



## wwPDB EM Validation Summary Report ⓘ

Feb 5, 2025 – 10:24 AM JST

PDB ID : 8Z6S  
EMDB ID : EMD-39803  
Title : Structure of XBB.1.16 S trimer with 2 down-RBDs complex with antibody CYFN1006-1.  
Authors : Wang, Y.J.; Sun, L.  
Deposited on : 2024-04-19  
Resolution : 2.84 Å(reported)

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

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<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
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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  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

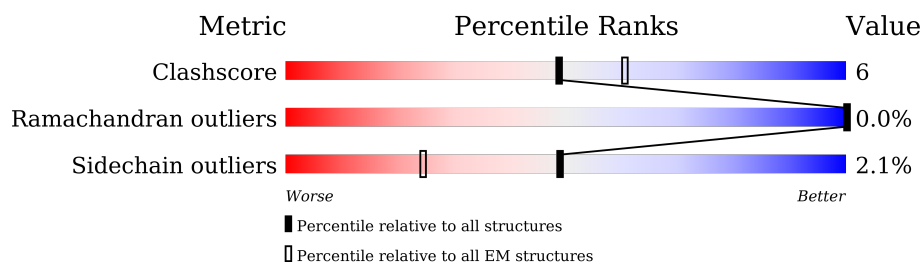
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.84 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	D	215	
1	F	215	
1	H	215	
2	E	451	
2	G	451	
2	I	451	
3	A	1299	
3	B	1299	

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Mol	Chain	Length	Quality of chain
3	C	1299	 A horizontal bar chart showing the quality of chain C. The bar is divided into three segments: a green segment representing 71%, a yellow segment representing 14%, and a grey segment representing 15%. A small black dot is located on the yellow segment.

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 35014 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 CYFN1006-1 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	194	Total	C	N	O	S	0	0
			1443	904	240	292	7		
1	F	192	Total	C	N	O	S	0	0
			1429	895	237	290	7		
1	H	192	Total	C	N	O	S	0	0
			1429	895	237	290	7		

- Molecule 2 is a protein called CYFN1006-1 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	202	Total	C	N	O	S	0	0
			1544	992	251	293	8		
2	G	202	Total	C	N	O	S	0	0
			1544	992	251	293	8		
2	I	202	Total	C	N	O	S	0	0
			1544	992	251	293	8		

- Molecule 3 is a protein called Spike glycoprotein,Fibritin,Expression Tag.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	1106	Total	C	N	O	S	0	0
			8662	5534	1445	1643	40		
3	B	1103	Total	C	N	O	S	0	0
			8650	5533	1440	1637	40		
3	A	1119	Total	C	N	O	S	0	0
			8769	5607	1462	1660	40		

There are 243 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	MET	-	initiating methionine	UNP P0DTC2
C	-5	PRO	-	expression tag	UNP P0DTC2
C	-4	MET	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP P0DTC2
C	-2	SER	-	expression tag	UNP P0DTC2
C	-1	LEU	-	expression tag	UNP P0DTC2
C	0	GLN	-	expression tag	UNP P0DTC2
C	1	PRO	-	expression tag	UNP P0DTC2
C	2	LEU	-	expression tag	UNP P0DTC2
C	3	ALA	-	expression tag	UNP P0DTC2
C	4	THR	-	expression tag	UNP P0DTC2
C	5	LEU	-	expression tag	UNP P0DTC2
C	6	TYR	-	expression tag	UNP P0DTC2
C	7	LEU	-	expression tag	UNP P0DTC2
C	8	LEU	-	expression tag	UNP P0DTC2
C	9	GLY	-	expression tag	UNP P0DTC2
C	10	MET	-	expression tag	UNP P0DTC2
C	11	LEU	-	expression tag	UNP P0DTC2
C	12	VAL	-	expression tag	UNP P0DTC2
C	13	ALA	-	expression tag	UNP P0DTC2
C	14	SER	-	expression tag	UNP P0DTC2
C	15	VAL	-	expression tag	UNP P0DTC2
C	16	LEU	-	expression tag	UNP P0DTC2
C	17	ALA	-	expression tag	UNP P0DTC2
C	23	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	28	SER	ALA	variant	UNP P0DTC2
C	84	ALA	VAL	variant	UNP P0DTC2
C	143	ASP	GLY	variant	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	146	GLN	HIS	variant	UNP P0DTC2
C	180	VAL	GLU	conflict	UNP P0DTC2
C	183	GLU	GLN	variant	UNP P0DTC2
C	213	GLU	VAL	variant	UNP P0DTC2
C	252	VAL	GLY	variant	UNP P0DTC2
C	339	HIS	GLY	variant	UNP P0DTC2
C	346	THR	ARG	variant	UNP P0DTC2
C	368	ILE	LEU	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	445	PRO	VAL	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	460	LYS	ASN	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	ARG	THR	conflict	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	486	PRO	PHE	variant	UNP P0DTC2
C	490	SER	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	-	insertion	UNP P0DTC2
C	686	SER	-	insertion	UNP P0DTC2
C	687	LYS	-	insertion	UNP P0DTC2
C	689	SER	-	insertion	UNP P0DTC2
C	768	LYS	ASN	variant	UNP P0DTC2
C	800	TYR	ASP	variant	UNP P0DTC2
C	821	PRO	PHE	conflict	UNP P0DTC2
C	896	PRO	ALA	conflict	UNP P0DTC2
C	903	PRO	ALA	conflict	UNP P0DTC2
C	946	PRO	ALA	conflict	UNP P0DTC2
C	958	HIS	GLN	variant	UNP P0DTC2
C	973	LYS	ASN	variant	UNP P0DTC2
C	990	PRO	LYS	variant	UNP P0DTC2
C	991	PRO	VAL	variant	UNP P0DTC2
C	1213	GLY	-	linker	UNP P0DTC2
C	1214	SER	-	linker	UNP P0DTC2
B	-6	MET	-	initiating methionine	UNP P0DTC2
B	-5	PRO	-	expression tag	UNP P0DTC2
B	-4	MET	-	expression tag	UNP P0DTC2
B	-3	GLY	-	expression tag	UNP P0DTC2
B	-2	SER	-	expression tag	UNP P0DTC2
B	-1	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLN	-	expression tag	UNP P0DTC2
B	1	PRO	-	expression tag	UNP P0DTC2
B	2	LEU	-	expression tag	UNP P0DTC2
B	3	ALA	-	expression tag	UNP P0DTC2
B	4	THR	-	expression tag	UNP P0DTC2
B	5	LEU	-	expression tag	UNP P0DTC2
B	6	TYR	-	expression tag	UNP P0DTC2
B	7	LEU	-	expression tag	UNP P0DTC2
B	8	LEU	-	expression tag	UNP P0DTC2
B	9	GLY	-	expression tag	UNP P0DTC2
B	10	MET	-	expression tag	UNP P0DTC2
B	11	LEU	-	expression tag	UNP P0DTC2
B	12	VAL	-	expression tag	UNP P0DTC2
B	13	ALA	-	expression tag	UNP P0DTC2
B	14	SER	-	expression tag	UNP P0DTC2
B	15	VAL	-	expression tag	UNP P0DTC2
B	16	LEU	-	expression tag	UNP P0DTC2
B	17	ALA	-	expression tag	UNP P0DTC2
B	23	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	28	SER	ALA	variant	UNP P0DTC2
B	84	ALA	VAL	variant	UNP P0DTC2
B	143	ASP	GLY	variant	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	146	GLN	HIS	variant	UNP P0DTC2
B	180	VAL	GLU	conflict	UNP P0DTC2
B	183	GLU	GLN	variant	UNP P0DTC2
B	213	GLU	VAL	variant	UNP P0DTC2
B	252	VAL	GLY	variant	UNP P0DTC2
B	339	HIS	GLY	variant	UNP P0DTC2
B	346	THR	ARG	variant	UNP P0DTC2
B	368	ILE	LEU	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	445	PRO	VAL	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	460	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	ARG	THR	conflict	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	PRO	PHE	variant	UNP P0DTC2
B	490	SER	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	-	insertion	UNP P0DTC2
B	686	SER	-	insertion	UNP P0DTC2
B	687	LYS	-	insertion	UNP P0DTC2
B	689	SER	-	insertion	UNP P0DTC2
B	768	LYS	ASN	variant	UNP P0DTC2
B	800	TYR	ASP	variant	UNP P0DTC2
B	821	PRO	PHE	conflict	UNP P0DTC2
B	896	PRO	ALA	conflict	UNP P0DTC2
B	903	PRO	ALA	conflict	UNP P0DTC2
B	946	PRO	ALA	conflict	UNP P0DTC2
B	958	HIS	GLN	variant	UNP P0DTC2
B	973	LYS	ASN	variant	UNP P0DTC2
B	990	PRO	LYS	variant	UNP P0DTC2
B	991	PRO	VAL	variant	UNP P0DTC2
B	1213	GLY	-	linker	UNP P0DTC2
B	1214	SER	-	linker	UNP P0DTC2
A	-6	MET	-	initiating methionine	UNP P0DTC2
A	-5	PRO	-	expression tag	UNP P0DTC2
A	-4	MET	-	expression tag	UNP P0DTC2
A	-3	GLY	-	expression tag	UNP P0DTC2
A	-2	SER	-	expression tag	UNP P0DTC2
A	-1	LEU	-	expression tag	UNP P0DTC2
A	0	GLN	-	expression tag	UNP P0DTC2
A	1	PRO	-	expression tag	UNP P0DTC2
A	2	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ALA	-	expression tag	UNP P0DTC2
A	4	THR	-	expression tag	UNP P0DTC2
A	5	LEU	-	expression tag	UNP P0DTC2
A	6	TYR	-	expression tag	UNP P0DTC2
A	7	LEU	-	expression tag	UNP P0DTC2
A	8	LEU	-	expression tag	UNP P0DTC2
A	9	GLY	-	expression tag	UNP P0DTC2
A	10	MET	-	expression tag	UNP P0DTC2
A	11	LEU	-	expression tag	UNP P0DTC2
A	12	VAL	-	expression tag	UNP P0DTC2
A	13	ALA	-	expression tag	UNP P0DTC2
A	14	SER	-	expression tag	UNP P0DTC2
A	15	VAL	-	expression tag	UNP P0DTC2
A	16	LEU	-	expression tag	UNP P0DTC2
A	17	ALA	-	expression tag	UNP P0DTC2
A	23	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	28	SER	ALA	variant	UNP P0DTC2
A	84	ALA	VAL	variant	UNP P0DTC2
A	143	ASP	GLY	variant	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	146	GLN	HIS	variant	UNP P0DTC2
A	180	VAL	GLU	conflict	UNP P0DTC2
A	183	GLU	GLN	variant	UNP P0DTC2
A	213	GLU	VAL	variant	UNP P0DTC2
A	252	VAL	GLY	variant	UNP P0DTC2
A	339	HIS	GLY	variant	UNP P0DTC2
A	346	THR	ARG	variant	UNP P0DTC2
A	368	ILE	LEU	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	445	PRO	VAL	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	460	LYS	ASN	variant	UNP P0DTC2

