C5-C6-O6
5	A	401	NAG	O5-C5-C6-O6
5	C	405	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	401	NAG	1	0

## 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.



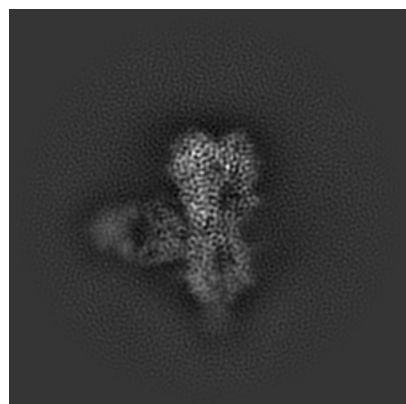
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42529. These allow visual inspection of the internal detail of the map and identification of artifacts.

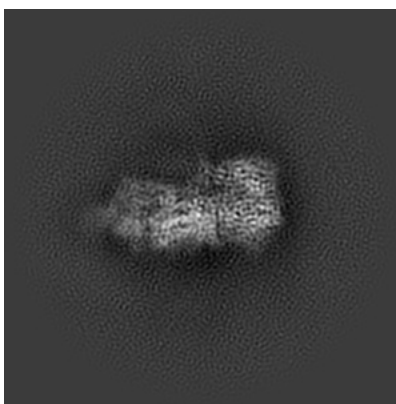
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

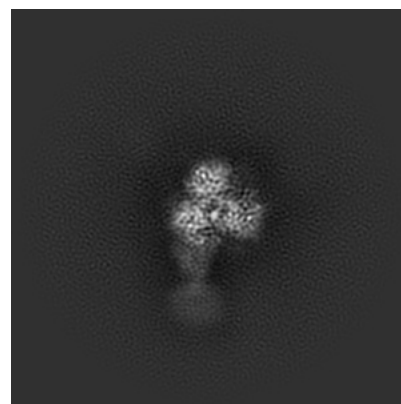
#### 6.1.1 Primary map



X

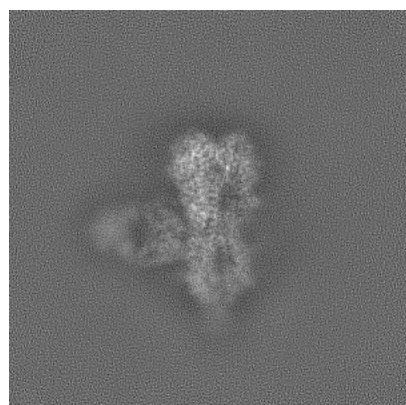


Y

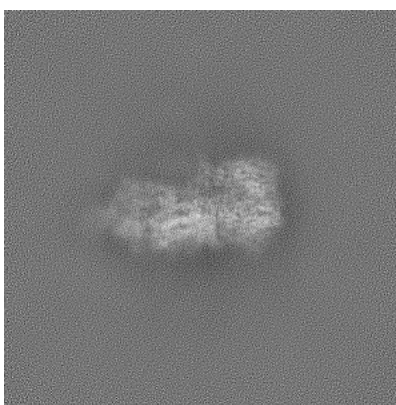


Z

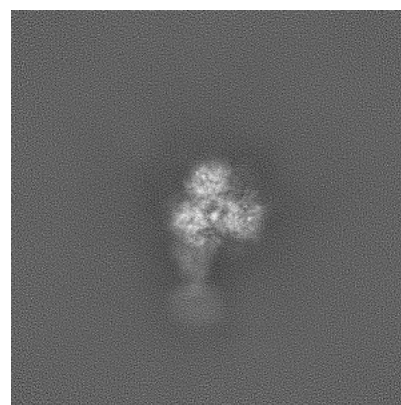
#### 6.1.2 Raw map



X



Y

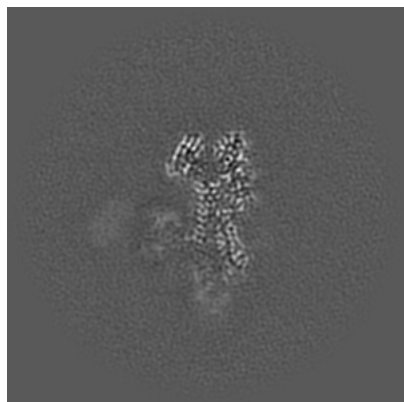


Z

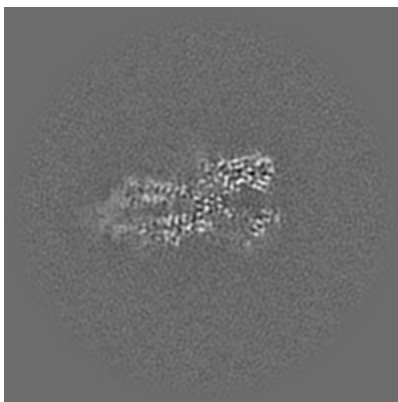
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

