



Full wwPDB EM Validation Report ⓘ

Sep 29, 2024 – 05:40 AM EDT

PDB ID : 8TVH
EMDB ID : EMD-41642
Title : Langya henipavirus postfusion F protein in complex with 4G5 Fab, local refinement of the viral membrane proximal region
Authors : Wang, Z.; Seattle Structural Genomics Center for Infectious Disease (SSG-CID); Veesler, D.
Deposited on : 2023-08-18
Resolution : 3.60 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

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>.

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

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

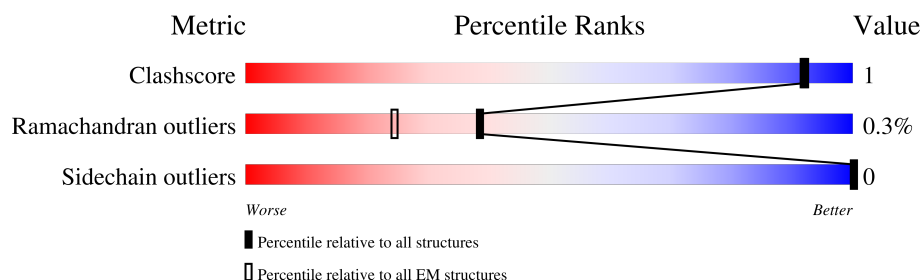
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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 ≥ 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	107	<div> <div>7%</div> <div>93%</div> <div>7%</div> </div>
1	E	107	<div> <div>7%</div> <div>93%</div> <div>7%</div> </div>
1	H	107	<div> <div>8%</div> <div>93%</div> <div>7%</div> </div>
2	F	120	<div> <div>9%</div> <div>100%</div> </div>
2	G	120	<div> <div>9%</div> <div>100%</div> </div>
2	I	120	<div> <div>8%</div> <div>100%</div> </div>
3	A	534	<div> <div>16%</div> <div>84%</div> </div>
3	B	534	<div> <div>16%</div> <div>84%</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	534	<div><div></div><div>16%</div><div>84%</div></div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6744 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 4G5 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	107	Total	C	N	O	S	0	0
			740	476	131	130	3		
1	D	107	Total	C	N	O	S	0	0
			740	476	131	130	3		
1	H	107	Total	C	N	O	S	0	0
			740	476	131	130	3		

- Molecule 2 is a protein called 4G5 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	120	Total	C	N	O	S	0	0
			870	558	147	163	2		
2	F	120	Total	C	N	O	S	0	0
			870	558	147	163	2		
2	I	120	Total	C	N	O	S	0	0
			870	558	147	163	2		

- Molecule 3 is a protein called Fusion glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	86	Total	C	N	O	S	0	0
			624	388	112	123	1		
3	B	86	Total	C	N	O	S	0	0
			624	388	112	123	1		
3	C	86	Total	C	N	O	S	0	0
			624	388	112	123	1		

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	479	ILE	-	expression tag	UNP A0AA82WPF7
A	480	ASN	-	expression tag	UNP A0AA82WPF7
A	481	PRO	-	expression tag	UNP A0AA82WPF7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	482	SER	-	expression tag	UNP A0AA82WPF7
A	483	MET	-	expression tag	UNP A0AA82WPF7
A	484	LYS	-	expression tag	UNP A0AA82WPF7
A	485	GLN	-	expression tag	UNP A0AA82WPF7
A	486	ILE	-	expression tag	UNP A0AA82WPF7
A	487	GLU	-	expression tag	UNP A0AA82WPF7
A	488	ASP	-	expression tag	UNP A0AA82WPF7
A	489	LYS	-	expression tag	UNP A0AA82WPF7
A	490	ILE	-	expression tag	UNP A0AA82WPF7
A	491	GLU	-	expression tag	UNP A0AA82WPF7
A	492	GLU	-	expression tag	UNP A0AA82WPF7
A	493	ILE	-	expression tag	UNP A0AA82WPF7
A	494	LEU	-	expression tag	UNP A0AA82WPF7
A	495	SER	-	expression tag	UNP A0AA82WPF7
A	496	LYS	-	expression tag	UNP A0AA82WPF7
A	497	ILE	-	expression tag	UNP A0AA82WPF7
A	498	TYR	-	expression tag	UNP A0AA82WPF7
A	499	HIS	-	expression tag	UNP A0AA82WPF7
A	500	ILE	-	expression tag	UNP A0AA82WPF7
A	501	GLU	-	expression tag	UNP A0AA82WPF7
A	502	ASN	-	expression tag	UNP A0AA82WPF7
A	503	GLU	-	expression tag	UNP A0AA82WPF7
A	504	ILE	-	expression tag	UNP A0AA82WPF7
A	505	ALA	-	expression tag	UNP A0AA82WPF7
A	506	ARG	-	expression tag	UNP A0AA82WPF7
A	507	ILE	-	expression tag	UNP A0AA82WPF7
A	508	LYS	-	expression tag	UNP A0AA82WPF7
A	509	LYS	-	expression tag	UNP A0AA82WPF7
A	510	LEU	-	expression tag	UNP A0AA82WPF7
A	511	ILE	-	expression tag	UNP A0AA82WPF7
A	512	GLY	-	expression tag	UNP A0AA82WPF7
A	513	GLU	-	expression tag	UNP A0AA82WPF7
A	514	ALA	-	expression tag	UNP A0AA82WPF7
A	515	PRO	-	expression tag	UNP A0AA82WPF7
A	516	GLY	-	expression tag	UNP A0AA82WPF7
A	517	GLY	-	expression tag	UNP A0AA82WPF7
A	518	SER	-	expression tag	UNP A0AA82WPF7
A	519	ILE	-	expression tag	UNP A0AA82WPF7
A	520	GLU	-	expression tag	UNP A0AA82WPF7
A	521	GLY	-	expression tag	UNP A0AA82WPF7
A	522	ARG	-	expression tag	UNP A0AA82WPF7
A	523	GLY	-	expression tag	UNP A0AA82WPF7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	524	SER	-	expression tag	UNP A0AA82WPF7
A	525	GLY	-	expression tag	UNP A0AA82WPF7
A	526	GLY	-	expression tag	UNP A0AA82WPF7
A	527	GLY	-	expression tag	UNP A0AA82WPF7
A	528	SER	-	expression tag	UNP A0AA82WPF7
A	529	HIS	-	expression tag	UNP A0AA82WPF7
A	530	HIS	-	expression tag	UNP A0AA82WPF7
A	531	HIS	-	expression tag	UNP A0AA82WPF7
A	532	HIS	-	expression tag	UNP A0AA82WPF7
A	533	HIS	-	expression tag	UNP A0AA82WPF7
A	534	HIS	-	expression tag	UNP A0AA82WPF7
B	479	ILE	-	expression tag	UNP A0AA82WPF7
B	480	ASN	-	expression tag	UNP A0AA82WPF7
B	481	PRO	-	expression tag	UNP A0AA82WPF7
B	482	SER	-	expression tag	UNP A0AA82WPF7
B	483	MET	-	expression tag	UNP A0AA82WPF7
B	484	LYS	-	expression tag	UNP A0AA82WPF7
B	485	GLN	-	expression tag	UNP A0AA82WPF7
B	486	ILE	-	expression tag	UNP A0AA82WPF7
B	487	GLU	-	expression tag	UNP A0AA82WPF7
B	488	ASP	-	expression tag	UNP A0AA82WPF7
B	489	LYS	-	expression tag	UNP A0AA82WPF7
B	490	ILE	-	expression tag	UNP A0AA82WPF7
B	491	GLU	-	expression tag	UNP A0AA82WPF7
B	492	GLU	-	expression tag	UNP A0AA82WPF7
B	493	ILE	-	expression tag	UNP A0AA82WPF7
B	494	LEU	-	expression tag	UNP A0AA82WPF7
B	495	SER	-	expression tag	UNP A0AA82WPF7
B	496	LYS	-	expression tag	UNP A0AA82WPF7
B	497	ILE	-	expression tag	UNP A0AA82WPF7
B	498	TYR	-	expression tag	UNP A0AA82WPF7
B	499	HIS	-	expression tag	UNP A0AA82WPF7
B	500	ILE	-	expression tag	UNP A0AA82WPF7
B	501	GLU	-	expression tag	UNP A0AA82WPF7
B	502	ASN	-	expression tag	UNP A0AA82WPF7
B	503	GLU	-	expression tag	UNP A0AA82WPF7
B	504	ILE	-	expression tag	UNP A0AA82WPF7
B	505	ALA	-	expression tag	UNP A0AA82WPF7
B	506	ARG	-	expression tag	UNP A0AA82WPF7
B	507	ILE	-	expression tag	UNP A0AA82WPF7
B	508	LYS	-	expression tag	UNP A0AA82WPF7
B	509	LYS	-	expression tag	UNP A0AA82WPF7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	510	LEU	-	expression tag	UNP A0AA82WPF7
B	511	ILE	-	expression tag	UNP A0AA82WPF7
B	512	GLY	-	expression tag	UNP A0AA82WPF7
B	513	GLU	-	expression tag	UNP A0AA82WPF7
B	514	ALA	-	expression tag	UNP A0AA82WPF7
B	515	PRO	-	expression tag	UNP A0AA82WPF7
B	516	GLY	-	expression tag	UNP A0AA82WPF7
B	517	GLY	-	expression tag	UNP A0AA82WPF7
B	518	SER	-	expression tag	UNP A0AA82WPF7
B	519	ILE	-	expression tag	UNP A0AA82WPF7
B	520	GLU	-	expression tag	UNP A0AA82WPF7
B	521	GLY	-	expression tag	UNP A0AA82WPF7
B	522	ARG	-	expression tag	UNP A0AA82WPF7
B	523	GLY	-	expression tag	UNP A0AA82WPF7
B	524	SER	-	expression tag	UNP A0AA82WPF7
B	525	GLY	-	expression tag	UNP A0AA82WPF7
B	526	GLY	-	expression tag	UNP A0AA82WPF7
B	527	GLY	-	expression tag	UNP A0AA82WPF7
B	528	SER	-	expression tag	UNP A0AA82WPF7
B	529	HIS	-	expression tag	UNP A0AA82WPF7
B	530	HIS	-	expression tag	UNP A0AA82WPF7
B	531	HIS	-	expression tag	UNP A0AA82WPF7
B	532	HIS	-	expression tag	UNP A0AA82WPF7
B	533	HIS	-	expression tag	UNP A0AA82WPF7
B	534	HIS	-	expression tag	UNP A0AA82WPF7
C	479	ILE	-	expression tag	UNP A0AA82WPF7
C	480	ASN	-	expression tag	UNP A0AA82WPF7
C	481	PRO	-	expression tag	UNP A0AA82WPF7
C	482	SER	-	expression tag	UNP A0AA82WPF7
C	483	MET	-	expression tag	UNP A0AA82WPF7
C	484	LYS	-	expression tag	UNP A0AA82WPF7
C	485	GLN	-	expression tag	UNP A0AA82WPF7
C	486	ILE	-	expression tag	UNP A0AA82WPF7
C	487	GLU	-	expression tag	UNP A0AA82WPF7
C	488	ASP	-	expression tag	UNP A0AA82WPF7
C	489	LYS	-	expression tag	UNP A0AA82WPF7
C	490	ILE	-	expression tag	UNP A0AA82WPF7
C	491	GLU	-	expression tag	UNP A0AA82WPF7
C	492	GLU	-	expression tag	UNP A0AA82WPF7
C	493	ILE	-	expression tag	UNP A0AA82WPF7
C	494	LEU	-	expression tag	UNP A0AA82WPF7
C	495	SER	-	expression tag	UNP A0AA82WPF7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	496	LYS	-	expression tag	UNP A0AA82WPF7
C	497	ILE	-	expression tag	UNP A0AA82WPF7
C	498	TYR	-	expression tag	UNP A0AA82WPF7
C	499	HIS	-	expression tag	UNP A0AA82WPF7
C	500	ILE	-	expression tag	UNP A0AA82WPF7
C	501	GLU	-	expression tag	UNP A0AA82WPF7
C	502	ASN	-	expression tag	UNP A0AA82WPF7
C	503	GLU	-	expression tag	UNP A0AA82WPF7
C	504	ILE	-	expression tag	UNP A0AA82WPF7
C	505	ALA	-	expression tag	UNP A0AA82WPF7
C	506	ARG	-	expression tag	UNP A0AA82WPF7
C	507	ILE	-	expression tag	UNP A0AA82WPF7
C	508	LYS	-	expression tag	UNP A0AA82WPF7
C	509	LYS	-	expression tag	UNP A0AA82WPF7
C	510	LEU	-	expression tag	UNP A0AA82WPF7
C	511	ILE	-	expression tag	UNP A0AA82WPF7
C	512	GLY	-	expression tag	UNP A0AA82WPF7
C	513	GLU	-	expression tag	UNP A0AA82WPF7
C	514	ALA	-	expression tag	UNP A0AA82WPF7
C	515	PRO	-	expression tag	UNP A0AA82WPF7
C	516	GLY	-	expression tag	UNP A0AA82WPF7
C	517	GLY	-	expression tag	UNP A0AA82WPF7
C	518	SER	-	expression tag	UNP A0AA82WPF7
C	519	ILE	-	expression tag	UNP A0AA82WPF7
C	520	GLU	-	expression tag	UNP A0AA82WPF7
C	521	GLY	-	expression tag	UNP A0AA82WPF7
C	522	ARG	-	expression tag	UNP A0AA82WPF7
C	523	GLY	-	expression tag	UNP A0AA82WPF7
C	524	SER	-	expression tag	UNP A0AA82WPF7
C	525	GLY	-	expression tag	UNP A0AA82WPF7
C	526	GLY	-	expression tag	UNP A0AA82WPF7
C	527	GLY	-	expression tag	UNP A0AA82WPF7
C	528	SER	-	expression tag	UNP A0AA82WPF7
C	529	HIS	-	expression tag	UNP A0AA82WPF7
C	530	HIS	-	expression tag	UNP A0AA82WPF7
C	531	HIS	-	expression tag	UNP A0AA82WPF7
C	532	HIS	-	expression tag	UNP A0AA82WPF7
C	533	HIS	-	expression tag	UNP A0AA82WPF7
C	534	HIS	-	expression tag	UNP A0AA82WPF7