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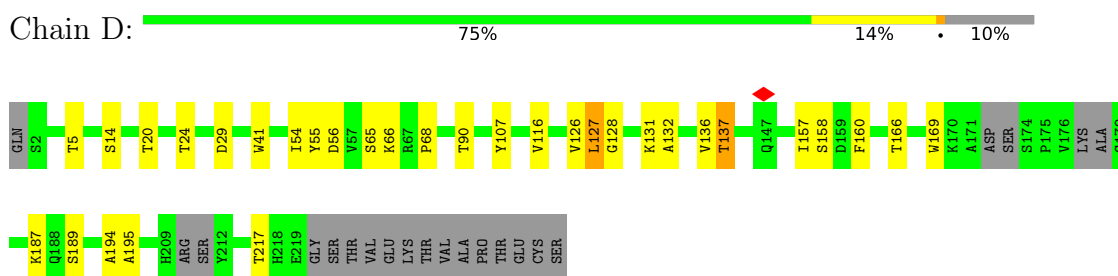
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Chain	Residue	Modelled	Actual	Comment	Reference
A	477	ASN	SER	variant	UNP P0DTC2
A	478	ARG	THR	conflict	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	PRO	PHE	variant	UNP P0DTC2
A	490	SER	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	-	insertion	UNP P0DTC2
A	686	SER	-	insertion	UNP P0DTC2
A	687	LYS	-	insertion	UNP P0DTC2
A	689	SER	-	insertion	UNP P0DTC2
A	768	LYS	ASN	variant	UNP P0DTC2
A	800	TYR	ASP	variant	UNP P0DTC2
A	821	PRO	PHE	conflict	UNP P0DTC2
A	896	PRO	ALA	conflict	UNP P0DTC2
A	903	PRO	ALA	conflict	UNP P0DTC2
A	946	PRO	ALA	conflict	UNP P0DTC2
A	958	HIS	GLN	variant	UNP P0DTC2
A	973	LYS	ASN	variant	UNP P0DTC2
A	990	PRO	LYS	variant	UNP P0DTC2
A	991	PRO	VAL	variant	UNP P0DTC2
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A	1214	SER	-	linker	UNP P0DTC2

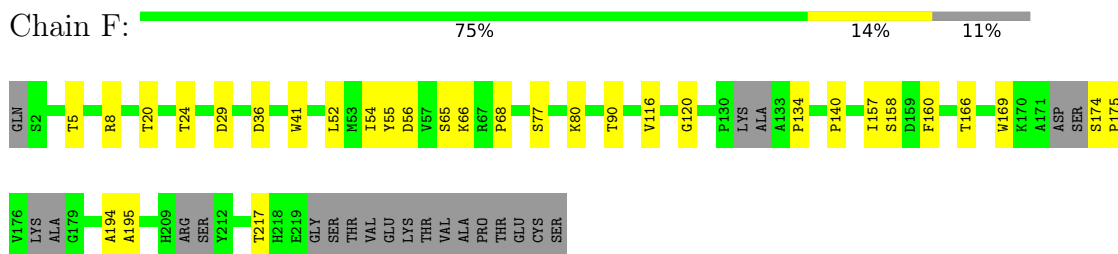
### 3 Residue-property plots [i](#)

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.

