



# wwPDB EM Validation Summary Report ⓘ

Oct 14, 2024 – 11:38 AM EDT

PDB ID : 8TOA  
EMDB ID : EMD-41441  
Title : CryoEM structure of H7 hemagglutinin from A/Shanghai2/2013 H7N9 in complex with a human neutralizing antibody H7.HK2  
Authors : Morano, N.C.; Becker, J.E.; Wu, X.; Shapiro, L.  
Deposited on : 2023-08-03  
Resolution : 3.69 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:

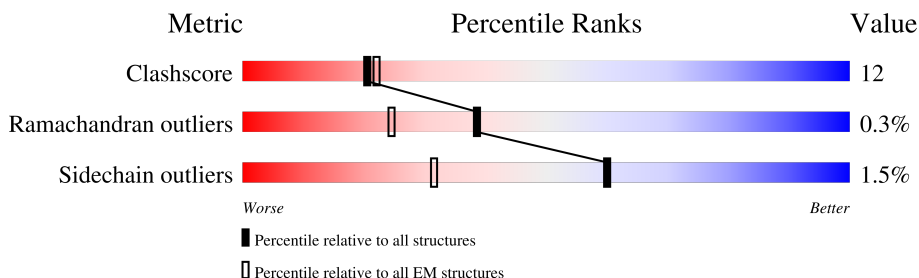
EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.69 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	119	
1	D	119	
1	H	119	
2	B	112	
2	E	112	
2	L	112	
3	C	566	
3	I	566	

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Mol	Chain	Length	Quality of chain
3	K	566	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment at the beginning labeled '7%', a large green segment labeled '70%', a yellow segment labeled '14%', and a grey segment at the end labeled '16%'.</p>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 16570 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 H7.HK2 Neutralizing Antibody Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	H	119	925	586	155	181	3	0	0
1	D	119	925	586	155	181	3	0	0
1	A	119	925	586	155	181	3	0	0

- Molecule 2 is a protein called H7.HK2 Neutralizing Antibody Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	L	111	848	535	145	164	4	0	0
2	E	111	848	535	145	164	4	0	0
2	B	111	848	535	145	164	4	0	0

- Molecule 3 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	473	3699	2296	652	727	24	0	0
3	I	473	3699	2296	652	727	24	0	0
3	K	473	3699	2296	652	727	24	0	0

There are 171 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	20	CYS	THR	conflict	UNP A0A067Y6L0
C	128	SER	ALA	conflict	UNP A0A067Y6L0
C	205	VAL	ALA	conflict	UNP A0A067Y6L0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	274	TYR	HIS	conflict	UNP A0A067Y6L0
C	316E	ARG	-	insertion	UNP A0A067Y6L0
C	316F	ARG	-	insertion	UNP A0A067Y6L0
C	316G	ARG	-	insertion	UNP A0A067Y6L0
C	316H	ARG	-	insertion	UNP A0A067Y6L0
C	316I	ARG	-	insertion	UNP A0A067Y6L0
C	368	CYS	GLN	conflict	UNP A0A067Y6L0
C	496	GLY	PRO	conflict	UNP A0A067Y6L0
C	498	SER	-	expression tag	UNP A0A067Y6L0
C	499	GLY	-	expression tag	UNP A0A067Y6L0
C	500	ARG	-	expression tag	UNP A0A067Y6L0
C	501	LEU	-	expression tag	UNP A0A067Y6L0
C	502	VAL	-	expression tag	UNP A0A067Y6L0
C	503	PRO	-	expression tag	UNP A0A067Y6L0
C	504	ARG	-	expression tag	UNP A0A067Y6L0
C	505	GLY	-	expression tag	UNP A0A067Y6L0
C	506	SER	-	expression tag	UNP A0A067Y6L0
C	507	PRO	-	expression tag	UNP A0A067Y6L0
C	508	GLY	-	expression tag	UNP A0A067Y6L0
C	509	SER	-	expression tag	UNP A0A067Y6L0
C	510	GLY	-	expression tag	UNP A0A067Y6L0
C	511	TYR	-	expression tag	UNP A0A067Y6L0
C	512	ILE	-	expression tag	UNP A0A067Y6L0
C	513	PRO	-	expression tag	UNP A0A067Y6L0
C	514	GLU	-	expression tag	UNP A0A067Y6L0
C	515	ALA	-	expression tag	UNP A0A067Y6L0
C	516	PRO	-	expression tag	UNP A0A067Y6L0
C	517	ARG	-	expression tag	UNP A0A067Y6L0
C	518	ASP	-	expression tag	UNP A0A067Y6L0
C	519	GLY	-	expression tag	UNP A0A067Y6L0
C	520	GLN	-	expression tag	UNP A0A067Y6L0
C	521	ALA	-	expression tag	UNP A0A067Y6L0
C	522	TYR	-	expression tag	UNP A0A067Y6L0
C	523	VAL	-	expression tag	UNP A0A067Y6L0
C	524	ARG	-	expression tag	UNP A0A067Y6L0
C	525	LYS	-	expression tag	UNP A0A067Y6L0
C	526	ASP	-	expression tag	UNP A0A067Y6L0
C	527	GLY	-	expression tag	UNP A0A067Y6L0
C	528	GLU	-	expression tag	UNP A0A067Y6L0
C	529	TRP	-	expression tag	UNP A0A067Y6L0
C	530	VAL	-	expression tag	UNP A0A067Y6L0
C	531	LEU	-	expression tag	UNP A0A067Y6L0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	532	LEU	-	expression tag	UNP A0A067Y6L0
C	533	SER	-	expression tag	UNP A0A067Y6L0
C	534	THR	-	expression tag	UNP A0A067Y6L0
C	535	PHE	-	expression tag	UNP A0A067Y6L0
C	536	LEU	-	expression tag	UNP A0A067Y6L0
C	537	GLY	-	expression tag	UNP A0A067Y6L0
C	538	HIS	-	expression tag	UNP A0A067Y6L0
C	539	HIS	-	expression tag	UNP A0A067Y6L0
C	540	HIS	-	expression tag	UNP A0A067Y6L0
C	541	HIS	-	expression tag	UNP A0A067Y6L0
C	542	HIS	-	expression tag	UNP A0A067Y6L0
C	543	HIS	-	expression tag	UNP A0A067Y6L0
I	20	CYS	THR	conflict	UNP A0A067Y6L0
I	128	SER	ALA	conflict	UNP A0A067Y6L0
I	205	VAL	ALA	conflict	UNP A0A067Y6L0
I	274	TYR	HIS	conflict	UNP A0A067Y6L0
I	316E	ARG	-	insertion	UNP A0A067Y6L0
I	316F	ARG	-	insertion	UNP A0A067Y6L0
I	316G	ARG	-	insertion	UNP A0A067Y6L0
I	316H	ARG	-	insertion	UNP A0A067Y6L0
I	316I	ARG	-	insertion	UNP A0A067Y6L0
I	368	CYS	GLN	conflict	UNP A0A067Y6L0
I	496	GLY	PRO	conflict	UNP A0A067Y6L0
I	498	SER	-	expression tag	UNP A0A067Y6L0
I	499	GLY	-	expression tag	UNP A0A067Y6L0
I	500	ARG	-	expression tag	UNP A0A067Y6L0
I	501	LEU	-	expression tag	UNP A0A067Y6L0
I	502	VAL	-	expression tag	UNP A0A067Y6L0
I	503	PRO	-	expression tag	UNP A0A067Y6L0
I	504	ARG	-	expression tag	UNP A0A067Y6L0
I	505	GLY	-	expression tag	UNP A0A067Y6L0
I	506	SER	-	expression tag	UNP A0A067Y6L0
I	507	PRO	-	expression tag	UNP A0A067Y6L0
I	508	GLY	-	expression tag	UNP A0A067Y6L0
I	509	SER	-	expression tag	UNP A0A067Y6L0
I	510	GLY	-	expression tag	UNP A0A067Y6L0
I	511	TYR	-	expression tag	UNP A0A067Y6L0
I	512	ILE	-	expression tag	UNP A0A067Y6L0
I	513	PRO	-	expression tag	UNP A0A067Y6L0
I	514	GLU	-	expression tag	UNP A0A067Y6L0
I	515	ALA	-	expression tag	UNP A0A067Y6L0
I	516	PRO	-	expression tag	UNP A0A067Y6L0

