



Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 11:22 AM EDT

PDB ID : 8TVB
EMDB ID : EMD-41636
Title : Ghanaian virus fusion glycoprotein (GhV F)
Authors : Park, Y.J.; Seattle Structural Genomics Center for Infectious Disease (SSG-CID); Veesler, D.
Deposited on : 2023-08-17
Resolution : 2.90 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

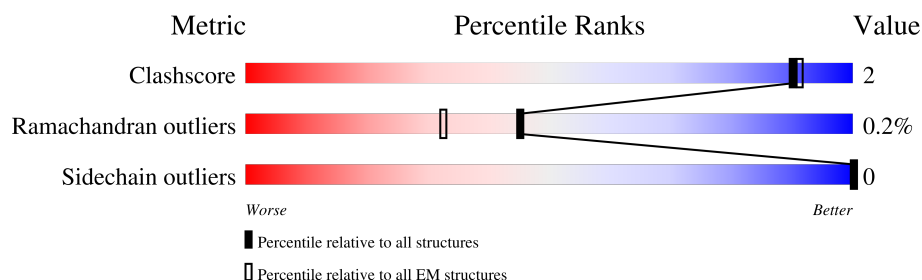
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	A	886	
1	B	886	
1	C	886	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9687 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 Fusion glycoprotein F0,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	422	Total	C	N	O	S	0	0
			3173	2030	531	592	20		
1	B	422	Total	C	N	O	S	0	0
			3173	2030	531	592	20		
1	C	422	Total	C	N	O	S	0	0
			3173	2030	531	592	20		

There are 315 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	587	MET	-	linker	UNP I0E092
A	588	LYS	-	linker	UNP I0E092
A	589	GLN	-	linker	UNP I0E092
A	590	ILE	-	linker	UNP I0E092
A	591	GLU	-	linker	UNP I0E092
A	592	ASP	-	linker	UNP I0E092
A	593	LYS	-	linker	UNP I0E092
A	594	ILE	-	linker	UNP I0E092
A	595	GLU	-	linker	UNP I0E092
A	596	GLU	-	linker	UNP I0E092
A	597	ILE	-	linker	UNP I0E092
A	598	LEU	-	linker	UNP I0E092
A	599	SER	-	linker	UNP I0E092
A	600	LYS	-	linker	UNP I0E092
A	601	ILE	-	linker	UNP I0E092
A	602	TYR	-	linker	UNP I0E092
A	603	HIS	-	linker	UNP I0E092
A	604	ILE	-	linker	UNP I0E092
A	605	GLU	-	linker	UNP I0E092
A	606	ASN	-	linker	UNP I0E092
A	607	GLU	-	linker	UNP I0E092
A	608	ILE	-	linker	UNP I0E092
A	609	ALA	-	linker	UNP I0E092

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Chain	Residue	Modelled	Actual	Comment	Reference
A	610	ARG	-	linker	UNP I0E092
A	611	ILE	-	linker	UNP I0E092
A	612	LYS	-	linker	UNP I0E092
A	613	LYS	-	linker	UNP I0E092
A	614	LEU	-	linker	UNP I0E092
A	615	ILE	-	linker	UNP I0E092
A	616	GLY	-	linker	UNP I0E092
A	617	GLU	-	linker	UNP I0E092
A	618	ALA	-	linker	UNP I0E092
A	619	PRO	-	linker	UNP I0E092
A	620	GLY	-	linker	UNP I0E092
A	621	GLY	-	linker	UNP I0E092
A	622	ILE	-	linker	UNP I0E092
A	623	GLU	-	linker	UNP I0E092
A	624	GLY	-	linker	UNP I0E092
A	625	ARG	-	linker	UNP I0E092
A	626	GLY	-	linker	UNP I0E092
A	627	GLY	-	linker	UNP I0E092
A	628	SER	-	linker	UNP I0E092
A	629	GLY	-	linker	UNP I0E092
A	630	SER	-	linker	UNP I0E092
A	631	GLY	-	linker	UNP I0E092
A	632	GLY	-	linker	UNP I0E092
A	633	SER	-	linker	UNP I0E092
A	634	GLY	-	linker	UNP I0E092
A	635	GLY	-	linker	UNP I0E092
A	636	SER	-	linker	UNP I0E092
A	637	GLY	-	linker	UNP I0E092
A	638	SER	-	linker	UNP I0E092
A	639	GLU	-	linker	UNP I0E092
A	640	LYS	-	linker	UNP I0E092
A	641	ALA	-	linker	UNP I0E092
A	642	ALA	-	linker	UNP I0E092
A	643	LYS	-	linker	UNP I0E092
A	644	ALA	-	linker	UNP I0E092
A	645	GLU	-	linker	UNP I0E092
A	646	GLU	-	linker	UNP I0E092
A	647	ALA	-	linker	UNP I0E092
A	648	ALA	-	linker	UNP I0E092
A	649	ARG	-	linker	UNP I0E092
A	673	ILE	LYS	conflict	UNP Q9WXS1
A	677	VAL	LEU	conflict	UNP Q9WXS1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	681	ALA	GLU	conflict	UNP Q9WXS1
A	702	ALA	GLU	conflict	UNP Q9WXS1
A	705	VAL	PHE	conflict	UNP Q9WXS1
A	724	ALA	CYS	conflict	UNP Q9WXS1
A	748	ALA	CYS	conflict	UNP Q9WXS1
A	813	ALA	CYS	conflict	UNP Q9WXS1
A	851	ALA	CYS	conflict	UNP Q9WXS1
A	854	GLY	-	expression tag	UNP Q9WXS1
A	855	GLY	-	expression tag	UNP Q9WXS1
A	856	SER	-	expression tag	UNP Q9WXS1
A	857	GLY	-	expression tag	UNP Q9WXS1
A	858	GLY	-	expression tag	UNP Q9WXS1
A	859	SER	-	expression tag	UNP Q9WXS1
A	860	HIS	-	expression tag	UNP Q9WXS1
A	861	HIS	-	expression tag	UNP Q9WXS1
A	862	HIS	-	expression tag	UNP Q9WXS1
A	863	HIS	-	expression tag	UNP Q9WXS1
A	864	HIS	-	expression tag	UNP Q9WXS1
A	865	HIS	-	expression tag	UNP Q9WXS1
A	866	GLY	-	expression tag	UNP Q9WXS1
A	867	SER	-	expression tag	UNP Q9WXS1
A	868	GLY	-	expression tag	UNP Q9WXS1
A	869	GLY	-	expression tag	UNP Q9WXS1
A	870	GLY	-	expression tag	UNP Q9WXS1
A	871	SER	-	expression tag	UNP Q9WXS1
A	872	GLY	-	expression tag	UNP Q9WXS1
A	873	LEU	-	expression tag	UNP Q9WXS1
A	874	ASN	-	expression tag	UNP Q9WXS1
A	875	ASP	-	expression tag	UNP Q9WXS1
A	876	ILE	-	expression tag	UNP Q9WXS1
A	877	PHE	-	expression tag	UNP Q9WXS1
A	878	GLU	-	expression tag	UNP Q9WXS1
A	879	ALA	-	expression tag	UNP Q9WXS1
A	880	GLN	-	expression tag	UNP Q9WXS1
A	881	LYS	-	expression tag	UNP Q9WXS1
A	882	ILE	-	expression tag	UNP Q9WXS1
A	883	GLU	-	expression tag	UNP Q9WXS1
A	884	TRP	-	expression tag	UNP Q9WXS1
A	885	HIS	-	expression tag	UNP Q9WXS1
A	886	GLU	-	expression tag	UNP Q9WXS1
B	587	MET	-	linker	UNP I0E092
B	588	LYS	-	linker	UNP I0E092

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Chain	Residue	Modelled	Actual	Comment	Reference
B	589	GLN	-	linker	UNP I0E092
B	590	ILE	-	linker	UNP I0E092
B	591	GLU	-	linker	UNP I0E092
B	592	ASP	-	linker	UNP I0E092
B	593	LYS	-	linker	UNP I0E092
B	594	ILE	-	linker	UNP I0E092
B	595	GLU	-	linker	UNP I0E092
B	596	GLU	-	linker	UNP I0E092
B	597	ILE	-	linker	UNP I0E092
B	598	LEU	-	linker	UNP I0E092
B	599	SER	-	linker	UNP I0E092
B	600	LYS	-	linker	UNP I0E092
B	601	ILE	-	linker	UNP I0E092
B	602	TYR	-	linker	UNP I0E092
B	603	HIS	-	linker	UNP I0E092
B	604	ILE	-	linker	UNP I0E092
B	605	GLU	-	linker	UNP I0E092
B	606	ASN	-	linker	UNP I0E092
B	607	GLU	-	linker	UNP I0E092
B	608	ILE	-	linker	UNP I0E092
B	609	ALA	-	linker	UNP I0E092
B	610	ARG	-	linker	UNP I0E092
B	611	ILE	-	linker	UNP I0E092
B	612	LYS	-	linker	UNP I0E092
B	613	LYS	-	linker	UNP I0E092
B	614	LEU	-	linker	UNP I0E092
B	615	ILE	-	linker	UNP I0E092
B	616	GLY	-	linker	UNP I0E092
B	617	GLU	-	linker	UNP I0E092
B	618	ALA	-	linker	UNP I0E092
B	619	PRO	-	linker	UNP I0E092
B	620	GLY	-	linker	UNP I0E092
B	621	GLY	-	linker	UNP I0E092
B	622	ILE	-	linker	UNP I0E092
B	623	GLU	-	linker	UNP I0E092
B	624	GLY	-	linker	UNP I0E092
B	625	ARG	-	linker	UNP I0E092
B	626	GLY	-	linker	UNP I0E092
B	627	GLY	-	linker	UNP I0E092
B	628	SER	-	linker	UNP I0E092
B	629	GLY	-	linker	UNP I0E092
B	630	SER	-	linker	UNP I0E092