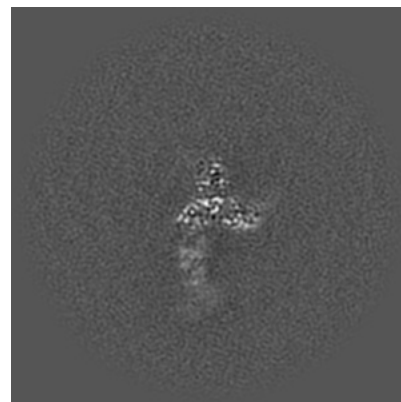
### 6.2.1 Primary map



X Index: 208

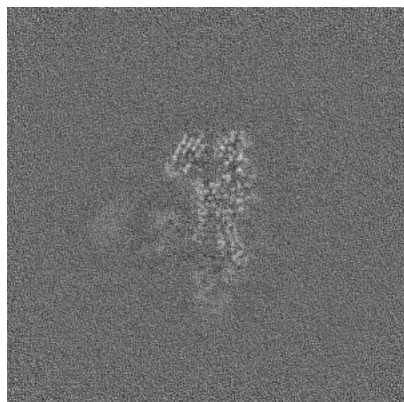


Y Index: 208

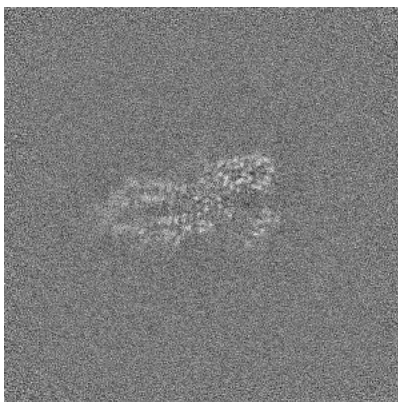


Z Index: 208

### 6.2.2 Raw map



X Index: 208



Y Index: 208

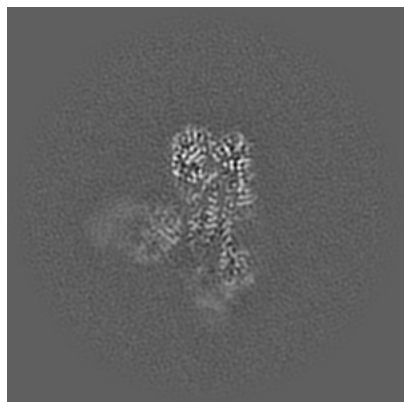


Z Index: 208

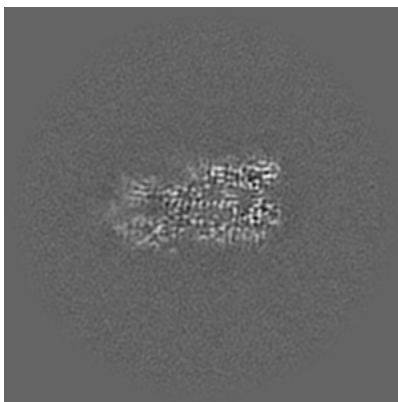
The images above show central slices of the map in three orthogonal directions.