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Chain	Residue	Modelled	Actual	Comment	Reference
I	517	ARG	-	expression tag	UNP A0A067Y6L0
I	518	ASP	-	expression tag	UNP A0A067Y6L0
I	519	GLY	-	expression tag	UNP A0A067Y6L0
I	520	GLN	-	expression tag	UNP A0A067Y6L0
I	521	ALA	-	expression tag	UNP A0A067Y6L0
I	522	TYR	-	expression tag	UNP A0A067Y6L0
I	523	VAL	-	expression tag	UNP A0A067Y6L0
I	524	ARG	-	expression tag	UNP A0A067Y6L0
I	525	LYS	-	expression tag	UNP A0A067Y6L0
I	526	ASP	-	expression tag	UNP A0A067Y6L0
I	527	GLY	-	expression tag	UNP A0A067Y6L0
I	528	GLU	-	expression tag	UNP A0A067Y6L0
I	529	TRP	-	expression tag	UNP A0A067Y6L0
I	530	VAL	-	expression tag	UNP A0A067Y6L0
I	531	LEU	-	expression tag	UNP A0A067Y6L0
I	532	LEU	-	expression tag	UNP A0A067Y6L0
I	533	SER	-	expression tag	UNP A0A067Y6L0
I	534	THR	-	expression tag	UNP A0A067Y6L0
I	535	PHE	-	expression tag	UNP A0A067Y6L0
I	536	LEU	-	expression tag	UNP A0A067Y6L0
I	537	GLY	-	expression tag	UNP A0A067Y6L0
I	538	HIS	-	expression tag	UNP A0A067Y6L0
I	539	HIS	-	expression tag	UNP A0A067Y6L0
I	540	HIS	-	expression tag	UNP A0A067Y6L0
I	541	HIS	-	expression tag	UNP A0A067Y6L0
I	542	HIS	-	expression tag	UNP A0A067Y6L0
I	543	HIS	-	expression tag	UNP A0A067Y6L0
K	20	CYS	THR	conflict	UNP A0A067Y6L0
K	128	SER	ALA	conflict	UNP A0A067Y6L0
K	205	VAL	ALA	conflict	UNP A0A067Y6L0
K	274	TYR	HIS	conflict	UNP A0A067Y6L0
K	316E	ARG	-	insertion	UNP A0A067Y6L0
K	316F	ARG	-	insertion	UNP A0A067Y6L0
K	316G	ARG	-	insertion	UNP A0A067Y6L0
K	316H	ARG	-	insertion	UNP A0A067Y6L0
K	316I	ARG	-	insertion	UNP A0A067Y6L0
K	368	CYS	GLN	conflict	UNP A0A067Y6L0
K	496	GLY	PRO	conflict	UNP A0A067Y6L0
K	498	SER	-	expression tag	UNP A0A067Y6L0
K	499	GLY	-	expression tag	UNP A0A067Y6L0
K	500	ARG	-	expression tag	UNP A0A067Y6L0
K	501	LEU	-	expression tag	UNP A0A067Y6L0

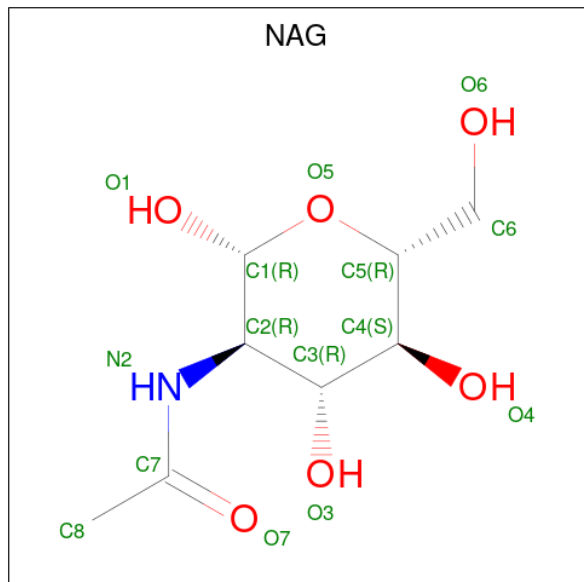
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Chain	Residue	Modelled	Actual	Comment	Reference
K	502	VAL	-	expression tag	UNP A0A067Y6L0
K	503	PRO	-	expression tag	UNP A0A067Y6L0
K	504	ARG	-	expression tag	UNP A0A067Y6L0
K	505	GLY	-	expression tag	UNP A0A067Y6L0
K	506	SER	-	expression tag	UNP A0A067Y6L0
K	507	PRO	-	expression tag	UNP A0A067Y6L0
K	508	GLY	-	expression tag	UNP A0A067Y6L0
K	509	SER	-	expression tag	UNP A0A067Y6L0
K	510	GLY	-	expression tag	UNP A0A067Y6L0
K	511	TYR	-	expression tag	UNP A0A067Y6L0
K	512	ILE	-	expression tag	UNP A0A067Y6L0
K	513	PRO	-	expression tag	UNP A0A067Y6L0
K	514	GLU	-	expression tag	UNP A0A067Y6L0
K	515	ALA	-	expression tag	UNP A0A067Y6L0
K	516	PRO	-	expression tag	UNP A0A067Y6L0
K	517	ARG	-	expression tag	UNP A0A067Y6L0
K	518	ASP	-	expression tag	UNP A0A067Y6L0
K	519	GLY	-	expression tag	UNP A0A067Y6L0
K	520	GLN	-	expression tag	UNP A0A067Y6L0
K	521	ALA	-	expression tag	UNP A0A067Y6L0
K	522	TYR	-	expression tag	UNP A0A067Y6L0
K	523	VAL	-	expression tag	UNP A0A067Y6L0
K	524	ARG	-	expression tag	UNP A0A067Y6L0
K	525	LYS	-	expression tag	UNP A0A067Y6L0
K	526	ASP	-	expression tag	UNP A0A067Y6L0
K	527	GLY	-	expression tag	UNP A0A067Y6L0
K	528	GLU	-	expression tag	UNP A0A067Y6L0
K	529	TRP	-	expression tag	UNP A0A067Y6L0
K	530	VAL	-	expression tag	UNP A0A067Y6L0
K	531	LEU	-	expression tag	UNP A0A067Y6L0
K	532	LEU	-	expression tag	UNP A0A067Y6L0
K	533	SER	-	expression tag	UNP A0A067Y6L0
K	534	THR	-	expression tag	UNP A0A067Y6L0
K	535	PHE	-	expression tag	UNP A0A067Y6L0
K	536	LEU	-	expression tag	UNP A0A067Y6L0
K	537	GLY	-	expression tag	UNP A0A067Y6L0
K	538	HIS	-	expression tag	UNP A0A067Y6L0
K	539	HIS	-	expression tag	UNP A0A067Y6L0
K	540	HIS	-	expression tag	UNP A0A067Y6L0
K	541	HIS	-	expression tag	UNP A0A067Y6L0
K	542	HIS	-	expression tag	UNP A0A067Y6L0
K	543	HIS	-	expression tag	UNP A0A067Y6L0



- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

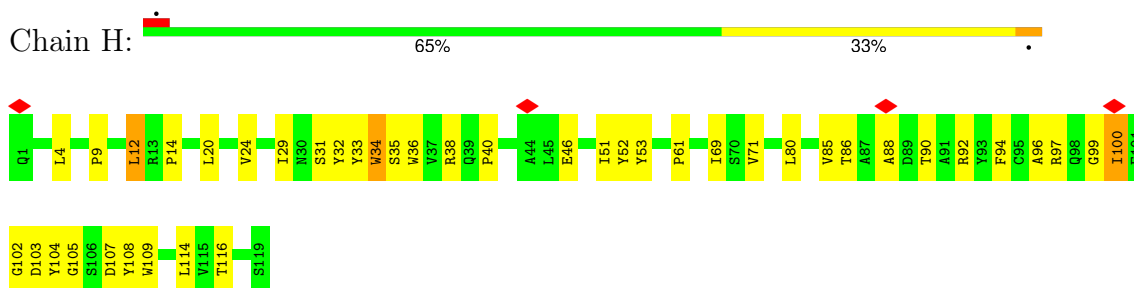


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	L	1	Total 14	8	1	5	0
4	E	1	Total 14	8	1	5	0
4	B	1	Total 14	8	1	5	0
4	C	1	Total 14	8	1	5	0
4	C	1	Total 14	8	1	5	0
4	C	1	Total 14	8	1	5	0
4	I	1	Total 14	8	1	5	0
4	I	1	Total 14	8	1	5	0
4	I	1	Total 14	8	1	5	0
4	K	1	Total 14	8	1	5	0
4	K	1	Total 14	8	1	5	0

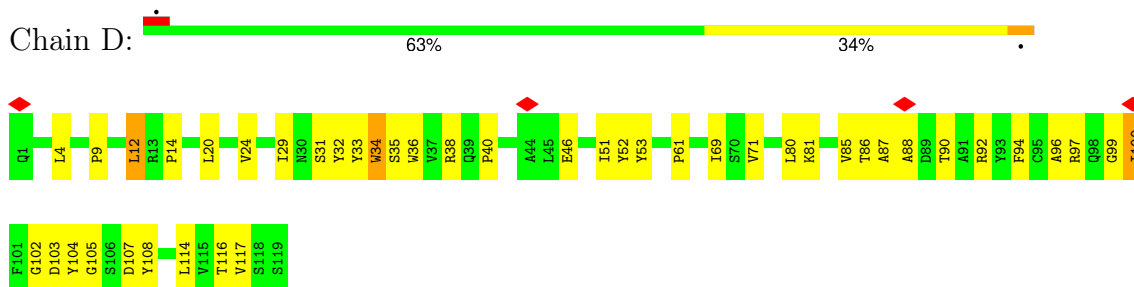
### 3 Residue-property plots [i](#)

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.