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

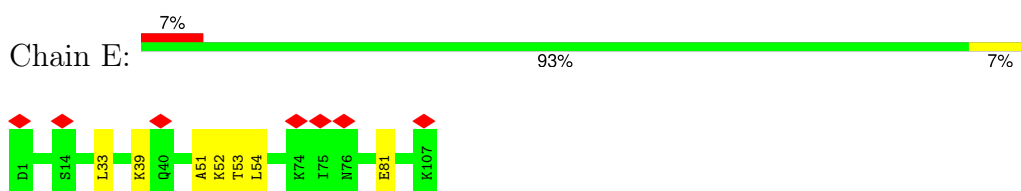


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

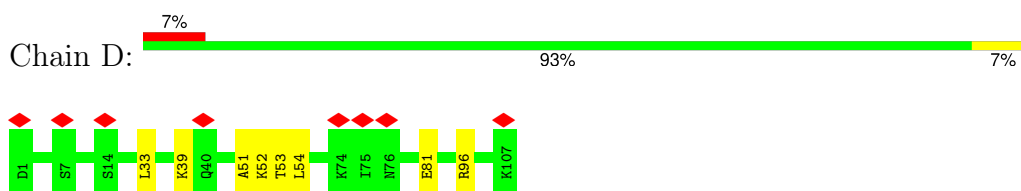
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

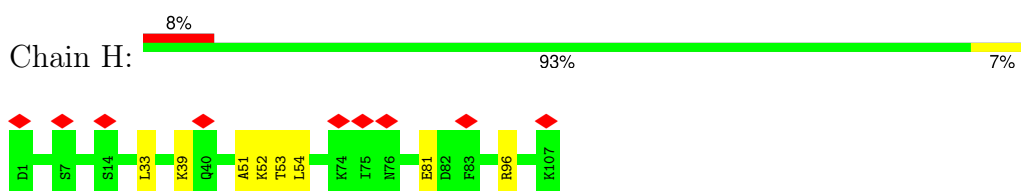
- Molecule 1: 4G5 light chain



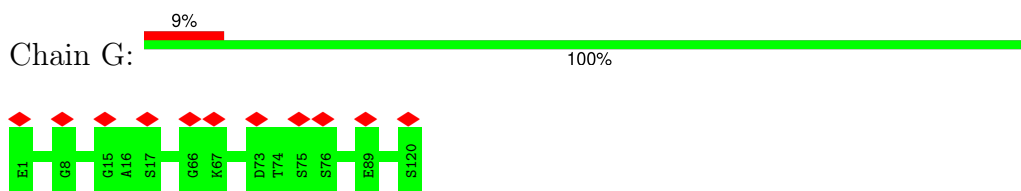
- Molecule 1: 4G5 light chain



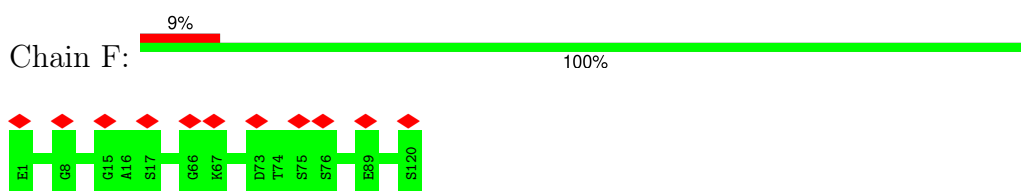
- Molecule 1: 4G5 light chain



- Molecule 2: 4G5 heavy chain



- Molecule 2: 4G5 heavy chain



- Molecule 3: Fusion glycoprotein



MET	ALA	ALA	PHE	LEU	LYS	SER	ALA	ILE	ILE	CYS	TYR	LEU	LEU	PHE	TYR	PRO	HIS	ILE	VAL	LYS	SER	SER	LEU	HIS	TYR	ASP	SER	SER	LYS	VAL	GLY	ILE	ILE	LYS	GLY	LEU	TYR	THR	ASN	TYR	LYS	ILE	LYS	GLY	SER	SER	PRO	PRO	THR	LEU	LYS	MET	VAL	VAL	LYS	LEU	ILE	ILE	PRO	ASN	ILE
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ASP	GLY	VAL	ARG	ASN	CYS	THR	GLN	LYS	GLN	PHE	ASP	GLU	TYR	LYS	ASN	LEU	VAL	PRO	VAL	LYS	VAL	LEU	ALA	ASN	ALA	MET	LEU	ASP	ASN	VAL	LYS	GLY	ASN	ASN	LYS	TYR	PHE	ARG	ALA	ALA	GLY	ALA	ILE	MET	ALA	ALA	GLY	VAL	VAL	ALA	LEU	GLY	VAL	ALA	ALA	THR	ALA
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ALA THR VAL THR ALA GLY ILE ALA LEU LEU ARG SER ASN GLU M135 A136 P180 V181 I182 M183 Q184 L185 S186 CYS ASP THR ILE GLY LEU SER SER VAL GLY ILE LYS LEU THR THR GLN TYR TYR SER SER GLU ILE LEU LEU THR ALA PHE GLY PRO PRO ALA LEU LEU GLN ASN ASN PRO VAL ASN THR ARG ILE THR