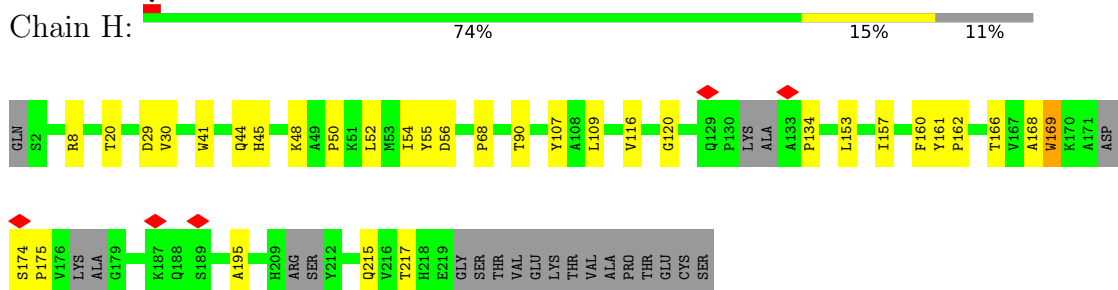
- Molecule 1: CYFN1006-1 light chain



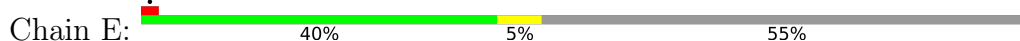
- Molecule 1: CYFN1006-1 light chain

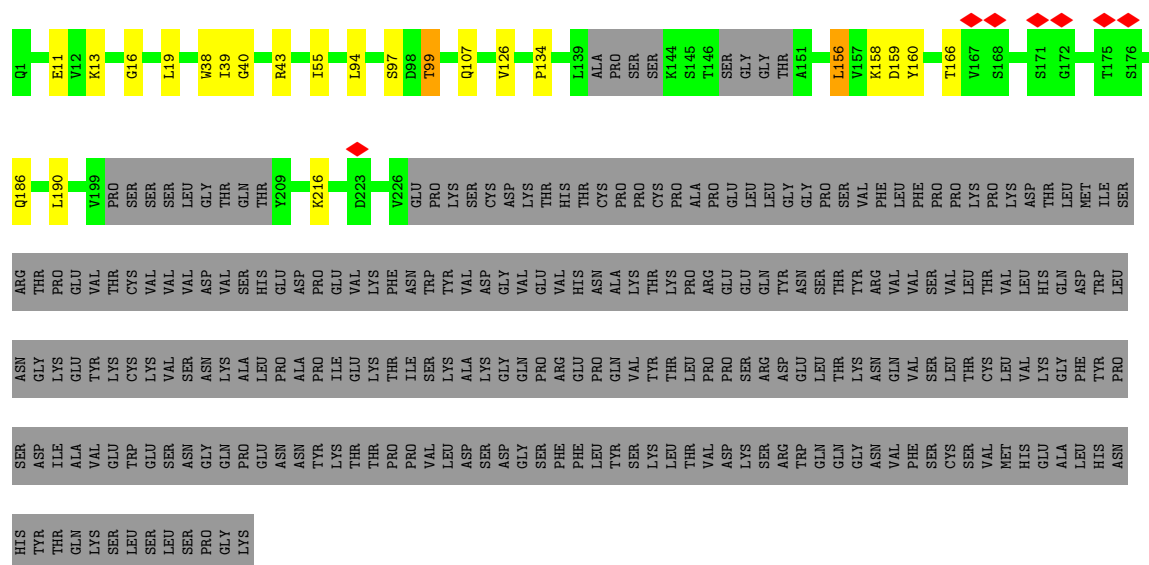


- Molecule 1: CYFN1006-1 light chain



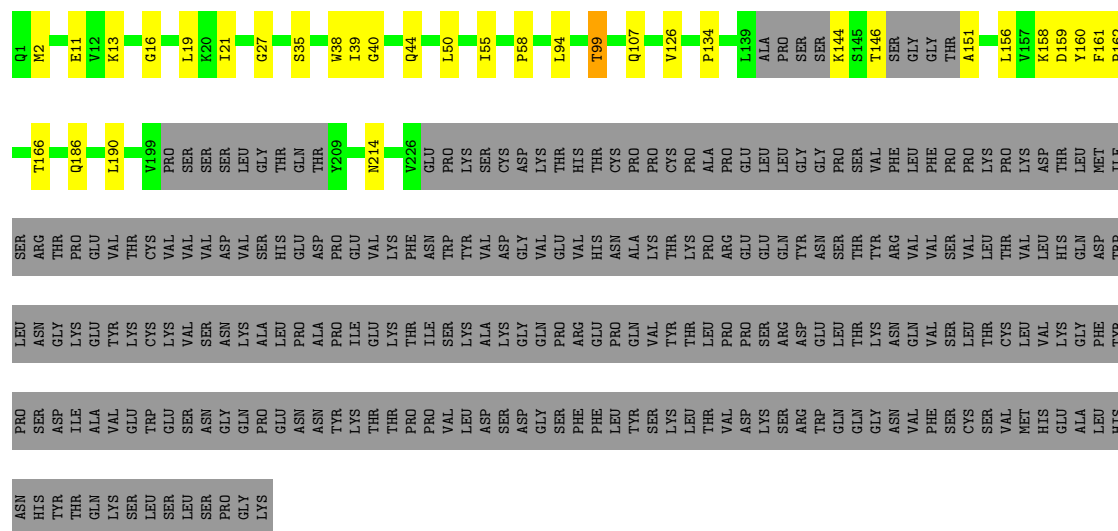
- Molecule 2: CYFN1006-1 heavy chain





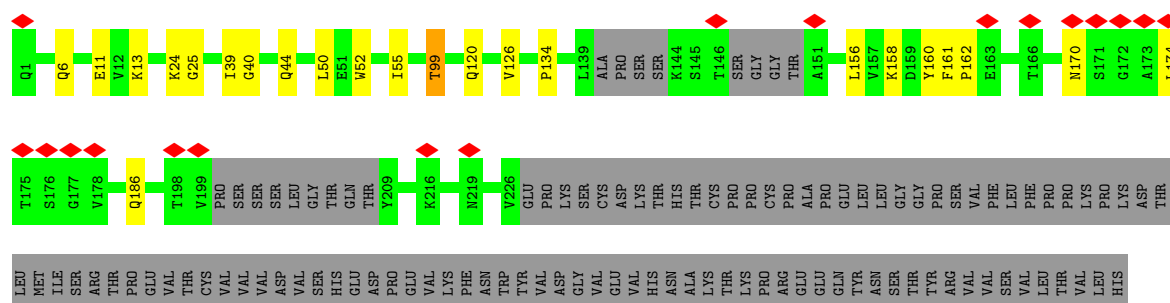
• Molecule 2: CYFN1006-1 heavy chain

Chain G: 37% 7% 55%



• Molecule 2: CYFN1006-1 heavy chain

Chain I: 40% 5% 55%





HIS	HIS	ASP	GLY	G1039	I809	Q644	F392	P230
		GLY	ILE	Q1040	L826	T645	F392	Q239
		TRP	GLY	S1041	L826	T645	V395	T240
		VAL	GLY	K1042	D834	G648	Y396	
		PHE	ILE	R1043				L244
		LEU	ASN	V1044	Y841	I651	N405	H245
		SER	ALA	D1045				R246
		THR	SER	F1046	I854	N658	I418	S247
		PHE	VAL					TYR
		LEU	VAL	Y1051	C855	I664	Y421	LEU
		SER	ASN		A856	P685	N422	THR
		GLY	ILE	Q1058	Q857	I666		
		LEU	GLN				C432	VAL
		GLY	LYS	V1065	N860	C671	L452	SER
		VAL	GLU					ASP
		LEU	ILE	H1068	L882	T676		SER
		PHE	ASP	V1069		GLN	R457	SER
		GLN	ARG	T1070	Q899	THR	K458	SER
		GLY	LEU	V1071		LYS	S459	GLY
		PRO	ASN	P1072	F910	SER	K460	
		GLY	GLU	P1073		HIS	L461	Y266
		GLY	VAL		I913	GLY		V267
		TRP	ALA	E1076		SER	I468	G268
		SER	LYS	K1077	T916	ALA		
		HIS	ASN	N1078		SER	R478	K278
		PRO	LEU	F1079	I938	SER		D294
		GLN	ASN	T1080		LYS	P486	P295
		PHE	GLU		L949	ARG	N487	L296
		GLU	SER	S1101		SER	G504	
		LYS	LEU		V955	SER		F306
		GLY	ILE	V1108		VAL	L517	
		GLY	ASP	T1109	N959	ALA		R319
		GLY	LEU	Q1110		SER	V524	V320
		SER	GLN		N964			Q321
		GLY	GLU	E1115	P965	G694		
		GLY	LEU		L966		K535	C336
		GLY	GLY	I1119			E554	
		SER	LYS	T1120	L988	V726		H339
		GLY	TYR		D989	I727	K557	E340
		GLY	GLU	N1129		T728		V341
		SER	GLN	C1130	A993	E729	R567	
		ALA	GLY	D1131		I730		V350
		TRP	SER	V1132	I997		D574	Y351
		SER	GLY		D998	M744	I598	
		HIS	TYR	Y1142		V745		R355
		PRO	ILE		R1004	I746		
		GLN	PRO	L1156	L1005		V608	I358
		PHE	GLU		Q1006	Y760		
		GLY	ALA	Y1159	S1007	F763	Q613	V367
		PRO	LYS		L1008		I368	I368
		GLY	ARG	N1162	Q1009	L767	N616	Y369
		GLY	ASP	H1163			C617	N370
		SER	GLY	T1164	V1012	I774		
		HIS	GLN	S1165			V620	F374
		HIS	ALA	P1166	R1023			
		HIS	TYR	ASP		Q778	L629	F377
		HIS	VAL	VAL	K1032		T630	K378
		HIS	ARG	ASP			R62	C379
		HIS	LYS	LEU	E1035	T806		

• Molecule 3: Spike glycoprotein,Fibritin,Expression Tag

Chain A:  71% 15% 14%

F1046	Q899	LYS	R457	ASP	F107
Y1051	I900	SER	K458	SER	T110
H1052	P901	HIS	S459	SER	L118
L1053	F902	GLY	K460	SER	N122
V1065	P903	SER	L461	W258	N126
V1069	M904	ALA	I468	Y266	N129
T1070	Q905	LYS	R478	L270	K130
Y1071	M906	ARG	N487	D294	E133
E1076	I913	SER	C488	R319	F134
K1077	T916	VAL	Y489	W320	C137
M1078	T916	ALA	G504	Q321	N138
F1079	L920	GLN	R509	R328	Y145
T1080	A934	S695	V512	C336	N149
K1090	I938	I696	L517	P337	K150
S1101	V955	P719	L518	R339	S151
V1108	N959	W726	H519	E340	F157
T1109	N959	I730	A520	T345	N164
Q1110	N964	M744	K529	V350	Y170
I1119	T965	Y745	S530	V351	P174
T1120	L966	I746	T531	I358	D178
M1123	V967	Y760	K535	A363	K182
V1126	K968	L767	E554	V369	E183
N1129	L988	I774	K558	F375	F186
D1131	E992	E777	R567	A376	F192
V1132	D998	Q778	T581	F377	H67
L1156	R1004	P796	L582	S383	M75
K1161	L1005	F806	E583	P384	GLY
N1162	S1007	F806	Q613	V395	THR
H1163	L1008	I809	N616	V401	LYS
T1164	Q1009	A833	C617	N405	ARG
S1165	V1012	D834	Q628	I418	F80
P1166	R1023	Y841	W633	T240	Y92
ASP	VAL	I	K1032	Y421	F93
ASP	LEU	I	E1035	N422	A94
GLY	GLY	I854	C855	W433	K98
ILE	ASP	A856	T645	I434	R103
SER	ILE	Q857	G649	A435	G104
GLY	SER	R358	Q675	W436	W105
ILE	GLY	Q1040	Q675	THR	I106
ASN	ASN	K1042	THR	GLN	VAL
ALA	ALA	V1044	THR	THR	VAL
SER	SER	D1045	THR	THR	VAL
VAL	VAL	D1045	THR	THR	VAL



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	936842	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.086	Depositor
Minimum map value	-0.344	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	298.24, 298.24, 298.24	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.932, 0.932, 0.932	Depositor

## 5 Model quality [i](#)

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

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	D	0.24	0/1475	0.43	0/2007
1	F	0.24	0/1460	0.42	0/1986
1	H	0.24	0/1460	0.42	0/1986
2	E	0.24	0/1584	0.43	0/2151
2	G	0.24	0/1584	0.43	0/2151
2	I	0.24	0/1584	0.43	0/2151
3	A	0.24	0/8983	0.41	0/12230
3	B	0.24	0/8860	0.41	0/12064
3	C	0.25	0/8870	0.41	0/12069
All	All	0.24	0/35860	0.41	0/48795

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1443	0	1394	15	0
1	F	1429	0	1375	18	0
1	H	1429	0	1375	19	0
2	E	1544	0	1519	12	0
2	G	1544	0	1519	16	0
2	I	1544	0	1519	11	0
3	A	8769	0	8563	106	0

*Continued on next page...*

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	8650	0	8445	109	0
3	C	8662	0	8458	111	0
All	All	35014	0	34167	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 6.

