



## Full wwPDB EM Validation Report ⓘ

Aug 4, 2025 – 05:20 PM EDT

PDB ID : 9MVU / pdb\_00009mvu  
EMDB ID : EMD-48671  
Title : C6 Herpes Virus Simplex Neutralizing Nanobody Bound to HSV Glycoprotein gB  
Authors : Viadiu, H.; Abernathy, E.; Lee, C.V.; Hung, M.; Yu, Y.; Xing, W.; Yu, X.  
Deposited on : 2025-01-16  
Resolution : 2.20 Å(reported)

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

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

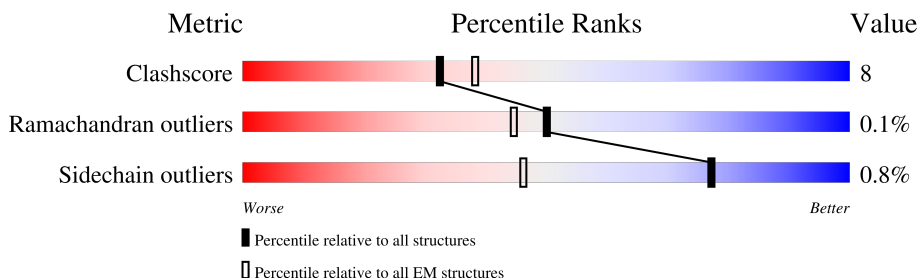
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.20 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	727	
1	B	727	
1	C	727	
2	D	131	
2	E	131	
2	F	131	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21199 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 Envelope glycoprotein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	576	Total	C	N	O	S	0	0
			4660	2945	818	874	23		
1	B	580	Total	C	N	O	S	0	0
			4689	2962	822	882	23		
1	C	574	Total	C	N	O	S	0	0
			4638	2931	810	874	23		

There are 288 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	PRO	SER	conflict	UNP P10211
A	33	ALA	SER	conflict	UNP P10211
A	34	ALA	SER	conflict	UNP P10211
A	36	ARG	GLY	conflict	UNP P10211
A	37	ALA	THR	conflict	UNP P10211
A	38	SER	PRO	conflict	UNP P10211
A	40	GLY	VAL	conflict	UNP P10211
A	41	VAL	ALA	conflict	UNP P10211
A	45	VAL	GLN	conflict	UNP P10211
A	53	SER	THR	conflict	UNP P10211
A	54	ARG	PRO	conflict	UNP P10211
A	55	PRO	ALA	conflict	UNP P10211
A	58	VAL	ALA	conflict	UNP P10211
A	60	SER	GLY	conflict	UNP P10211
A	61	PRO	ALA	conflict	UNP P10211
A	62	ALA	PRO	conflict	UNP P10211
A	63	THR	PRO	conflict	UNP P10211
A	65	LYS	GLY	conflict	UNP P10211
A	66	ALA	ASP	conflict	UNP P10211
A	67	ARG	PRO	conflict	UNP P10211
A	69	ARG	PRO	conflict	UNP P10211
A	71	THR	LYS	conflict	UNP P10211
A	72	LYS	ASN	conflict	UNP P10211
A	73	LYS	ARG	variant	UNP P10211

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Chain	Residue	Modelled	Actual	Comment	Reference
A	74	PRO	LYS	conflict	UNP P10211
A	77	ARG	PRO	conflict	UNP P10211
A	79	GLU	LYS	conflict	UNP P10211
A	80	ALA	PRO	conflict	UNP P10211
A	81	THR	PRO	conflict	UNP P10211
A	82	PRO	ARG	conflict	UNP P10211
A	84	PRO	ALA	conflict	UNP P10211
A	85	ASP	GLY	conflict	UNP P10211
A	86	ALA	ASP	conflict	UNP P10211
A	99	ALA	GLU	conflict	UNP P10211
A	103	GLU	ASP	conflict	UNP P10211
A	106	VAL	ALA	conflict	UNP P10211
A	109	ALA	THR	conflict	UNP P10211
A	218	MET	LEU	conflict	UNP P10211
A	238	LYS	ASN	conflict	UNP P10211
A	239	VAL	ALA	conflict	UNP P10211
A	338	SER	ALA	conflict	UNP P10211
A	362	ALA	SER	conflict	UNP P10211
A	378	ALA	SER	conflict	UNP P10211
A	403	SER	PRO	conflict	UNP P10211
A	415	ARG	LYS	conflict	UNP P10211
A	419	GLU	ASP	conflict	UNP P10211
A	421	ILE	MET	conflict	UNP P10211
A	424	MET	ILE	conflict	UNP P10211
A	428	LYS	ARG	conflict	UNP P10211
A	445	THR	ASN	conflict	UNP P10211
A	459I	TYR	HIS	conflict	UNP P10211
A	459J	MET	LEU	conflict	UNP P10211
A	459N	ASP	SER	conflict	UNP P10211
A	459Q	PRO	-	insertion	UNP P10211
A	459R	ARG	-	insertion	UNP P10211
A	459S	ASN	PRO	conflict	UNP P10211
A	459T	ALA	PRO	conflict	UNP P10211
A	459U	THR	ASN	conflict	UNP P10211
A	459W	ALA	THR	conflict	UNP P10211
A	459Y	LEU	PRO	conflict	UNP P10211
A	459Z	ARG	PRO	conflict	UNP P10211
A	460A	GLU	PRO	conflict	UNP P10211
A	460B	ALA	GLY	conflict	UNP P10211
A	460C	PRO	ALA	conflict	UNP P10211
A	524	ILE	VAL	conflict	UNP P10211
A	526	VAL	ILE	conflict	UNP P10211

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Chain	Residue	Modelled	Actual	Comment	Reference
A	578	PRO	ALA	conflict	UNP P10211
A	589	VAL	ILE	conflict	UNP P10211
A	595	THR	ALA	conflict	UNP P10211
A	613	ILE	VAL	conflict	UNP P10211
A	630	LEU	ILE	conflict	UNP P10211
A	642	ILE	THR	conflict	UNP P10211
A	664	VAL	ILE	conflict	UNP P10211
A	724	ARG	HIS	conflict	UNP P10211
A	731	GLY	-	expression tag	UNP P10211
A	732	GLY	-	expression tag	UNP P10211
A	733	GLY	-	expression tag	UNP P10211
A	734	SER	-	expression tag	UNP P10211
A	735	HIS	-	expression tag	UNP P10211
A	736	HIS	-	expression tag	UNP P10211
A	737	HIS	-	expression tag	UNP P10211
A	738	HIS	-	expression tag	UNP P10211
A	739	HIS	-	expression tag	UNP P10211
A	740	HIS	-	expression tag	UNP P10211
A	741	HIS	-	expression tag	UNP P10211
A	742	HIS	-	expression tag	UNP P10211
A	743	GLY	-	expression tag	UNP P10211
A	744	SER	-	expression tag	UNP P10211
A	745	ASP	-	expression tag	UNP P10211
A	746	TYR	-	expression tag	UNP P10211
A	747	LYS	-	expression tag	UNP P10211
A	748	ASP	-	expression tag	UNP P10211
A	749	ASP	-	expression tag	UNP P10211
A	750	ASP	-	expression tag	UNP P10211
A	751	ASP	-	expression tag	UNP P10211
A	752	LYS	-	expression tag	UNP P10211
B	29	PRO	SER	conflict	UNP P10211
B	33	ALA	SER	conflict	UNP P10211
B	34	ALA	SER	conflict	UNP P10211
B	36	ARG	GLY	conflict	UNP P10211
B	37	ALA	THR	conflict	UNP P10211
B	38	SER	PRO	conflict	UNP P10211
B	40	GLY	VAL	conflict	UNP P10211
B	41	VAL	ALA	conflict	UNP P10211
B	45	VAL	GLN	conflict	UNP P10211
B	53	SER	THR	conflict	UNP P10211
B	54	ARG	PRO	conflict	UNP P10211
B	55	PRO	ALA	conflict	UNP P10211

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Chain	Residue	Modelled	Actual	Comment	Reference
B	58	VAL	ALA	conflict	UNP P10211
B	60	SER	GLY	conflict	UNP P10211
B	61	PRO	ALA	conflict	UNP P10211
B	62	ALA	PRO	conflict	UNP P10211
B	63	THR	PRO	conflict	UNP P10211
B	65	LYS	GLY	conflict	UNP P10211
B	66	ALA	ASP	conflict	UNP P10211
B	67	ARG	PRO	conflict	UNP P10211
B	69	ARG	PRO	conflict	UNP P10211
B	71	THR	LYS	conflict	UNP P10211
B	72	LYS	ASN	conflict	UNP P10211
B	73	LYS	ARG	variant	UNP P10211
B	74	PRO	LYS	conflict	UNP P10211
B	77	ARG	PRO	conflict	UNP P10211
B	79	GLU	LYS	conflict	UNP P10211
B	80	ALA	PRO	conflict	UNP P10211
B	81	THR	PRO	conflict	UNP P10211
B	82	PRO	ARG	conflict	UNP P10211
B	84	PRO	ALA	conflict	UNP P10211
B	85	ASP	GLY	conflict	UNP P10211
B	86	ALA	ASP	conflict	UNP P10211
B	99	ALA	GLU	conflict	UNP P10211
B	103	GLU	ASP	conflict	UNP P10211
B	106	VAL	ALA	conflict	UNP P10211
B	109	ALA	THR	conflict	UNP P10211
B	218	MET	LEU	conflict	UNP P10211
B	238	LYS	ASN	conflict	UNP P10211
B	239	VAL	ALA	conflict	UNP P10211
B	338	SER	ALA	conflict	UNP P10211
B	362	ALA	SER	conflict	UNP P10211
B	378	ALA	SER	conflict	UNP P10211
B	403	SER	PRO	conflict	UNP P10211
B	415	ARG	LYS	conflict	UNP P10211
B	419	GLU	ASP	conflict	UNP P10211
B	421	ILE	MET	conflict	UNP P10211
B	424	MET	ILE	conflict	UNP P10211
B	428	LYS	ARG	conflict	UNP P10211
B	445	THR	ASN	conflict	UNP P10211
B	461G	TYR	HIS	conflict	UNP P10211
B	461H	MET	LEU	conflict	UNP P10211
B	461L	ASP	SER	conflict	UNP P10211
B	461O	PRO	-	insertion	UNP P10211

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Chain	Residue	Modelled	Actual	Comment	Reference
B	461P	ARG	-	insertion	UNP P10211
B	461Q	ASN	PRO	conflict	UNP P10211
B	461R	ALA	PRO	conflict	UNP P10211
B	461S	THR	ASN	conflict	UNP P10211
B	461U	ALA	THR	conflict	UNP P10211
B	461W	LEU	PRO	conflict	UNP P10211
B	461X	ARG	PRO	conflict	UNP P10211
B	461Y	GLU	PRO	conflict	UNP P10211
B	461Z	ALA	GLY	conflict	UNP P10211
B	462A	PRO	ALA	conflict	UNP P10211
B	524	ILE	VAL	conflict	UNP P10211
B	526	VAL	ILE	conflict	UNP P10211
B	578	PRO	ALA	conflict	UNP P10211
B	589	VAL	ILE	conflict	UNP P10211
B	595	THR	ALA	conflict	UNP P10211
B	613	ILE	VAL	conflict	UNP P10211
B	630	LEU	ILE	conflict	UNP P10211
B	642	ILE	THR	conflict	UNP P10211
B	664	VAL	ILE	conflict	UNP P10211
B	724	ARG	HIS	conflict	UNP P10211
B	731	GLY	-	expression tag	UNP P10211
B	732	GLY	-	expression tag	UNP P10211
B	733	GLY	-	expression tag	UNP P10211
B	734	SER	-	expression tag	UNP P10211
B	735	HIS	-	expression tag	UNP P10211
B	736	HIS	-	expression tag	UNP P10211
B	737	HIS	-	expression tag	UNP P10211
B	738	HIS	-	expression tag	UNP P10211
B	739	HIS	-	expression tag	UNP P10211
B	740	HIS	-	expression tag	UNP P10211
B	741	HIS	-	expression tag	UNP P10211
B	742	HIS	-	expression tag	UNP P10211
B	743	GLY	-	expression tag	UNP P10211
B	744	SER	-	expression tag	UNP P10211
B	745	ASP	-	expression tag	UNP P10211
B	746	TYR	-	expression tag	UNP P10211
B	747	LYS	-	expression tag	UNP P10211
B	748	ASP	-	expression tag	UNP P10211
B	749	ASP	-	expression tag	UNP P10211
B	750	ASP	-	expression tag	UNP P10211
B	751	ASP	-	expression tag	UNP P10211
B	752	LYS	-	expression tag	UNP P10211