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Chain	Residue	Modelled	Actual	Comment	Reference
B	631	GLY	-	linker	UNP I0E092
B	632	GLY	-	linker	UNP I0E092
B	633	SER	-	linker	UNP I0E092
B	634	GLY	-	linker	UNP I0E092
B	635	GLY	-	linker	UNP I0E092
B	636	SER	-	linker	UNP I0E092
B	637	GLY	-	linker	UNP I0E092
B	638	SER	-	linker	UNP I0E092
B	639	GLU	-	linker	UNP I0E092
B	640	LYS	-	linker	UNP I0E092
B	641	ALA	-	linker	UNP I0E092
B	642	ALA	-	linker	UNP I0E092
B	643	LYS	-	linker	UNP I0E092
B	644	ALA	-	linker	UNP I0E092
B	645	GLU	-	linker	UNP I0E092
B	646	GLU	-	linker	UNP I0E092
B	647	ALA	-	linker	UNP I0E092
B	648	ALA	-	linker	UNP I0E092
B	649	ARG	-	linker	UNP I0E092
B	673	ILE	LYS	conflict	UNP Q9WXS1
B	677	VAL	LEU	conflict	UNP Q9WXS1
B	681	ALA	GLU	conflict	UNP Q9WXS1
B	702	ALA	GLU	conflict	UNP Q9WXS1
B	705	VAL	PHE	conflict	UNP Q9WXS1
B	724	ALA	CYS	conflict	UNP Q9WXS1
B	748	ALA	CYS	conflict	UNP Q9WXS1
B	813	ALA	CYS	conflict	UNP Q9WXS1
B	851	ALA	CYS	conflict	UNP Q9WXS1
B	854	GLY	-	expression tag	UNP Q9WXS1
B	855	GLY	-	expression tag	UNP Q9WXS1
B	856	SER	-	expression tag	UNP Q9WXS1
B	857	GLY	-	expression tag	UNP Q9WXS1
B	858	GLY	-	expression tag	UNP Q9WXS1
B	859	SER	-	expression tag	UNP Q9WXS1
B	860	HIS	-	expression tag	UNP Q9WXS1
B	861	HIS	-	expression tag	UNP Q9WXS1
B	862	HIS	-	expression tag	UNP Q9WXS1
B	863	HIS	-	expression tag	UNP Q9WXS1
B	864	HIS	-	expression tag	UNP Q9WXS1
B	865	HIS	-	expression tag	UNP Q9WXS1
B	866	GLY	-	expression tag	UNP Q9WXS1
B	867	SER	-	expression tag	UNP Q9WXS1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	868	GLY	-	expression tag	UNP Q9WXS1
B	869	GLY	-	expression tag	UNP Q9WXS1
B	870	GLY	-	expression tag	UNP Q9WXS1
B	871	SER	-	expression tag	UNP Q9WXS1
B	872	GLY	-	expression tag	UNP Q9WXS1
B	873	LEU	-	expression tag	UNP Q9WXS1
B	874	ASN	-	expression tag	UNP Q9WXS1
B	875	ASP	-	expression tag	UNP Q9WXS1
B	876	ILE	-	expression tag	UNP Q9WXS1
B	877	PHE	-	expression tag	UNP Q9WXS1
B	878	GLU	-	expression tag	UNP Q9WXS1
B	879	ALA	-	expression tag	UNP Q9WXS1
B	880	GLN	-	expression tag	UNP Q9WXS1
B	881	LYS	-	expression tag	UNP Q9WXS1
B	882	ILE	-	expression tag	UNP Q9WXS1
B	883	GLU	-	expression tag	UNP Q9WXS1
B	884	TRP	-	expression tag	UNP Q9WXS1
B	885	HIS	-	expression tag	UNP Q9WXS1
B	886	GLU	-	expression tag	UNP Q9WXS1
C	587	MET	-	linker	UNP I0E092
C	588	LYS	-	linker	UNP I0E092
C	589	GLN	-	linker	UNP I0E092
C	590	ILE	-	linker	UNP I0E092
C	591	GLU	-	linker	UNP I0E092
C	592	ASP	-	linker	UNP I0E092
C	593	LYS	-	linker	UNP I0E092
C	594	ILE	-	linker	UNP I0E092
C	595	GLU	-	linker	UNP I0E092
C	596	GLU	-	linker	UNP I0E092
C	597	ILE	-	linker	UNP I0E092
C	598	LEU	-	linker	UNP I0E092
C	599	SER	-	linker	UNP I0E092
C	600	LYS	-	linker	UNP I0E092
C	601	ILE	-	linker	UNP I0E092
C	602	TYR	-	linker	UNP I0E092
C	603	HIS	-	linker	UNP I0E092
C	604	ILE	-	linker	UNP I0E092
C	605	GLU	-	linker	UNP I0E092
C	606	ASN	-	linker	UNP I0E092
C	607	GLU	-	linker	UNP I0E092
C	608	ILE	-	linker	UNP I0E092
C	609	ALA	-	linker	UNP I0E092

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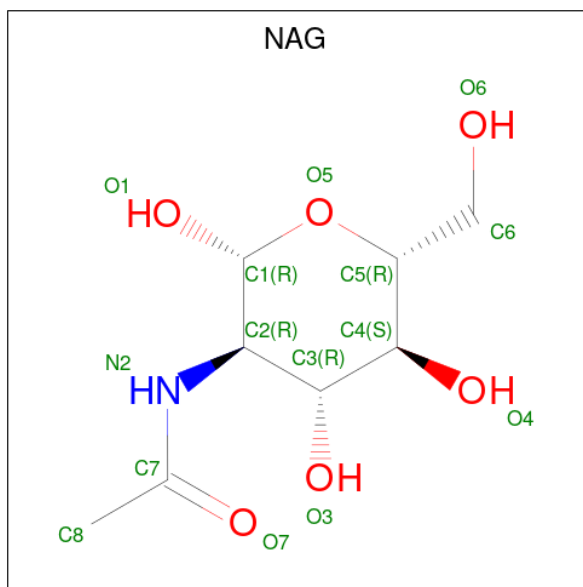
Chain	Residue	Modelled	Actual	Comment	Reference
C	610	ARG	-	linker	UNP I0E092
C	611	ILE	-	linker	UNP I0E092
C	612	LYS	-	linker	UNP I0E092
C	613	LYS	-	linker	UNP I0E092
C	614	LEU	-	linker	UNP I0E092
C	615	ILE	-	linker	UNP I0E092
C	616	GLY	-	linker	UNP I0E092
C	617	GLU	-	linker	UNP I0E092
C	618	ALA	-	linker	UNP I0E092
C	619	PRO	-	linker	UNP I0E092
C	620	GLY	-	linker	UNP I0E092
C	621	GLY	-	linker	UNP I0E092
C	622	ILE	-	linker	UNP I0E092
C	623	GLU	-	linker	UNP I0E092
C	624	GLY	-	linker	UNP I0E092
C	625	ARG	-	linker	UNP I0E092
C	626	GLY	-	linker	UNP I0E092
C	627	GLY	-	linker	UNP I0E092
C	628	SER	-	linker	UNP I0E092
C	629	GLY	-	linker	UNP I0E092
C	630	SER	-	linker	UNP I0E092
C	631	GLY	-	linker	UNP I0E092
C	632	GLY	-	linker	UNP I0E092
C	633	SER	-	linker	UNP I0E092
C	634	GLY	-	linker	UNP I0E092
C	635	GLY	-	linker	UNP I0E092
C	636	SER	-	linker	UNP I0E092
C	637	GLY	-	linker	UNP I0E092
C	638	SER	-	linker	UNP I0E092
C	639	GLU	-	linker	UNP I0E092
C	640	LYS	-	linker	UNP I0E092
C	641	ALA	-	linker	UNP I0E092
C	642	ALA	-	linker	UNP I0E092
C	643	LYS	-	linker	UNP I0E092
C	644	ALA	-	linker	UNP I0E092
C	645	GLU	-	linker	UNP I0E092
C	646	GLU	-	linker	UNP I0E092
C	647	ALA	-	linker	UNP I0E092
C	648	ALA	-	linker	UNP I0E092
C	649	ARG	-	linker	UNP I0E092
C	673	ILE	LYS	conflict	UNP Q9WXS1
C	677	VAL	LEU	conflict	UNP Q9WXS1