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)
3:A:767:LEU:HG	3:A:1012:VAL:HG21	1.74	0.70
3:B:629:LEU:HG	3:B:631:PRO:HD2	1.72	0.70
1:H:41:TRP:HB2	1:H:54:ILE:HB	1.75	0.69
3:B:767:LEU:HG	3:B:1012:VAL:HG21	1.75	0.68
3:B:478:ARG:HE	3:B:487:ASN:HD21	1.41	0.67

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	D	186/215 (86%)	178 (96%)	6 (3%)	2 (1%)	12	24
1	F	182/215 (85%)	176 (97%)	6 (3%)	0	100	100
1	H	182/215 (85%)	179 (98%)	3 (2%)	0	100	100
2	E	194/451 (43%)	187 (96%)	7 (4%)	0	100	100
2	G	194/451 (43%)	186 (96%)	8 (4%)	0	100	100
2	I	194/451 (43%)	186 (96%)	8 (4%)	0	100	100
3	A	1111/1299 (86%)	1074 (97%)	37 (3%)	0	100	100
3	B	1091/1299 (84%)	1066 (98%)	25 (2%)	0	100	100

*Continued on next page...*

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	1096/1299 (84%)	1060 (97%)	36 (3%)	0	100	100
All	All	4430/5895 (75%)	4292 (97%)	136 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	137	THR
1	D	128	GLY

### 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	D	163/181 (90%)	156 (96%)	7 (4%)	25	48
1	F	162/181 (90%)	159 (98%)	3 (2%)	52	75
1	H	162/181 (90%)	160 (99%)	2 (1%)	67	85
2	E	171/399 (43%)	168 (98%)	3 (2%)	54	76
2	G	171/399 (43%)	167 (98%)	4 (2%)	45	70
2	I	171/399 (43%)	168 (98%)	3 (2%)	54	76
3	A	977/1122 (87%)	956 (98%)	21 (2%)	48	72
3	B	965/1122 (86%)	949 (98%)	16 (2%)	56	78
3	C	966/1122 (86%)	944 (98%)	22 (2%)	45	70
All	All	3908/5106 (76%)	3827 (98%)	81 (2%)	49	72

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	1129	ASN
3	A	558	LYS
3	B	1165	SER
3	A	336	CYS
3	A	696	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	370	ASN
3	A	876	GLN
3	B	917	GLN
3	A	675	GLN
3	A	1139	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](#)

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.

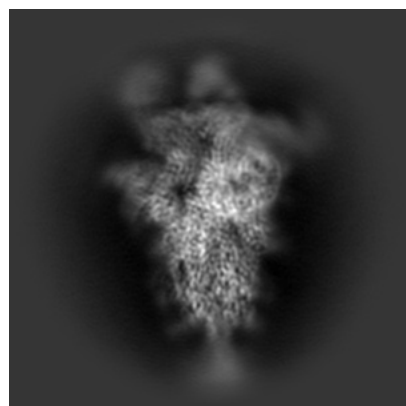
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39803. These allow visual inspection of the internal detail of the map and identification of artifacts.

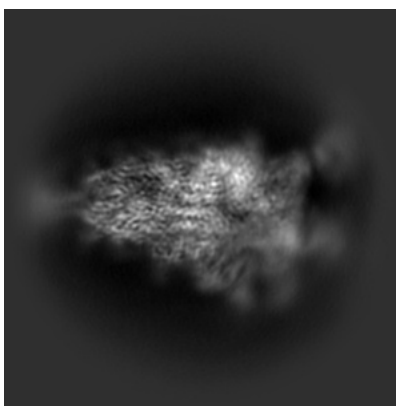
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

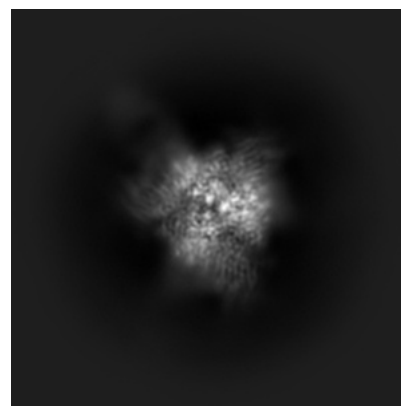
#### 6.1.1 Primary map



X

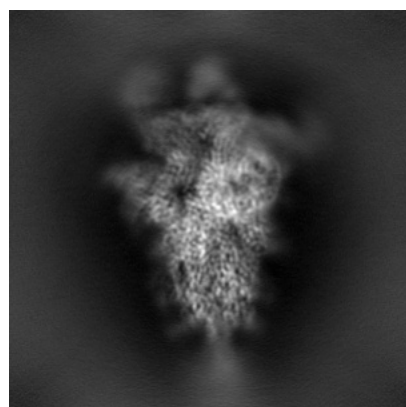


Y

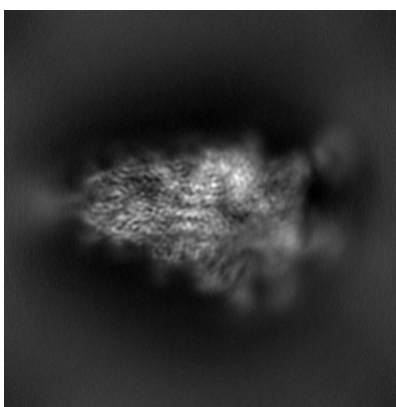


Z

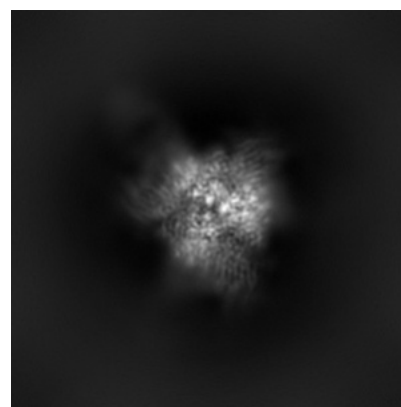
#### 6.1.2 Raw map



X



Y

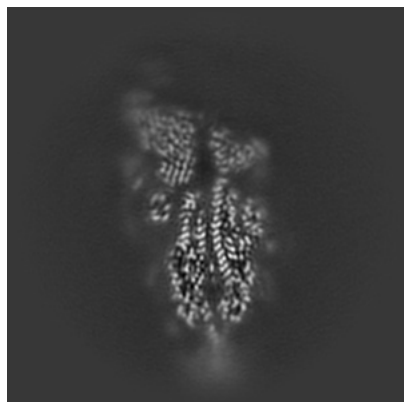


Z

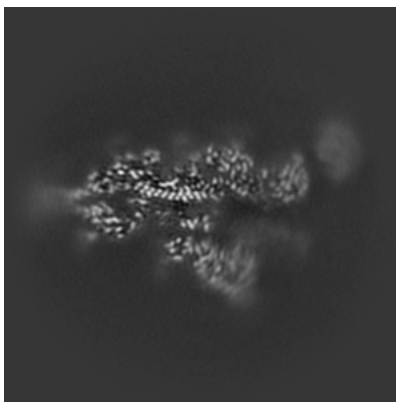
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