ILE	GLN	ALA	ALA	ILE	SER	SER	VAL	PHE	ASN	ARG	ASN	PHE	ASP	GLU	LEU	LEU	LYS	ILE	MET	GLY	TYR	THR	SER	SER	GLY	ASP	LEU	TYR	GLU	ILE	LEU	HIS	GLY	SER	ASN	ILE	ILE	ILE	ASP	VAL	ASP	VAL	GLU	ALA	GLU	GLY	TYR	ILE	LEU	LEU	GLU	GLU	PHE	PRO	ASN	ASN	LEU	LEU	THR	LEU	LEU
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VAL	PRO	ASN	ALA	VAL	VAL	GLN	GLU	LEU	MET	PRO	ILE	SER	TYR	ASN	ASP	VAL	GLY	ASP	GLU	TRP	VAL	THR	LEU	VAL	ARG	ARG	PHE	VAL	VAL	LEU	THR	THR	THR	LEU	LEU	SER	SER	ASN	ILE	SER	THR	THR	THR	VAL	VAL	CYS	SER	VAL	VAL	THR	THR	THR	GLU	SER	ASP	ASN	TYR	ALA	LEU	PRO
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MET	SER	TYR	GLU	LEU	ILE	GLY	CYS	LEU	GLN	GLY	ASP	THR	THR	SER	LYS	CYS	ALA	ALA	ARG	GLU	LYS	VAL	VAL	SER	SER	TYR	VAL	VAL	PRO	ARG	PHE	ALA	ALA	LEU	SER	SER	ASP	GLY	LEU	VAL	VAL	TYR	ALA	ASN	CYS	LYS	LEU	ASN	THR	ILE	CYS	ARG	CYS	MET	THR	PRO	ILE	SER	GLN	SER	LEU	GLY
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[illegible]

GLU	GLU	ILE	LEU	SER	LYS	ILE	TYR	HIS	ILE	GLU	ASN	GLU	ILE	ALA	ARG	ILE	LYS	LYS	LEU	ILE	GLY	GLU	ALA	PRO	GLY	GLY	SER	ILE	GLU	GLY	ARG	GLY	SER	GLY	GLY	GLY	SER	HIS	HIS	HIS	HIS	HIS
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- Molecule 3: Fusion glycoprotein



MET	ALA	PHE	LEU	LYS	SER	ALA	ILE	ILE	CYS	TYR	LEU	LEU	PHE	TYR	PRO	HIS	ILE	VAL	LYS	SER	SER	LEU	LEU	HIS	TYR	ASP	SER	SER	LYS	VAL	GLY	ILE	ILE	LYS	GLY	TYR	THR	ASN	TYR	LYS	ILE	LYS	GLY	SER	SER	PRO	SER	THR	LYS	LEU	ILE	ILE	PRO	ASN	ILE
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ASP	GLY	VAL	ARG	ASN	CYS	THR	GLN	LYS	PHE	ASP	GLU	TYR	LYS	ASN	LEU	LEU	VAL	VAL	LYS	ASN	ALA	MET	LEU	LEU	ALA	ALA	ASP	ASN	VAL	VAL	LYS	SER	GLY	ASN	ASN	LYS	TYR	ARG	PHE	ALA	ALA	GLY	GLY	ILE	MET	ALA	ALA	VAL	VAL	LEU	GLY	ALA	ALA	THR	ALA
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ALA	THR	VAL	THR	THR	ALA	GLY	ILE	ALA	ALA	LEU	HIS	ARG	SER	ASN	GLU	M135	A136	P180	V181	I182	M183	Q184	I185	S186	CYS	ASP	THR	THR	ILE	GLY	LEU	SER	SER	VAL	GLY	ILE	LYS	THR	LEU	THR	GLN	TYR	TVR	TVR	SER	SER	GLU	ILE	LEU	LEU	THR	ALA	ALA	PHE	GLY	PRO	PRO	ALA	ALA	LEU	LEU	GLN	GLN	ASN	ASN	PRO	VAL	ASN	ASN	THR	ARG	THR	ILE	LEU	THR
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ILE	GLN	ALA	ALA	ILE	SER	SER	VAL	PHE	ASN	ASN	ARG	ASN	ASN	PHE	ASP	GLU	LEU	LEU	LYS	ILE	ILE	MET	GLY	TYR	THR	SER	GLY	ASP	ASP	LEU	TYR	GLU	ILE	LEU	HIS	SER	SER	GLY	LEU	ILE	ILE	ARG	GLY	ASN	ASN	ILE	ILE	ILE	ASP	VAL	VAL	ASP	GLU	GLY	ALA	ALA	GLY	TYR	GLY	ILE	ILE	GLU	GLU	PHE	PRO	ASN	ASN	LEU	LEU	THR	LEU	LEU
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VAL	PRO	ASN	ALA	VAL	VAL	GLN	GLU	LEU	MET	PRO	ILE	SER	TYR	ASN	ASP	GLY	ASP	GLU	TRP	VAL	THR	LEU	VAL	ARG	PHE	ARG	VAL	VAL	LEU	THR	THR	THR	THR	LEU	SER	SER	ASN	ILE	THR	THR	VAL	THR	THR	GLU	SER	VAL	CYS	ASP	ASN	TYR	ALA	LEU	PRO
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GLU	GLU	TLE	LEU	SER	LYS	TLE	TVR	HIS	TLE	GLU	ASN	GLU	TLE	ALA	ARG	TLE	LYS	LYS	LEU	TLE	GLY	GLU	ALA	PRO	GLY	GLY	SER	TLE	GLU	GLY	ARG	GLY	SER	GLY	GLY	SER	HIS	HIS	HIS	HIS	HIS	HIS
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- Molecule 3: Fusion glycoprotein



ASP	GLY	VAL	ARG	ASN	CYS	THR	GLN	LYS	GLN	PHE	ASP	GLU	TYR	LYS	ASN	LEU	VAL	GLU	PRO	VAL	LYS	LEU	ALA	ALA	ASN	ALA	ALA	LEU	ASP	ASN	VAL	LYS	SER	GLY	ASN	ASN	LYS	TYR	ARG	PHE	ALA	ALA	GLY	ALA	ILE	MET	ALA	ALA	GLY	VAL	VAL	GLY	ALA	ALA	THR	ALA
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ALA	THR	VAL	THR	ALA	GLY	ILE	LEU	LEU	ARG	SER	ASN	GLU	M135	A136	P180	V181	I182	N183	L185	S186	CYS	ASP	THR	ILE	GLY	LEU	SER	VAL	GLY	ILE	LYS	LEU	THR	GLN	TYR	TYR	SER	GLU	ILE	LEU	THR	ALA	PHE	GLY	PRO	ALA	LEU	GLN	ASN	PRO	VAL	ASN	THR	ARG	ILE
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ILE	GLN	ALA	ALA	ILE	SER	SER	VAL	PHE	ASN	ARG	ASN	PHE	ASP	GLU	LEU	LEU	LEU	LYS	ILE	MET	GLY	TYR	THR	SER	GLY	ASP	LEU	GLU	LEU	HIS	SER	GLY	LEU	ILE	ILE	ARG	GLY	ASN	ILE	ILE	ILE	ASP	VAL	ASP	VAL	GLU	ALA	GLY	TYR	ILE	ALA	LEU	GLU	ILE	GLU	PHE	PRO	ASN	LEU	THR	LEU
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VAL	PRO	ASN	ALA	VAL	VAL	GLN	GLU	LEU	MET	PRO	ILE	SER	TYR	ASN	VAL	ASP	GLY	ASP	GLU	TRP	THR	THR	LEU	VAL	ARG	ARG	PHE	VAL	VAL	LEU	THR	THR	LEU	LEU	SER	ASN	ILE	ASP	THR	SER	THR	THR	VAL	VAL	CYS	ARG	SER	GLU	SER	VAL	ILE	CYS	ASP	ASN	TYR	ALA	LEU	PRO
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MET	SER	TYR	GLU	LEU	ILE	GLY	CYS	LEU	GLN	GLY	ASP	THR	SER	LYS	CYS	ALA	ARG	GLU	LYS	VAL	VAL	SER	SER	TYR	VAL	PRO	ARG	PHE	ALA	ALA	LEU	SER	SER	ASP	GLY	LEU	VAL	TYR	ALA	ASN	CYS	LEU	ASN	THR	ILE	CYS	ARG	CYS	MET	ASP	THR	ASP	THR	PRO	ILE	SER	GLN	SER	LEU	GLY	THR
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THR	VAL	SER	LEU	LEU	ASN	ASP	LYS	LYS	CYS	LEU	VAL	TYR	GLN	VAL	GLY	ASP	ILE	LEU	SER	VAL	GLY	SER	TYR	LEU	GLY	GLU	GLU	TYR	SER	ALA	ASP	ASN	VAL	GLU	LEU	GLY	PRO	PRO	VAL	VAL	ILE	ASP	N448	I449	D450	N480	P481	SER	MET	LYS	GLN	ILE	GLU	ASP	LYS	ILE
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	60440	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	63	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.398	Depositor
Minimum map value	-2.098	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.5	Depositor
Map size (\AA)	472.08002, 472.08002, 472.08002	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.98350006, 0.98350006, 0.98350006	Depositor