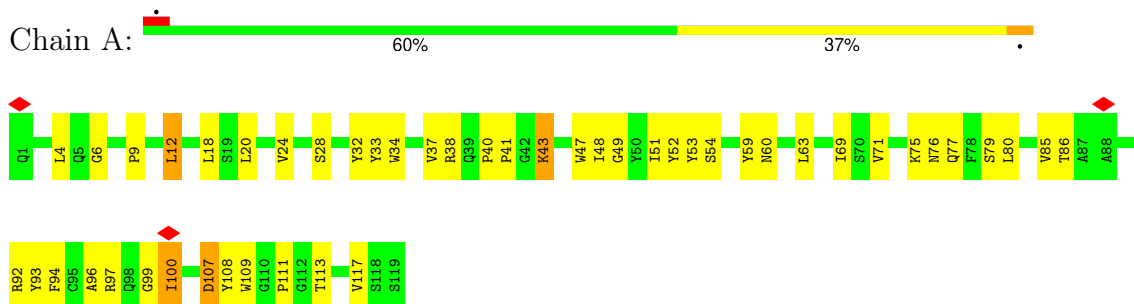
- Molecule 1: H7.HK2 Neutralizing Antibody Heavy Chain



- Molecule 1: H7.HK2 Neutralizing Antibody Heavy Chain

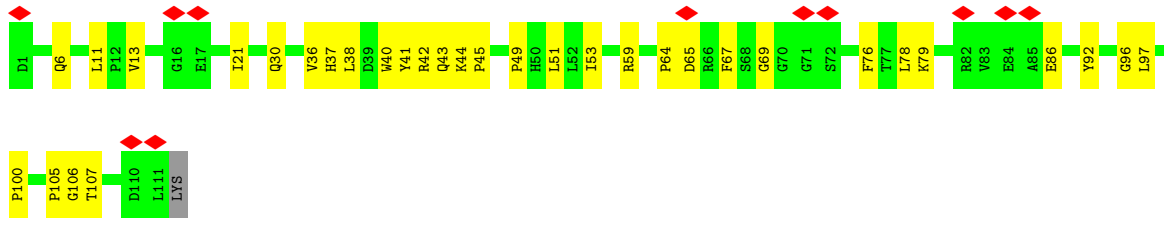


- Molecule 1: H7.HK2 Neutralizing Antibody Heavy Chain



- Molecule 2: H7.HK2 Neutralizing Antibody Light Chain





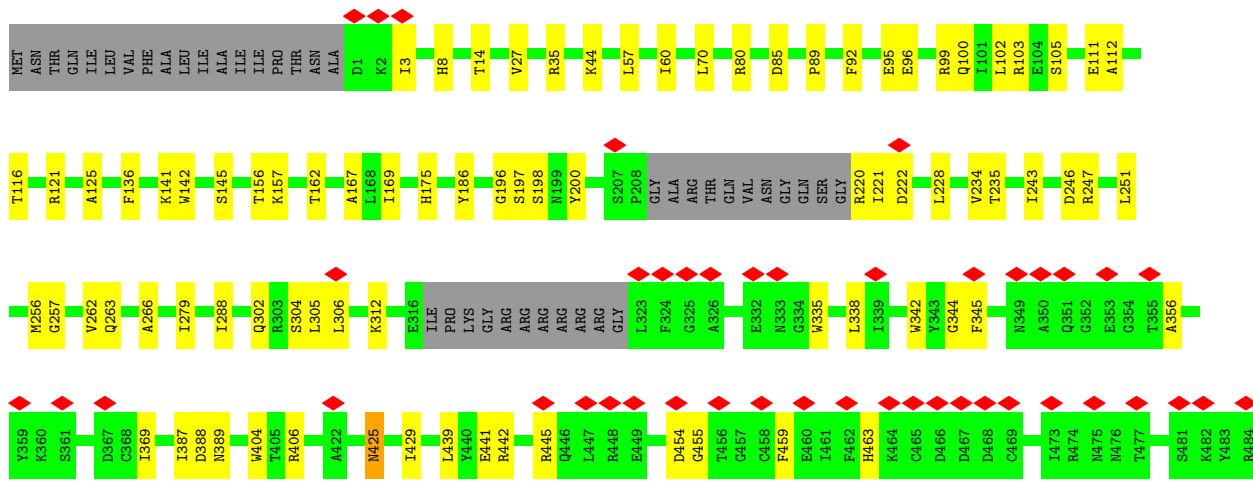
● Molecule 2: H7.HK2 Neutralizing Antibody Light Chain

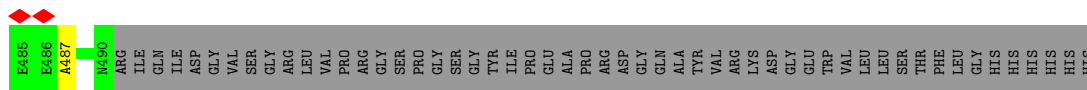


● Molecule 2: H7.HK2 Neutralizing Antibody Light Chain

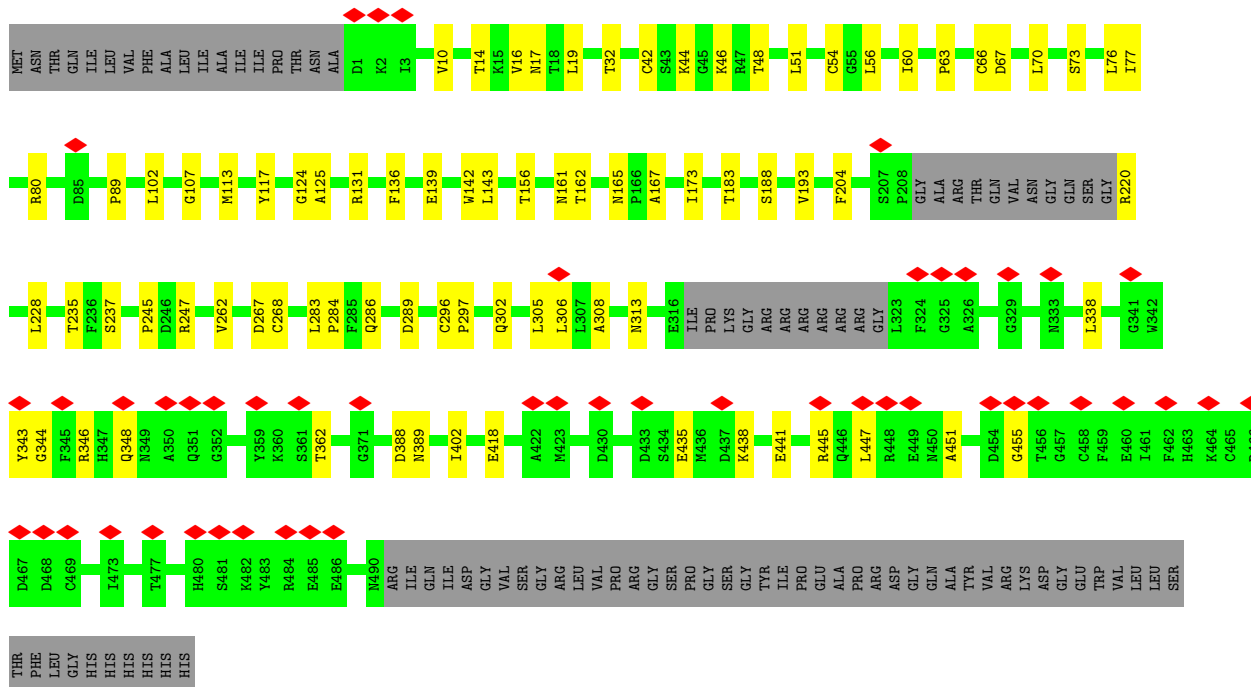


● Molecule 3: Hemagglutinin

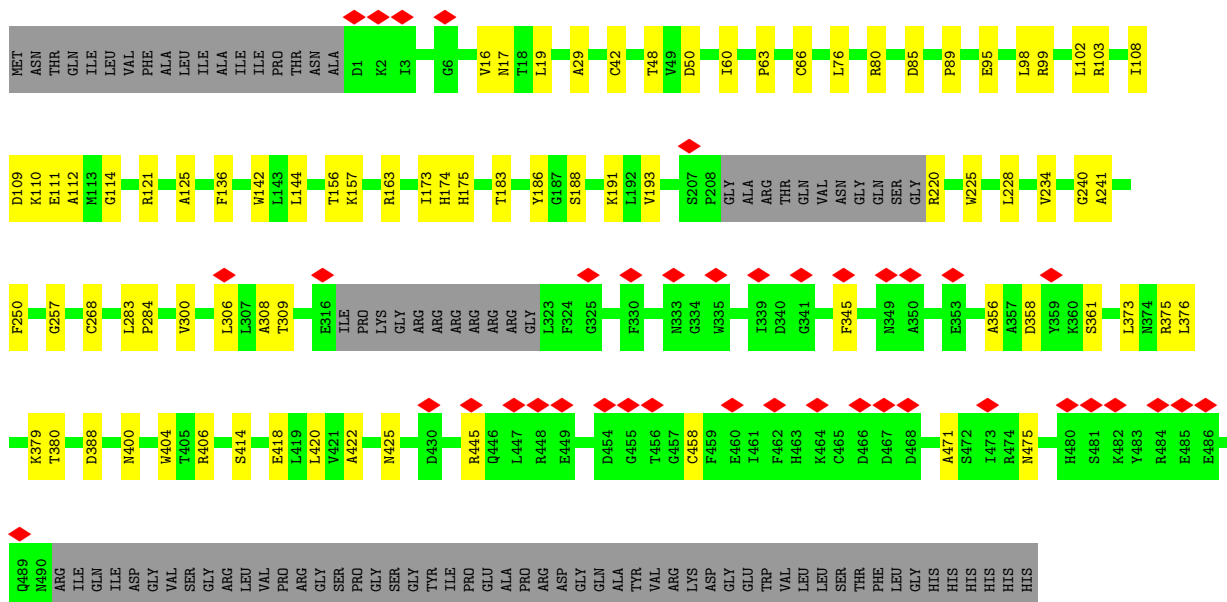




• Molecule 3: Hemagglutinin



• Molecule 3: Hemagglutinin



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	191469	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	58.06	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.597	Depositor
Minimum map value	-0.399	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.0829	Depositor
Map size (Å)	318.72, 318.72, 318.72	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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	0.62	0/950	0.66	0/1294
1	D	0.48	0/950	0.69	0/1294
1	H	0.48	0/950	0.70	0/1294
2	B	0.63	0/871	0.62	0/1186
2	E	0.33	0/871	0.63	0/1186
2	L	0.33	0/871	0.63	0/1186
3	C	0.29	0/3767	0.60	0/5084
3	I	0.29	0/3767	0.60	0/5084
3	K	0.31	0/3767	0.60	0/5084
All	All	0.37	0/16764	0.62	0/22692

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	99	THR	Peptide

## 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	925	0	887	43	0
1	D	925	0	886	71	0
1	H	925	0	886	69	0
2	B	848	0	814	34	0
2	E	848	0	814	38	0
2	L	848	0	814	37	0
3	C	3699	0	3545	78	0
3	I	3699	0	3547	49	0
3	K	3699	0	3548	72	0
4	B	14	0	13	1	0
4	C	42	0	39	0	0
4	E	14	0	13	0	0
4	I	42	0	39	0	0
4	K	28	0	26	0	0
4	L	14	0	13	0	0
All	All	16570	0	15884	387	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 12.