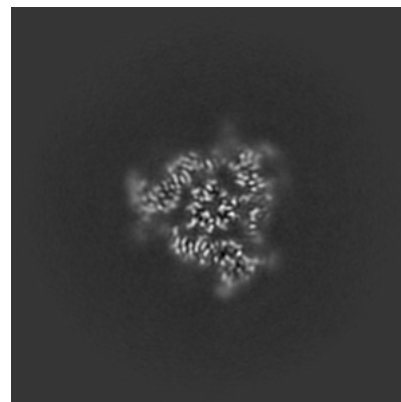
### 6.2.1 Primary map



X Index: 160

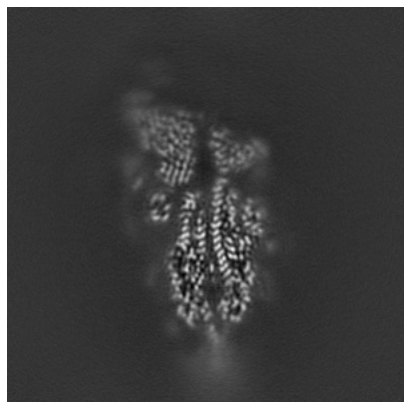


Y Index: 160

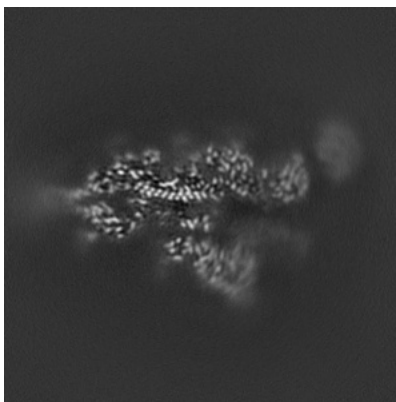


Z Index: 160

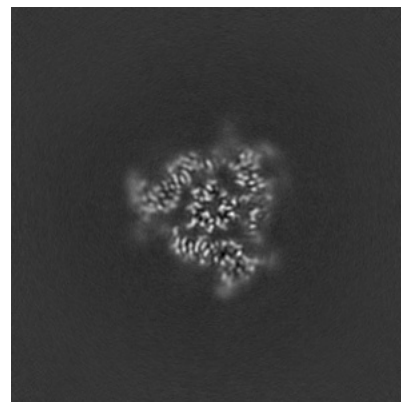
### 6.2.2 Raw map



X Index: 160



Y Index: 160

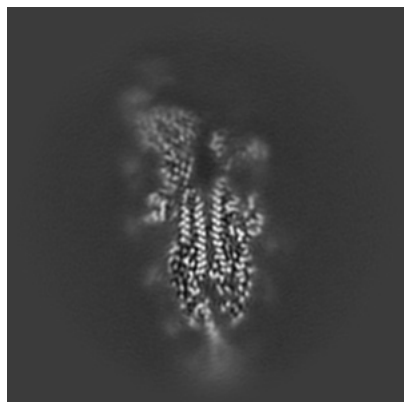


Z Index: 160

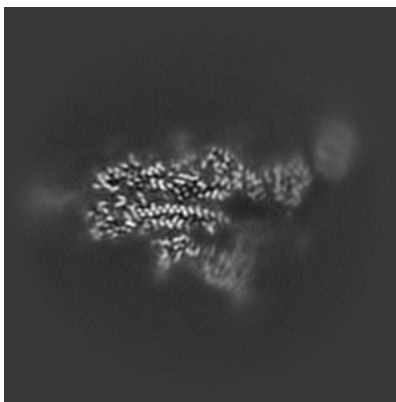
The images above show central slices of the map in three orthogonal directions.

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

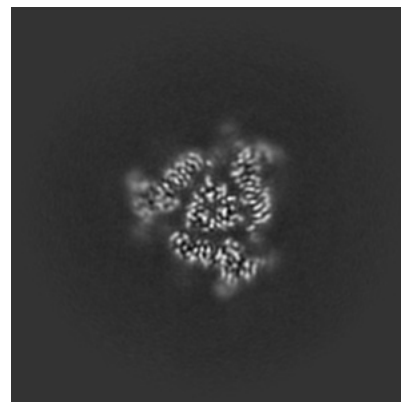
### 6.3.1 Primary map



X Index: 157

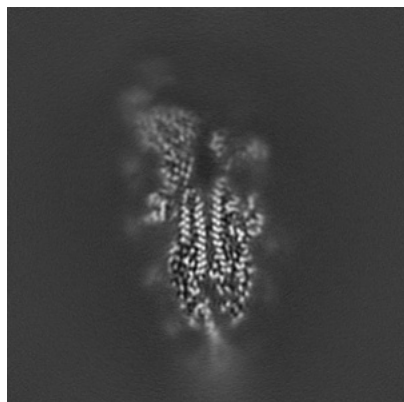


Y Index: 155

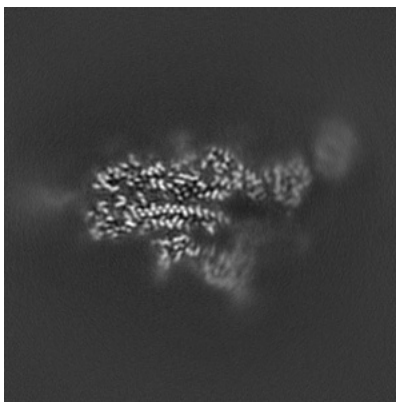


Z Index: 163

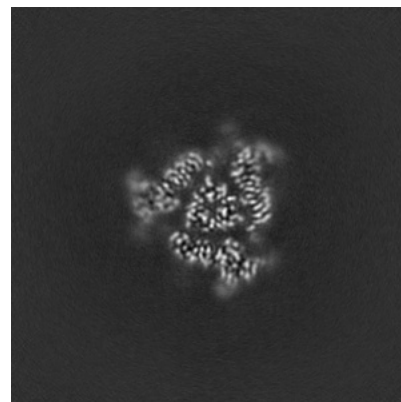
### 6.3.2 Raw map



X Index: 157



Y Index: 155

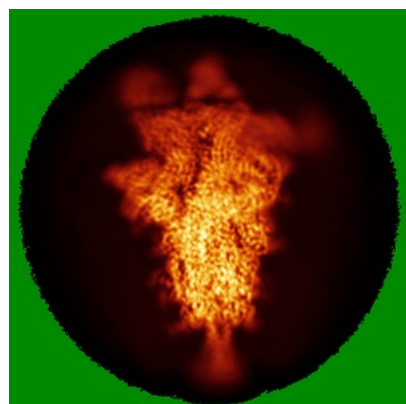


Z Index: 163

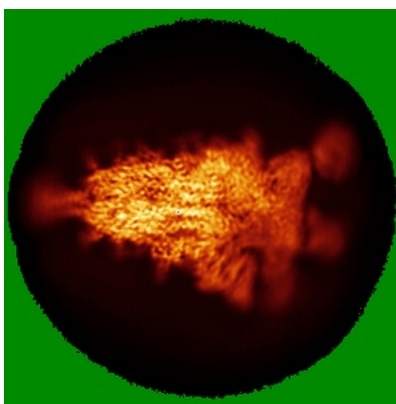
The images above show the largest variance slices of the map in three orthogonal directions.

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

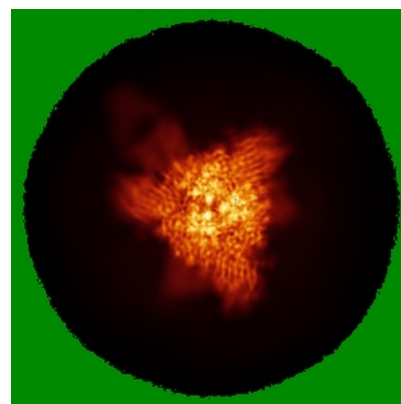
### 6.4.1 Primary map



X

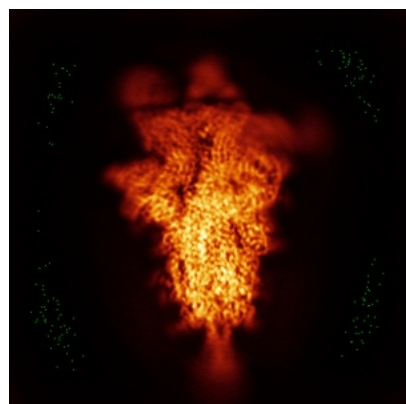


Y

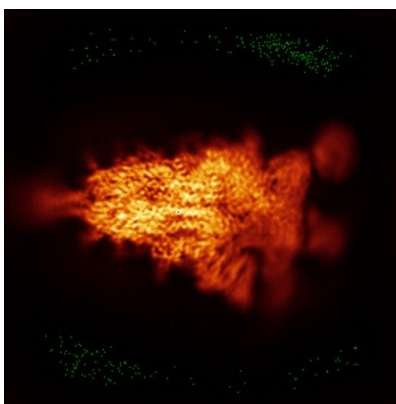


Z

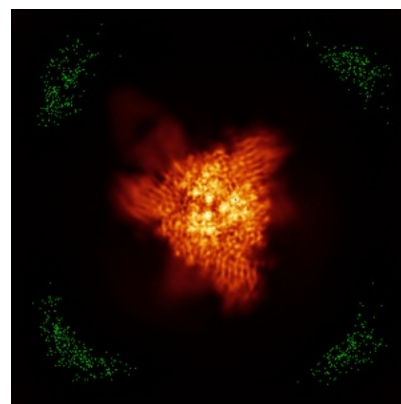
### 6.4.2 Raw map



X



Y

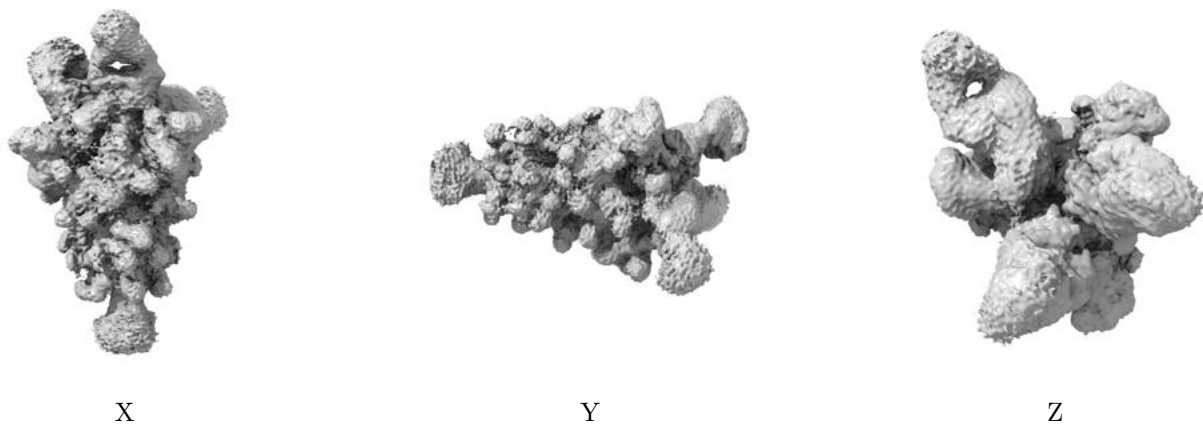


Z

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.