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Chain	Residue	Modelled	Actual	Comment	Reference
C	29	PRO	SER	conflict	UNP P10211
C	33	ALA	SER	conflict	UNP P10211
C	34	ALA	SER	conflict	UNP P10211
C	36	ARG	GLY	conflict	UNP P10211
C	37	ALA	THR	conflict	UNP P10211
C	38	SER	PRO	conflict	UNP P10211
C	40	GLY	VAL	conflict	UNP P10211
C	41	VAL	ALA	conflict	UNP P10211
C	45	VAL	GLN	conflict	UNP P10211
C	53	SER	THR	conflict	UNP P10211
C	54	ARG	PRO	conflict	UNP P10211
C	55	PRO	ALA	conflict	UNP P10211
C	58	VAL	ALA	conflict	UNP P10211
C	60	SER	GLY	conflict	UNP P10211
C	61	PRO	ALA	conflict	UNP P10211
C	62	ALA	PRO	conflict	UNP P10211
C	63	THR	PRO	conflict	UNP P10211
C	65	LYS	GLY	conflict	UNP P10211
C	66	ALA	ASP	conflict	UNP P10211
C	67	ARG	PRO	conflict	UNP P10211
C	69	ARG	PRO	conflict	UNP P10211
C	71	THR	LYS	conflict	UNP P10211
C	72	LYS	ASN	conflict	UNP P10211
C	73	LYS	ARG	variant	UNP P10211
C	74	PRO	LYS	conflict	UNP P10211
C	77	ARG	PRO	conflict	UNP P10211
C	79	GLU	LYS	conflict	UNP P10211
C	80	ALA	PRO	conflict	UNP P10211
C	81	THR	PRO	conflict	UNP P10211
C	82	PRO	ARG	conflict	UNP P10211
C	84	PRO	ALA	conflict	UNP P10211
C	85	ASP	GLY	conflict	UNP P10211
C	86	ALA	ASP	conflict	UNP P10211
C	99	ALA	GLU	conflict	UNP P10211
C	103	GLU	ASP	conflict	UNP P10211
C	106	VAL	ALA	conflict	UNP P10211
C	109	ALA	THR	conflict	UNP P10211
C	218	MET	LEU	conflict	UNP P10211
C	238	LYS	ASN	conflict	UNP P10211
C	239	VAL	ALA	conflict	UNP P10211
C	338	SER	ALA	conflict	UNP P10211
C	362	ALA	SER	conflict	UNP P10211

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Chain	Residue	Modelled	Actual	Comment	Reference
C	378	ALA	SER	conflict	UNP P10211
C	403	SER	PRO	conflict	UNP P10211
C	415	ARG	LYS	conflict	UNP P10211
C	419	GLU	ASP	conflict	UNP P10211
C	421	ILE	MET	conflict	UNP P10211
C	424	MET	ILE	conflict	UNP P10211
C	428	LYS	ARG	conflict	UNP P10211
C	445	THR	ASN	conflict	UNP P10211
C	459I	TYR	HIS	conflict	UNP P10211
C	459J	MET	LEU	conflict	UNP P10211
C	459N	ASP	SER	conflict	UNP P10211
C	459Q	PRO	-	insertion	UNP P10211
C	459R	ARG	-	insertion	UNP P10211
C	459S	ASN	PRO	conflict	UNP P10211
C	459T	ALA	PRO	conflict	UNP P10211
C	459U	THR	ASN	conflict	UNP P10211
C	459W	ALA	THR	conflict	UNP P10211
C	459Y	LEU	PRO	conflict	UNP P10211
C	459Z	ARG	PRO	conflict	UNP P10211
C	460A	GLU	PRO	conflict	UNP P10211
C	460B	ALA	GLY	conflict	UNP P10211
C	460C	PRO	ALA	conflict	UNP P10211
C	524	ILE	VAL	conflict	UNP P10211
C	526	VAL	ILE	conflict	UNP P10211
C	578	PRO	ALA	conflict	UNP P10211
C	589	VAL	ILE	conflict	UNP P10211
C	595	THR	ALA	conflict	UNP P10211
C	613	ILE	VAL	conflict	UNP P10211
C	630	LEU	ILE	conflict	UNP P10211
C	642	ILE	THR	conflict	UNP P10211
C	664	VAL	ILE	conflict	UNP P10211
C	724	ARG	HIS	conflict	UNP P10211
C	731	GLY	-	expression tag	UNP P10211
C	732	GLY	-	expression tag	UNP P10211
C	733	GLY	-	expression tag	UNP P10211
C	734	SER	-	expression tag	UNP P10211
C	735	HIS	-	expression tag	UNP P10211
C	736	HIS	-	expression tag	UNP P10211
C	737	HIS	-	expression tag	UNP P10211
C	738	HIS	-	expression tag	UNP P10211
C	739	HIS	-	expression tag	UNP P10211
C	740	HIS	-	expression tag	UNP P10211

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Chain	Residue	Modelled	Actual	Comment	Reference
C	741	HIS	-	expression tag	UNP P10211
C	742	HIS	-	expression tag	UNP P10211
C	743	GLY	-	expression tag	UNP P10211
C	744	SER	-	expression tag	UNP P10211
C	745	ASP	-	expression tag	UNP P10211
C	746	TYR	-	expression tag	UNP P10211
C	747	LYS	-	expression tag	UNP P10211
C	748	ASP	-	expression tag	UNP P10211
C	749	ASP	-	expression tag	UNP P10211
C	750	ASP	-	expression tag	UNP P10211
C	751	ASP	-	expression tag	UNP P10211
C	752	LYS	-	expression tag	UNP P10211

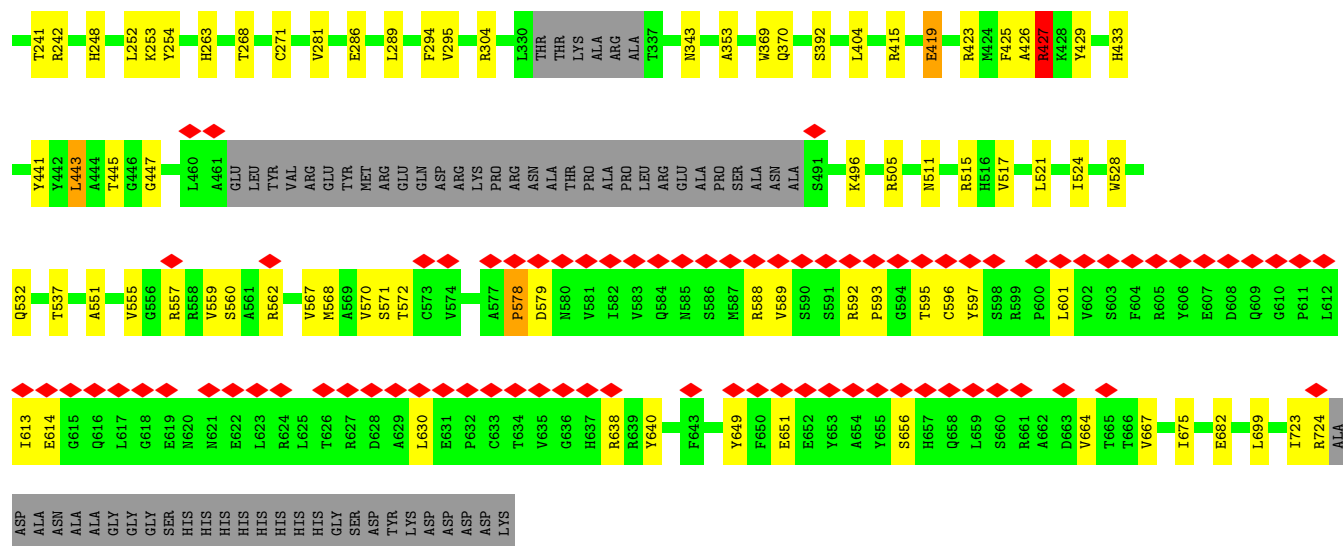
- Molecule 2 is a protein called C6 Neutralizing Nanobody.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	125	Total	C	N	O	S	0	0
			950	590	173	183	4		
2	E	125	Total	C	N	O	S	0	0
			950	590	173	183	4		
2	F	125	Total	C	N	O	S	0	0
			950	590	173	183	4		

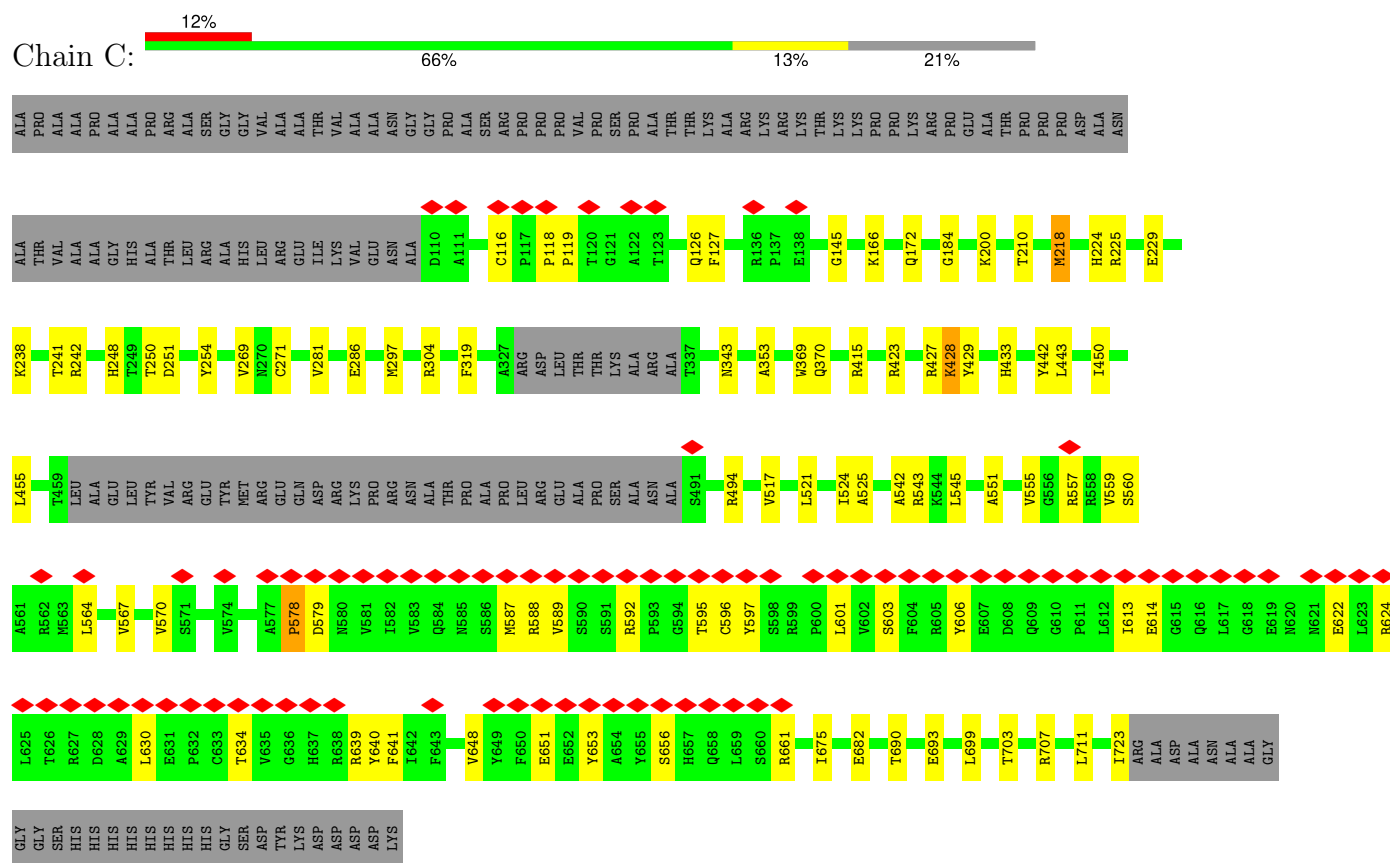
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A	1240	Total	O	0
			1240	1240	
3	B	1238	Total	O	0
			1238	1238	
3	C	1250	Total	O	0
			1250	1250	
3	D	213	Total	O	0
			213	213	
3	E	214	Total	O	0
			214	214	
3	F	207	Total	O	0
			207	207	