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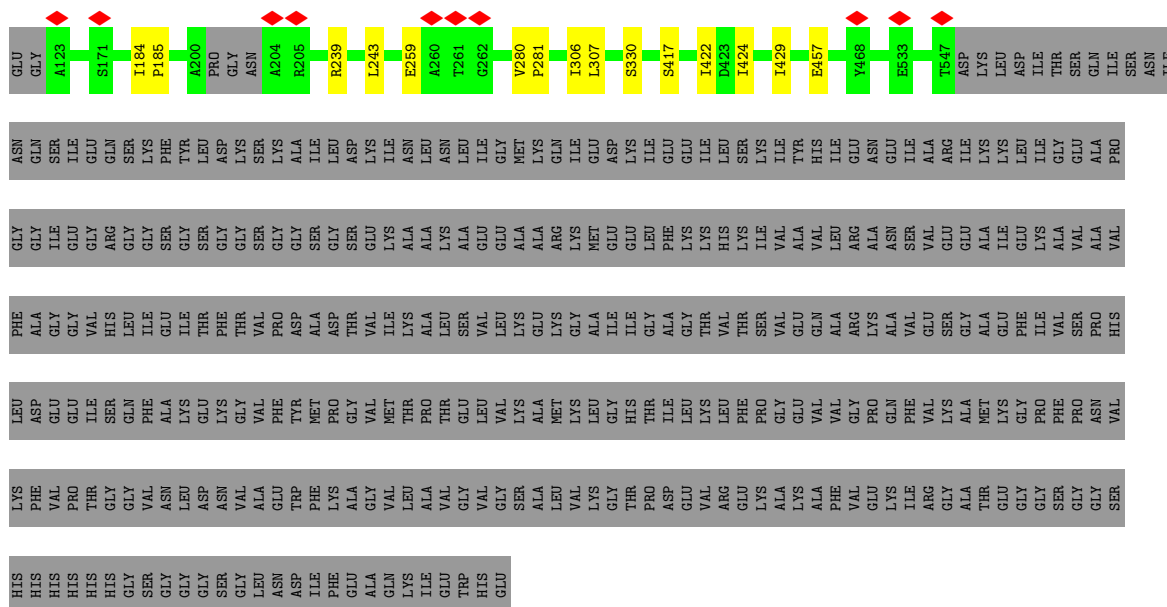
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Chain	Residue	Modelled	Actual	Comment	Reference
C	681	ALA	GLU	conflict	UNP Q9WXS1
C	702	ALA	GLU	conflict	UNP Q9WXS1
C	705	VAL	PHE	conflict	UNP Q9WXS1
C	724	ALA	CYS	conflict	UNP Q9WXS1
C	748	ALA	CYS	conflict	UNP Q9WXS1
C	813	ALA	CYS	conflict	UNP Q9WXS1
C	851	ALA	CYS	conflict	UNP Q9WXS1
C	854	GLY	-	expression tag	UNP Q9WXS1
C	855	GLY	-	expression tag	UNP Q9WXS1
C	856	SER	-	expression tag	UNP Q9WXS1
C	857	GLY	-	expression tag	UNP Q9WXS1
C	858	GLY	-	expression tag	UNP Q9WXS1
C	859	SER	-	expression tag	UNP Q9WXS1
C	860	HIS	-	expression tag	UNP Q9WXS1
C	861	HIS	-	expression tag	UNP Q9WXS1
C	862	HIS	-	expression tag	UNP Q9WXS1
C	863	HIS	-	expression tag	UNP Q9WXS1
C	864	HIS	-	expression tag	UNP Q9WXS1
C	865	HIS	-	expression tag	UNP Q9WXS1
C	866	GLY	-	expression tag	UNP Q9WXS1
C	867	SER	-	expression tag	UNP Q9WXS1
C	868	GLY	-	expression tag	UNP Q9WXS1
C	869	GLY	-	expression tag	UNP Q9WXS1
C	870	GLY	-	expression tag	UNP Q9WXS1
C	871	SER	-	expression tag	UNP Q9WXS1
C	872	GLY	-	expression tag	UNP Q9WXS1
C	873	LEU	-	expression tag	UNP Q9WXS1
C	874	ASN	-	expression tag	UNP Q9WXS1
C	875	ASP	-	expression tag	UNP Q9WXS1
C	876	ILE	-	expression tag	UNP Q9WXS1
C	877	PHE	-	expression tag	UNP Q9WXS1
C	878	GLU	-	expression tag	UNP Q9WXS1
C	879	ALA	-	expression tag	UNP Q9WXS1
C	880	GLN	-	expression tag	UNP Q9WXS1
C	881	LYS	-	expression tag	UNP Q9WXS1
C	882	ILE	-	expression tag	UNP Q9WXS1
C	883	GLU	-	expression tag	UNP Q9WXS1
C	884	TRP	-	expression tag	UNP Q9WXS1
C	885	HIS	-	expression tag	UNP Q9WXS1
C	886	GLU	-	expression tag	UNP Q9WXS1

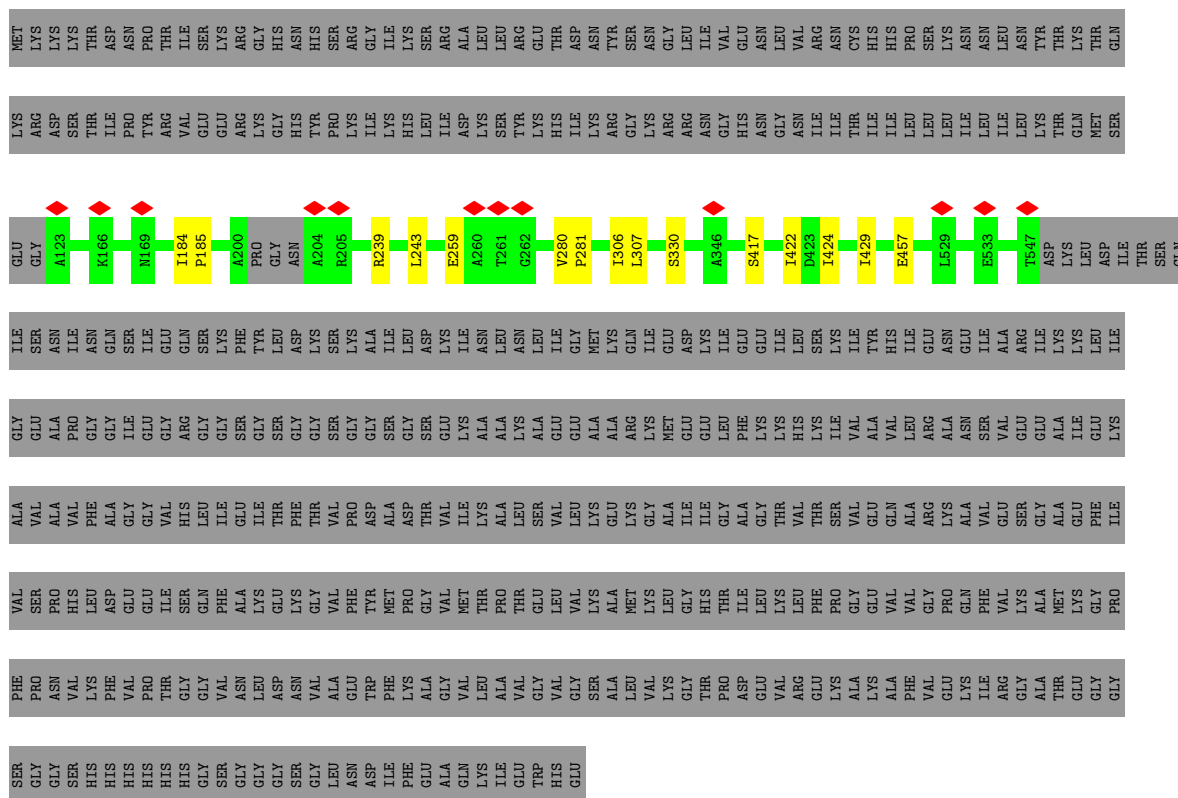
- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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



- Molecule 1: Fusion glycoprotein F0,2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	60207	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 ($e^-/\text{\AA}^2$)	63	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.679	Depositor
Minimum map value	-4.300	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.152	Depositor
Recommended contour level	0.9	Depositor
Map size (Å)	260.0, 260.0, 260.0	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	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	A	0.55	0/3219	0.57	0/4378
1	B	0.55	0/3219	0.57	0/4378
1	C	0.55	0/3219	0.57	0/4378
All	All	0.55	0/9657	0.57	0/13134

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	1
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	239	ARG	Sidechain
1	B	239	ARG	Sidechain
1	C	239	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3173	0	3158	10	0
1	B	3173	0	3158	10	0
1	C	3173	0	3158	10	0
2	A	56	0	52	0	0
2	B	56	0	52	0	0
2	C	56	0	52	0	0
All	All	9687	0	9630	30	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 2.

All (30) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:ILE:HG23	1:C:429:ILE:HD11	1.78	0.66
1:A:424:ILE:HG23	1:A:429:ILE:HD11	1.78	0.65
1:B:424:ILE:HG23	1:B:429:ILE:HD11	1.78	0.65
1:C:424:ILE:CG2	1:C:429:ILE:HD11	2.32	0.60
1:A:424:ILE:CG2	1:A:429:ILE:HD11	2.32	0.59
1:B:424:ILE:CG2	1:B:429:ILE:HD11	2.32	0.58
1:B:280:VAL:N	1:B:281:PRO:CD	2.72	0.52
1:C:280:VAL:N	1:C:281:PRO:CD	2.72	0.52
1:A:280:VAL:N	1:A:281:PRO:CD	2.72	0.52
1:B:422:ILE:HG12	1:B:424:ILE:HD13	1.94	0.49
1:A:306:ILE:HG13	1:A:307:LEU:N	2.28	0.49
1:C:306:ILE:HG13	1:C:307:LEU:N	2.28	0.49
1:C:422:ILE:HG12	1:C:424:ILE:HD13	1.94	0.48
1:A:422:ILE:HG12	1:A:424:ILE:HD13	1.94	0.48
1:B:306:ILE:HG13	1:B:307:LEU:N	2.28	0.47
1:A:306:ILE:HG22	1:A:330:SER:HA	1.99	0.45
1:C:306:ILE:HG22	1:C:330:SER:HA	1.99	0.45
1:B:306:ILE:HG22	1:B:330:SER:HA	1.99	0.44
1:B:184:ILE:N	1:B:185:PRO:CD	2.82	0.43
1:A:184:ILE:N	1:A:185:PRO:CD	2.82	0.43
1:B:457:GLU:OE1	1:B:457:GLU:N	2.51	0.43

Continued on next page...