5 Model quality

5.1 Standard geometry

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	D	0.63	0/760	0.74	1/1039 (0.1%)
1	E	0.63	0/760	0.74	0/1039
1	H	0.63	0/760	0.74	1/1039 (0.1%)
2	F	0.66	0/890	0.72	0/1219
2	G	0.66	0/890	0.72	0/1219
2	I	0.66	0/890	0.72	0/1219
3	A	0.71	0/626	0.55	0/848
3	B	0.71	0/626	0.55	0/848
3	C	0.71	0/626	0.55	0/848
All	All	0.66	0/6828	0.68	2/9318 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	H	96	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	D	96	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	740	0	613	6	0
1	E	740	0	613	6	0
1	H	740	0	613	6	0
2	F	870	0	781	0	0
2	G	870	0	781	0	0
2	I	870	0	781	0	0
3	A	624	0	601	0	0
3	B	624	0	601	0	0
3	C	624	0	601	0	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
All	All	6744	0	6024	18	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 1.

All (18) 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:53:THR:HG22	1:D:54:LEU:N	1.95	0.81
1:H:53:THR:HG22	1:H:54:LEU:N	1.95	0.80
1:E:53:THR:HG22	1:E:54:LEU:N	1.95	0.79
1:D:53:THR:CG2	1:D:54:LEU:N	2.60	0.64
1:H:53:THR:CG2	1:H:54:LEU:N	2.60	0.64
1:D:53:THR:HG22	1:D:54:LEU:H	1.64	0.62
1:H:53:THR:HG22	1:H:54:LEU:H	1.63	0.62
1:E:53:THR:HG22	1:E:54:LEU:H	1.63	0.62
1:E:53:THR:CG2	1:E:54:LEU:N	2.60	0.62
1:D:33:LEU:HB3	1:D:51:ALA:HB2	1.81	0.62
1:H:33:LEU:HB3	1:H:51:ALA:HB2	1.81	0.61
1:E:33:LEU:HB3	1:E:51:ALA:HB2	1.80	0.61
1:E:53:THR:CG2	1:E:54:LEU:H	2.18	0.56
1:D:53:THR:CG2	1:D:54:LEU:H	2.18	0.56
1:H:53:THR:CG2	1:H:54:LEU:H	2.18	0.55
1:E:39:LYS:NZ	1:E:81:GLU:O	2.49	0.46
1:H:39:LYS:NZ	1:H:81:GLU:O	2.49	0.46
1:D:39:LYS:NZ	1:D:81:GLU:O	2.49	0.45

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	D	105/107 (98%)	101 (96%)	3 (3%)	1 (1%)	13	46
1	E	105/107 (98%)	101 (96%)	3 (3%)	1 (1%)	13	46
1	H	105/107 (98%)	101 (96%)	3 (3%)	1 (1%)	13	46
2	F	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
2	G	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
2	I	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
3	A	82/534 (15%)	82 (100%)	0	0	100	100
3	B	82/534 (15%)	82 (100%)	0	0	100	100
3	C	82/534 (15%)	82 (100%)	0	0	100	100
All	All	915/2283 (40%)	891 (97%)	21 (2%)	3 (0%)	38	67

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	52	LYS
1	D	52	LYS
1	H	52	LYS

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	55/90 (61%)	55 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	55/90 (61%)	55 (100%)	0	100	100
1	H	55/90 (61%)	55 (100%)	0	100	100
2	F	77/102 (76%)	77 (100%)	0	100	100
2	G	77/102 (76%)	77 (100%)	0	100	100
2	I	77/102 (76%)	77 (100%)	0	100	100
3	A	60/460 (13%)	60 (100%)	0	100	100
3	B	60/460 (13%)	60 (100%)	0	100	100
3	C	60/460 (13%)	60 (100%)	0	100	100
All	All	576/1956 (29%)	576 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

3 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	A	601	3	14,14,15	1.77	3 (21%)	17,19,21	1.05	1 (5%)
4	NAG	B	601	3	14,14,15	1.77	3 (21%)	17,19,21	1.05	1 (5%)
4	NAG	C	601	3	14,14,15	1.77	3 (21%)	17,19,21	1.05	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	A	601	3	-	0/6/23/26	0/1/1/1
4	NAG	B	601	3	-	0/6/23/26	0/1/1/1
4	NAG	C	601	3	-	0/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	601	NAG	C1-C2	4.96	1.59	1.52
4	A	601	NAG	C1-C2	4.96	1.59	1.52
4	B	601	NAG	C1-C2	4.94	1.59	1.52
4	C	601	NAG	O5-C5	2.29	1.47	1.43
4	A	601	NAG	O5-C5	2.27	1.47	1.43
4	B	601	NAG	O5-C5	2.27	1.47	1.43
4	B	601	NAG	O5-C1	2.13	1.47	1.43
4	A	601	NAG	O5-C1	2.11	1.47	1.43
4	C	601	NAG	O5-C1	2.10	1.47	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	601	NAG	C8-C7-N2	2.64	120.49	116.12
4	B	601	NAG	C8-C7-N2	2.61	120.44	116.12
4	A	601	NAG	C8-C7-N2	2.59	120.42	116.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

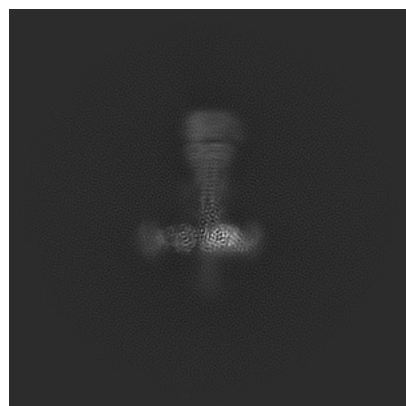
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41642. These allow visual inspection of the internal detail of the map and identification of artifacts.

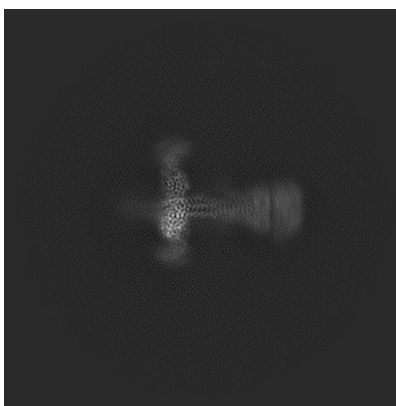
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

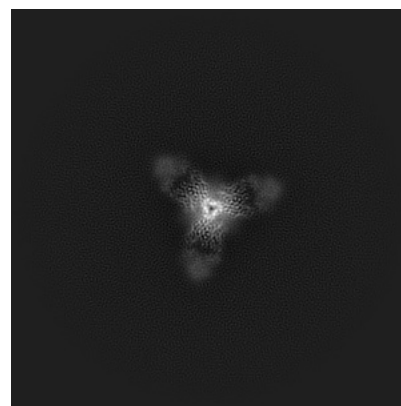
6.1.1 Primary map



X

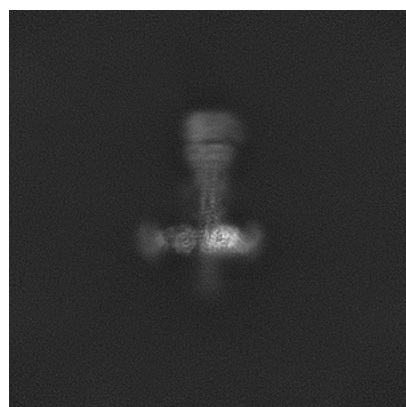


Y

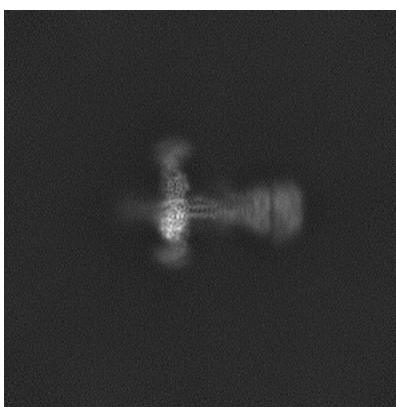


Z

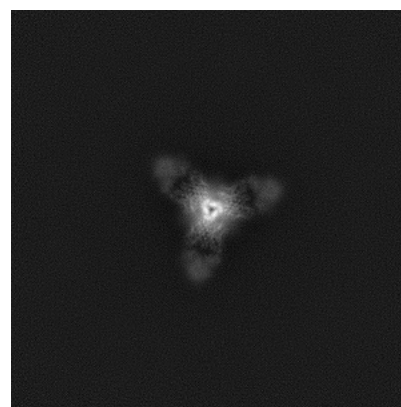
6.1.2 Raw map



X



Y



Z

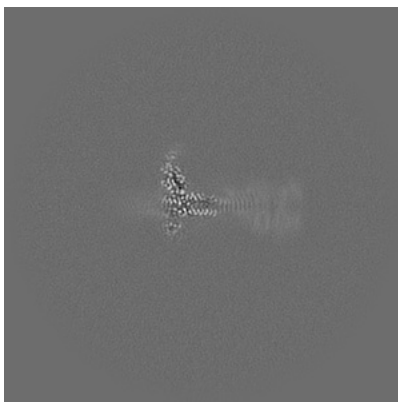
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