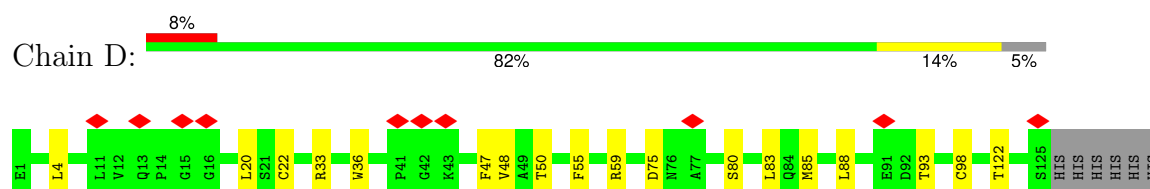




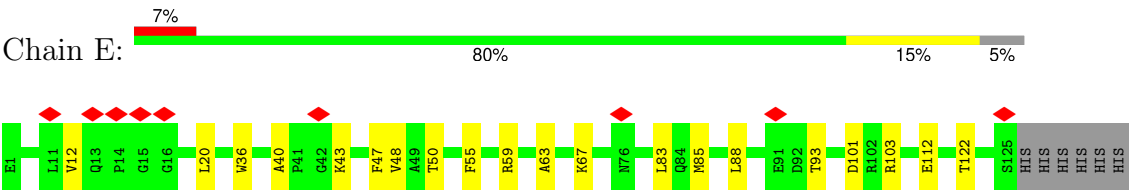
### • Molecule 1: Envelope glycoprotein B



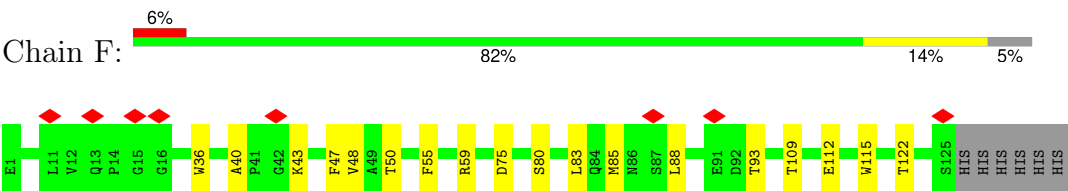
### • Molecule 2: C6 Neutralizing Nanobody



● Molecule 2: C6 Neutralizing Nanobody



● Molecule 2: C6 Neutralizing Nanobody



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	149170	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	52	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	165000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.457	Depositor
Minimum map value	-0.838	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	262.44, 262.44, 262.44	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.72900003, 0.72900003, 0.72900003	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.27	0/4776	0.48	2/6486 (0.0%)
1	B	0.24	0/4805	0.47	3/6526 (0.0%)
1	C	0.24	0/4754	0.44	2/6458 (0.0%)
2	D	0.16	0/970	0.40	0/1313
2	E	0.15	0/970	0.39	0/1313
2	F	0.15	0/970	0.38	0/1313
All	All	0.24	0/17245	0.45	7/23409 (0.0%)

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
1	A	0	4
1	B	0	2
1	C	0	2
All	All	0	8

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	578	PRO	CA-N-CD	-9.08	99.29	112.00
1	C	578	PRO	CA-N-CD	-9.08	99.29	112.00
1	B	578	PRO	CA-N-CD	-9.05	99.32	112.00
1	B	419	GLU	CB-CG-CD	-8.22	98.63	112.60
1	A	419	GLU	CB-CG-CD	-7.26	100.26	112.60
1	C	428	LYS	N-CA-CB	-5.46	103.73	111.00
1	B	419	GLU	N-CA-CB	5.26	117.94	110.16

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	418	ARG	Sidechain
1	A	423	ARG	Sidechain
1	A	427	ARG	Sidechain
1	A	724	ARG	Sidechain
1	B	423	ARG	Sidechain
1	B	427	ARG	Sidechain
1	C	423	ARG	Sidechain
1	C	427	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4660	0	4486	82	0
1	B	4689	0	4513	91	0
1	C	4638	0	4456	86	0
2	D	950	0	910	11	0
2	E	950	0	910	13	0
2	F	950	0	910	13	0
3	A	1240	0	0	20	0
3	B	1238	0	0	24	0
3	C	1250	0	0	18	0
3	D	213	0	0	0	0
3	E	214	0	0	0	0
3	F	207	0	0	0	0
All	All	21199	0	16185	273	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 8.