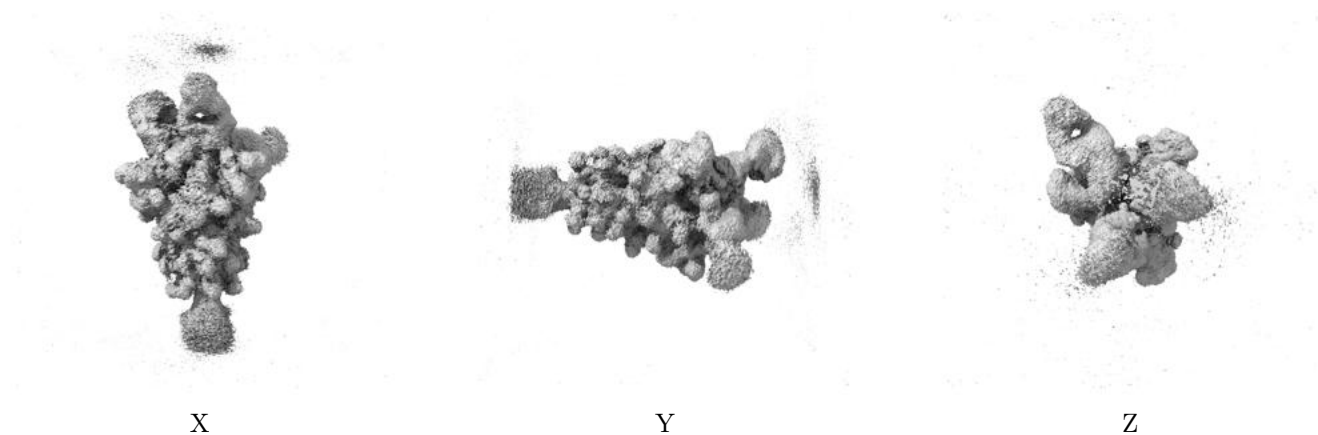
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

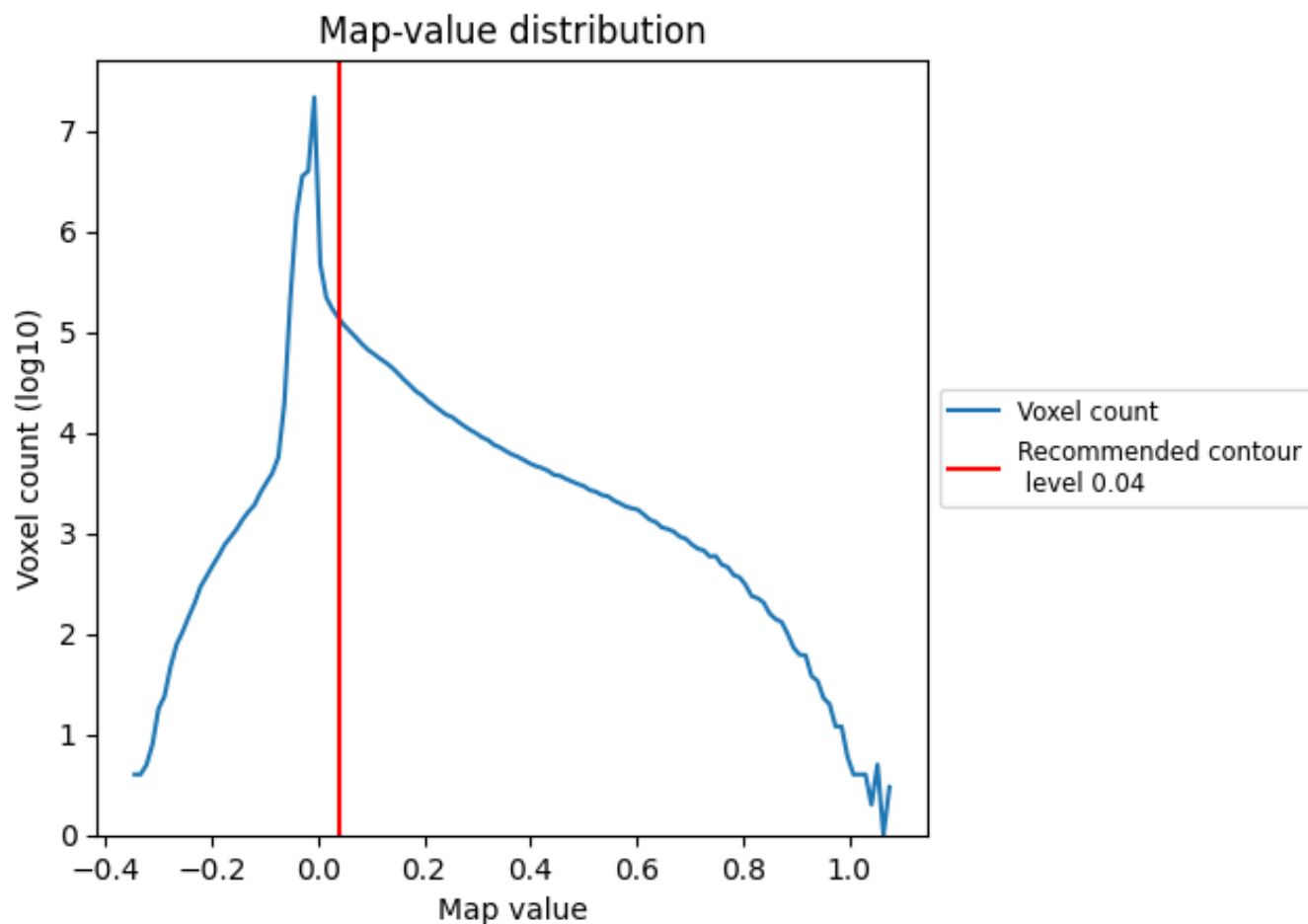
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

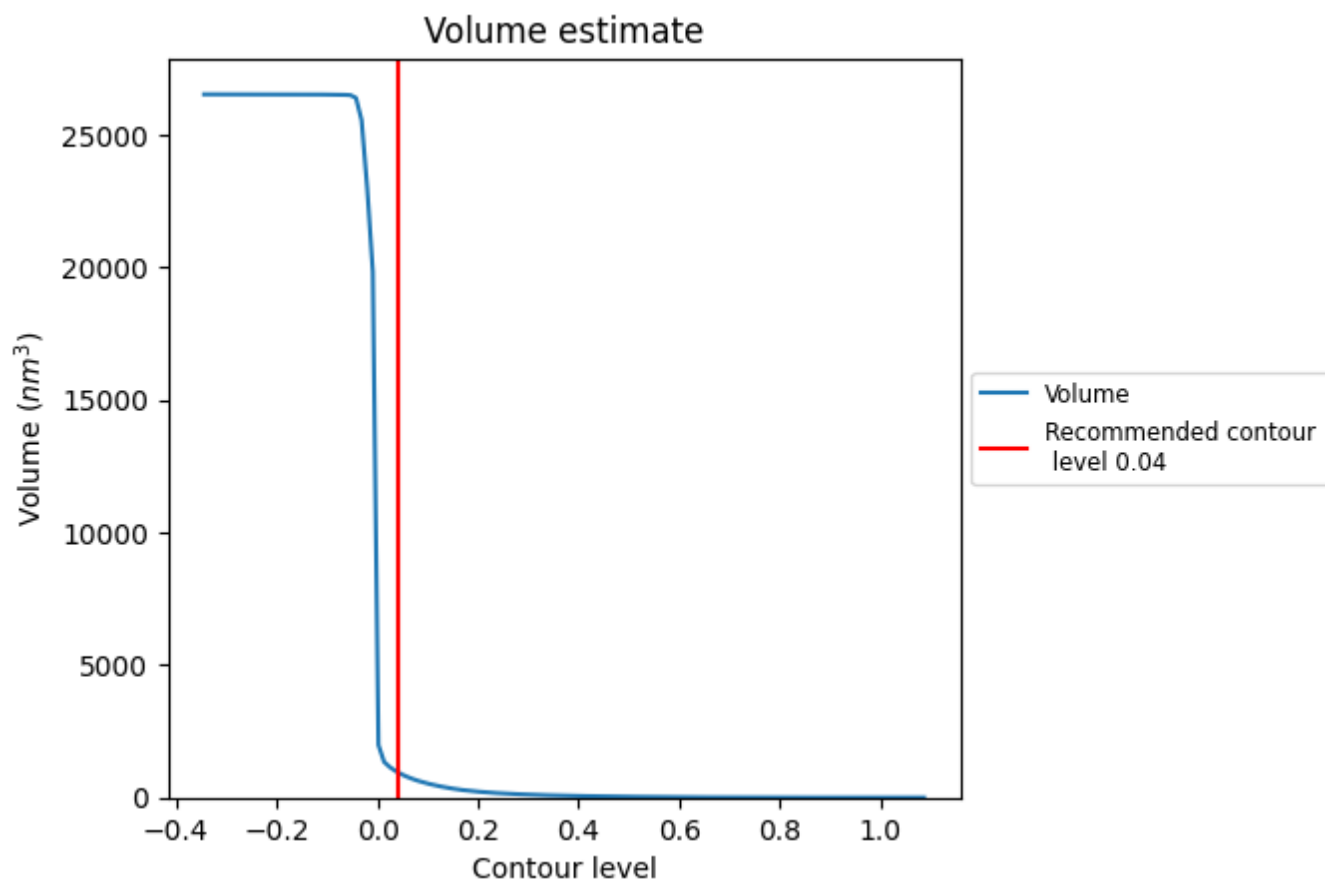
This section contains the results of statistical analysis of the map.