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

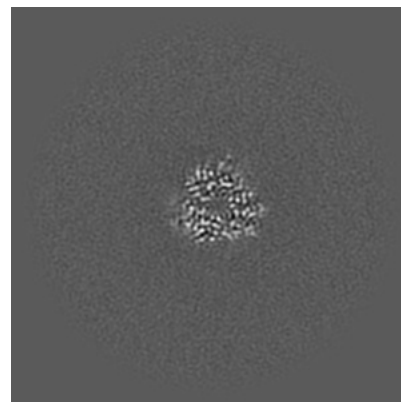
### 6.3.1 Primary map



X Index: 199

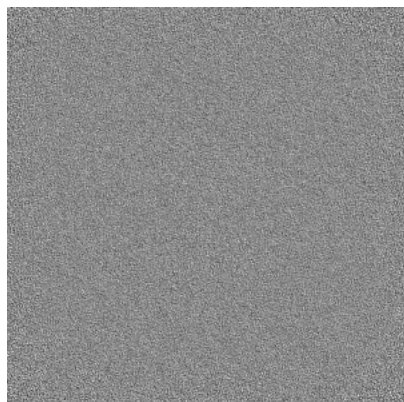


Y Index: 198

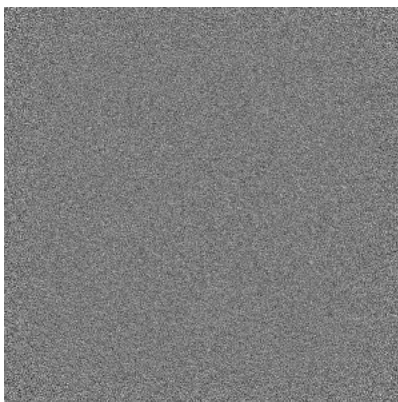


Z Index: 260

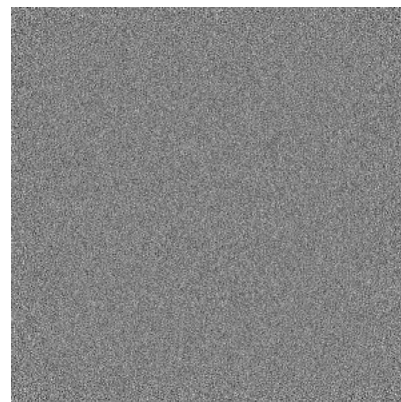
### 6.3.2 Raw map



X Index: 0



Y Index: 0



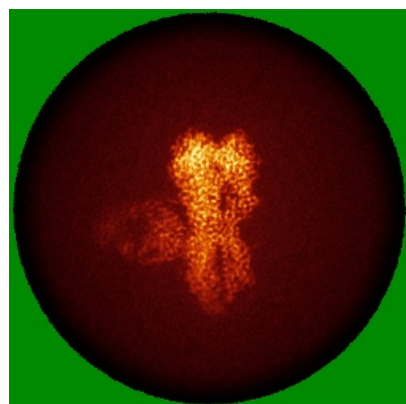
Z Index: 0

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

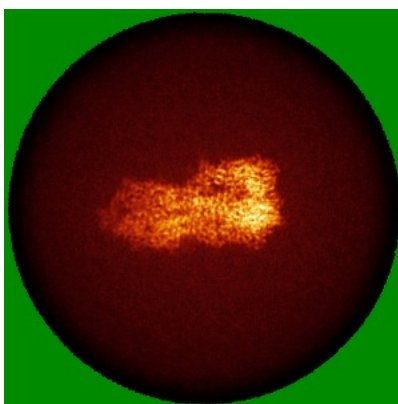