All (273) 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:B:589:VAL:HG22	1:B:597:TYR:CE2	1.66	1.29
1:C:589:VAL:HG22	1:C:597:TYR:CE2	1.73	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:589:VAL:CG2	1:C:597:TYR:CE2	2.22	1.22
1:B:238:LYS:HE3	3:B:1236:HOH:O	1.40	1.21
1:A:724:ARG:NH1	3:A:802:HOH:O	1.79	1.14
1:A:578:PRO:HD2	1:A:579:ASP:H	1.20	1.06
1:C:578:PRO:HD2	1:C:579:ASP:H	1.20	1.04
1:C:597:TYR:CE1	1:C:630:LEU:HD21	1.93	1.03
1:B:238:LYS:CE	3:B:1236:HOH:O	2.01	1.00
1:B:589:VAL:CG2	1:B:597:TYR:CE2	2.45	1.00
1:B:578:PRO:HD2	1:B:579:ASP:H	1.22	1.00
1:C:592:ARG:HB3	1:C:595:THR:OG1	1.69	0.93
1:C:415:ARG:NH1	3:C:802:HOH:O	2.02	0.91
1:C:589:VAL:HG21	1:C:597:TYR:CZ	2.06	0.90
1:B:429:TYR:HB3	1:B:433:HIS:HB2	1.55	0.89
1:A:578:PRO:HD2	1:A:579:ASP:N	1.92	0.84
1:C:592:ARG:CB	1:C:595:THR:OG1	2.24	0.84
1:C:578:PRO:HD2	1:C:579:ASP:N	1.92	0.83
1:B:578:PRO:HD2	1:B:579:ASP:N	1.92	0.83
1:C:589:VAL:CG2	1:C:597:TYR:CZ	2.62	0.82
1:C:589:VAL:CG2	1:C:597:TYR:CD2	2.64	0.81
1:C:597:TYR:CD1	1:C:630:LEU:HD23	2.16	0.80
1:C:597:TYR:CD1	1:C:630:LEU:CD2	2.64	0.80
1:A:241:THR:HG22	1:A:242:ARG:HG3	1.64	0.79
1:B:415:ARG:CZ	3:B:806:HOH:O	2.30	0.78
1:C:116:CYS:HB3	1:C:560:SER:HB2	1.64	0.78
1:C:241:THR:HG22	1:C:242:ARG:HG3	1.67	0.76
1:B:238:LYS:HD2	3:C:808:HOH:O	1.88	0.74
1:A:415:ARG:CZ	3:A:803:HOH:O	2.34	0.74
1:C:597:TYR:CE1	1:C:630:LEU:CD2	2.69	0.74
1:B:595:THR:HG23	3:B:809:HOH:O	1.89	0.73
1:A:589:VAL:HG12	1:A:592:ARG:H	1.52	0.73
1:B:116:CYS:HB3	1:B:560:SER:HB2	1.69	0.73
1:C:592:ARG:NE	1:C:630:LEU:HD13	2.04	0.72
2:E:93:THR:HG23	2:E:122:THR:HA	1.72	0.72
2:F:93:THR:HG23	2:F:122:THR:HA	1.72	0.72
1:B:521:LEU:HD23	1:B:524:ILE:HD12	1.72	0.72
1:B:415:ARG:NE	3:B:803:HOH:O	2.22	0.71
1:A:597:TYR:CE1	1:A:630:LEU:HD21	2.25	0.71
1:C:589:VAL:HG23	1:C:597:TYR:CD2	2.26	0.71
1:A:578:PRO:CD	1:A:579:ASP:H	2.02	0.69
1:A:521:LEU:HD23	1:A:524:ILE:HD12	1.76	0.68
2:F:85:MET:HB3	2:F:88:LEU:HD21	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:578:PRO:CD	1:C:579:ASP:H	2.02	0.67
1:A:699:LEU:HD13	1:C:281:VAL:HG13	1.77	0.67
1:A:297:MET:HE1	1:A:319:PHE:CD1	2.29	0.67
1:C:521:LEU:HD23	1:C:524:ILE:HD12	1.76	0.66
1:B:238:LYS:NZ	3:B:802:HOH:O	2.01	0.66
2:F:75:ASP:HB2	2:F:80:SER:HB3	1.78	0.66
1:A:238:LYS:CE	3:A:1531:HOH:O	2.43	0.66
1:B:589:VAL:CG2	1:B:597:TYR:CD2	2.79	0.66
2:D:85:MET:HB3	2:D:88:LEU:HD21	1.77	0.66
1:B:578:PRO:CD	1:B:579:ASP:H	2.03	0.64
1:A:578:PRO:CD	1:A:579:ASP:N	2.61	0.64
1:B:281:VAL:HG13	1:C:699:LEU:HD13	1.80	0.64
1:A:415:ARG:NH1	3:A:803:HOH:O	2.31	0.63
1:B:200:LYS:HG2	3:B:812:HOH:O	1.98	0.63
1:C:172:GLN:HG3	3:C:843:HOH:O	1.98	0.63
2:D:93:THR:HG23	2:D:122:THR:HA	1.81	0.63
1:B:415:ARG:NH1	3:B:806:HOH:O	2.31	0.63
1:B:241:THR:HG22	1:B:242:ARG:HG3	1.80	0.62
1:A:156:PRO:HG2	1:A:279:ARG:HH21	1.64	0.62
1:B:252:LEU:HD13	1:C:723:ILE:HD11	1.82	0.62
1:B:578:PRO:CD	1:B:579:ASP:N	2.60	0.61
1:B:589:VAL:HG22	1:B:597:TYR:CZ	2.31	0.61
1:C:578:PRO:CD	1:C:579:ASP:N	2.60	0.61
2:E:12:VAL:HG11	2:E:88:LEU:HD12	1.82	0.61
1:A:597:TYR:CD1	1:A:630:LEU:HD21	2.36	0.61
1:A:238:LYS:HE3	3:A:1531:HOH:O	2.00	0.61
1:C:592:ARG:HB2	1:C:595:THR:OG1	2.01	0.59
1:A:597:TYR:CD1	1:A:630:LEU:CD2	2.85	0.59
1:C:597:TYR:CD1	1:C:630:LEU:HD21	2.30	0.59
2:E:40:ALA:HB3	2:E:43:LYS:HD3	1.83	0.59
1:A:116:CYS:HB3	1:A:560:SER:HB2	1.84	0.59
1:C:415:ARG:NH2	3:C:803:HOH:O	2.36	0.59
1:C:238:LYS:HE2	3:C:1563:HOH:O	2.03	0.59
1:A:525:ALA:HA	3:A:1560:HOH:O	2.02	0.58
1:A:232:MET:HE1	1:A:250:THR:HG22	1.85	0.58
1:B:415:ARG:CD	3:B:803:HOH:O	2.51	0.58
1:B:172:GLN:HG3	3:B:861:HOH:O	2.03	0.58
1:A:543:ARG:HA	1:A:550:ILE:HG13	1.86	0.58
1:A:238:LYS:HE2	3:A:1531:HOH:O	2.02	0.58
2:D:20:LEU:HD13	2:D:85:MET:HE2	1.86	0.58
1:C:218:MET:SD	3:C:1273:HOH:O	2.57	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:LEU:HB3	1:C:675:ILE:HG21	1.87	0.57
1:C:651:GLU:OE1	1:C:656:SER:HB2	2.04	0.57
1:C:238:LYS:CE	3:C:1563:HOH:O	2.53	0.56
2:D:75:ASP:HB2	2:D:80:SER:HB3	1.86	0.56
1:C:559:VAL:HG11	1:C:570:VAL:HB	1.87	0.56
1:C:622:GLU:HG2	1:C:624:ARG:HG3	1.87	0.56
1:A:111:ALA:O	1:A:112:ASN:OD1	2.24	0.56
1:C:606:TYR:HE1	1:C:613:ILE:HG13	1.71	0.55
1:A:172:GLN:HG3	3:A:836:HOH:O	2.06	0.55
1:A:634:THR:H	1:A:653:TYR:HE2	1.55	0.55
1:C:589:VAL:HG22	1:C:597:TYR:HE2	1.56	0.55
1:B:588:ARG:HG2	1:B:596:CYS:SG	2.47	0.55
1:A:639:ARG:HB3	1:A:641:PHE:CE2	2.42	0.55
1:B:675:ILE:HG21	1:C:521:LEU:HB3	1.87	0.55
2:F:109:THR:HG21	2:F:115:TRP:CZ2	2.42	0.55
1:A:620:ASN:HA	1:A:642:ILE:HG21	1.90	0.54
1:B:199:ASP:HB2	3:B:812:HOH:O	2.07	0.54
1:A:535:GLU:OE1	1:A:538:LEU:HD12	2.07	0.54
1:B:119:PRO:HA	1:B:571:SER:HB3	1.88	0.54
2:F:47:PHE:HE1	2:F:50:THR:HG23	1.73	0.54
2:F:109:THR:HG21	2:F:115:TRP:HZ2	1.73	0.53
2:F:40:ALA:HB3	2:F:43:LYS:HB2	1.91	0.52
2:E:47:PHE:HE1	2:E:50:THR:HG23	1.73	0.52
1:A:605:ARG:NH2	1:A:612:LEU:HD13	2.24	0.52
2:E:101:ASP:OD2	2:E:103:ARG:HD2	2.09	0.52
1:B:589:VAL:HG23	1:B:597:TYR:CD2	2.44	0.51
1:C:542:ALA:HA	1:C:545:LEU:HD12	1.93	0.51
1:C:587:MET:HE2	1:C:653:TYR:HA	1.93	0.51
1:A:119:PRO:HA	1:A:571:SER:HB3	1.92	0.51
1:A:343:ASN:O	1:A:353:ALA:HA	2.11	0.51
1:B:640:TYR:HB2	1:C:567:VAL:HG22	1.94	0.50
1:B:557:ARG:HG3	1:B:559:VAL:HG23	1.92	0.50
1:A:580:ASN:HB3	1:A:605:ARG:HG2	1.93	0.50
1:A:659:LEU:HD21	1:A:663:ASP:HB2	1.94	0.50
1:A:415:ARG:HG2	3:A:1678:HOH:O	2.12	0.50
1:A:659:LEU:HD23	1:A:660:SER:O	2.11	0.50
2:E:36:TRP:CD1	2:E:83:LEU:HB2	2.47	0.50
1:C:603:SER:HB2	3:C:811:HOH:O	2.12	0.49
1:C:525:ALA:HA	3:C:1505:HOH:O	2.12	0.49
1:B:425:PHE:C	1:B:427:ARG:H	2.20	0.49
1:C:343:ASN:O	1:C:353:ALA:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:HIS:HA	1:B:271:CYS:O	2.12	0.49
2:D:36:TRP:CD1	2:D:83:LEU:HB2	2.48	0.49
1:C:639:ARG:HB3	1:C:641:PHE:CE2	2.48	0.49
2:E:85:MET:HB3	2:E:88:LEU:HD21	1.94	0.49
1:A:528:TRP:O	1:A:532:GLN:HG2	2.13	0.48
1:B:589:VAL:CG2	1:B:597:TYR:CZ	2.94	0.48
1:B:592:ARG:HG3	1:B:595:THR:OG1	2.13	0.48
1:C:557:ARG:HG3	1:C:559:VAL:HG23	1.93	0.48
2:F:85:MET:CB	2:F:88:LEU:HD21	2.41	0.48
1:B:343:ASN:O	1:B:353:ALA:HA	2.12	0.48
1:A:126:GLN:CD	1:C:661:ARG:HE	2.22	0.48
1:A:199:ASP:HB2	3:A:845:HOH:O	2.12	0.48
1:A:300:PHE:HB2	1:A:310:GLU:OE1	2.14	0.48
1:C:224:HIS:HB2	1:C:269:VAL:HB	1.94	0.48
2:E:63:ALA:O	2:E:67:LYS:HG3	2.12	0.48
1:A:281:VAL:HG13	1:B:699:LEU:HD13	1.94	0.48
1:C:494:ARG:HG3	1:C:494:ARG:HH11	1.79	0.48
1:A:517:VAL:HA	3:A:1152:HOH:O	2.13	0.48
1:B:724:ARG:C	1:C:218:MET:HE1	2.39	0.48
1:C:450:ILE:HB	3:C:1684:HOH:O	2.13	0.48
1:C:690:THR:OG1	1:C:693:GLU:HG3	2.13	0.47
1:C:200:LYS:HD2	3:C:820:HOH:O	2.13	0.47
1:A:640:TYR:HA	1:A:648:VAL:O	2.13	0.47
1:B:517:VAL:HA	3:B:1204:HOH:O	2.13	0.47
1:B:597:TYR:CG	1:B:601:LEU:HD21	2.50	0.47
1:C:588:ARG:HG2	1:C:596:CYS:SG	2.55	0.47
1:A:597:TYR:CD1	1:A:630:LEU:HD23	2.49	0.47
2:E:20:LEU:HD13	2:E:85:MET:HE3	1.97	0.47
1:A:603:SER:HB3	1:A:612:LEU:HG	1.95	0.47
2:D:47:PHE:HE1	2:D:50:THR:HG23	1.80	0.47
1:A:604:PHE:O	1:A:612:LEU:HD12	2.15	0.47
1:A:297:MET:HE1	1:A:319:PHE:CE1	2.50	0.46
1:B:392:SER:HB2	1:B:505:ARG:HH21	1.79	0.46
1:B:638:ARG:HG2	1:B:651:GLU:HG3	1.97	0.46
1:B:238:LYS:HE2	3:B:1236:HOH:O	1.88	0.46
1:C:442:TYR:HB2	3:C:1684:HOH:O	2.16	0.46
1:B:559:VAL:HG11	1:B:570:VAL:HB	1.96	0.46
1:C:248:HIS:HA	1:C:271:CYS:O	2.16	0.46
1:C:517:VAL:HA	3:C:1148:HOH:O	2.14	0.46
2:D:22:CYS:O	2:D:80:SER:HA	2.16	0.46
1:A:119:PRO:HD2	1:A:562:ARG:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:HIS:HA	1:A:271:CYS:O	2.16	0.46
1:A:500:SER:HB3	3:A:914:HOH:O	2.16	0.46
1:B:295:VAL:HG23	3:B:846:HOH:O	2.16	0.46
1:B:404:LEU:HD11	1:B:441:TYR:CZ	2.51	0.46
1:B:169:THR:HG22	1:B:268:THR:HB	1.98	0.45
1:C:429:TYR:HB3	1:C:433:HIS:HB2	1.97	0.45
1:C:640:TYR:HA	1:C:648:VAL:O	2.17	0.45
1:C:166:LYS:HG2	1:C:271:CYS:HA	1.98	0.45
1:A:601:LEU:HD13	1:A:627:ARG:HH21	1.80	0.45
3:A:814:HOH:O	1:C:281:VAL:HG11	2.16	0.45
1:A:439:PRO:HB2	3:A:817:HOH:O	2.16	0.45
1:B:597:TYR:CE2	1:B:601:LEU:HD11	2.52	0.45
1:A:174:TRP:HB3	1:A:183:MET:HE3	1.98	0.45
1:A:232:MET:HE2	1:A:249:THR:HB	1.97	0.45
1:B:682:GLU:HB3	3:B:1389:HOH:O	2.16	0.45
1:A:225:ARG:HA	1:A:254:TYR:CD2	2.51	0.45
1:B:196:GLU:HA	3:B:812:HOH:O	2.17	0.45
1:B:281:VAL:HG11	3:C:812:HOH:O	2.16	0.45
1:A:589:VAL:HG22	1:A:597:TYR:CE2	2.52	0.45
1:B:597:TYR:CE1	1:B:630:LEU:HD21	2.51	0.45
1:C:248:HIS:HE1	1:C:251:ASP:HB3	1.82	0.45
2:F:36:TRP:O	2:F:48:VAL:HB	2.17	0.45
1:A:723:ILE:HD12	1:B:217:ASN:HB3	1.99	0.44
1:B:515:ARG:HG3	3:B:889:HOH:O	2.16	0.44
2:E:85:MET:CB	2:E:88:LEU:HD21	2.47	0.44
1:A:118:PRO:HA	1:A:119:PRO:HD3	1.90	0.44
1:B:592:ARG:HA	1:B:593:PRO:HD3	1.84	0.44
1:C:145:GLY:HA2	1:C:455:LEU:HG	1.99	0.44
2:E:36:TRP:O	2:E:48:VAL:HB	2.17	0.44
1:A:294:PHE:CZ	1:C:707:ARG:HB2	2.52	0.44
1:C:127:PHE:CE2	1:C:543:ARG:HD3	2.53	0.44
1:C:297:MET:HE1	1:C:319:PHE:CD1	2.53	0.44
1:B:119:PRO:HD2	1:B:562:ARG:HD3	2.00	0.44
1:B:289:LEU:HG	3:B:846:HOH:O	2.16	0.44
1:B:169:THR:CG2	1:B:268:THR:HB	2.48	0.43
1:A:286:GLU:HB2	3:A:916:HOH:O	2.18	0.43
1:B:304:ARG:HD3	2:F:112:GLU:HB2	1.99	0.43
1:B:169:THR:HG21	1:B:253:LYS:HD2	2.01	0.43
1:B:589:VAL:HG22	1:B:597:TYR:HE2	1.60	0.43
2:D:36:TRP:O	2:D:48:VAL:HB	2.18	0.43
1:A:369:TRP:CD2	1:A:370:GLN:HG2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:ARG:HH11	1:B:121:GLY:HA3	1.83	0.43
1:A:640:TYR:HB2	1:B:567:VAL:HG22	1.99	0.43
1:C:597:TYR:HD1	1:C:630:LEU:HD23	1.77	0.43
1:B:286:GLU:HB2	3:B:841:HOH:O	2.18	0.43
1:C:210:THR:HG23	1:C:229:GLU:HG3	2.01	0.43
1:C:238:LYS:HE3	3:C:1563:HOH:O	2.17	0.43
1:A:281:VAL:HG11	3:B:814:HOH:O	2.18	0.43
1:C:304:ARG:HD3	2:E:112:GLU:HB2	2.01	0.43
1:A:577:ALA:HB1	1:A:578:PRO:HD3	1.99	0.43
1:B:186:PHE:CG	1:C:184:GLY:HA2	2.54	0.43
1:A:224:HIS:HB2	1:A:269:VAL:HB	2.01	0.42
1:B:699:LEU:HB3	1:C:703:THR:HG21	2.00	0.42
1:C:224:HIS:CE1	1:C:250:THR:HG21	2.54	0.42
1:A:496:LYS:HD2	3:C:888:HOH:O	2.18	0.42
1:A:625:LEU:HD23	3:A:1439:HOH:O	2.19	0.42
1:B:443:LEU:HD23	1:B:443:LEU:HA	1.89	0.42
2:F:40:ALA:HB3	2:F:43:LYS:HD3	2.01	0.42
1:A:443:LEU:HD23	1:A:443:LEU:HA	1.94	0.42
1:B:592:ARG:HG3	3:B:809:HOH:O	2.19	0.42
1:B:638:ARG:O	1:C:564:LEU:HD22	2.18	0.42
1:A:200:LYS:HD2	3:A:934:HOH:O	2.19	0.42
1:B:723:ILE:O	1:B:724:ARG:HB2	2.20	0.42
1:B:369:TRP:CD2	1:B:370:GLN:HG2	2.55	0.42
1:A:695:LYS:HE3	3:A:1685:HOH:O	2.20	0.42
1:B:404:LEU:HB3	3:B:838:HOH:O	2.19	0.42
1:B:183:MET:HG3	1:B:263:HIS:CE1	2.55	0.42
1:B:649:TYR:O	1:B:656:SER:HB3	2.20	0.42
1:A:601:LEU:CD1	1:A:627:ARG:HH21	2.33	0.41
1:B:447:GLY:HA3	1:B:496:LYS:O	2.20	0.41
1:C:118:PRO:HA	1:C:119:PRO:HD3	1.88	0.41
1:C:606:TYR:CE1	1:C:613:ILE:HG13	2.54	0.41
2:F:36:TRP:CD1	2:F:83:LEU:HB2	2.55	0.41
1:A:511:ASN:HB3	1:A:515:ARG:NH1	2.35	0.41
1:B:667:VAL:HG11	1:C:555:VAL:HG12	2.02	0.41
1:C:369:TRP:CD2	1:C:370:GLN:HG2	2.54	0.41
1:A:296:TYR:CZ	1:C:711:LEU:HG	2.55	0.41
1:B:511:ASN:HB3	1:B:515:ARG:NH1	2.35	0.41
1:B:555:VAL:HG12	1:B:557:ARG:HG2	2.02	0.41
1:C:551:ALA:O	1:C:555:VAL:HG22	2.20	0.41
1:A:707:ARG:HB2	1:B:294:PHE:CZ	2.55	0.41
1:B:415:ARG:O	1:B:419:GLU:CD	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4:LEU:HD13	2:D:98:CYS:SG	2.61	0.41
1:B:294:PHE:HD2	3:B:841:HOH:O	2.02	0.41
1:A:183:MET:HG3	1:A:263:HIS:CE1	2.55	0.41
1:B:559:VAL:HG22	1:B:572:THR:HA	2.03	0.41
2:D:55:PHE:HB2	2:D:59:ARG:HG3	2.03	0.41
1:A:297:MET:HE3	1:A:301:TYR:CD2	2.56	0.41
1:A:514:GLN:HA	3:A:1449:HOH:O	2.21	0.41
1:B:225:ARG:HA	1:B:254:TYR:CD2	2.56	0.41
1:B:528:TRP:O	1:B:532:GLN:HG2	2.21	0.41
1:C:286:GLU:HB2	3:C:904:HOH:O	2.20	0.41
2:D:33:ARG:HD2	2:D:50:THR:HG21	2.03	0.41
1:C:634:THR:H	1:C:653:TYR:HE2	1.69	0.41
1:B:551:ALA:HB2	1:B:568:MET:SD	2.61	0.40
1:A:297:MET:SD	1:A:345:LEU:HD22	2.61	0.40
1:B:537:THR:HG23	3:B:819:HOH:O	2.20	0.40
1:C:682:GLU:HB3	3:C:1336:HOH:O	2.21	0.40
1:A:392:SER:HB2	1:A:505:ARG:HH21	1.86	0.40
1:A:670:PHE:CE2	1:B:128:GLU:HG2	2.56	0.40
1:B:664:VAL:HG11	1:C:126:GLN:HB3	2.02	0.40
3:A:1500:HOH:O	1:B:699:LEU:HD21	2.21	0.40
1:B:118:PRO:HA	1:B:119:PRO:HD3	1.91	0.40
1:C:225:ARG:HA	1:C:254:TYR:CD2	2.57	0.40
1:C:597:TYR:CE2	1:C:601:LEU:HD11	2.55	0.40
2:E:55:PHE:HB2	2:E:59:ARG:HG3	2.02	0.40
2:F:55:PHE:CD2	2:F:59:ARG:HD2	2.57	0.40