The worst 5 of 387 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:D:104:TYR:CD2	3:K:157:LYS:HD2	1.44	1.50
1:D:104:TYR:CG	3:K:157:LYS:CE	2.30	1.15
1:D:104:TYR:HB2	3:K:157:LYS:HD3	1.24	1.13
1:D:104:TYR:CG	3:K:157:LYS:HD2	1.84	1.13
1:D:104:TYR:HB2	3:K:157:LYS:CD	1.71	1.12

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	117/119 (98%)	101 (86%)	13 (11%)	3 (3%)	4	29
1	D	117/119 (98%)	99 (85%)	17 (14%)	1 (1%)	14	47
1	H	117/119 (98%)	99 (85%)	17 (14%)	1 (1%)	14	47
2	B	109/112 (97%)	99 (91%)	9 (8%)	1 (1%)	14	47
2	E	109/112 (97%)	103 (94%)	6 (6%)	0	100	100
2	L	109/112 (97%)	103 (94%)	6 (6%)	0	100	100
3	C	467/566 (82%)	446 (96%)	21 (4%)	0	100	100
3	I	467/566 (82%)	435 (93%)	32 (7%)	0	100	100
3	K	467/566 (82%)	434 (93%)	33 (7%)	0	100	100
All	All	2079/2391 (87%)	1919 (92%)	154 (7%)	6 (0%)	38	67

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	100	ILE
1	D	100	ILE
1	A	100	ILE
1	A	107	ASP
2	B	8	PRO

### 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	102/102 (100%)	96 (94%)	6 (6%)	16	44
1	D	102/102 (100%)	99 (97%)	3 (3%)	37	59
1	H	102/102 (100%)	99 (97%)	3 (3%)	37	59
2	B	95/96 (99%)	83 (87%)	12 (13%)	3	19
2	E	95/96 (99%)	95 (100%)	0	100	100
2	L	95/96 (99%)	95 (100%)	0	100	100
3	C	401/476 (84%)	400 (100%)	1 (0%)	92	96
3	I	401/476 (84%)	401 (100%)	0	100	100
3	K	401/476 (84%)	399 (100%)	2 (0%)	86	92
All	All	1794/2022 (89%)	1767 (98%)	27 (2%)	60	75

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	36	VAL
2	B	59	ARG
3	C	425	ASN
2	B	57	PHE
2	B	79	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
3	K	400	ASN
3	K	426	GLN
1	D	30	ASN
1	A	1	GLN
1	A	30	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 [i](#)

11 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
4	NAG	K	601	3	14,14,15	0.27	0	17,19,21	0.48	0
4	NAG	C	601	3	14,14,15	0.34	0	17,19,21	0.46	0
4	NAG	L	201	2	14,14,15	0.46	0	17,19,21	0.64	1 (5%)
4	NAG	E	201	2	14,14,15	0.46	0	17,19,21	0.63	1 (5%)
4	NAG	C	603	3	14,14,15	0.31	0	17,19,21	0.49	0
4	NAG	I	602	3	14,14,15	0.42	0	17,19,21	0.92	1 (5%)
4	NAG	B	201	2	14,14,15	0.47	0	17,19,21	0.64	1 (5%)
4	NAG	C	602	3	14,14,15	0.26	0	17,19,21	0.47	0
4	NAG	I	601	3	14,14,15	0.31	0	17,19,21	0.53	0
4	NAG	I	603	3	14,14,15	0.31	0	17,19,21	0.49	0
4	NAG	K	602	3	14,14,15	0.41	0	17,19,21	0.94	1 (5%)

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
4	NAG	K	601	3	-	2/6/23/26	0/1/1/1
4	NAG	C	601	3	-	0/6/23/26	0/1/1/1
4	NAG	L	201	2	-	2/6/23/26	0/1/1/1
4	NAG	E	201	2	-	2/6/23/26	0/1/1/1
4	NAG	C	603	3	-	0/6/23/26	0/1/1/1
4	NAG	I	602	3	-	3/6/23/26	0/1/1/1

*Continued on next page...*

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	201	2	-	2/6/23/26	0/1/1/1
4	NAG	C	602	3	-	2/6/23/26	0/1/1/1
4	NAG	I	601	3	-	2/6/23/26	0/1/1/1
4	NAG	I	603	3	-	0/6/23/26	0/1/1/1
4	NAG	K	602	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	602	NAG	C2-N2-C7	3.05	126.99	122.90
4	I	602	NAG	C2-N2-C7	3.00	126.92	122.90
4	B	201	NAG	C1-O5-C5	2.20	115.14	112.19
4	E	201	NAG	C1-O5-C5	2.20	115.13	112.19
4	L	201	NAG	C1-O5-C5	2.19	115.12	112.19

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	201	NAG	C4-C5-C6-O6
4	E	201	NAG	C4-C5-C6-O6
4	B	201	NAG	C4-C5-C6-O6
4	I	601	NAG	O5-C5-C6-O6
4	K	601	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
4	B	201	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

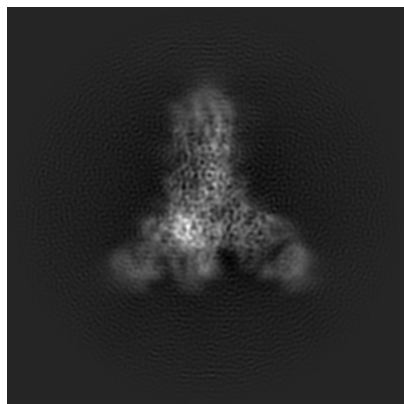
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41441. These allow visual inspection of the internal detail of the map and identification of artifacts.

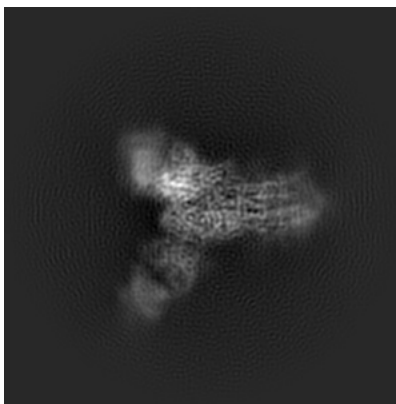
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

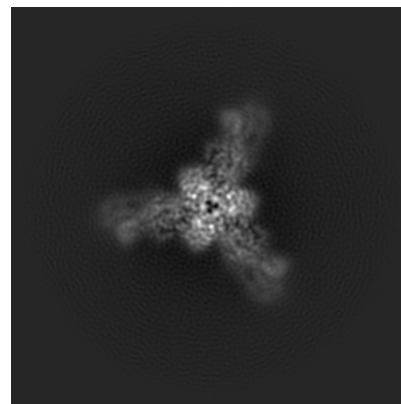
#### 6.1.1 Primary map



X

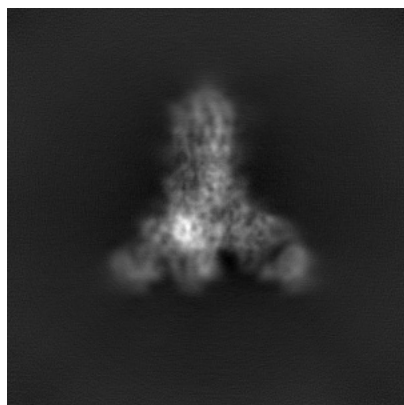


Y

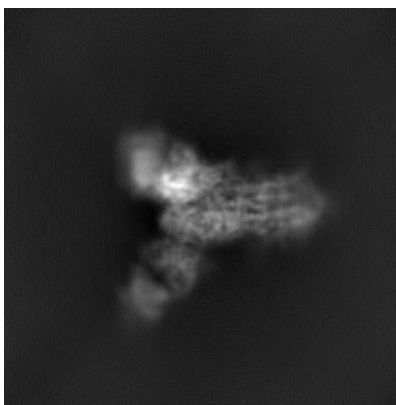


Z

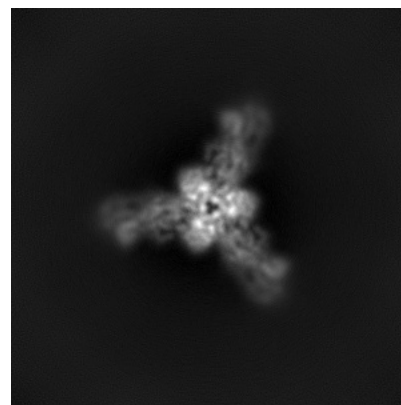
#### 6.1.2 Raw map



X



Y

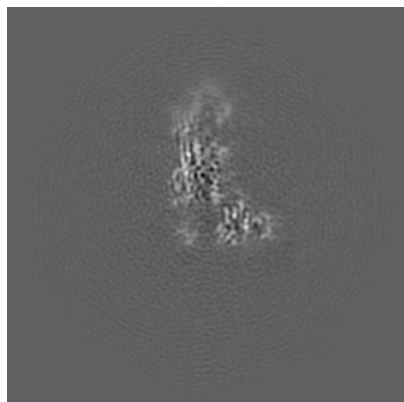


Z

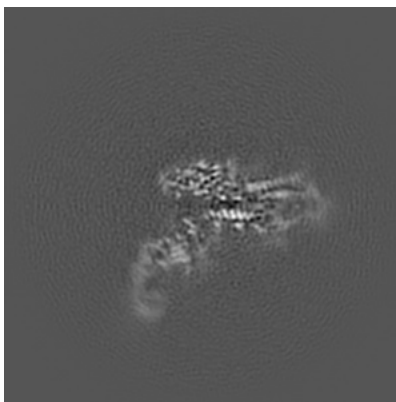
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