### 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.

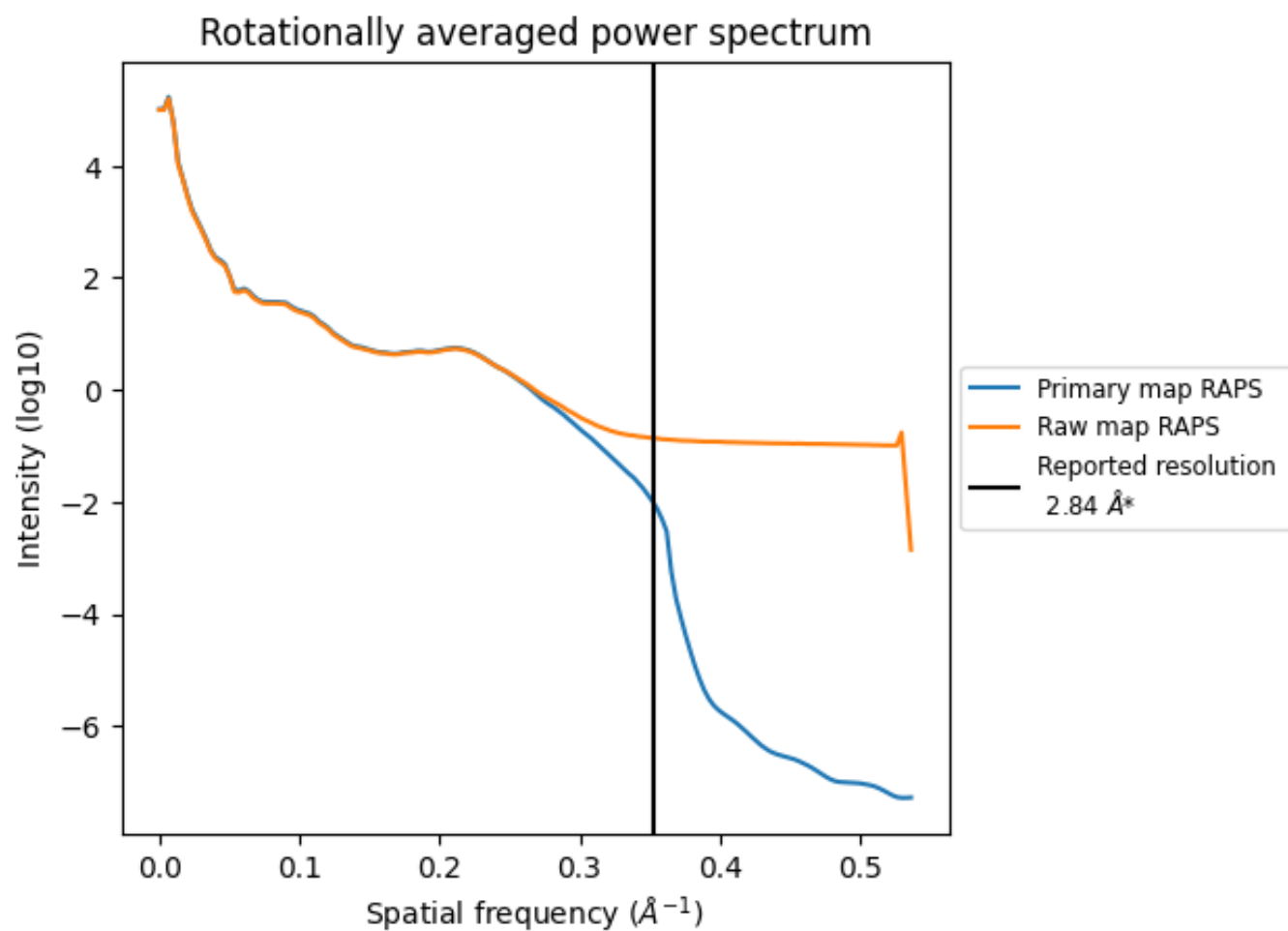
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 962  $\text{nm}^3$ ; this corresponds to an approximate mass of 869 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 ⓘ

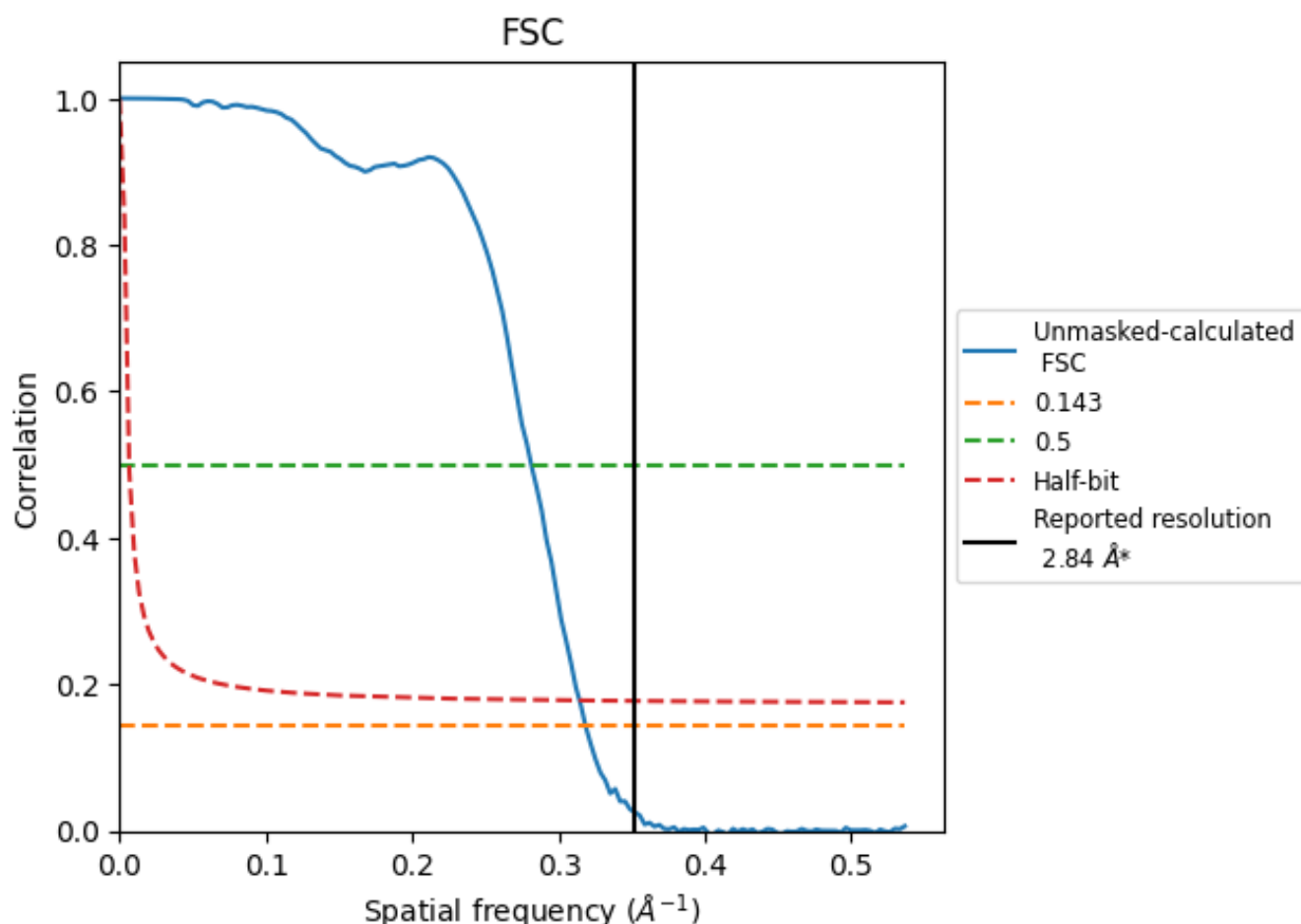


\*Reported resolution corresponds to spatial frequency of 0.352 Å⁻¹

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.352 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

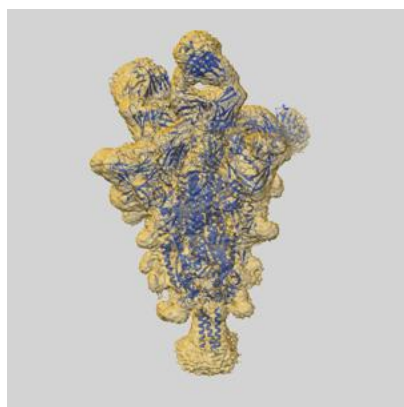
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.14	3.55	3.18

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.14 differs from the reported value 2.84 by more than 10 %

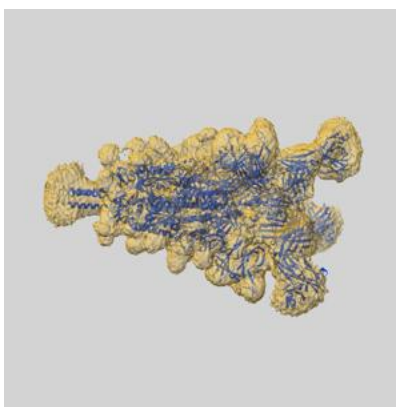
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39803 and PDB model 8Z6S. Per-residue inclusion information can be found in section 3 on page 11.