## 6.4 Orthogonal standard-deviation projections (False-color) ⓘ

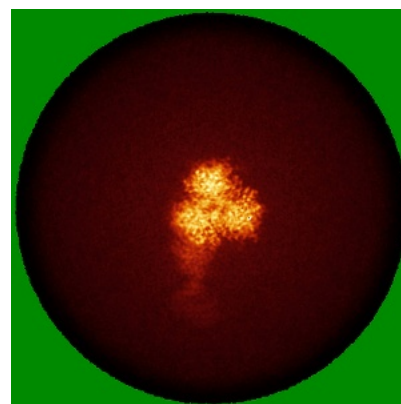
### 6.4.1 Primary map



X

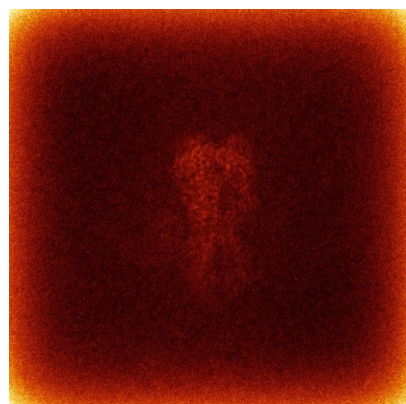


Y

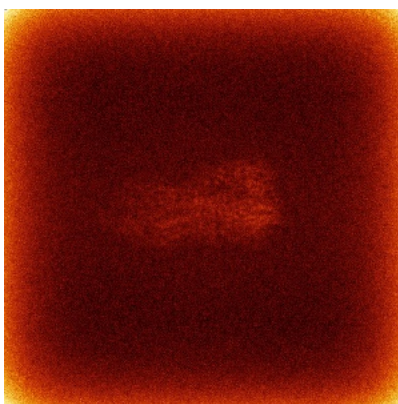


Z

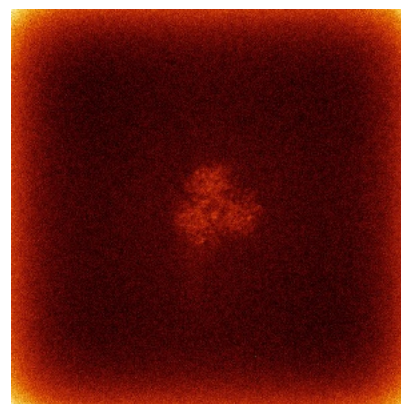
### 6.4.2 Raw map



X



Y

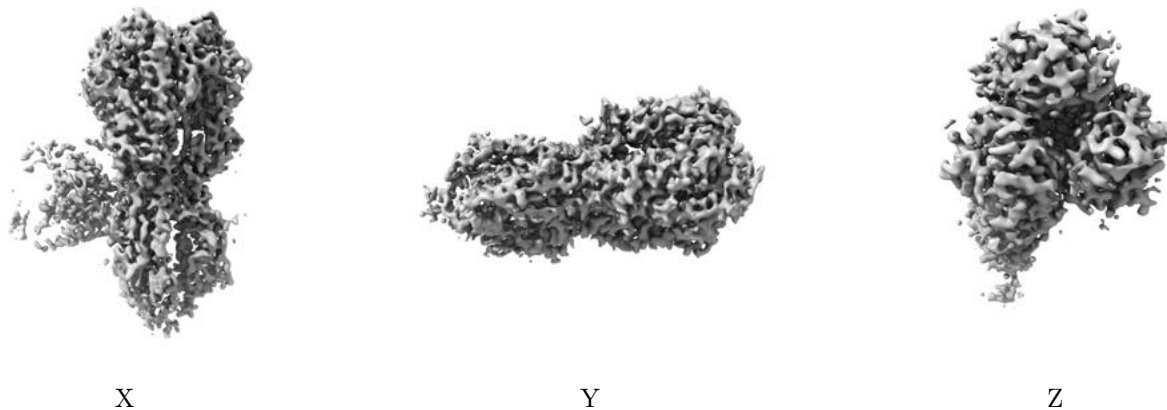


Z

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

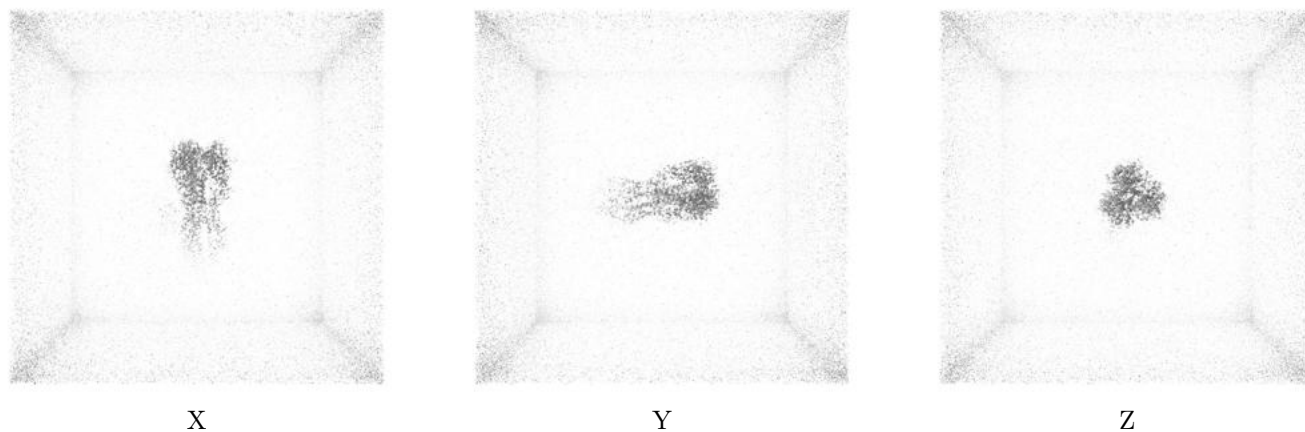
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

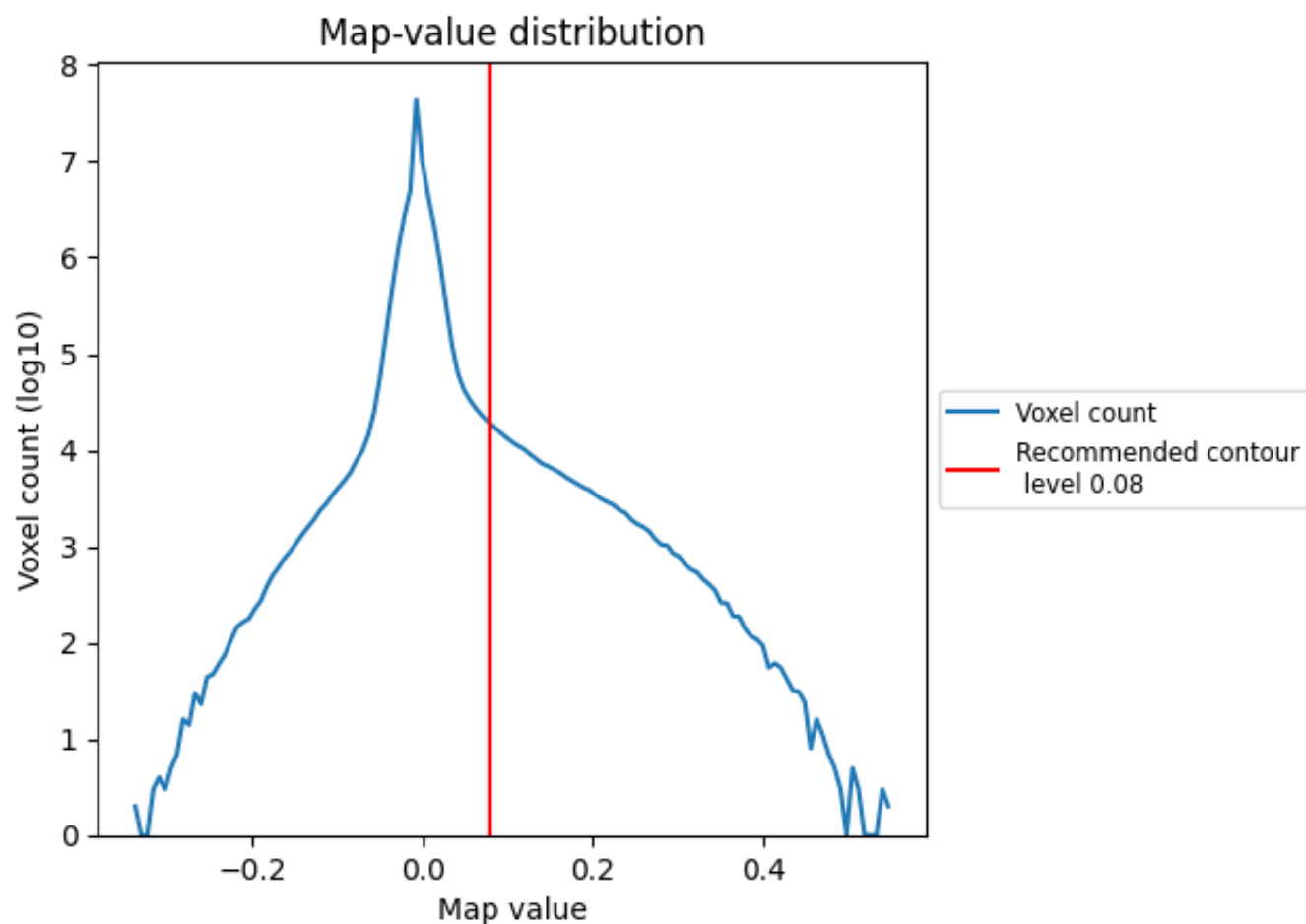
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