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:ILE:N	1:C:185:PRO:CD	2.82	0.42
1:C:243:LEU:HD11	1:C:259:GLU:HG2	2.02	0.42
1:C:457:GLU:OE1	1:C:457:GLU:N	2.51	0.42
1:B:184:ILE:HB	1:B:185:PRO:HD3	2.02	0.42
1:A:243:LEU:HD11	1:A:259:GLU:HG2	2.02	0.41
1:A:457:GLU:OE1	1:A:457:GLU:N	2.51	0.41
1:C:184:ILE:HB	1:C:185:PRO:HD3	2.02	0.41
1:B:243:LEU:HD11	1:B:259:GLU:HG2	2.02	0.41
1:A:184:ILE:HB	1:A:185:PRO:HD3	2.02	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	418/886 (47%)	412 (99%)	5 (1%)	1 (0%)	44	73
1	B	418/886 (47%)	412 (99%)	5 (1%)	1 (0%)	44	73
1	C	418/886 (47%)	412 (99%)	5 (1%)	1 (0%)	44	73
All	All	1254/2658 (47%)	1236 (99%)	15 (1%)	3 (0%)	45	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	417	SER
1	B	417	SER
1	C	417	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	335/750 (45%)	335 (100%)	0	100	100
1	B	335/750 (45%)	335 (100%)	0	100	100
1	C	335/750 (45%)	335 (100%)	0	100	100
All	All	1005/2250 (45%)	1005 (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. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	438	HIS
1	C	438	HIS

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](#)

12 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
2	NAG	B	903	1	14,14,15	1.19	1 (7%)	17,19,21	1.11	1 (5%)
2	NAG	A	904	1	14,14,15	0.40	0	17,19,21	0.76	0
2	NAG	B	902	1	14,14,15	1.23	1 (7%)	17,19,21	1.13	1 (5%)
2	NAG	A	902	1	14,14,15	1.24	1 (7%)	17,19,21	1.13	1 (5%)
2	NAG	B	901	1	14,14,15	1.23	1 (7%)	17,19,21	1.07	1 (5%)
2	NAG	C	903	1	14,14,15	1.19	1 (7%)	17,19,21	1.11	1 (5%)
2	NAG	A	903	1	14,14,15	1.19	1 (7%)	17,19,21	1.11	1 (5%)
2	NAG	C	904	1	14,14,15	0.39	0	17,19,21	0.76	0
2	NAG	C	901	1	14,14,15	1.21	1 (7%)	17,19,21	1.07	1 (5%)
2	NAG	C	902	1	14,14,15	1.25	1 (7%)	17,19,21	1.14	1 (5%)
2	NAG	A	901	1	14,14,15	1.22	1 (7%)	17,19,21	1.08	1 (5%)
2	NAG	B	904	1	14,14,15	0.40	0	17,19,21	0.75	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	903	1	-	0/6/23/26	0/1/1/1
2	NAG	A	904	1	-	1/6/23/26	0/1/1/1
2	NAG	B	902	1	-	0/6/23/26	0/1/1/1
2	NAG	A	902	1	-	0/6/23/26	0/1/1/1
2	NAG	B	901	1	-	0/6/23/26	0/1/1/1
2	NAG	C	903	1	-	0/6/23/26	0/1/1/1
2	NAG	A	903	1	-	0/6/23/26	0/1/1/1
2	NAG	C	904	1	-	1/6/23/26	0/1/1/1
2	NAG	C	901	1	-	0/6/23/26	0/1/1/1
2	NAG	C	902	1	-	0/6/23/26	0/1/1/1
2	NAG	A	901	1	-	0/6/23/26	0/1/1/1
2	NAG	B	904	1	-	1/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	902	NAG	C1-C2	3.69	1.57	1.52
2	B	901	NAG	C1-C2	3.69	1.57	1.52
2	A	902	NAG	C1-C2	3.68	1.57	1.52
2	B	902	NAG	C1-C2	3.66	1.57	1.52
2	A	901	NAG	C1-C2	3.65	1.57	1.52
2	C	901	NAG	C1-C2	3.61	1.57	1.52
2	A	903	NAG	C1-C2	3.59	1.57	1.52
2	C	903	NAG	C1-C2	3.56	1.57	1.52
2	B	903	NAG	C1-C2	3.56	1.57	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	902	NAG	C8-C7-N2	2.71	120.61	116.12
2	C	902	NAG	C8-C7-N2	2.71	120.61	116.12
2	A	902	NAG	C8-C7-N2	2.70	120.60	116.12
2	C	901	NAG	C8-C7-N2	2.58	120.39	116.12
2	A	901	NAG	C8-C7-N2	2.57	120.39	116.12
2	B	901	NAG	C8-C7-N2	2.56	120.36	116.12
2	C	903	NAG	C8-C7-N2	2.52	120.30	116.12
2	A	903	NAG	C8-C7-N2	2.50	120.26	116.12
2	B	903	NAG	C8-C7-N2	2.49	120.25	116.12

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	904	NAG	C1-C2-N2-C7
2	B	904	NAG	C1-C2-N2-C7
2	C	904	NAG	C1-C2-N2-C7

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.

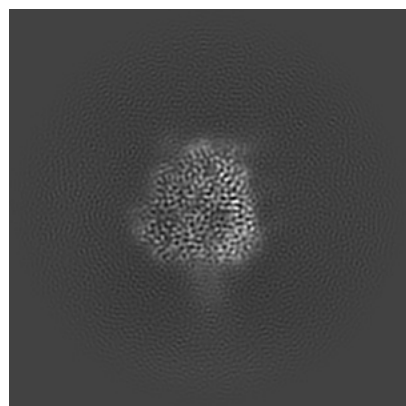
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41636. These allow visual inspection of the internal detail of the map and identification of artifacts.

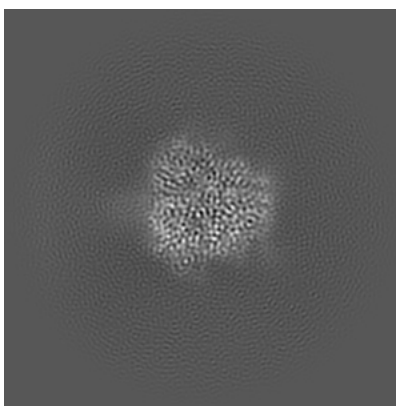
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

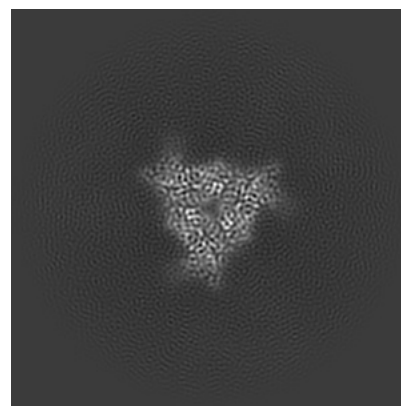
6.1.1 Primary map



X

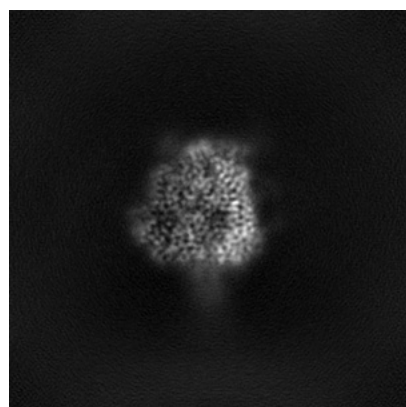


Y

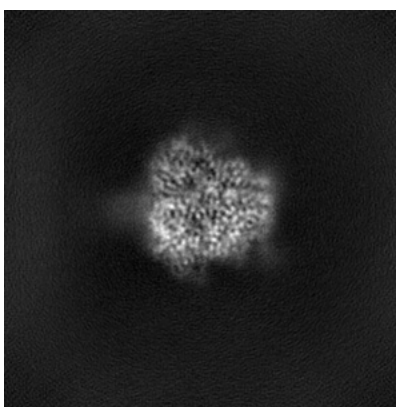


Z

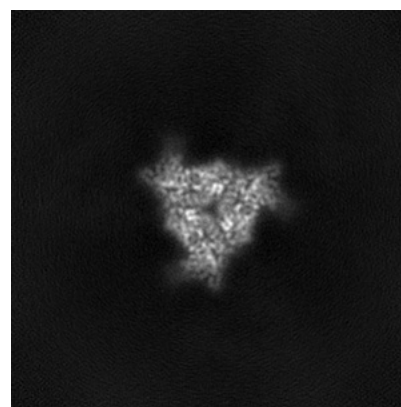
6.1.2 Raw map



X



Y

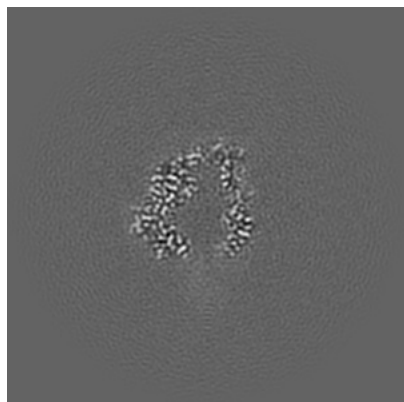


Z

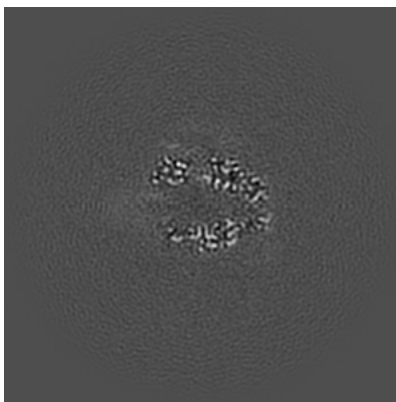
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