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	570/727 (78%)	562 (99%)	7 (1%)	1 (0%)	44	52

Continued on next page...



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	574/727 (79%)	568 (99%)	5 (1%)	1 (0%)	44	52
1	C	568/727 (78%)	559 (98%)	9 (2%)	0	100	100
2	D	123/131 (94%)	123 (100%)	0	0	100	100
2	E	123/131 (94%)	122 (99%)	1 (1%)	0	100	100
2	F	123/131 (94%)	119 (97%)	4 (3%)	0	100	100
All	All	2081/2574 (81%)	2053 (99%)	26 (1%)	2 (0%)	50	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	724	ARG
1	B	426	ALA

### 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	503/613 (82%)	498 (99%)	5 (1%)	73	84
1	B	507/613 (83%)	502 (99%)	5 (1%)	73	84
1	C	502/613 (82%)	498 (99%)	4 (1%)	79	88
2	D	99/105 (94%)	99 (100%)	0	100	100
2	E	99/105 (94%)	99 (100%)	0	100	100
2	F	99/105 (94%)	99 (100%)	0	100	100
All	All	1809/2154 (84%)	1795 (99%)	14 (1%)	77	88

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	419	GLU
1	A	443	LEU
1	A	613	ILE
1	A	642	ILE

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Mol	Chain	Res	Type
1	A	724	ARG
1	B	427	ARG
1	B	443	LEU
1	B	445	THR
1	B	613	ILE
1	B	614	GLU
1	C	218	MET
1	C	428	LYS
1	C	443	LEU
1	C	614	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	658	GLN
1	B	129	GLN
1	B	140	GLN
1	B	584	GLN
1	B	658	GLN
1	B	706	GLN
1	C	255	ASN
1	C	580	ASN
1	C	616	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

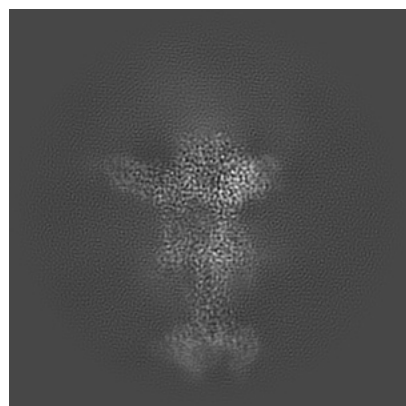
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48671. These allow visual inspection of the internal detail of the map and identification of artifacts.

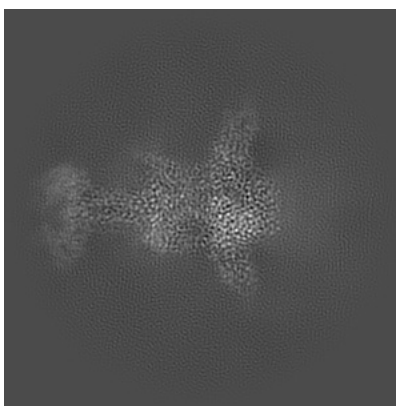
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

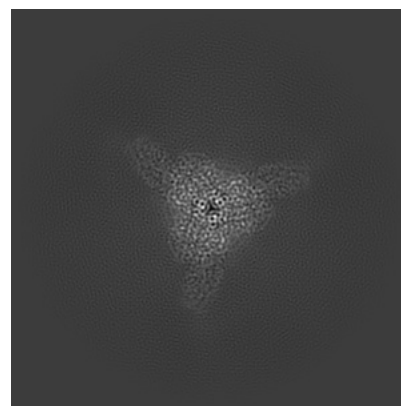
#### 6.1.1 Primary map



X

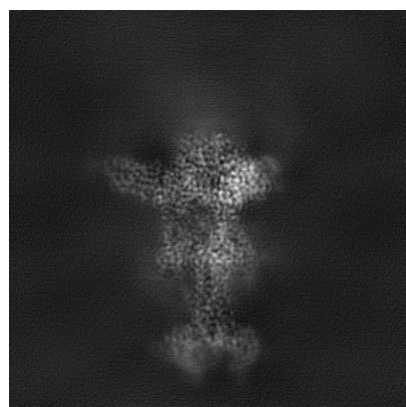


Y

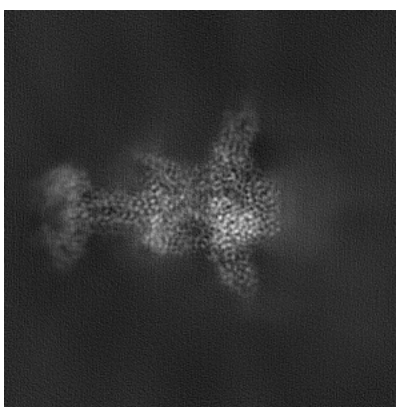


Z

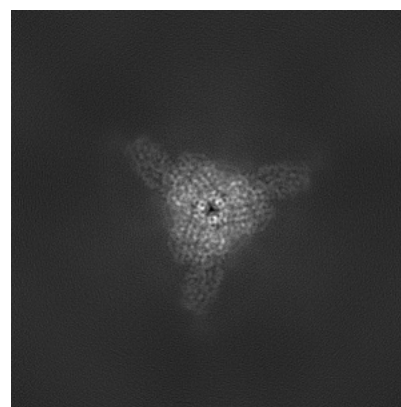
#### 6.1.2 Raw map



X



Y

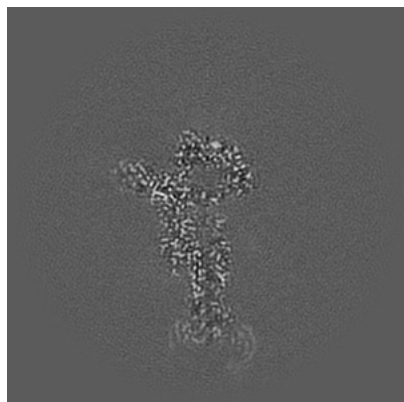


Z

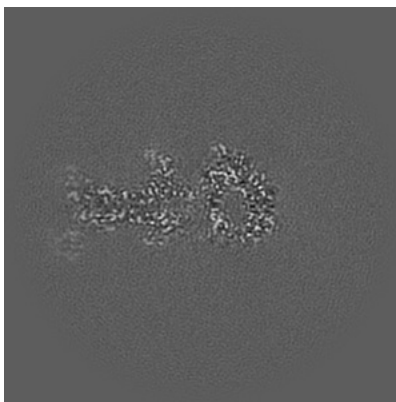
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