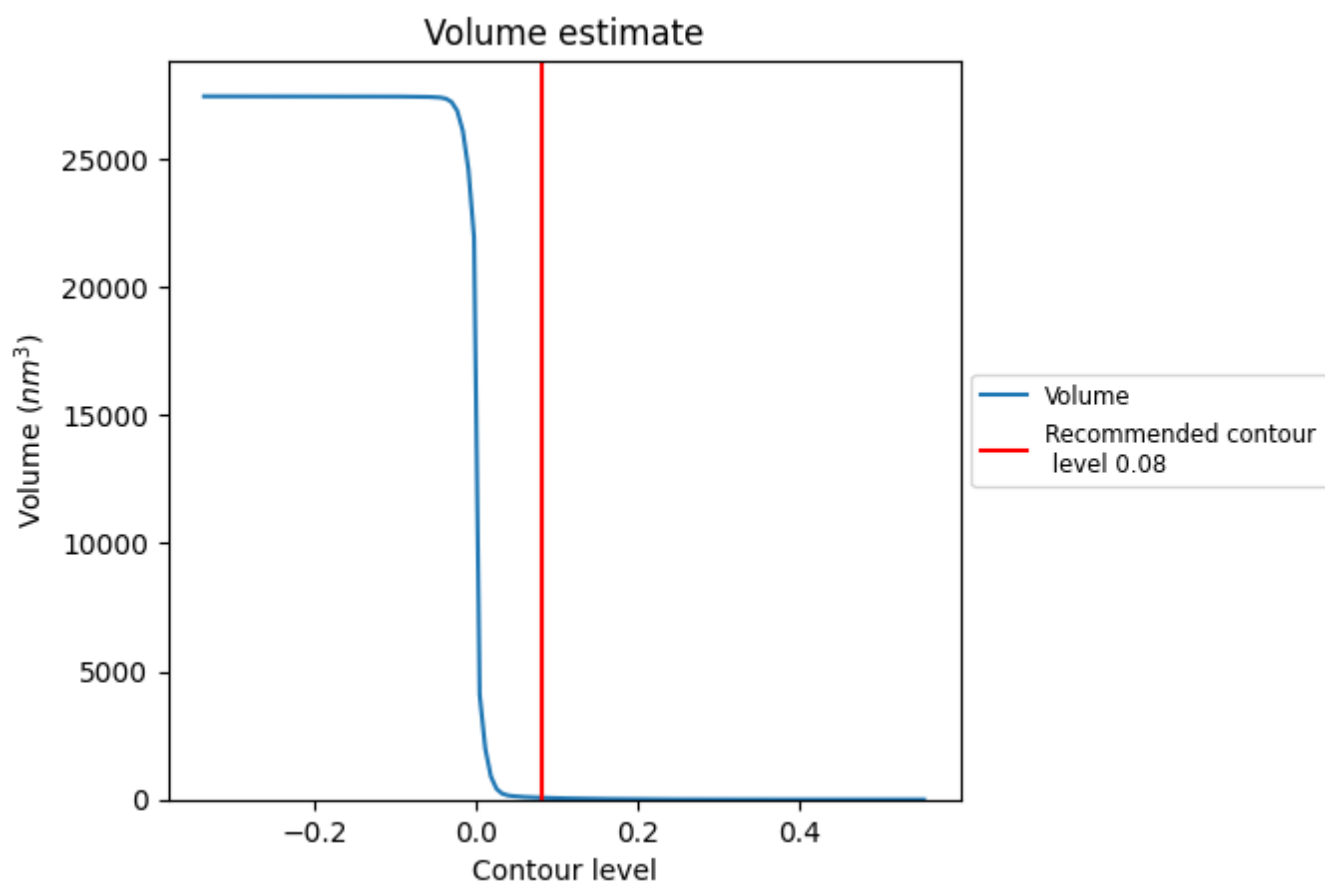
### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