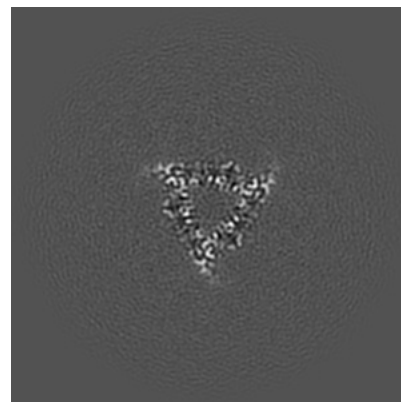
6.2.1 Primary map



X Index: 130

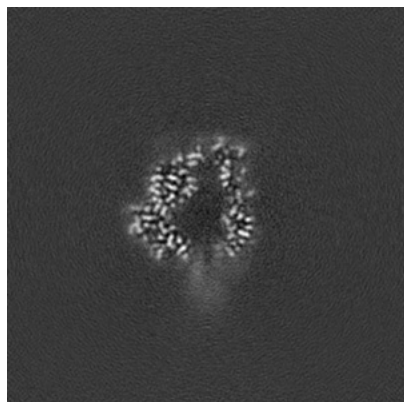


Y Index: 130

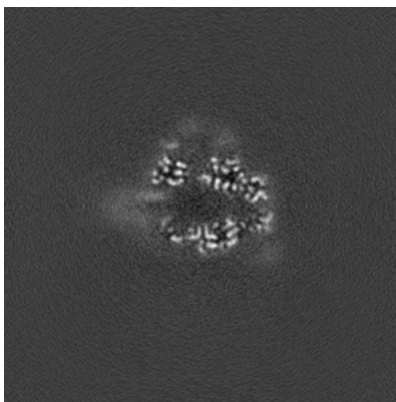


Z Index: 130

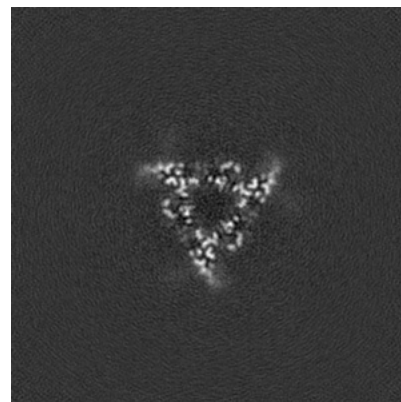
6.2.2 Raw map



X Index: 130



Y Index: 130

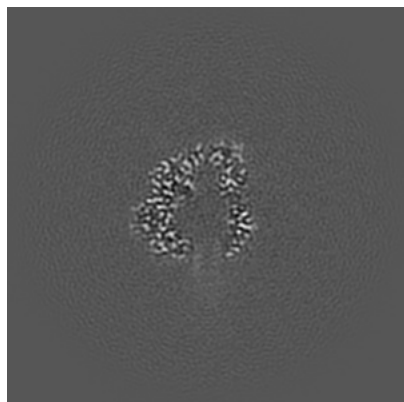


Z Index: 130

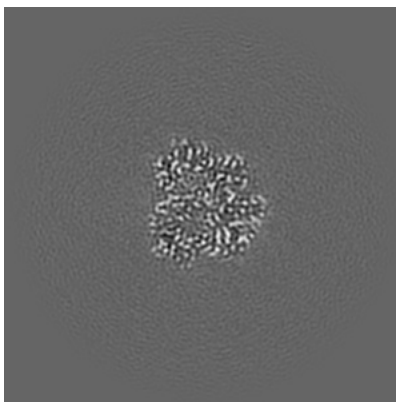
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

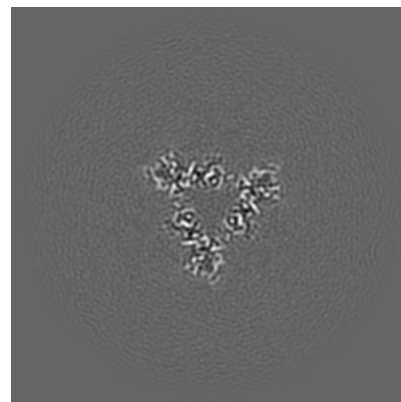
6.3.1 Primary map



X Index: 128

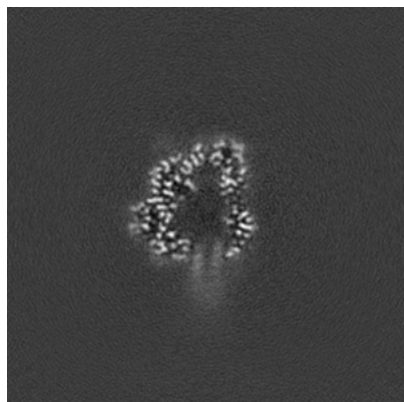


Y Index: 145

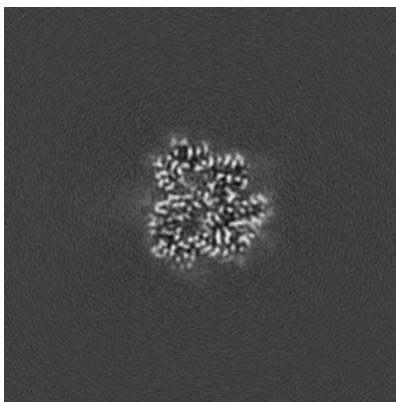


Z Index: 113

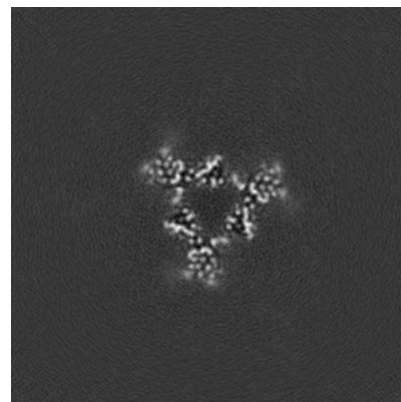
6.3.2 Raw map



X Index: 128



Y Index: 145

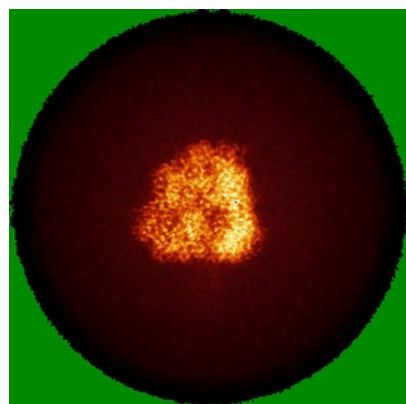


Z Index: 116

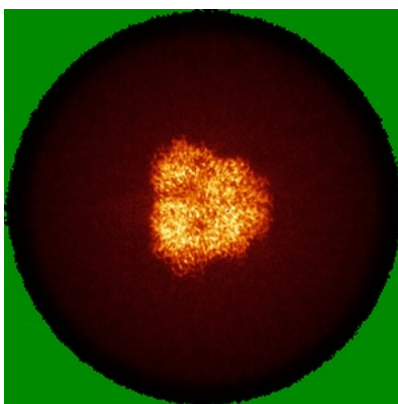
The images above show the largest variance slices of the map in three orthogonal directions.