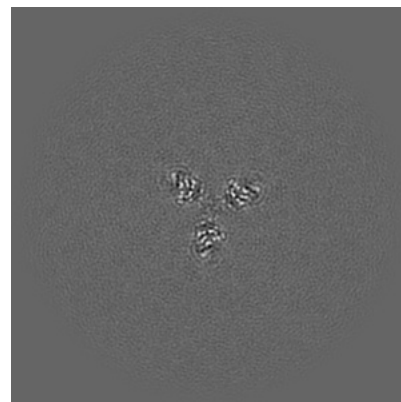
### 6.2.1 Primary map



X Index: 180

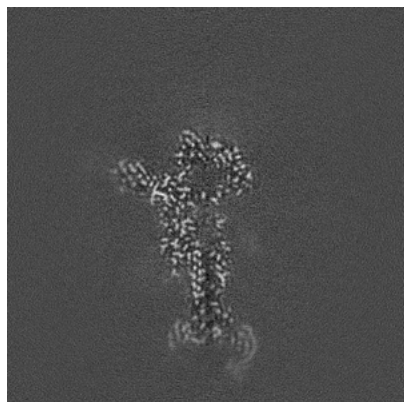


Y Index: 180

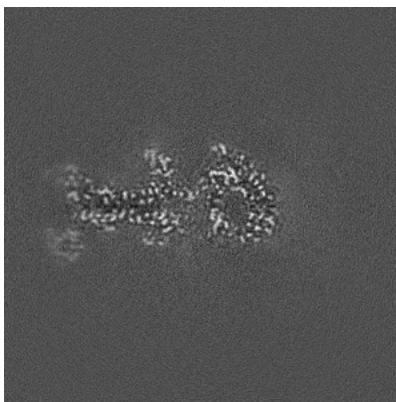


Z Index: 180

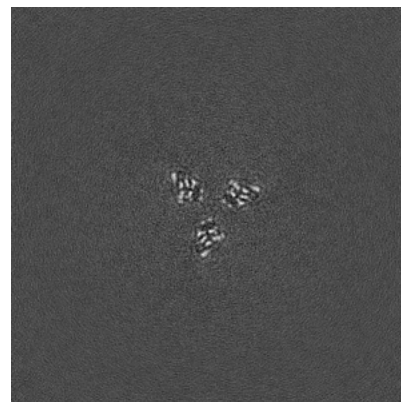
### 6.2.2 Raw map



X Index: 180



Y Index: 180

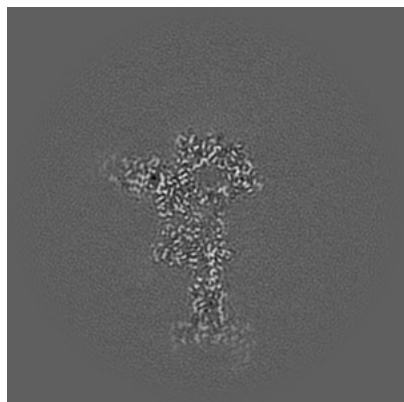


Z Index: 180

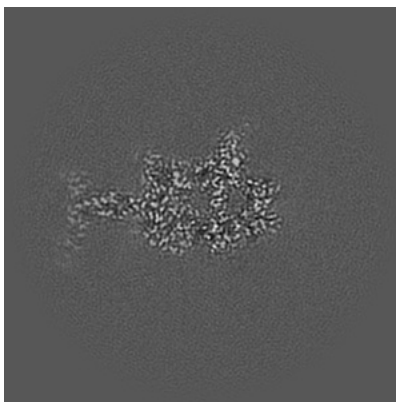
The images above show central slices of the map in three orthogonal directions.

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

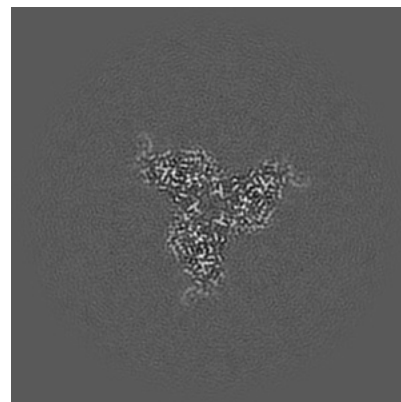
### 6.3.1 Primary map



X Index: 174

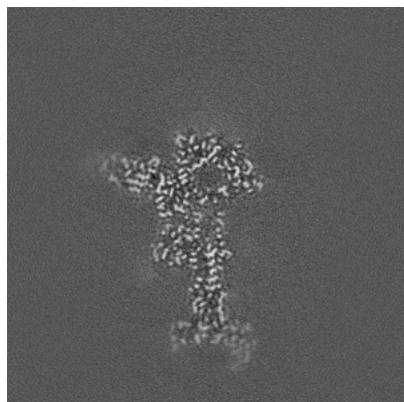


Y Index: 191

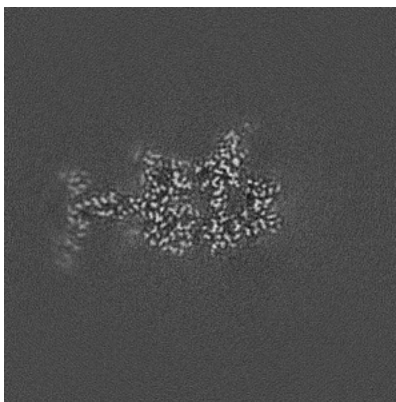


Z Index: 199

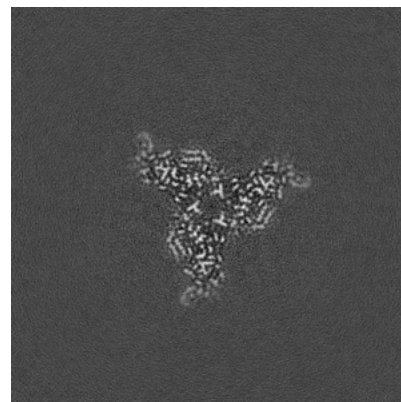
### 6.3.2 Raw map



X Index: 174



Y Index: 191



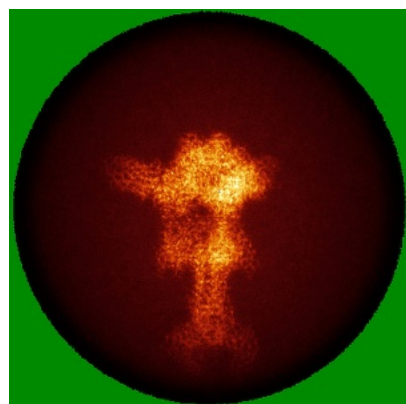
Z Index: 199

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

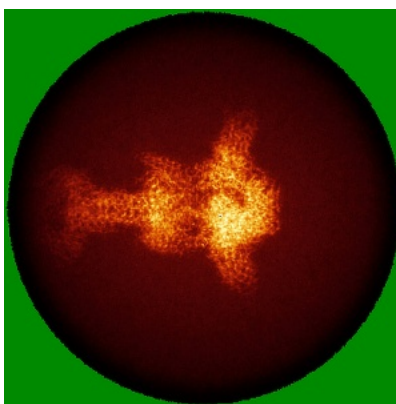


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

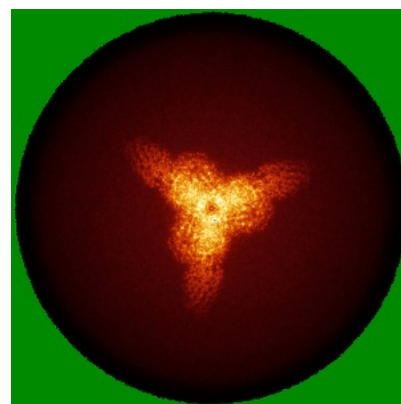
### 6.4.1 Primary map



X

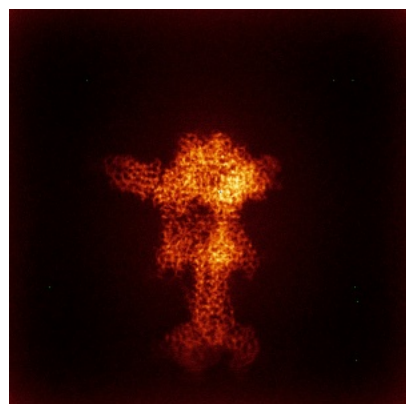


Y

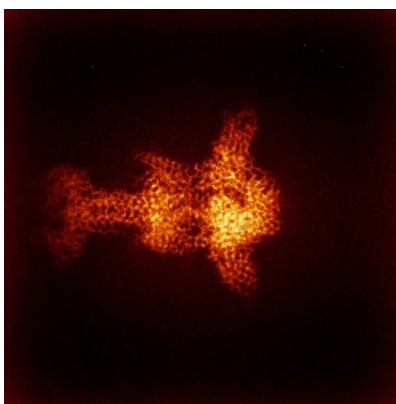


Z

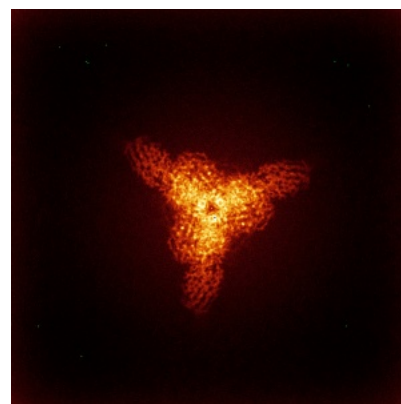
### 6.4.2 Raw map



X



Y

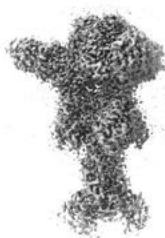


Z

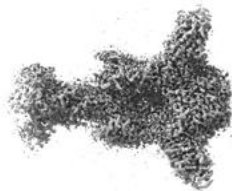
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

### 6.5.1 Primary map



X



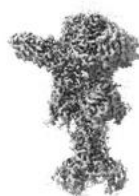
Y



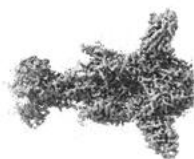
Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