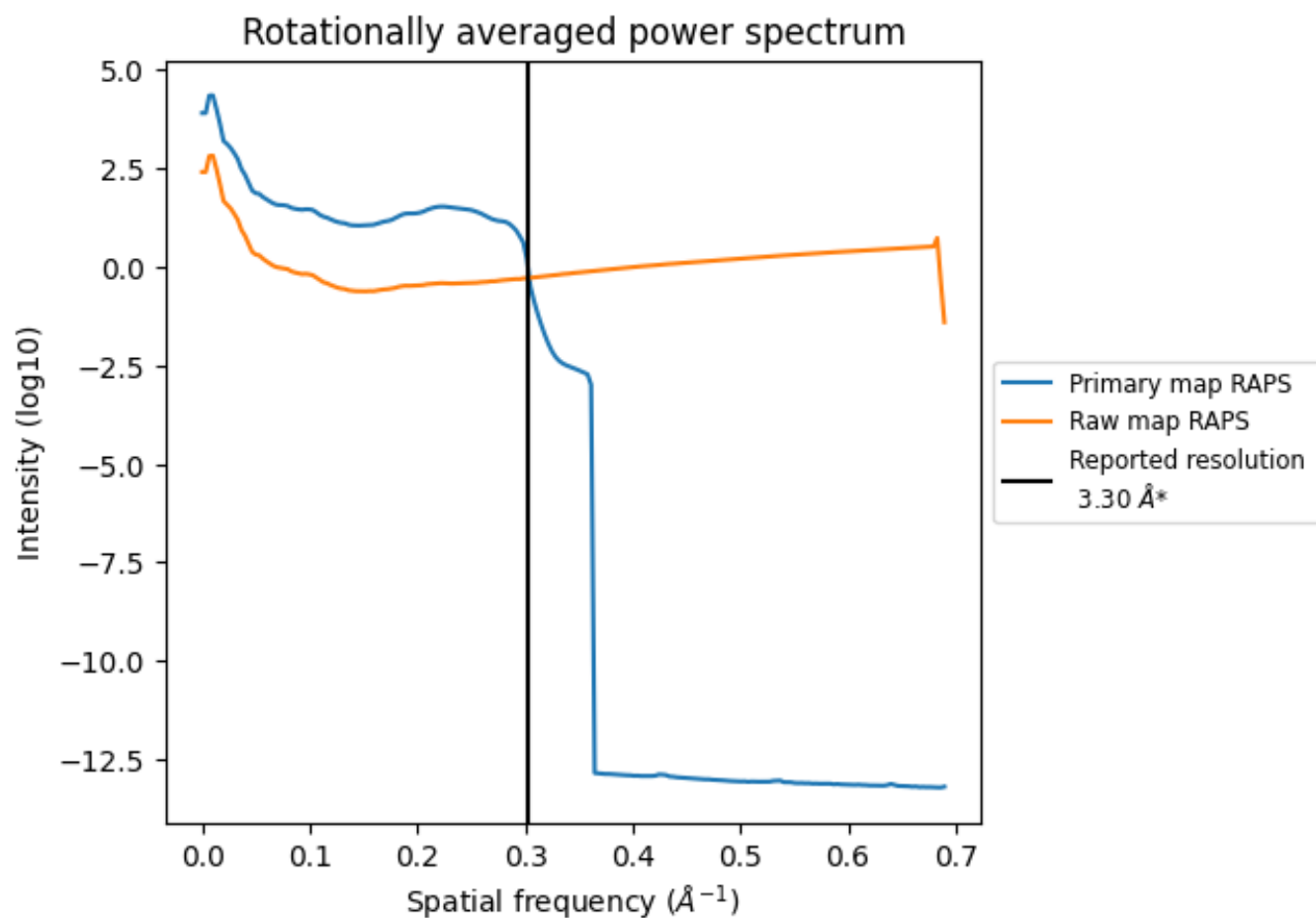
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 73 nm<sup>3</sup>; this corresponds to an approximate mass of 66 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 ⓘ