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

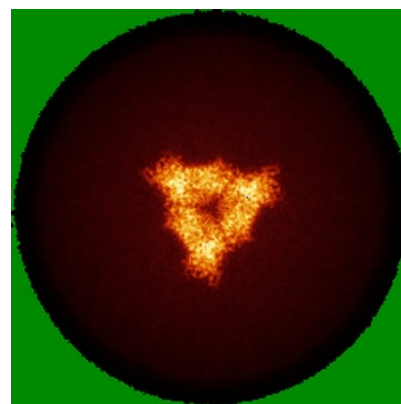
6.4.1 Primary map



X

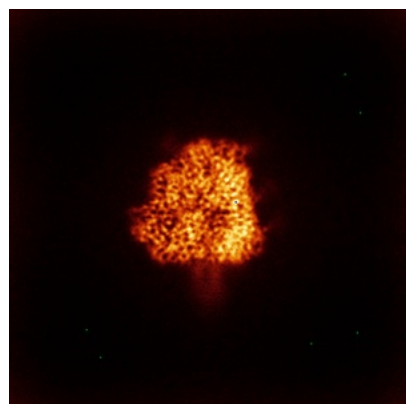


Y

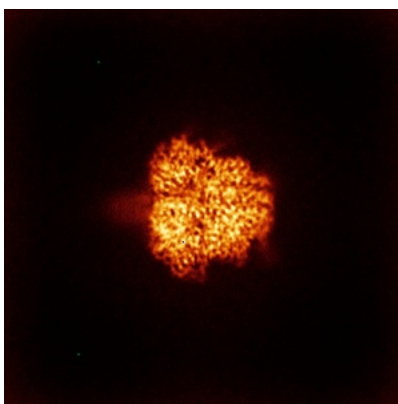


Z

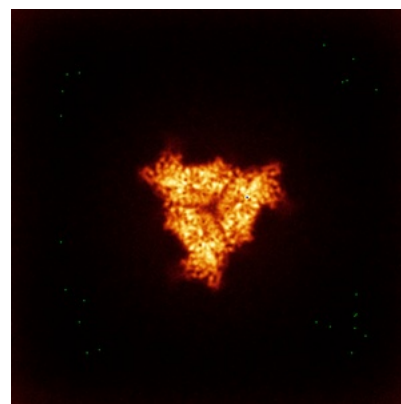
6.4.2 Raw map



X



Y

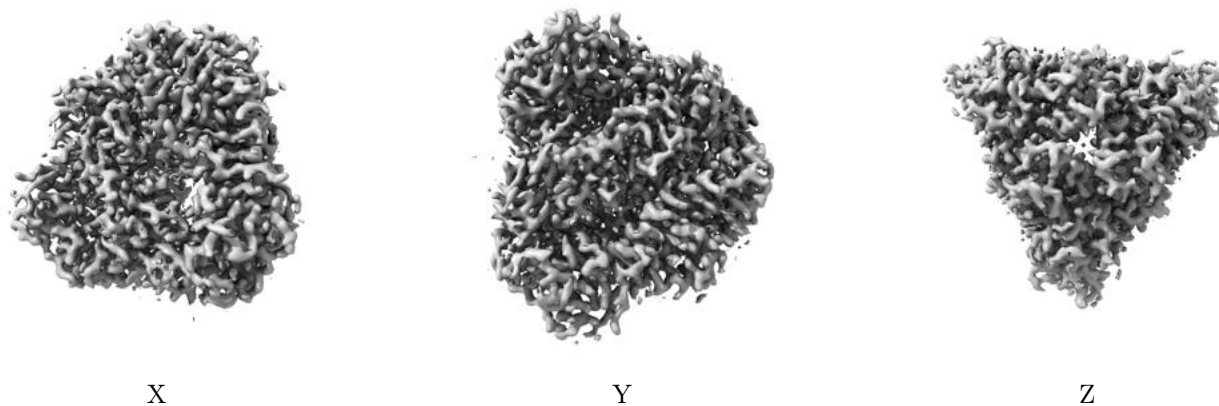


Z

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.

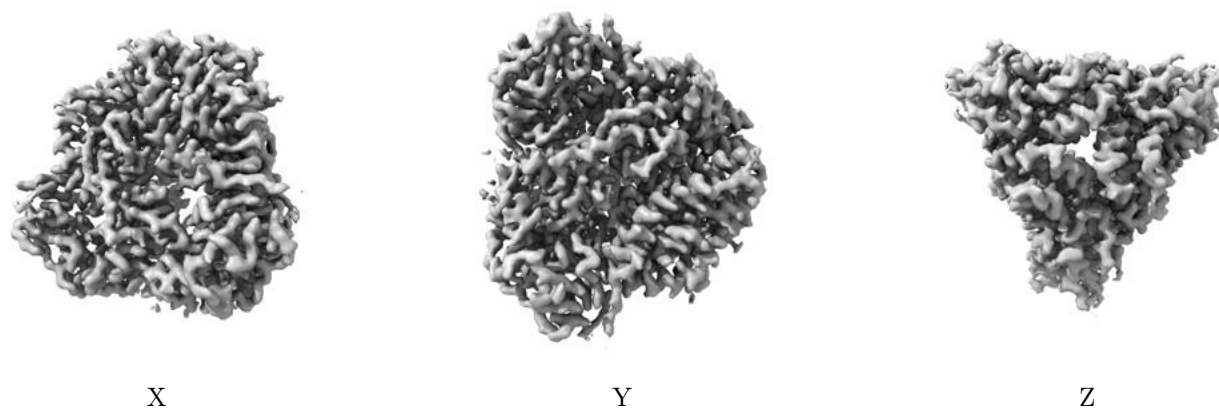
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.9. 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.

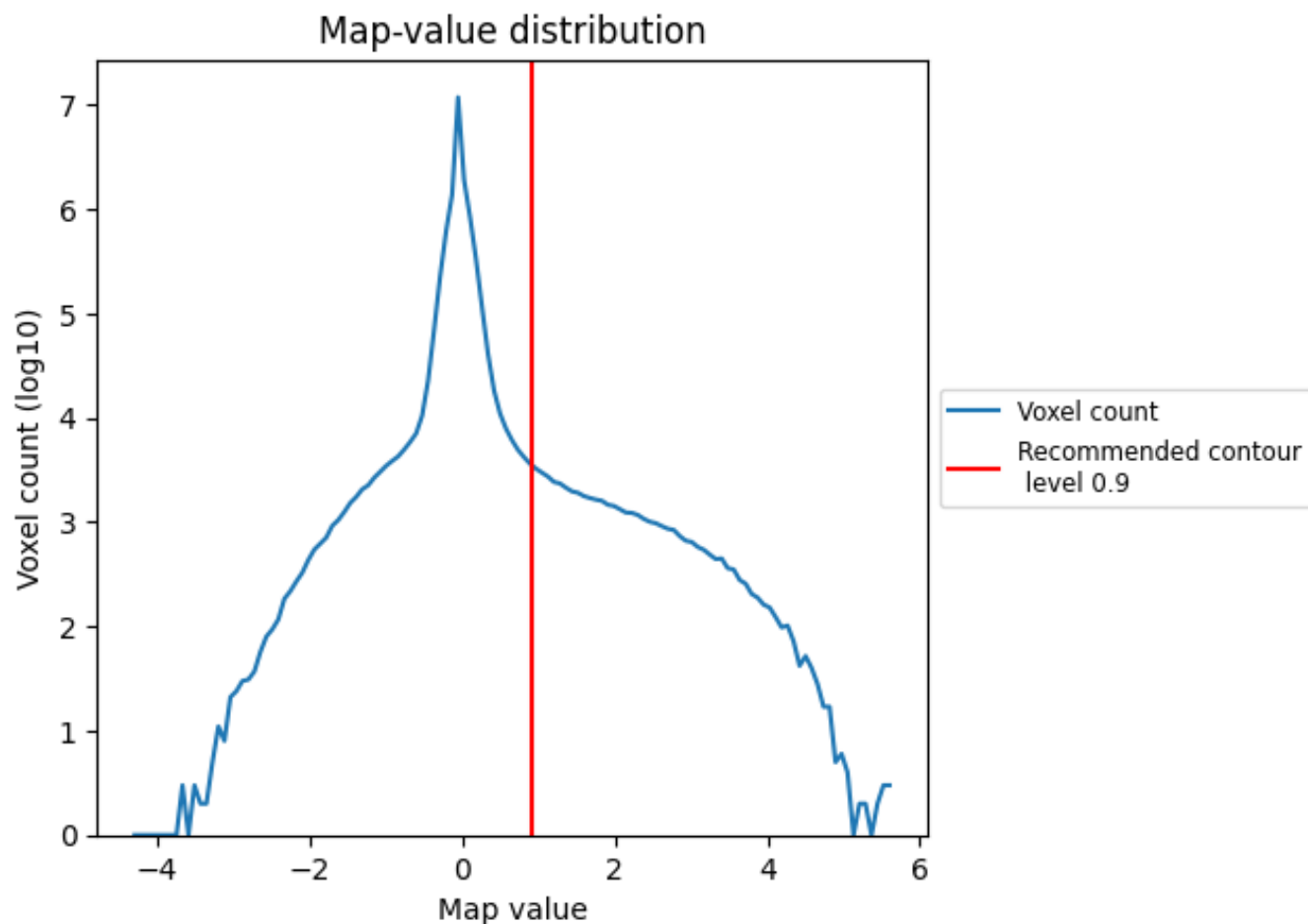
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

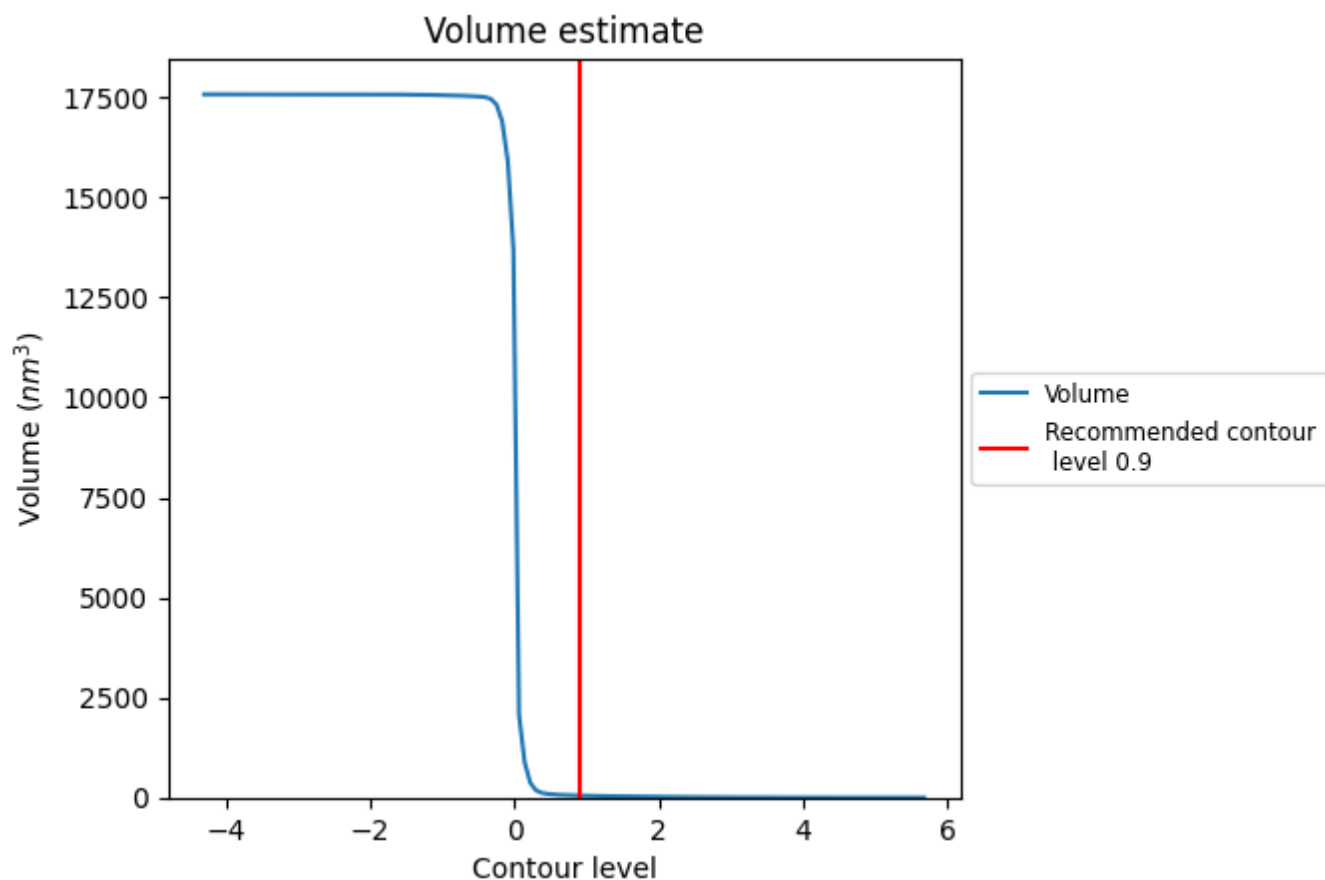
This section contains the results of statistical analysis of the map.