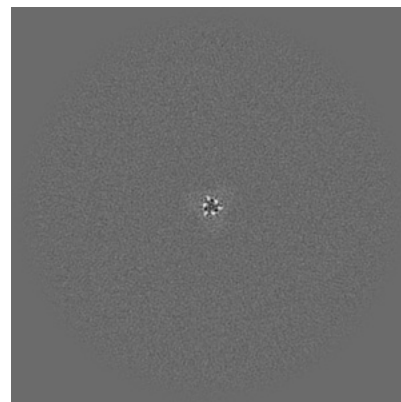
6.2.1 Primary map



X Index: 240



Y Index: 240

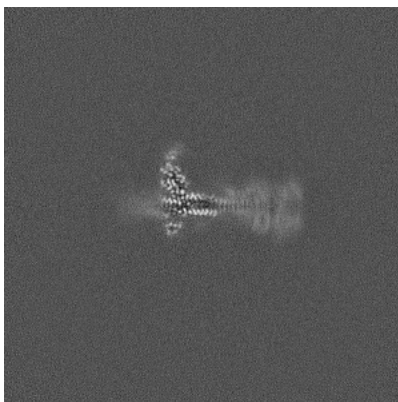


Z Index: 240

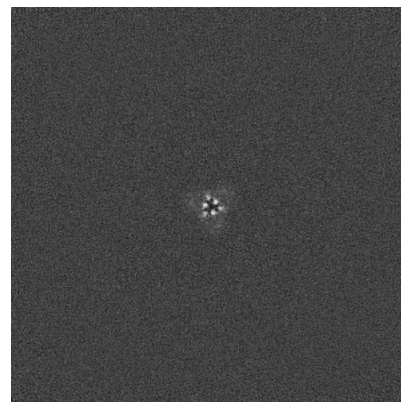
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

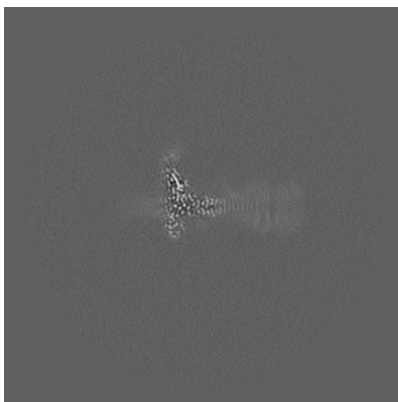
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

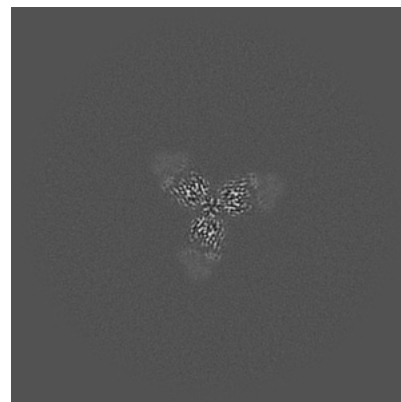
6.3.1 Primary map



X Index: 233



Y Index: 243



Z Index: 207

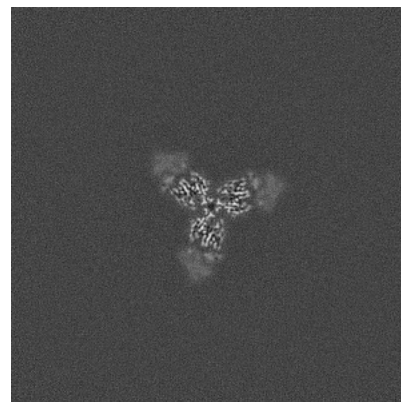
6.3.2 Raw map



X Index: 233



Y Index: 246

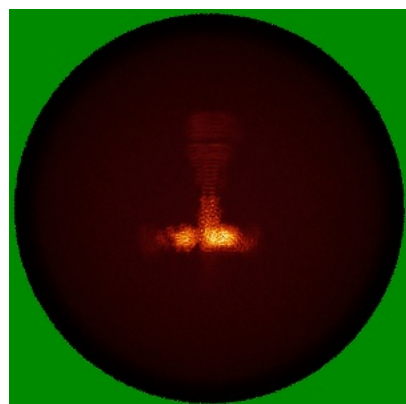


Z Index: 208

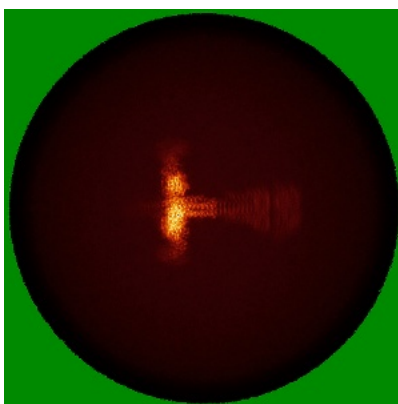
The images above show the largest variance slices of the map in three orthogonal directions.

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

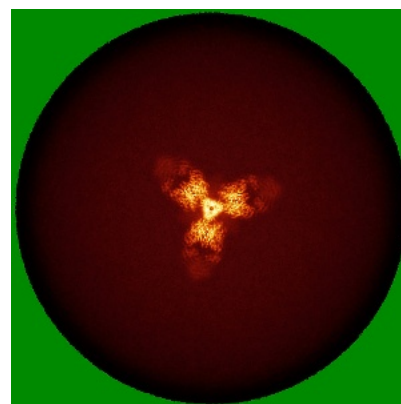
6.4.1 Primary map



X

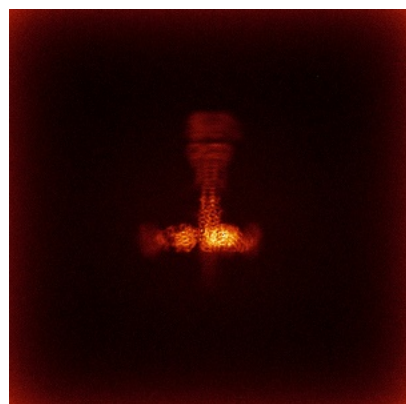


Y

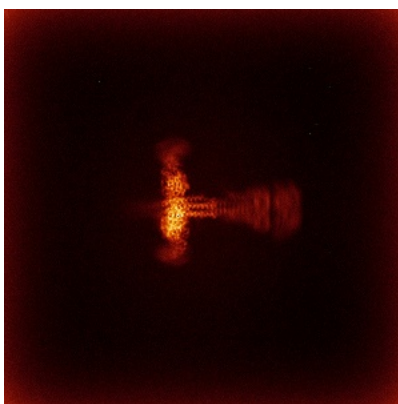


Z

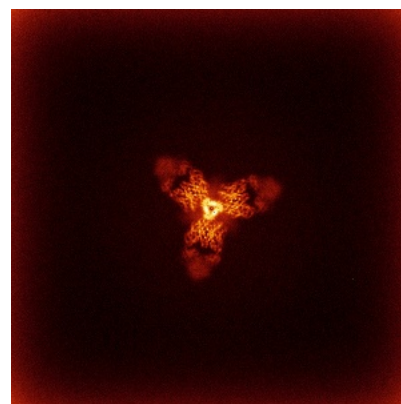
6.4.2 Raw map



X



Y

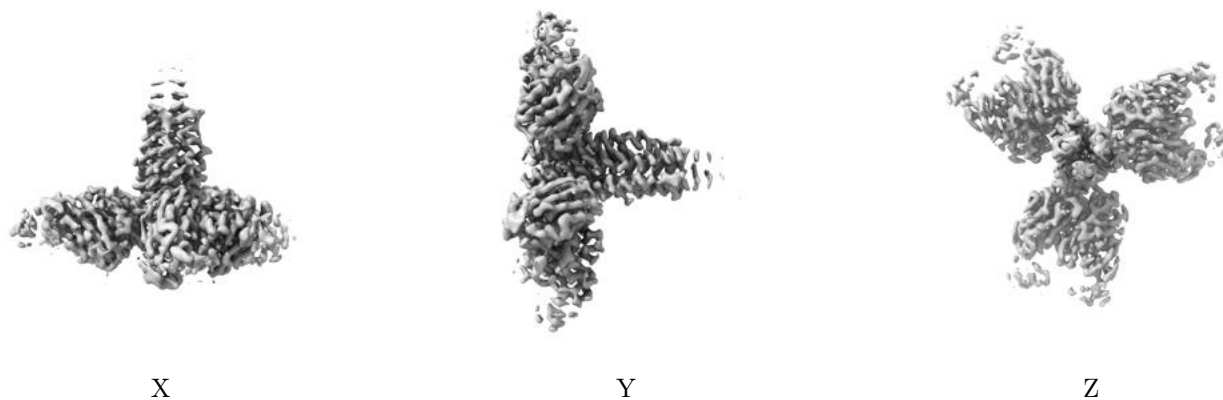


Z

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.