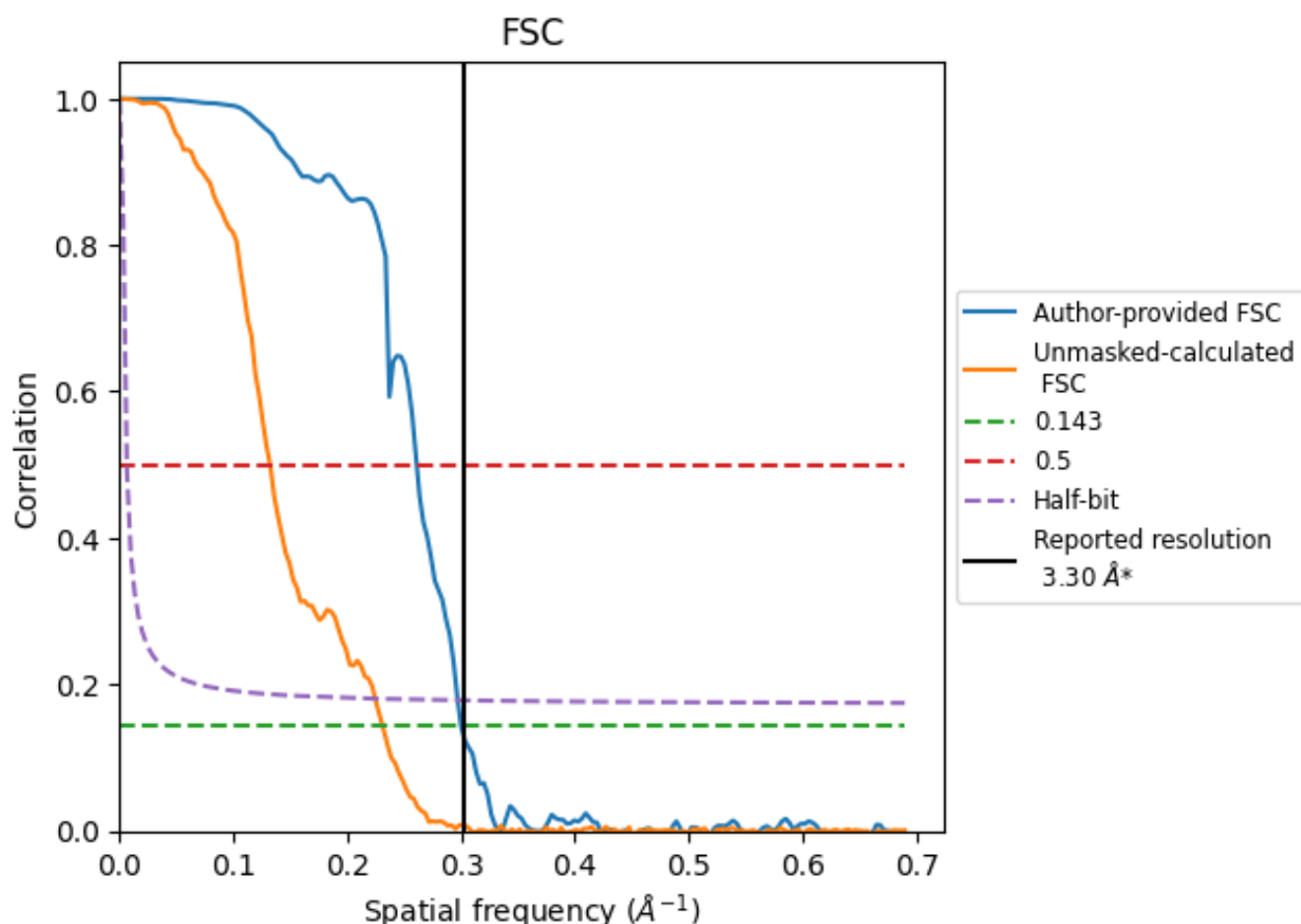


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 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 0.303 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

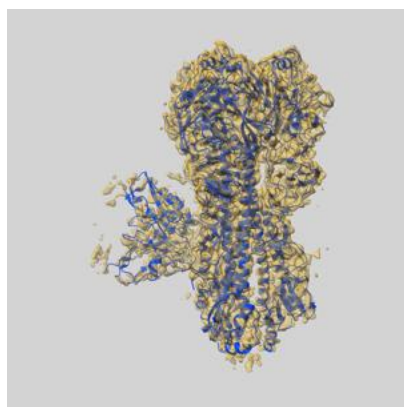
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.33	3.83	3.37
Unmasked-calculated*	4.33	7.56	4.45

\*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 4.33 differs from the reported value 3.3 by more than 10 %

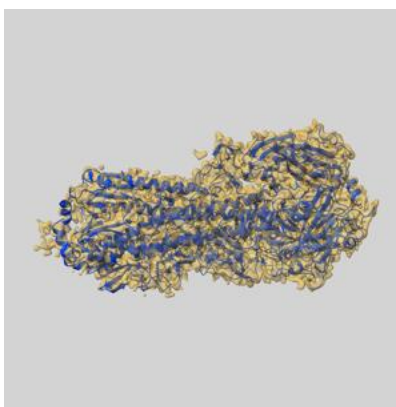
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42529 and PDB model 8UT4. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

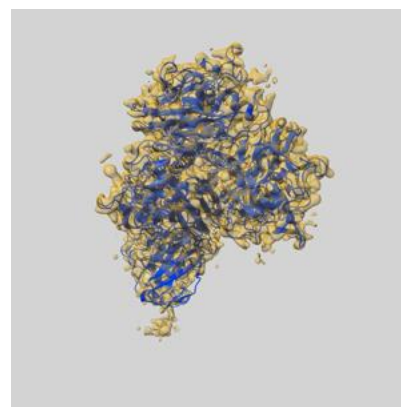
### 9.1 Map-model overlay [i](#)