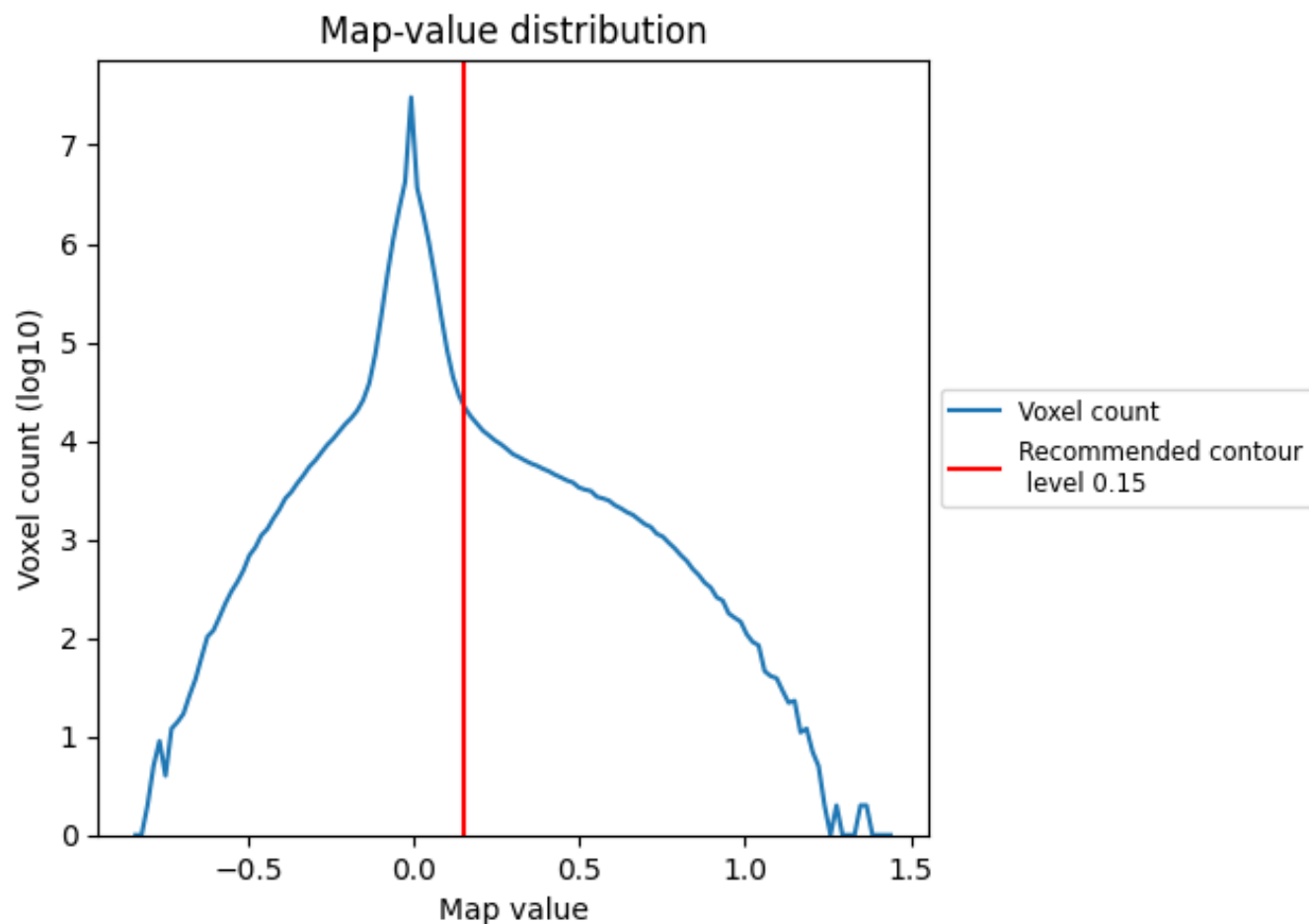
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

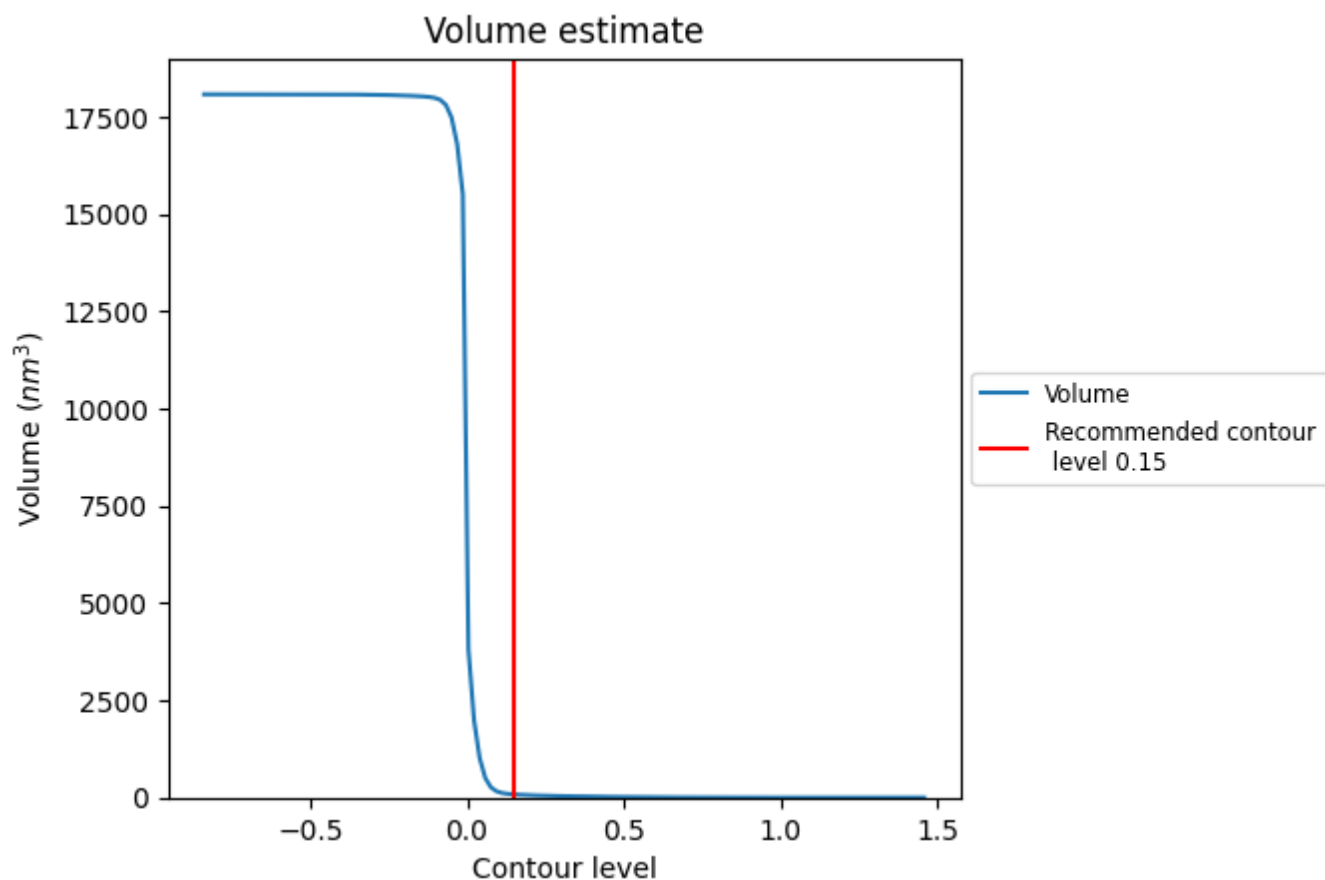
### 7.1 Map-value distribution [i](#)



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.



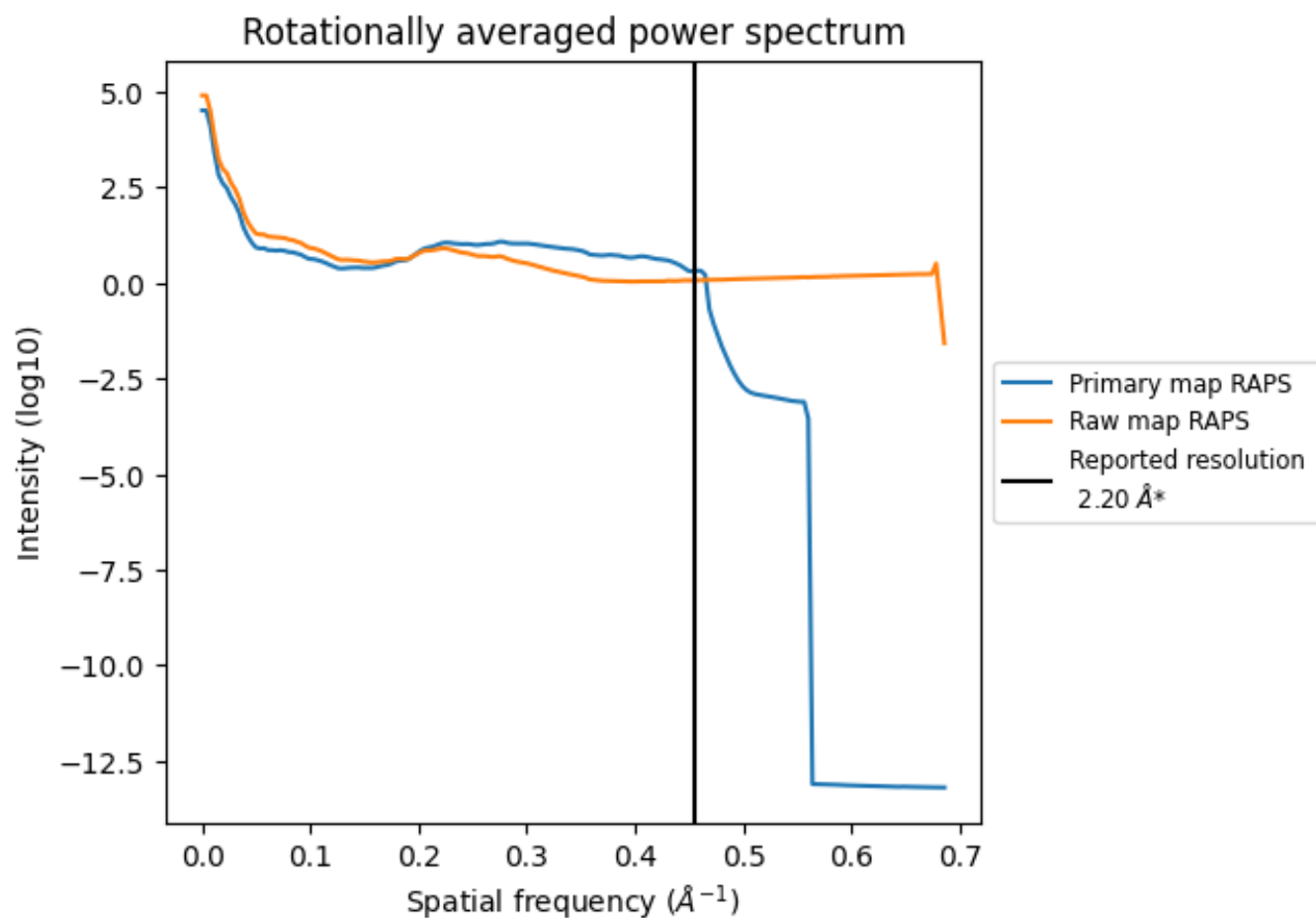
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 81 nm<sup>3</sup>; this corresponds to an approximate mass of 73 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 ⓘ