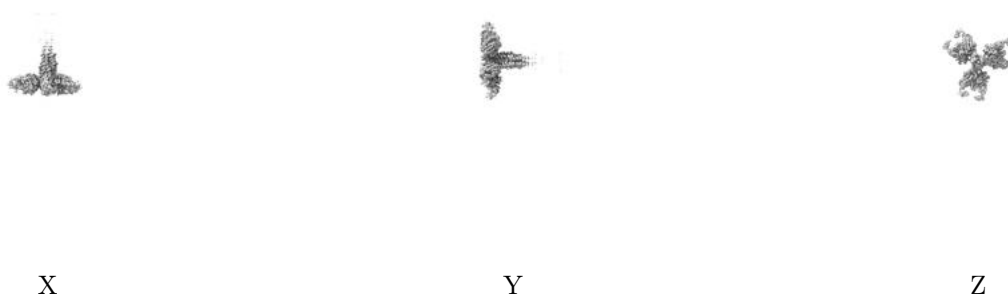
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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.

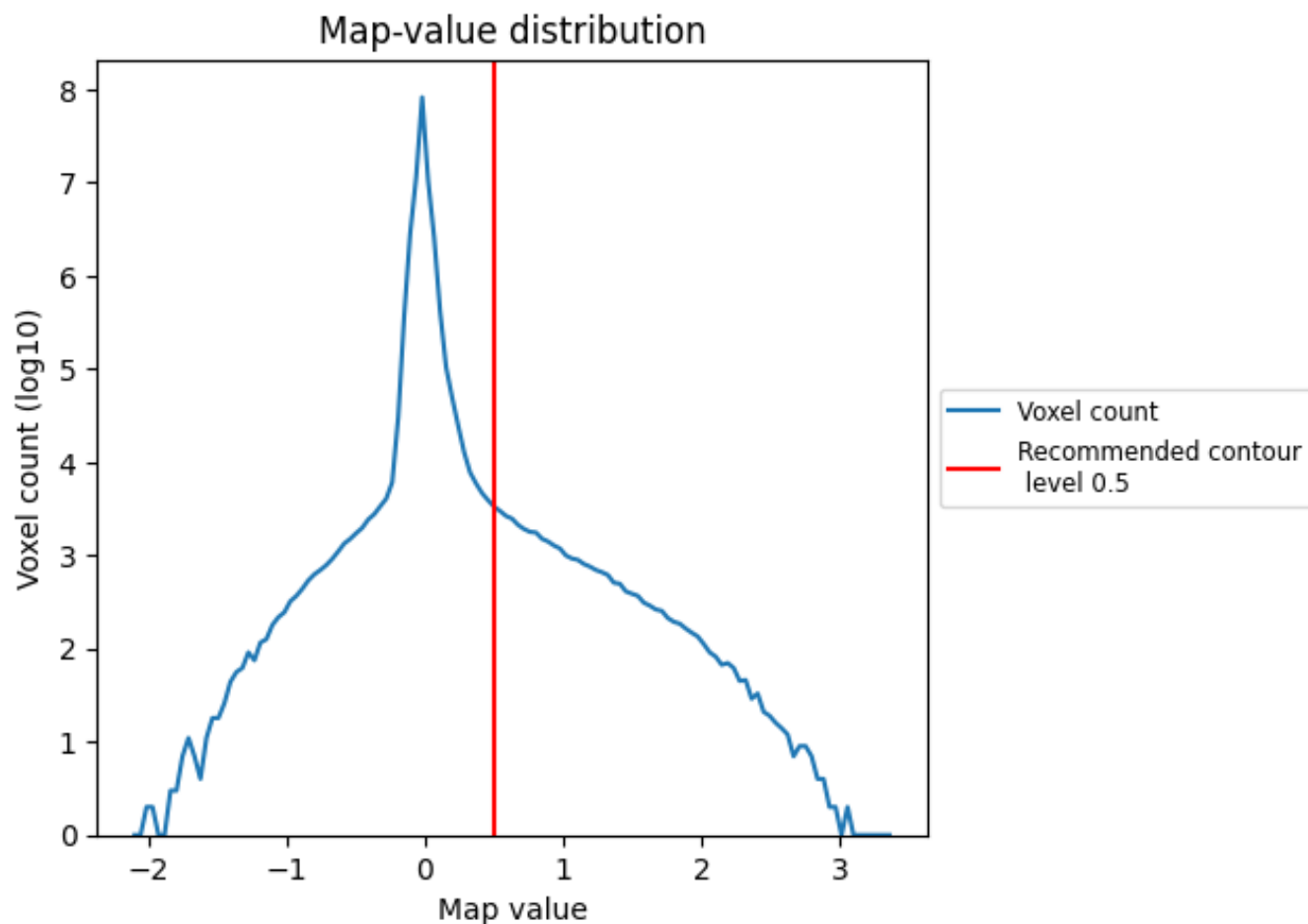
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

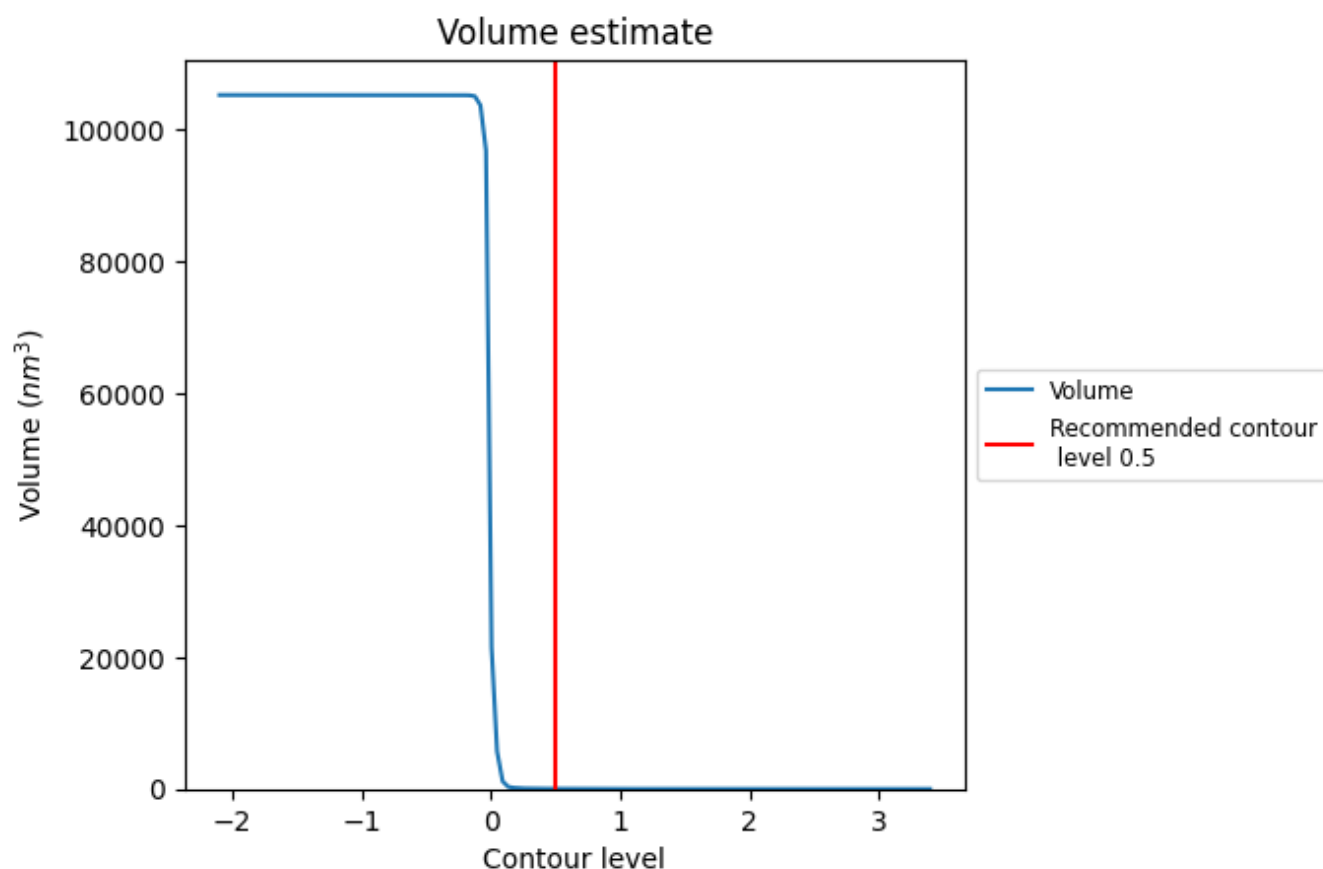
This section contains the results of statistical analysis of the map.