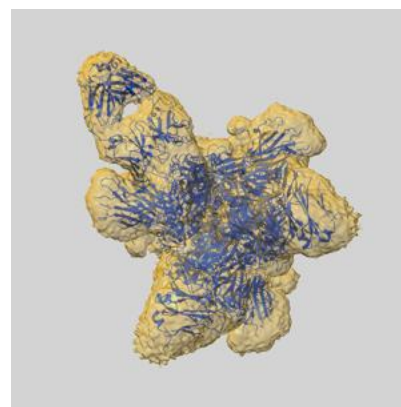
### 9.1 Map-model overlay [i](#)



X



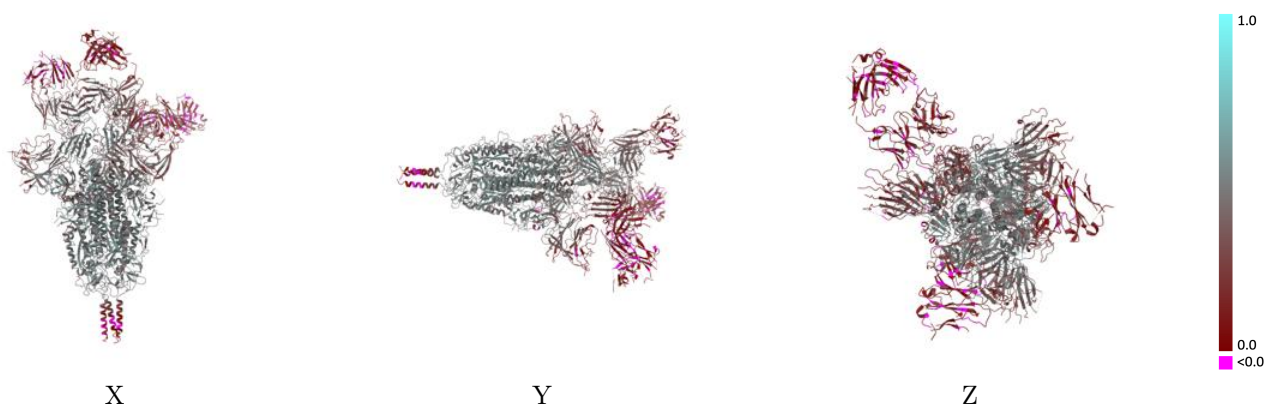
Y



Z

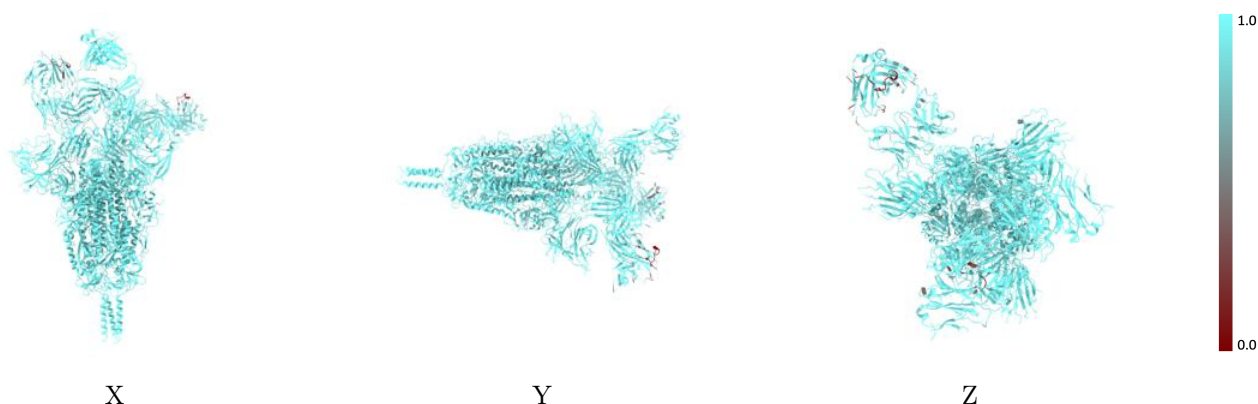
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



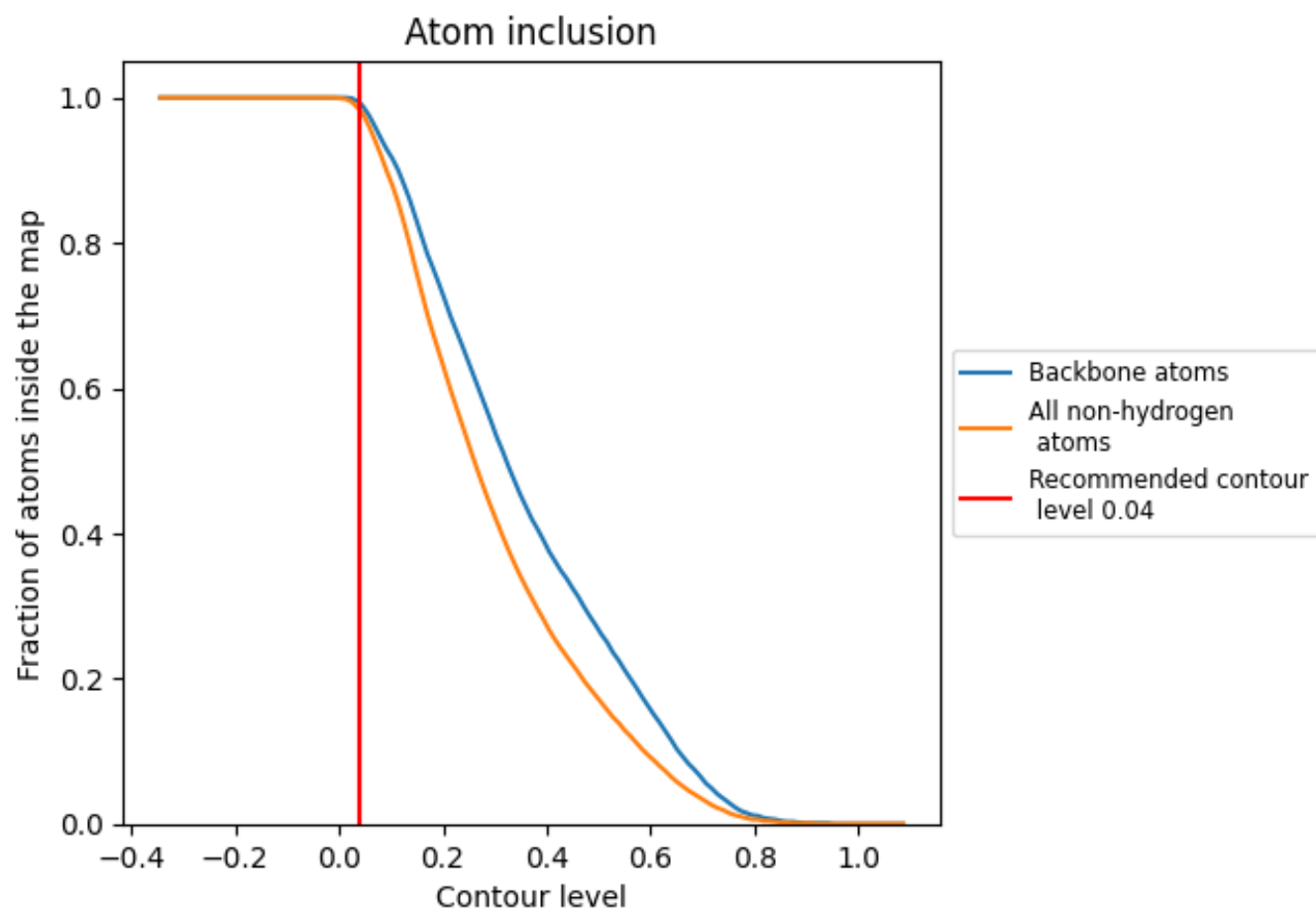
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9830	<div><div></div></div> 0.3790
A	<div><div></div></div> 0.9940	<div><div></div></div> 0.4310
B	<div><div></div></div> 0.9950	<div><div></div></div> 0.4550
C	<div><div></div></div> 0.9910	<div><div></div></div> 0.4050
D	<div><div></div></div> 0.9730	<div><div></div></div> 0.2590
E	<div><div></div></div> 0.9260	<div><div></div></div> 0.2900
F	<div><div></div></div> 0.9950	<div><div></div></div> 0.2780
G	<div><div></div></div> 0.9830	<div><div></div></div> 0.3040
H	<div><div></div></div> 0.9490	<div><div></div></div> 0.1230
I	<div><div></div></div> 0.8950	<div><div></div></div> 0.1120

1.0

0.0

<0.0