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.

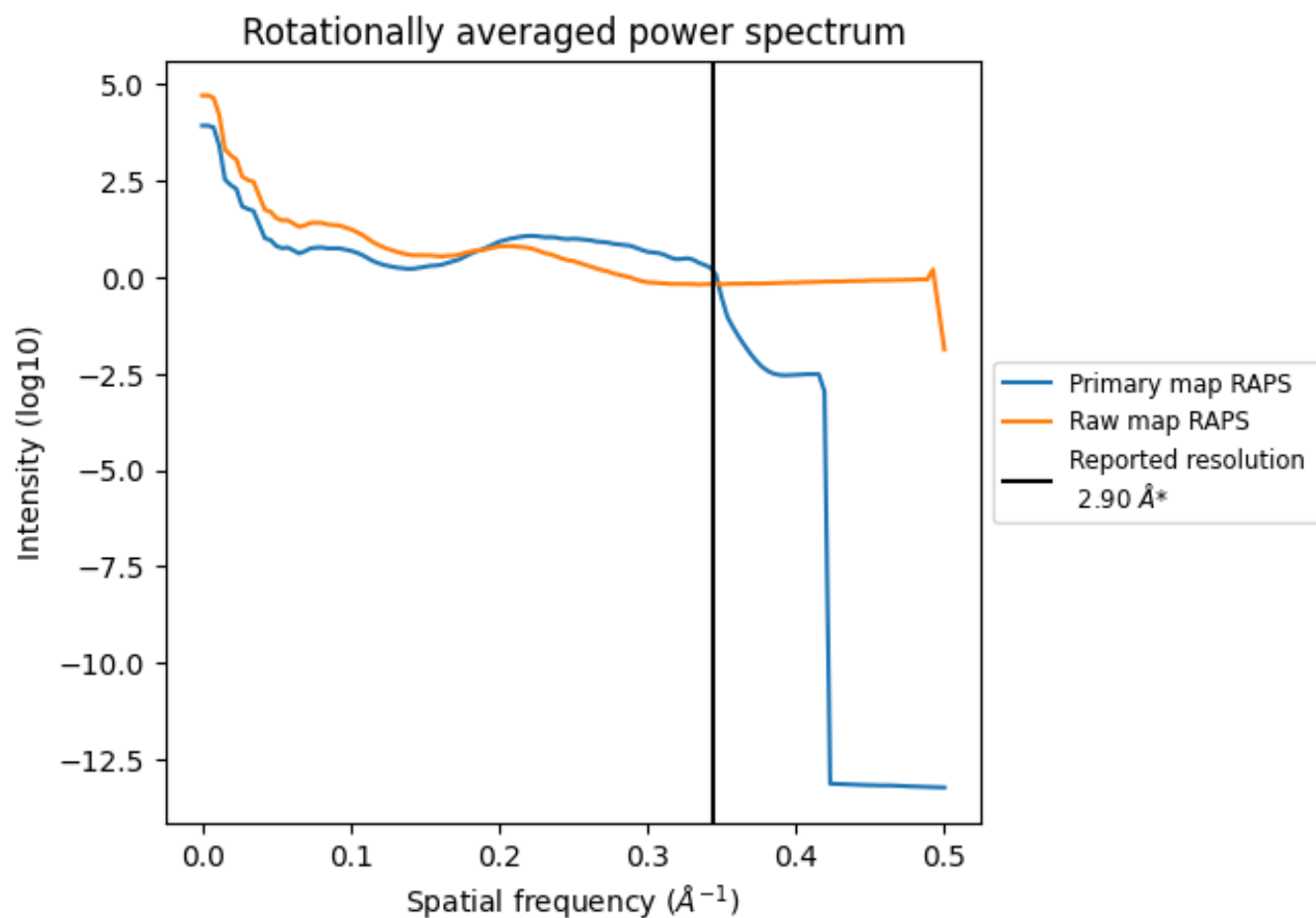
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 50 nm³; this corresponds to an approximate mass of 45 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 ⓘ

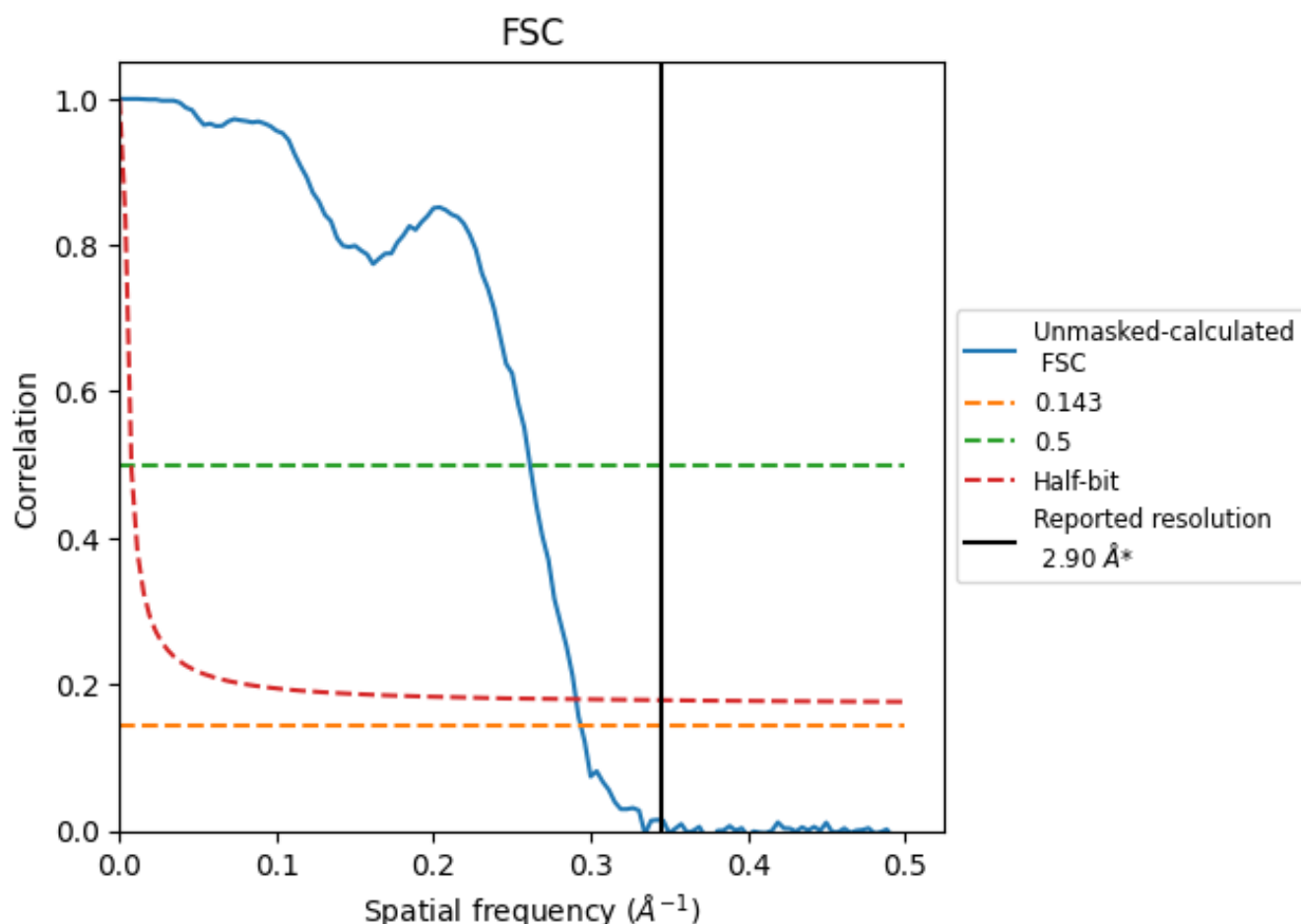


*Reported resolution corresponds to spatial frequency of 0.345 \AA^{-1}

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

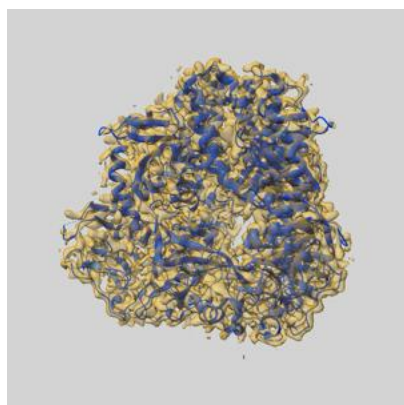
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.40	3.82	3.44

*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 3.40 differs from the reported value 2.9 by more than 10 %

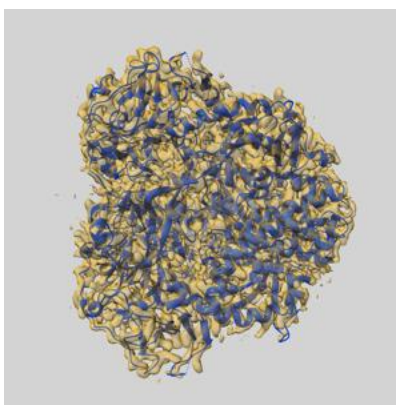
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41636 and PDB model 8TVB. Per-residue inclusion information can be found in section 3 on page 12.