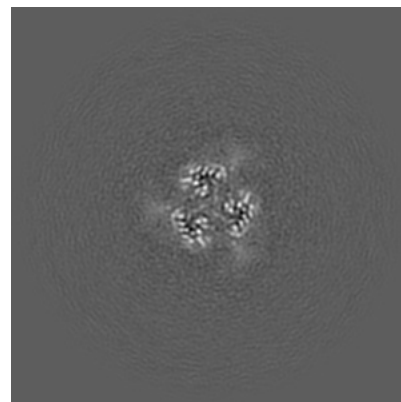
### 6.2.1 Primary map



X Index: 192

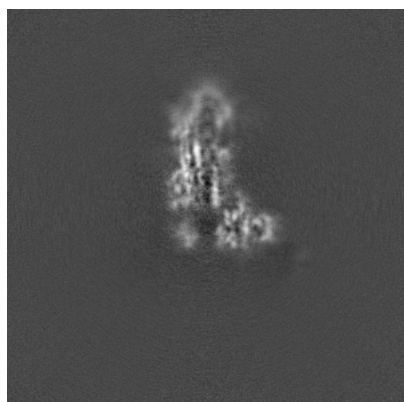


Y Index: 192

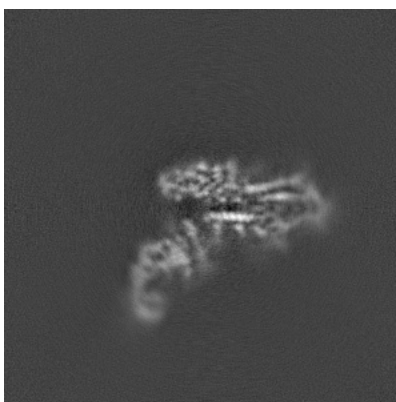


Z Index: 192

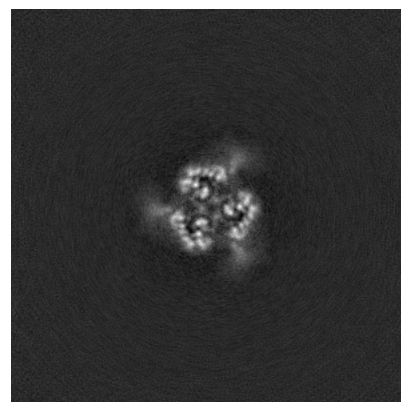
### 6.2.2 Raw map



X Index: 192



Y Index: 192

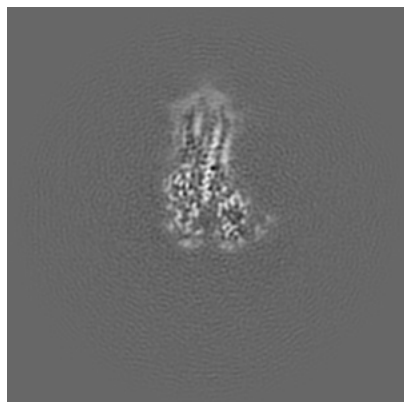


Z Index: 192

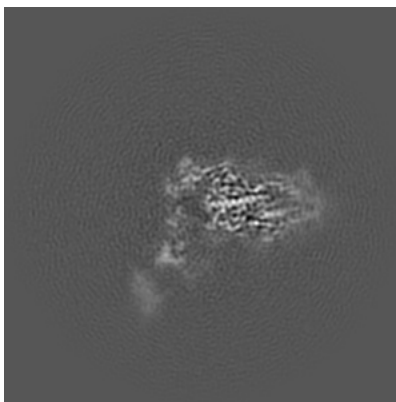
The images above show central slices of the map in three orthogonal directions.

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

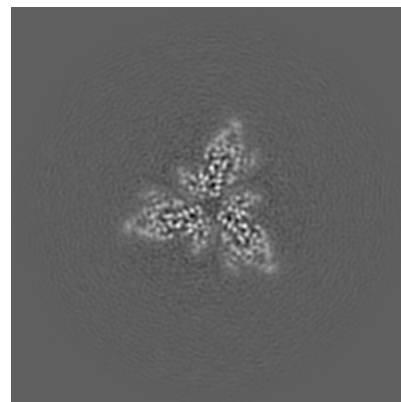
### 6.3.1 Primary map



X Index: 185

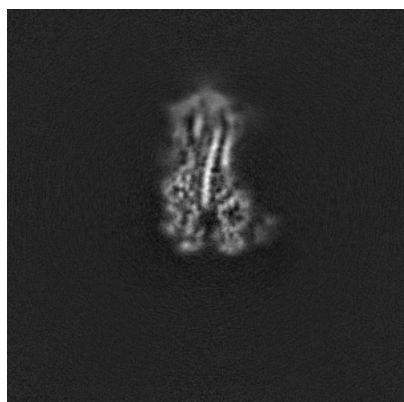


Y Index: 200

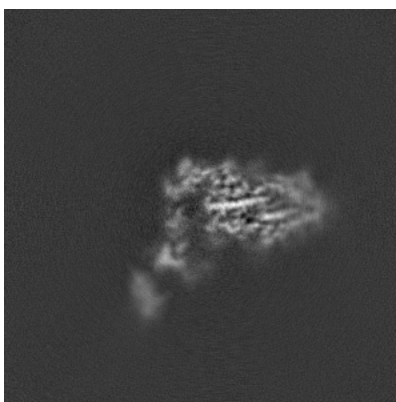


Z Index: 173

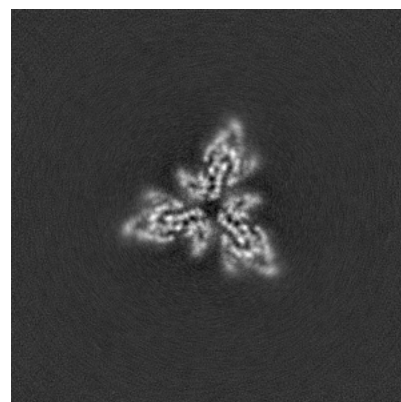
### 6.3.2 Raw map



X Index: 184



Y Index: 200

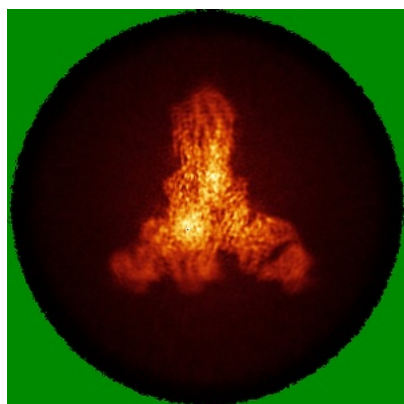


Z Index: 172

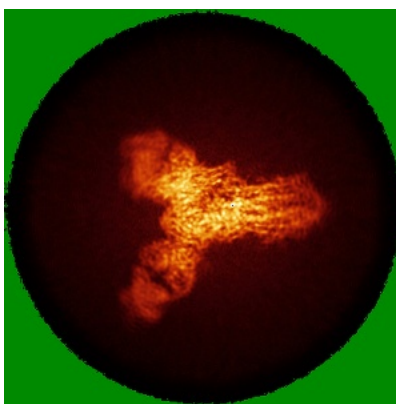
The images above show the largest variance slices of the map in three orthogonal directions.