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.

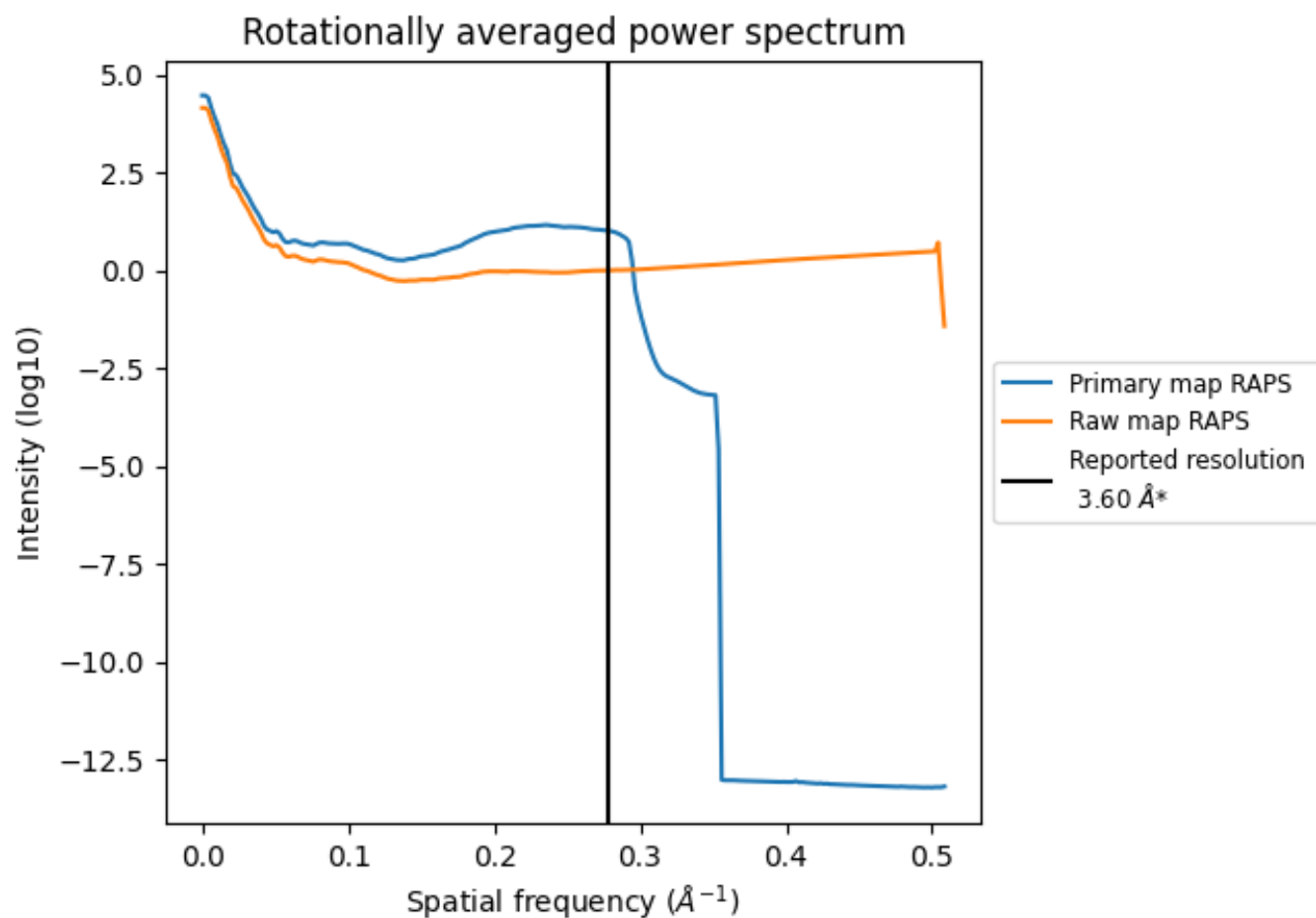
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 34 nm^3 ; this corresponds to an approximate mass of 31 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 ⓘ

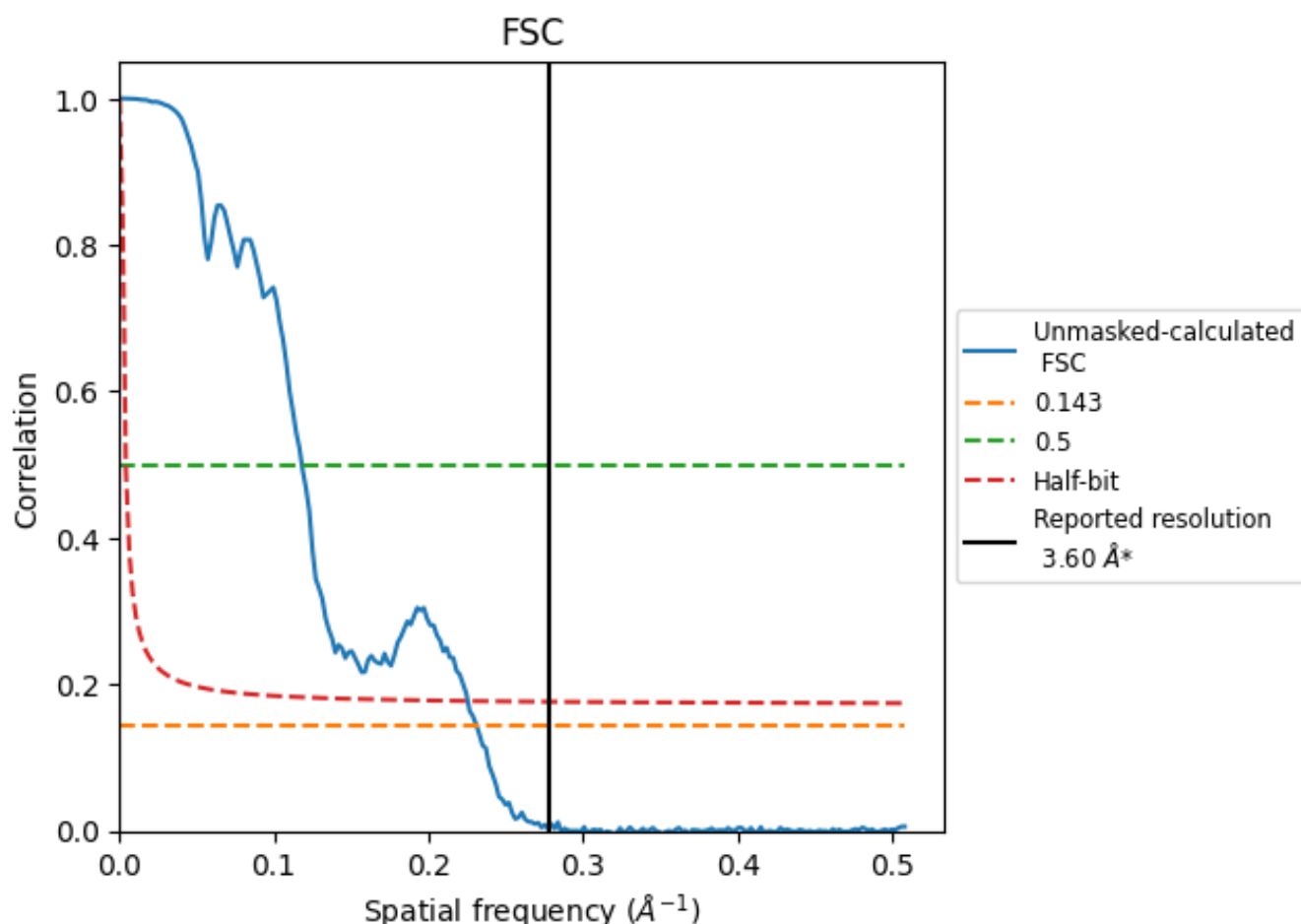


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 \AA^{-1}

8.2 Resolution estimates [i](#)

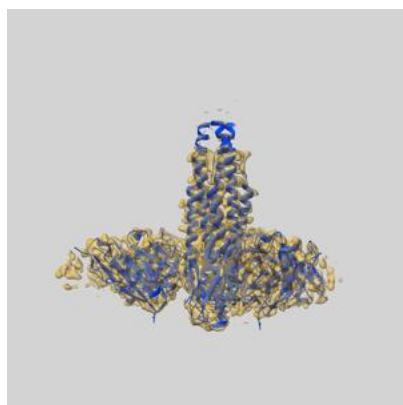
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.33	8.47	4.43

*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 3.6 by more than 10 %

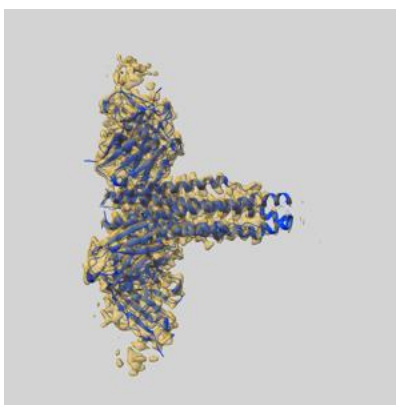
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41642 and PDB model 8TVH. Per-residue inclusion information can be found in section [3](#) on page [10](#).