X



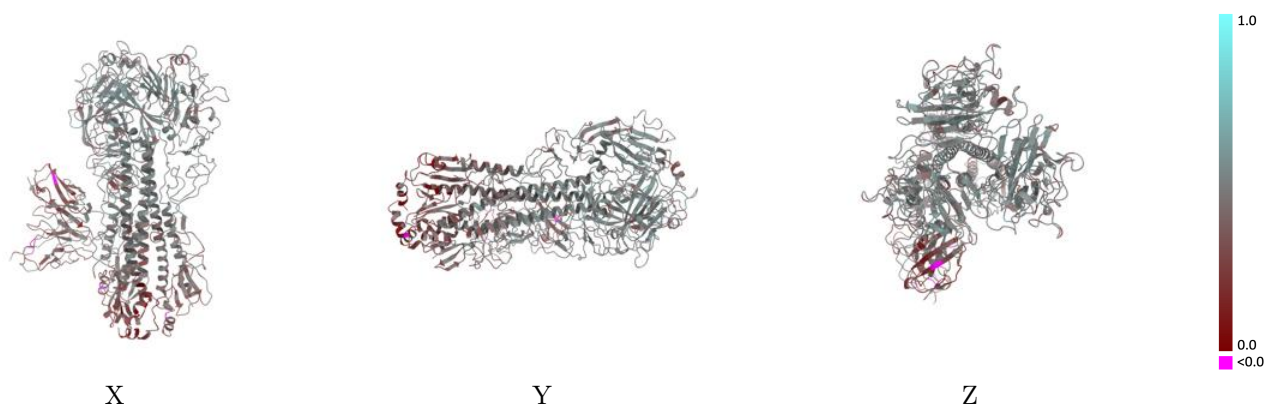
Y



Z

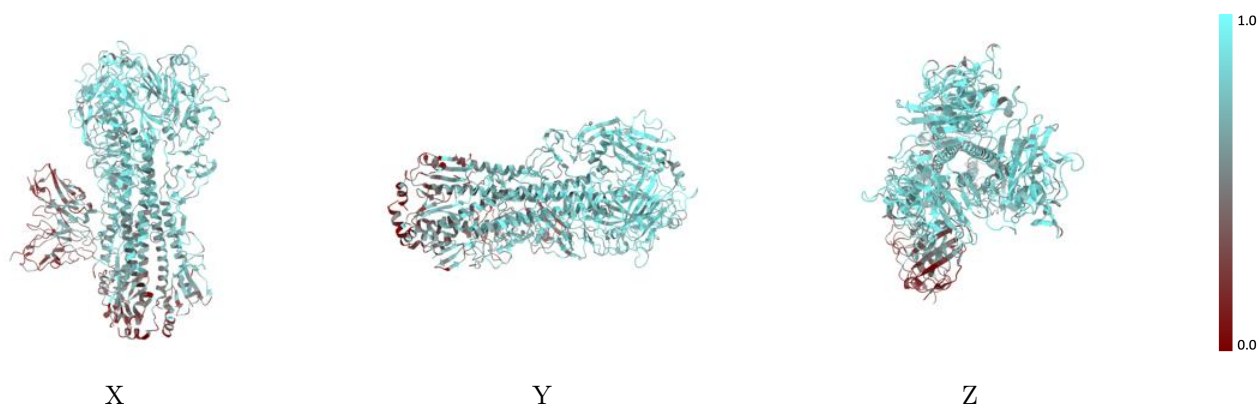
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

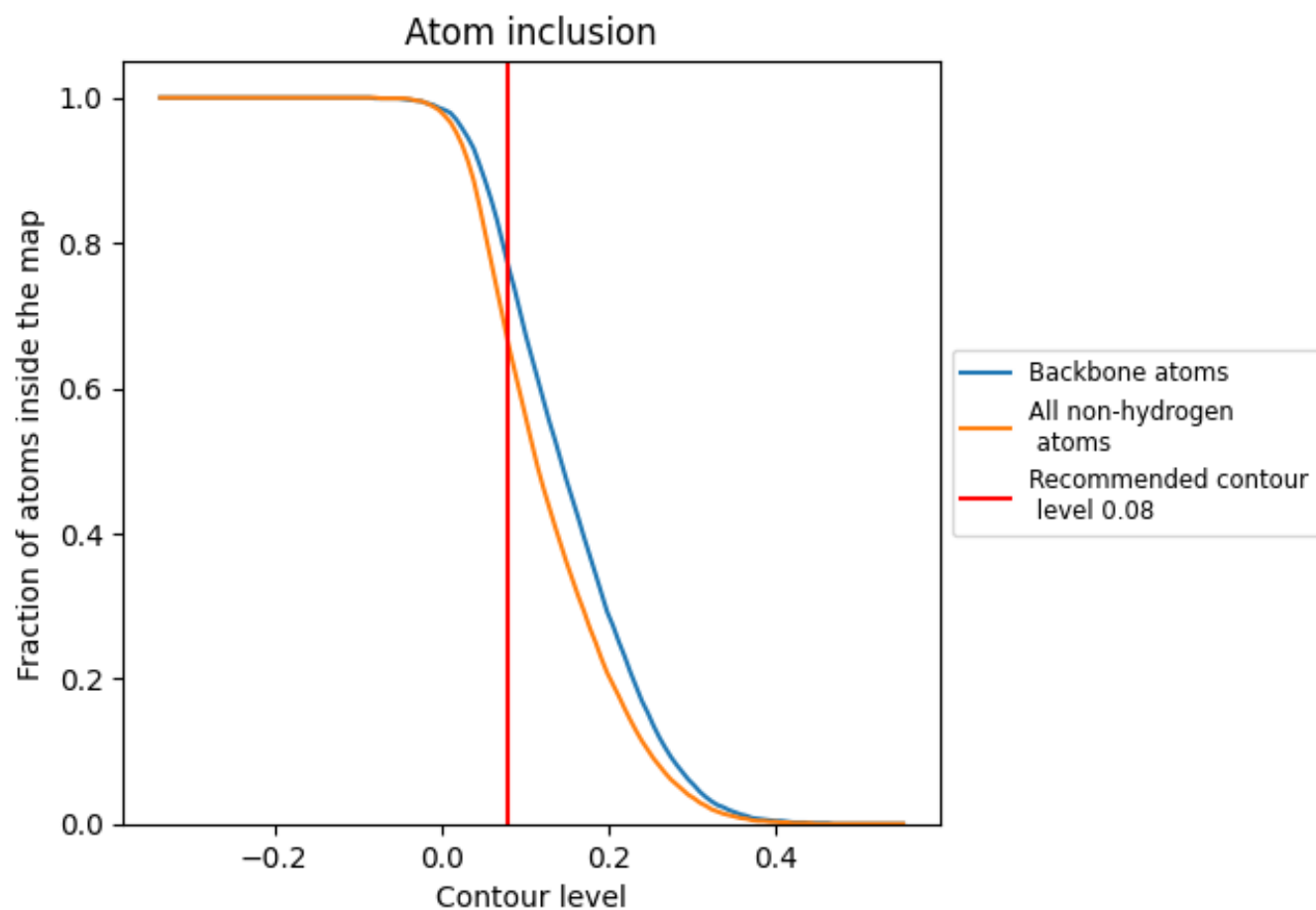
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.08).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 66% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6650	<div></div> 0.4330
A	<div></div> 0.7550	<div></div> 0.4770
B	<div></div> 0.5630	<div></div> 0.3760
C	<div></div> 0.7650	<div></div> 0.4770
D	<div></div> 0.6200	<div></div> 0.4050
E	<div></div> 0.7650	<div></div> 0.4750
F	<div></div> 0.6320	<div></div> 0.4150
H	<div></div> 0.3980	<div></div> 0.3260
I	<div></div> 0.3630	<div></div> 0.3260

1.0

0.0

<0.0