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

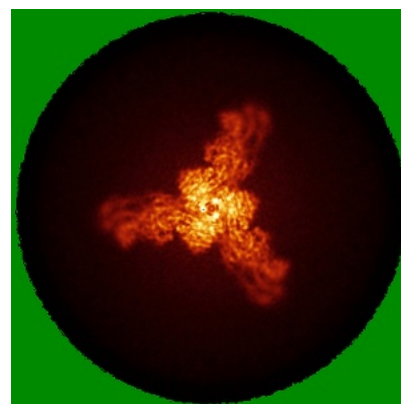
### 6.4.1 Primary map



X

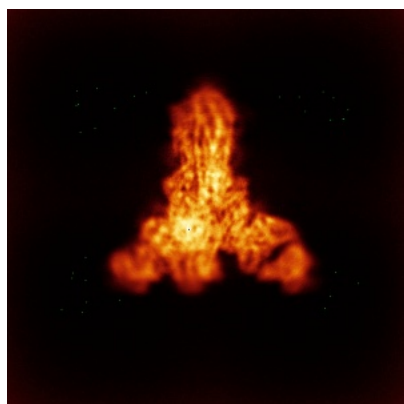


Y

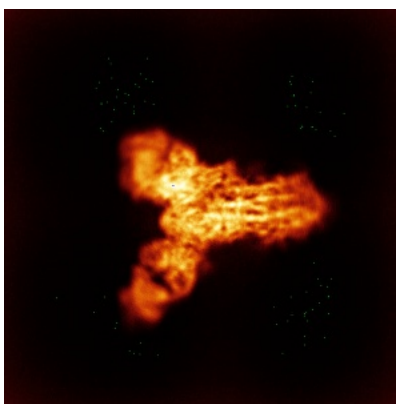


Z

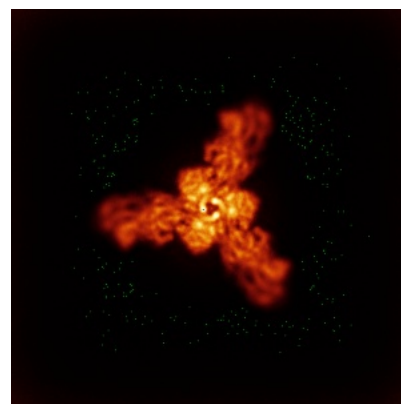
### 6.4.2 Raw map



X



Y



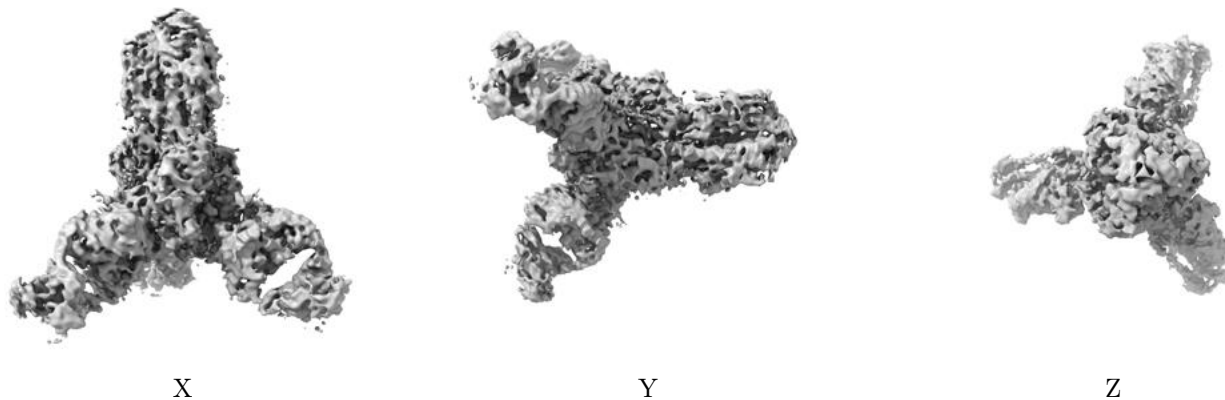
Z

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



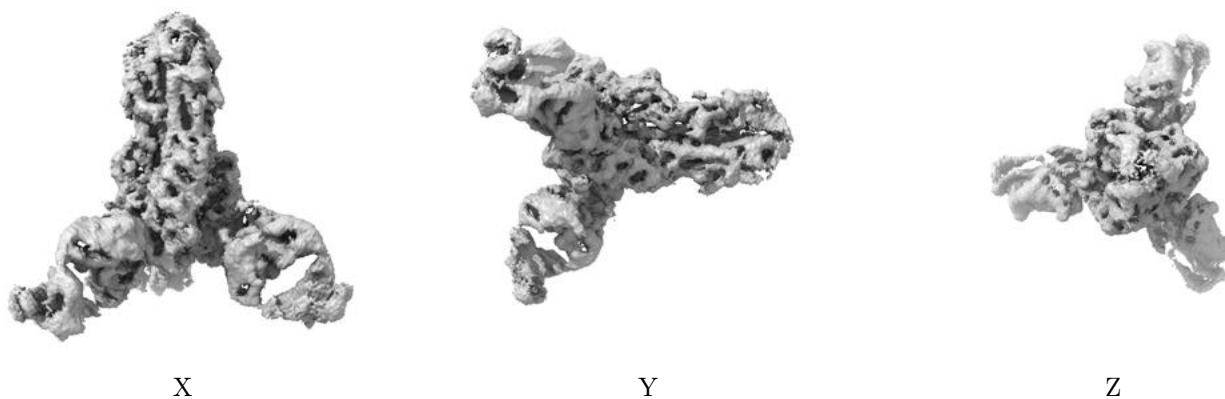
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0829. 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.

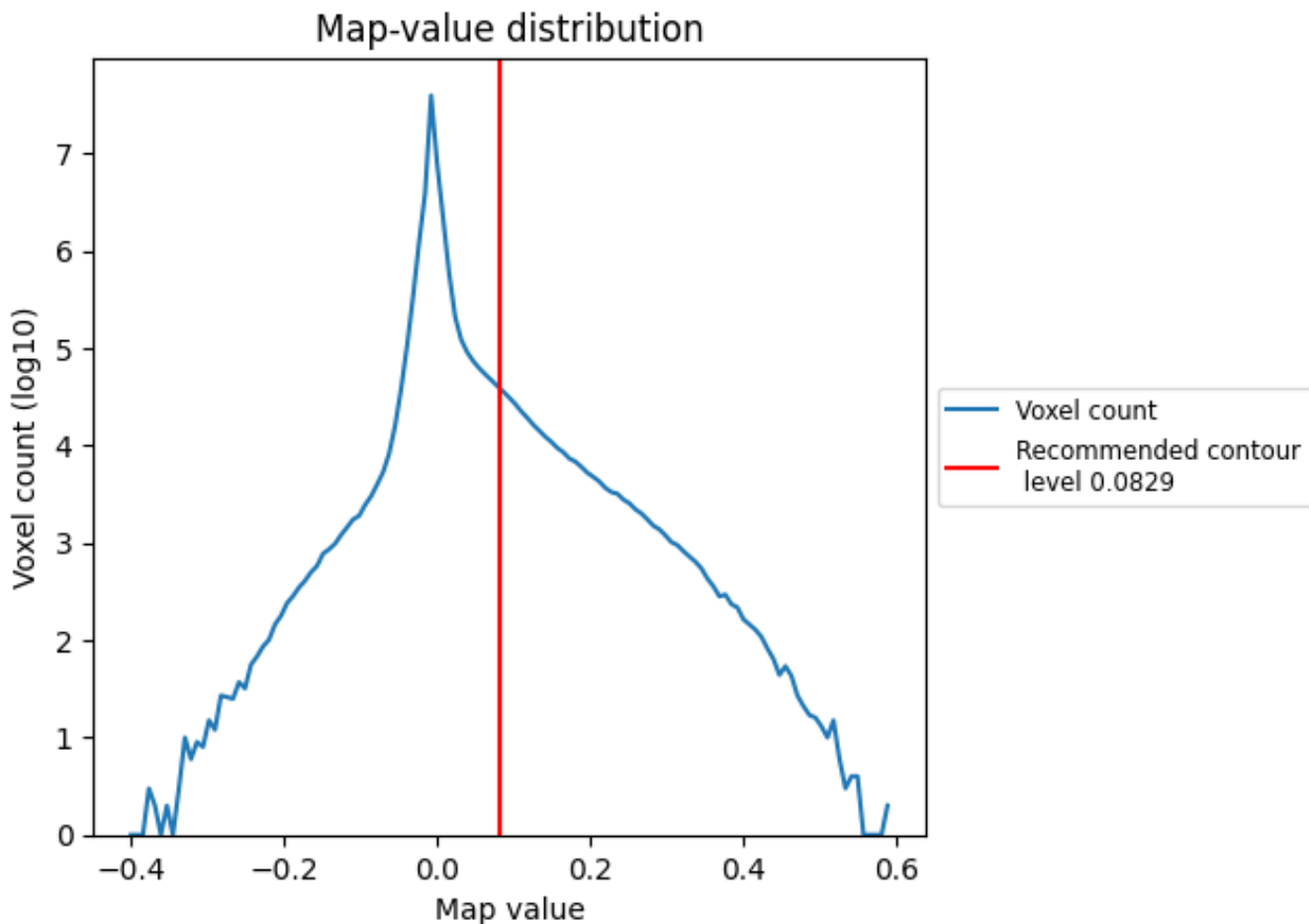
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

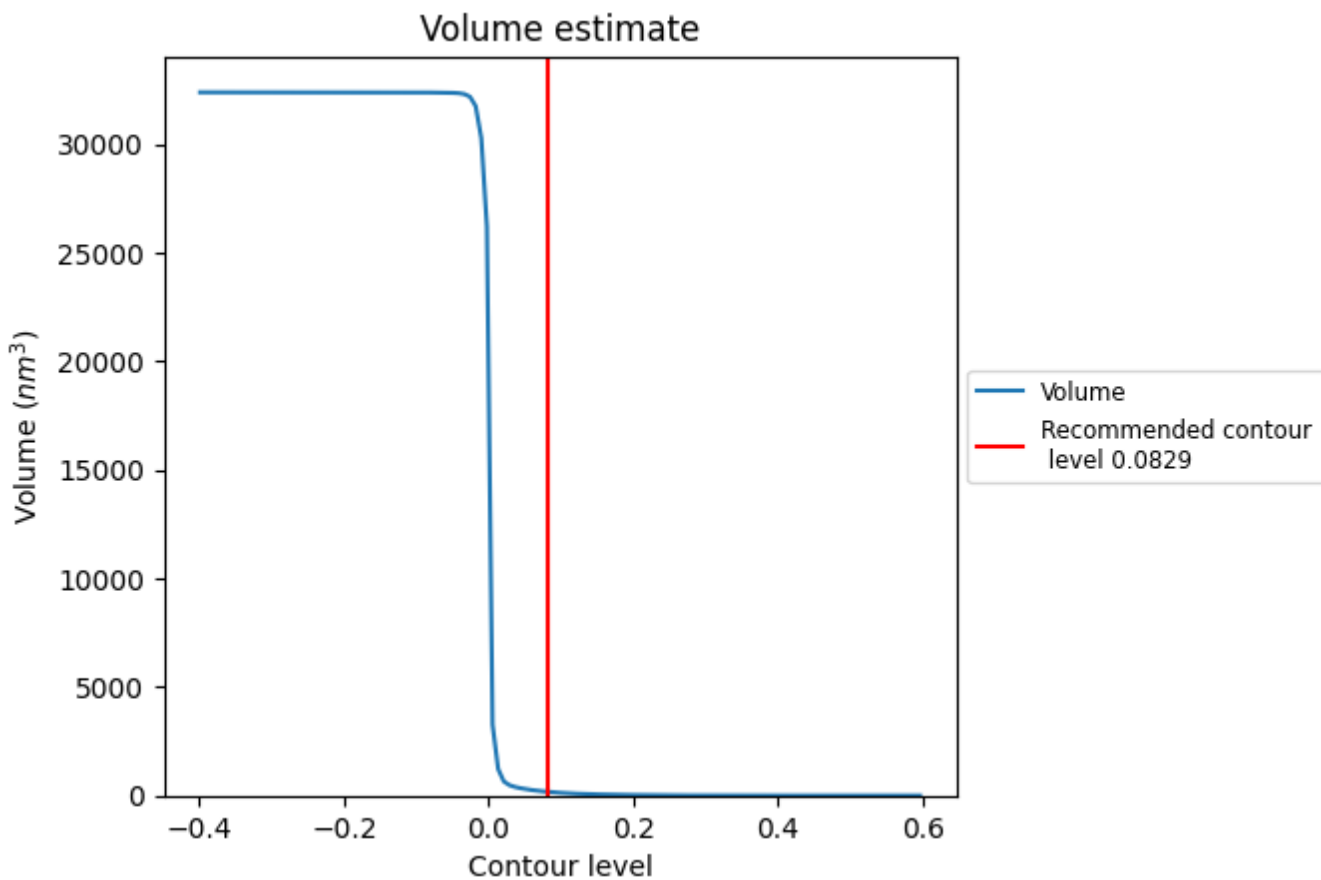
This section contains the results of statistical analysis of the map.