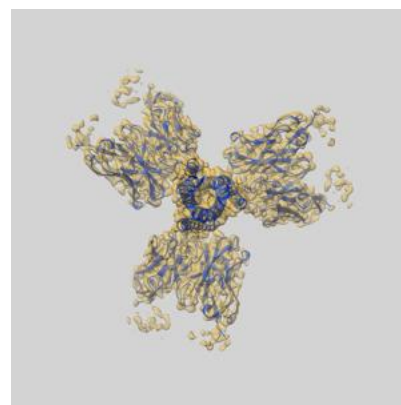
9.1 Map-model overlay [i](#)



X



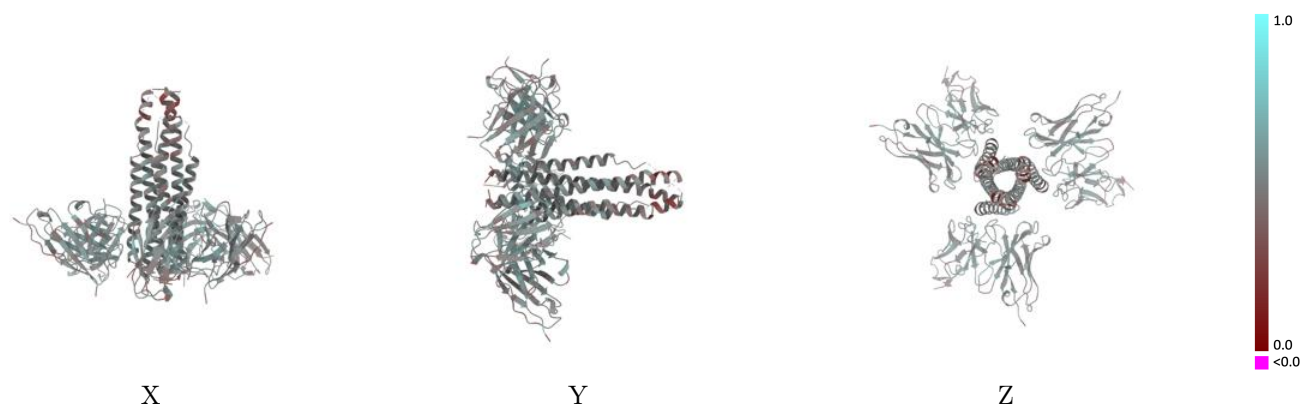
Y



Z

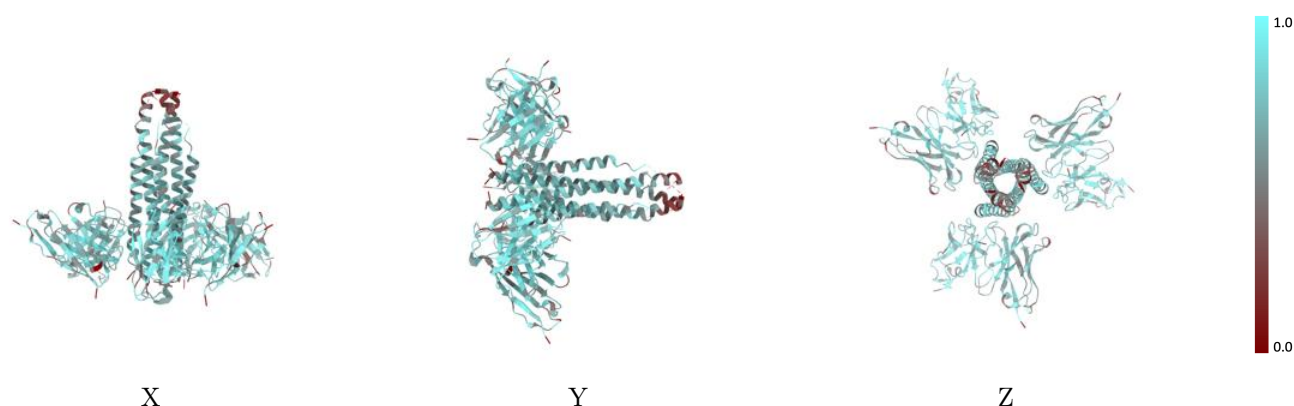
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



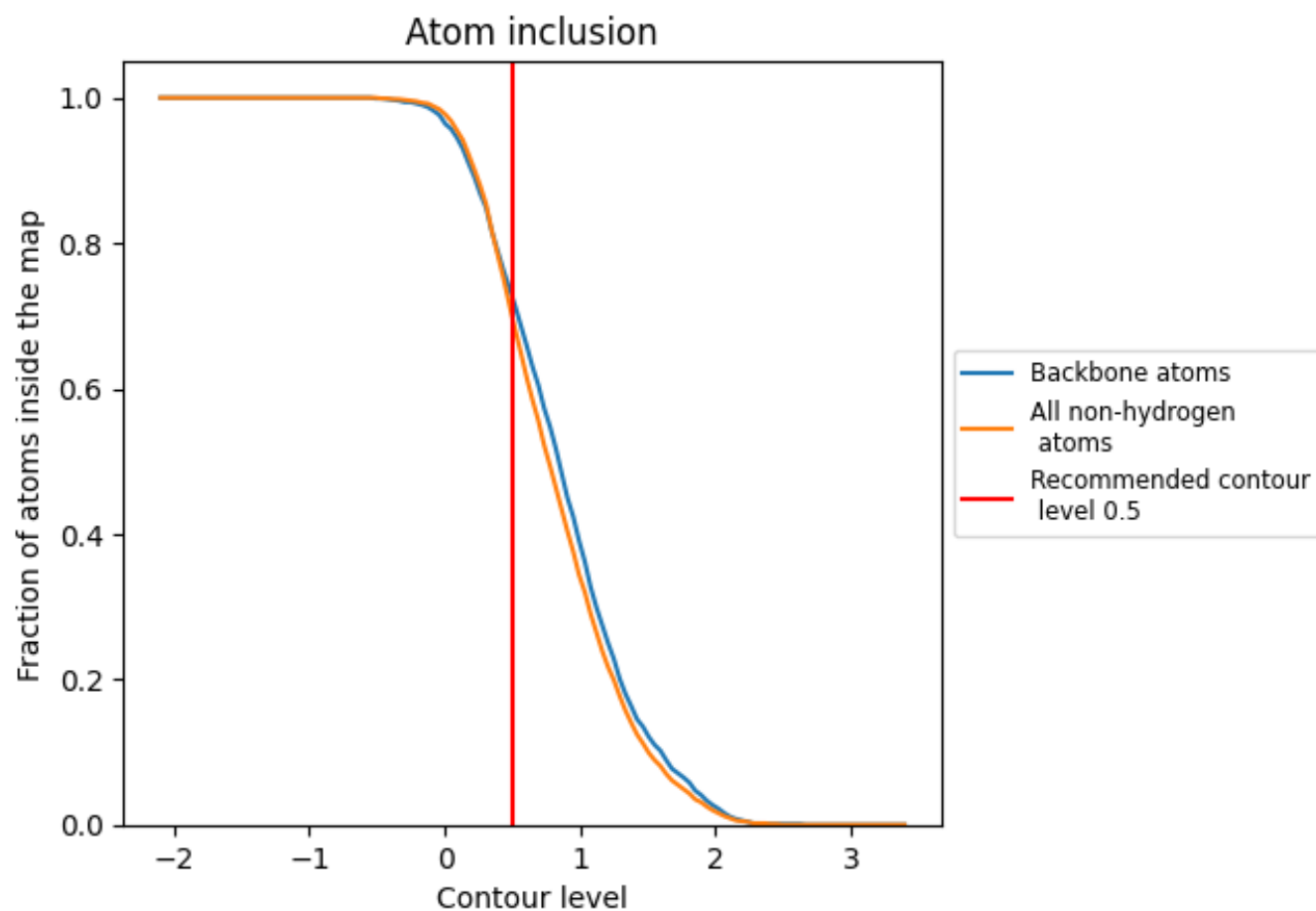
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.6980	<div><div></div></div> 0.4980
A	<div><div></div></div> 0.6460	<div><div></div></div> 0.4720
B	<div><div></div></div> 0.6470	<div><div></div></div> 0.4720
C	<div><div></div></div> 0.6490	<div><div></div></div> 0.4740
D	<div><div></div></div> 0.7430	<div><div></div></div> 0.5090
E	<div><div></div></div> 0.7490	<div><div></div></div> 0.5070
F	<div><div></div></div> 0.6970	<div><div></div></div> 0.5070
G	<div><div></div></div> 0.7010	<div><div></div></div> 0.5060
H	<div><div></div></div> 0.7360	<div><div></div></div> 0.5090
I	<div><div></div></div> 0.6970	<div><div></div></div> 0.5110

1.0

0.0

<0.0