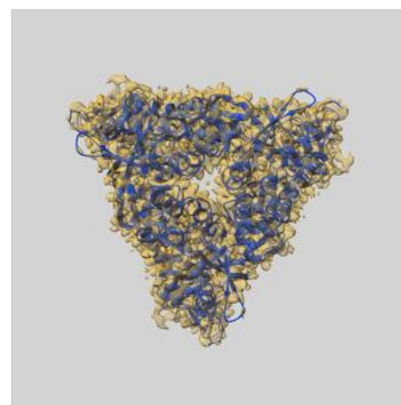
9.1 Map-model overlay [i](#)



X



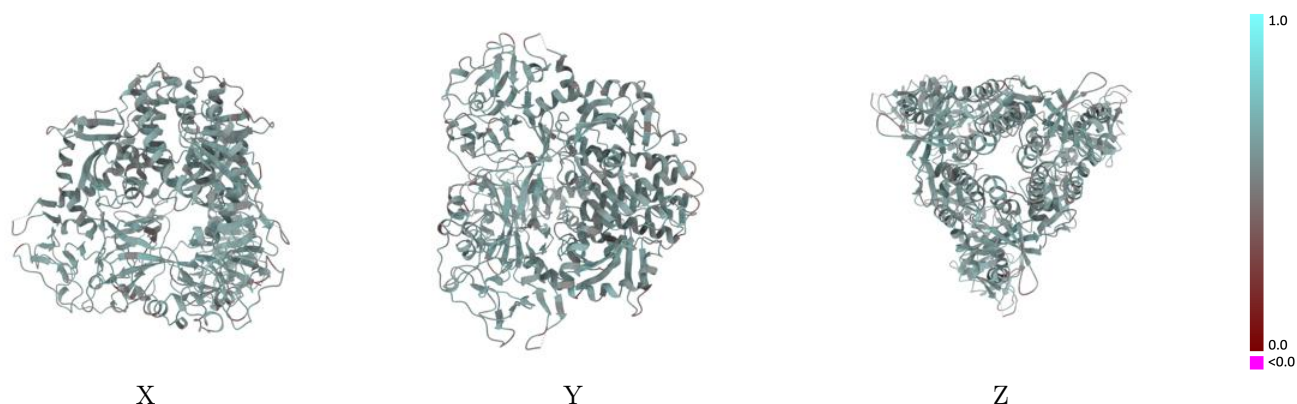
Y



Z

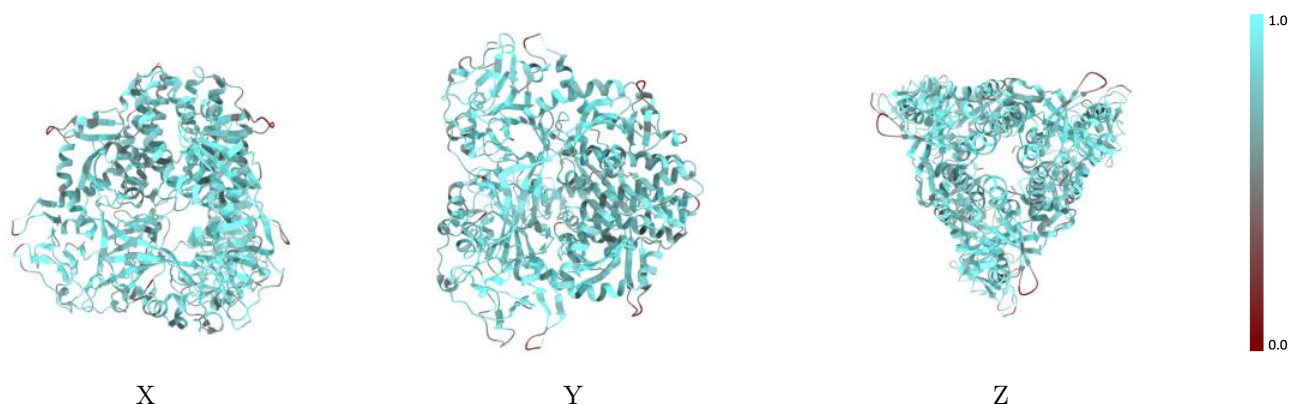
The images above show the 3D surface view of the map at the recommended contour level 0.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



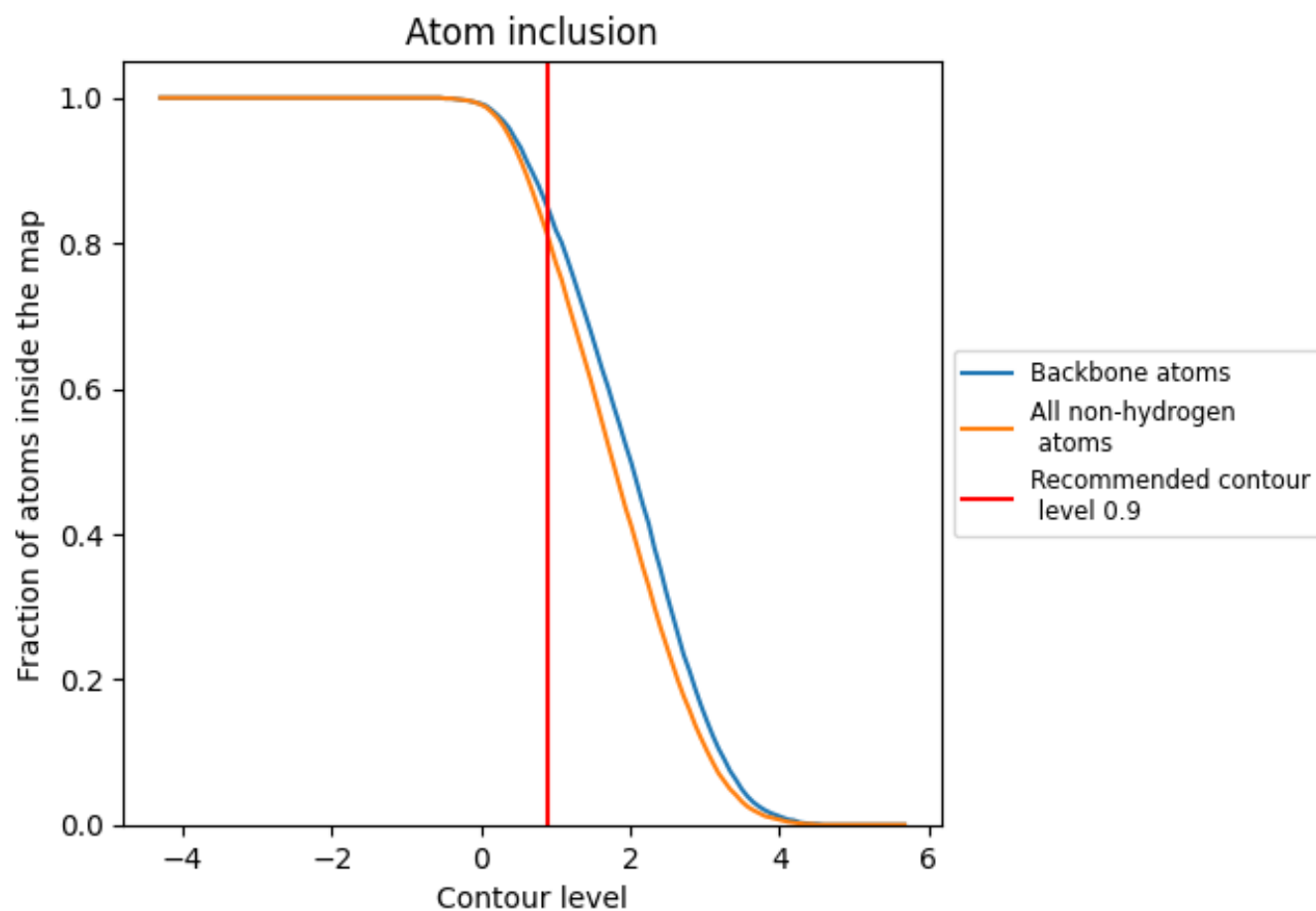
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.9).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% 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 (0.9) 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> 0.5600
A	<div><div></div></div> 0.8110	<div><div></div></div> 0.5640
B	<div><div></div></div> 0.8040	<div><div></div></div> 0.5570
C	<div><div></div></div> 0.8080	<div><div></div></div> 0.5610