### 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.

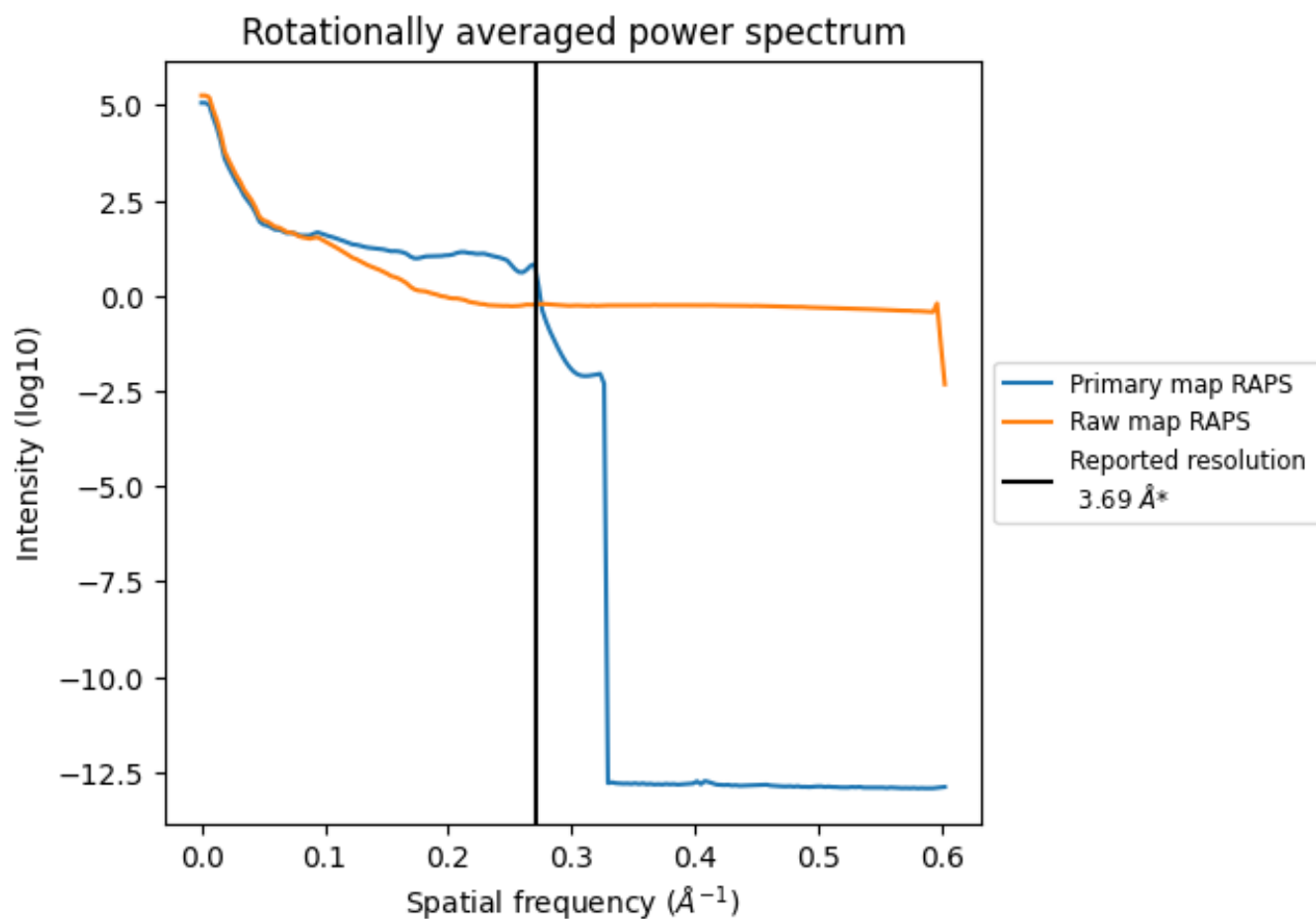
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 169  $\text{nm}^3$ ; this corresponds to an approximate mass of 153 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)

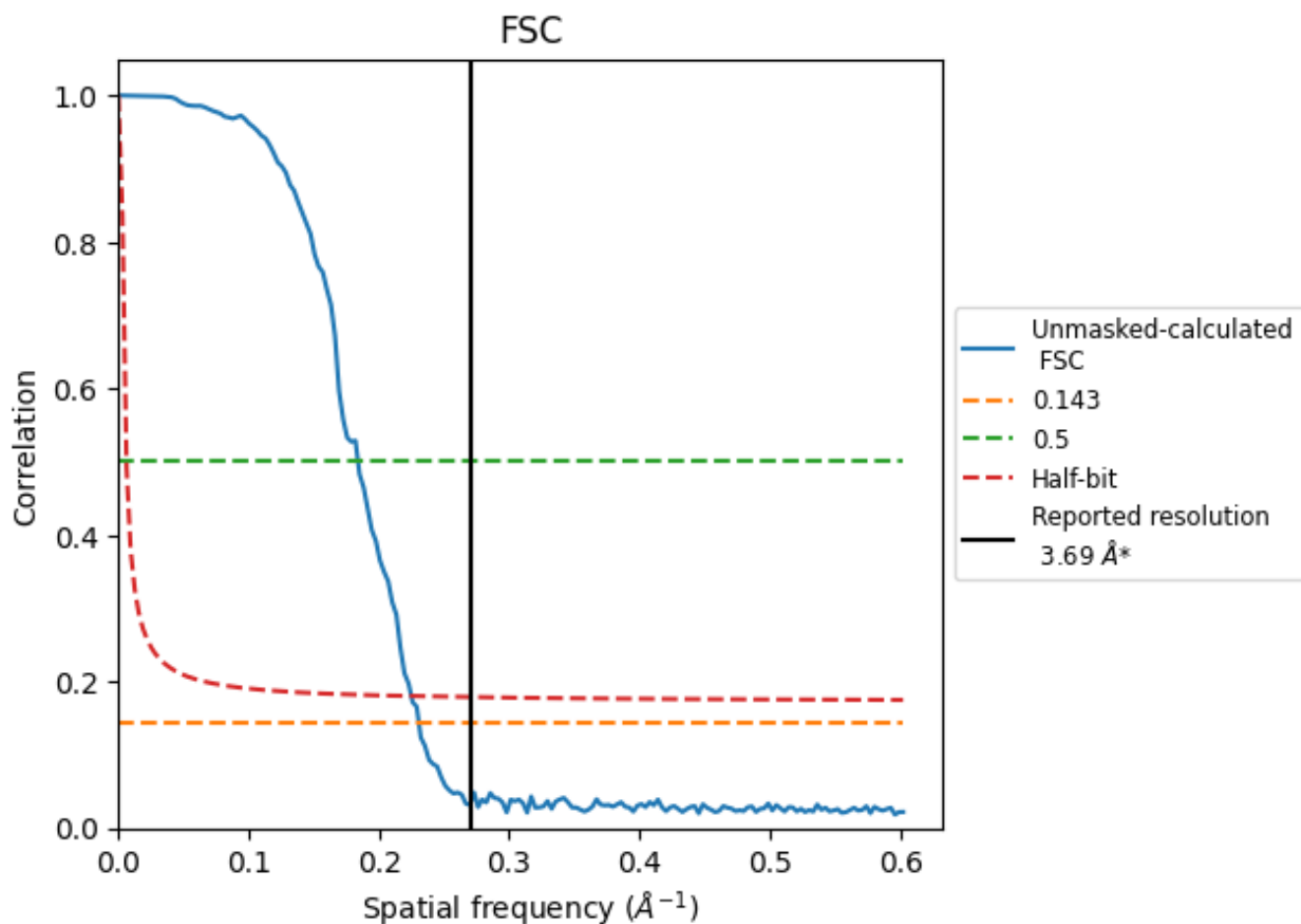


\*Reported resolution corresponds to spatial frequency of 0.271 Å<sup>-1</sup>

## 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 0.271 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

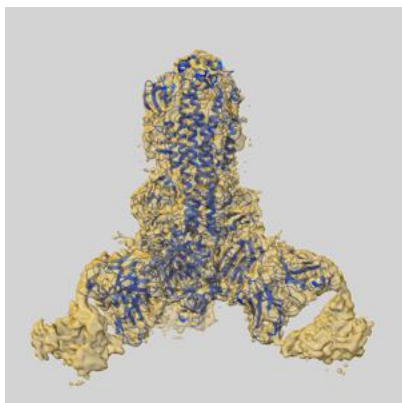
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.69	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.33	5.44	4.45

\*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 3.69 by more than 10 %

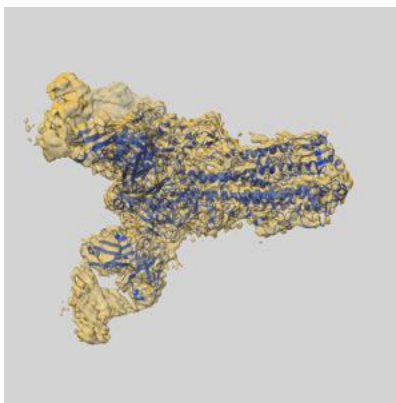
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41441 and PDB model 8TOA. Per-residue inclusion information can be found in section 3 on page 10.