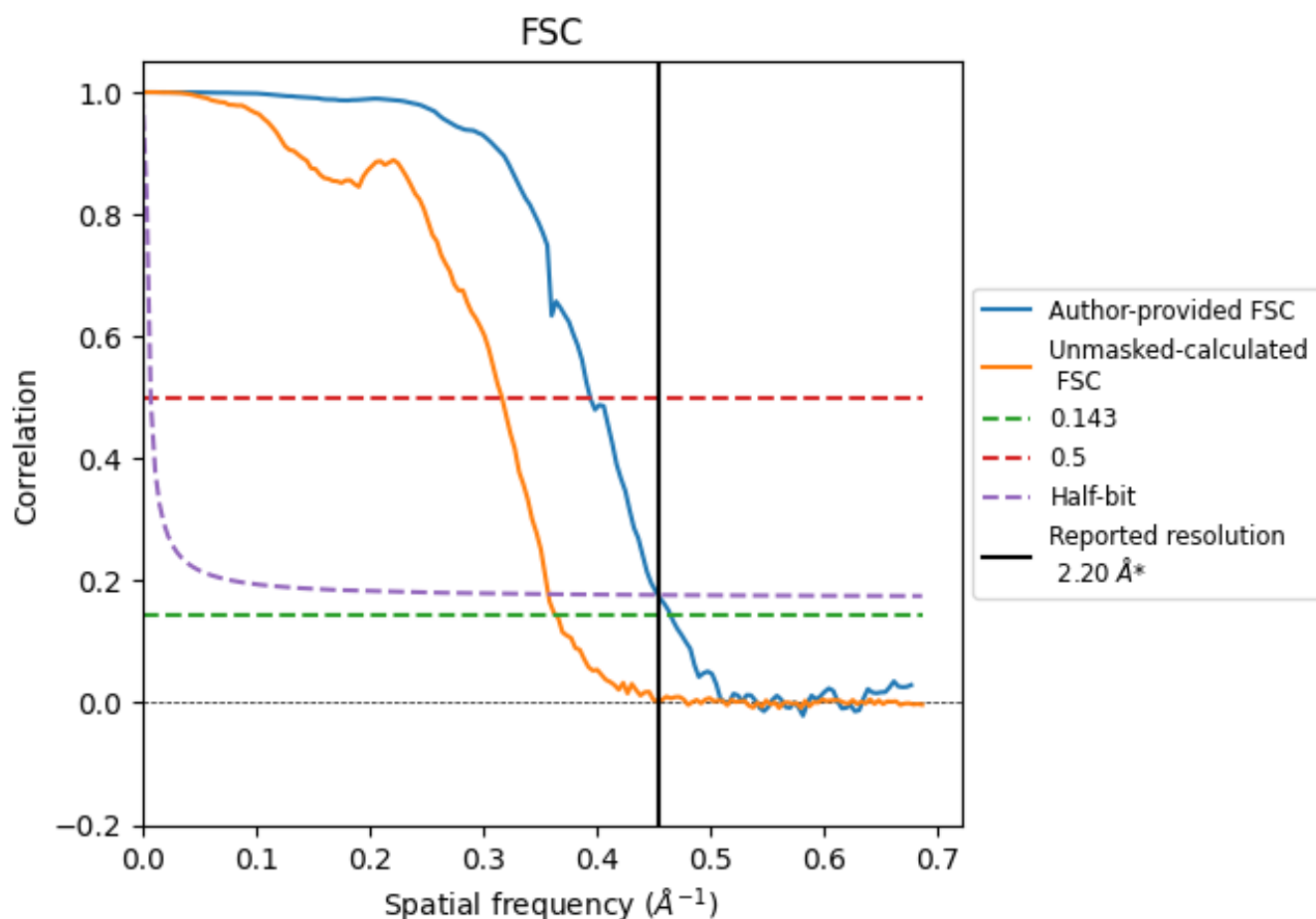


\*Reported resolution corresponds to spatial frequency of 0.455 Å<sup>-1</sup>

## 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 0.455  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

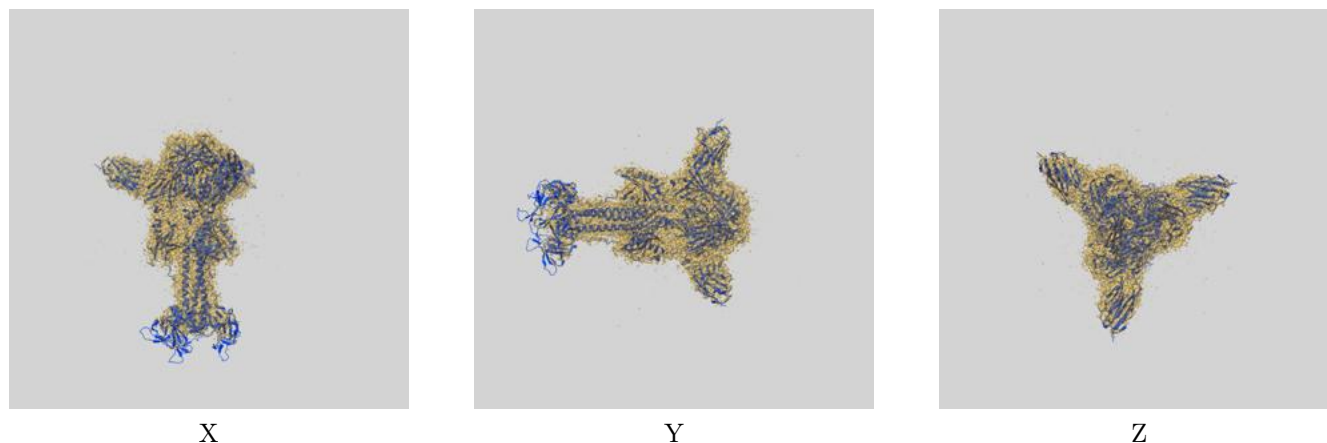
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.15	2.54	2.20
Unmasked-calculated*	2.75	3.16	2.80

\*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 2.75 differs from the reported value 2.2 by more than 10 %

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

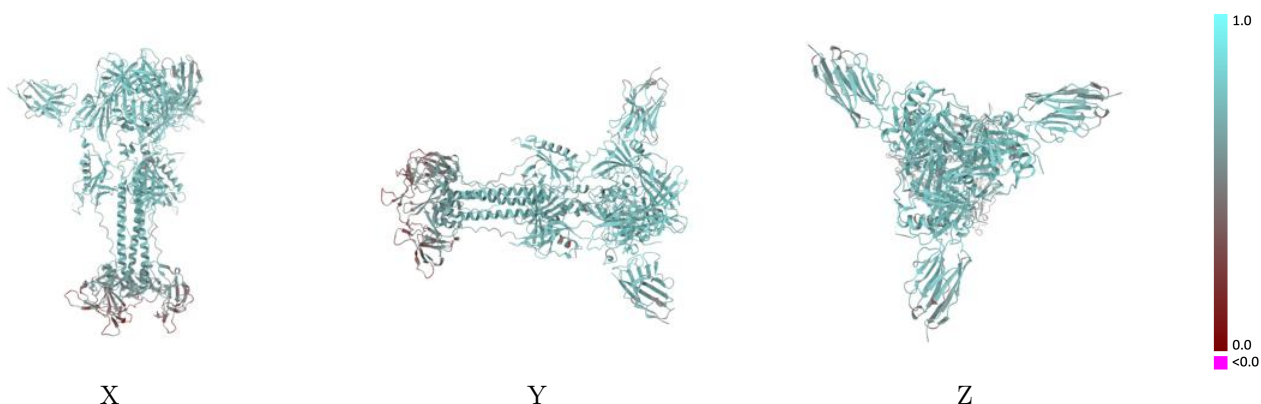
This section contains information regarding the fit between EMDB map EMD-48671 and PDB model 9MVU. Per-residue inclusion information can be found in section [3](#) on page [11](#).

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



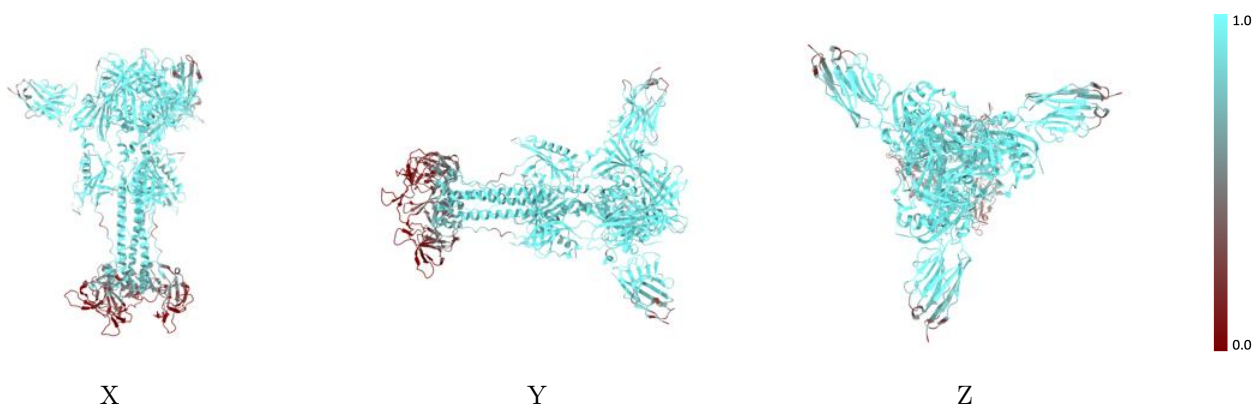
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



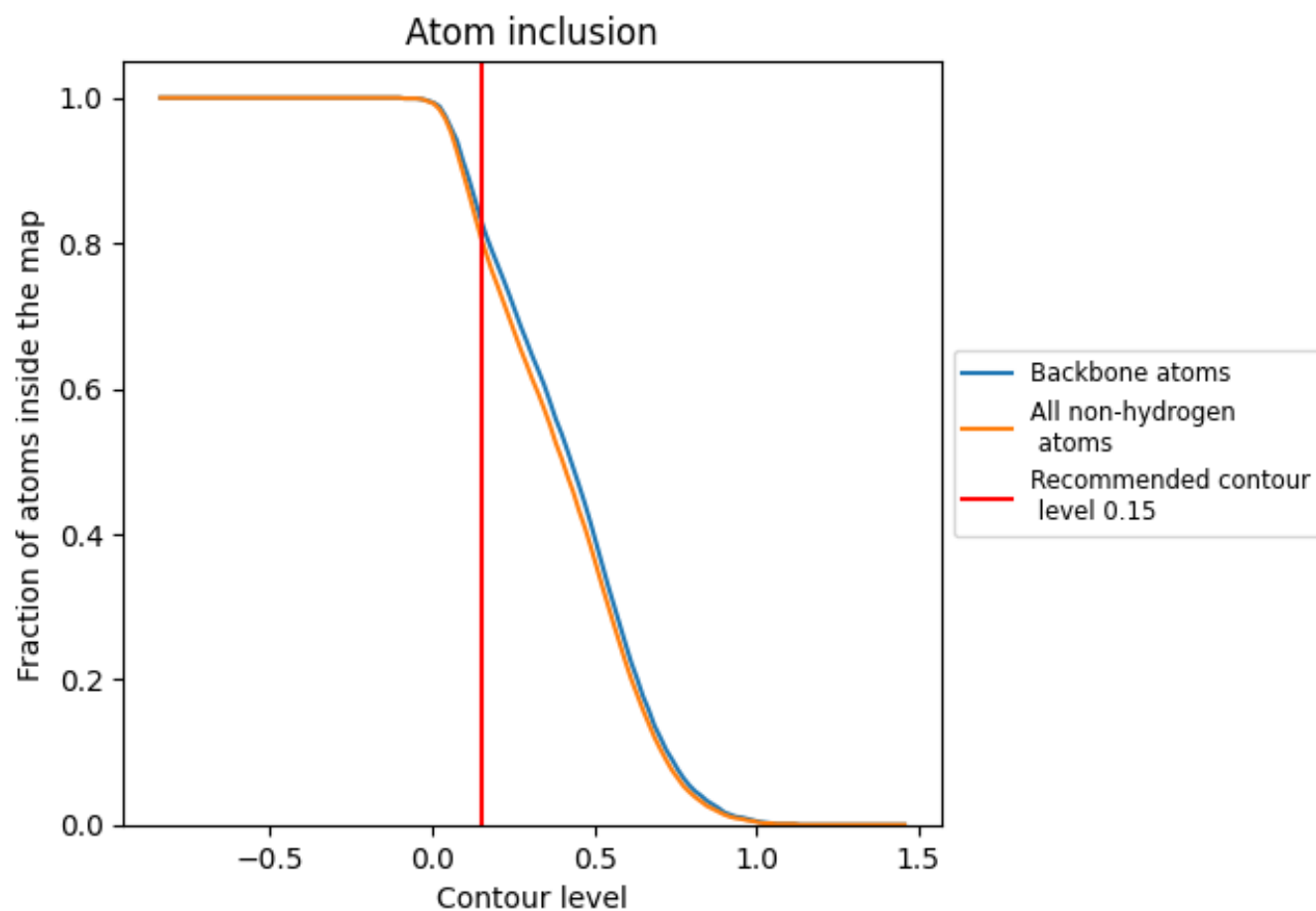
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 81% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8080	<div><div></div></div> 0.6580
A	<div><div></div></div> 0.8070	<div><div></div></div> 0.6570
B	<div><div></div></div> 0.8030	<div><div></div></div> 0.6620
C	<div><div></div></div> 0.8030	<div><div></div></div> 0.6590
D	<div><div></div></div> 0.8350	<div><div></div></div> 0.6530
E	<div><div></div></div> 0.8370	<div><div></div></div> 0.6460
F	<div><div></div></div> 0.8400	<div><div></div></div> 0.6520