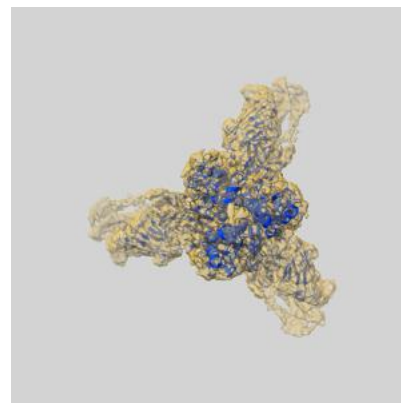
### 9.1 Map-model overlay [i](#)



X



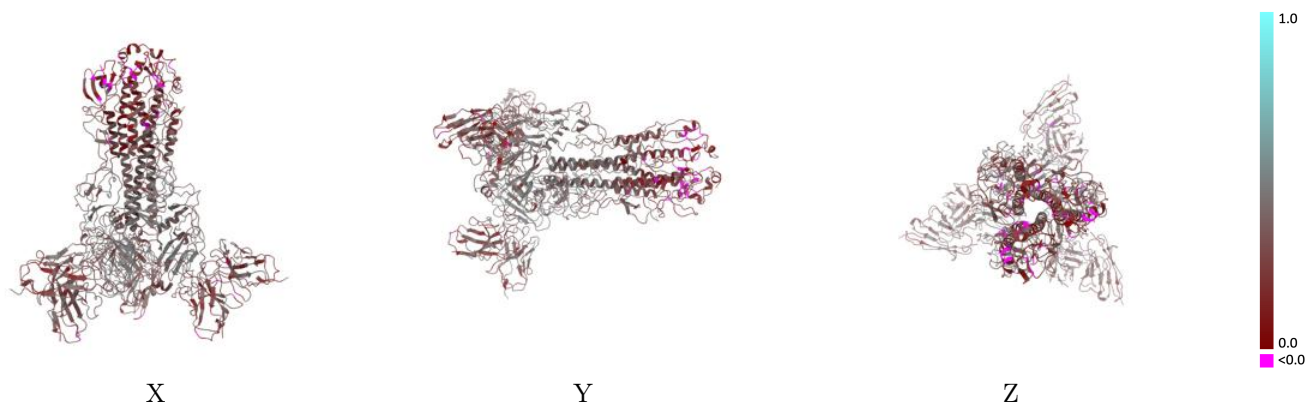
Y



Z

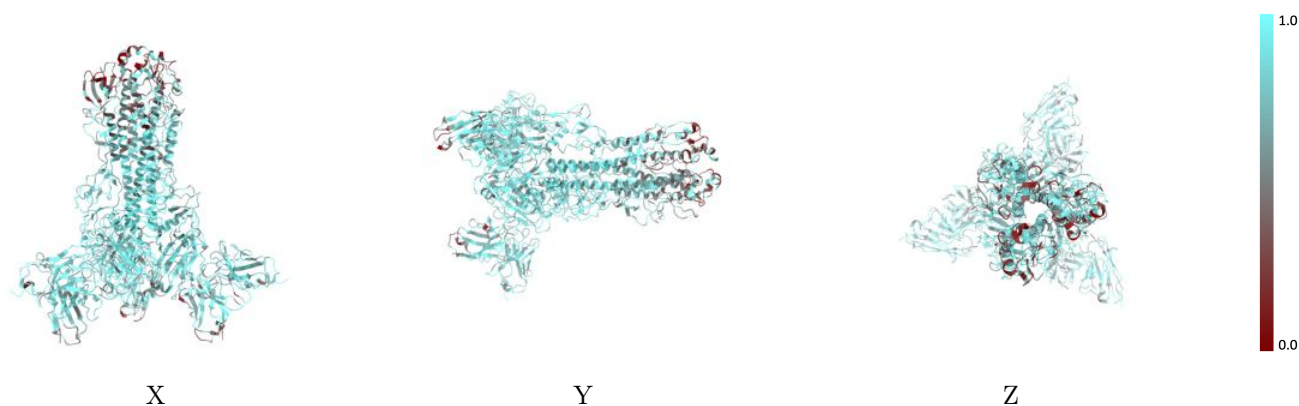
The images above show the 3D surface view of the map at the recommended contour level 0.0829 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

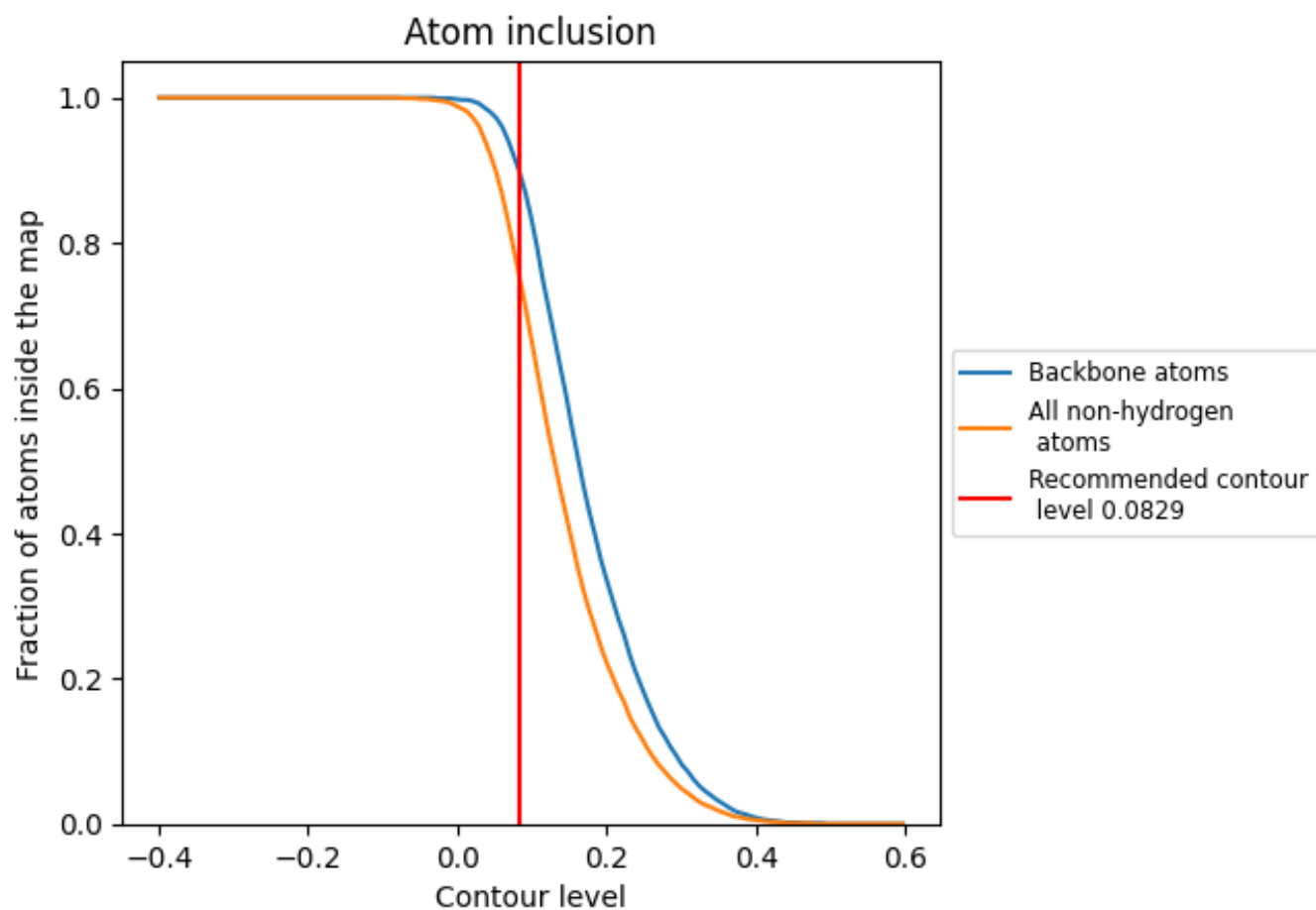
## 9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



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 (0.0829).























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 76% 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 (0.0829) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7550	 0.3420
A	 0.7970	 0.3200
B	 0.7360	 0.3380
C	 0.7500	 0.3490
D	 0.7970	 0.3170
E	 0.7210	 0.3030
H	 0.8030	 0.3240
I	 0.7510	 0.3480
K	 0.7510	 0.3580
L	 0.7310	 0.3190

