



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 07:23 AM UTC

PDB ID : 8TVH / pdb_00008tvh
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 wwPDB EM Validation Summary 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:

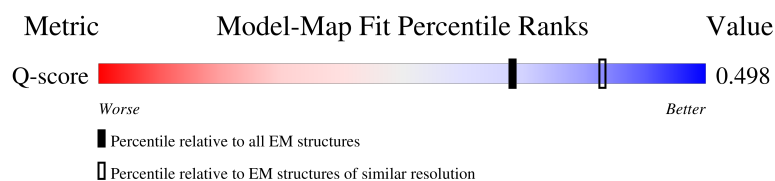
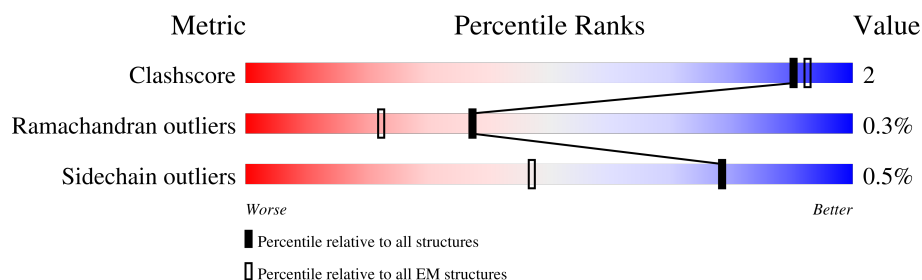
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	7% 91% 9%
1	E	107	7% 91% 9%
1	H	107	8% 91% 9%
2	F	120	9% 98% ..

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Mol	Chain	Length	Quality of chain
2	G	120	9% 96% ..
2	I	120	8% 98% ..
3	A	534	16% 84%
3	B	534	16% 84%
3	C	534	16% 84%

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 (CCD ID: NAG) (formula: C₈H₁₅NO₆).

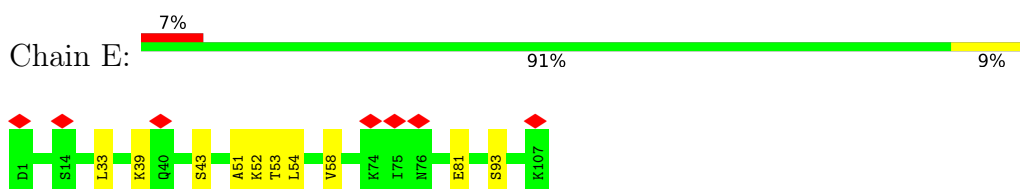


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

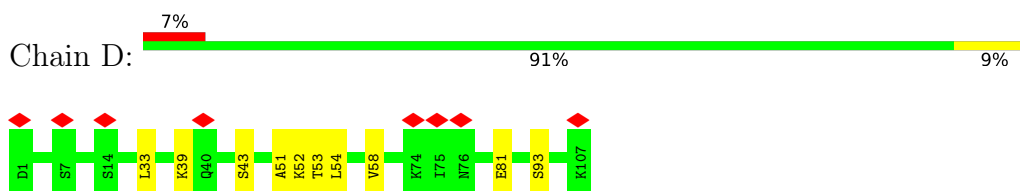
3 Residue-property plots [i](#)

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.

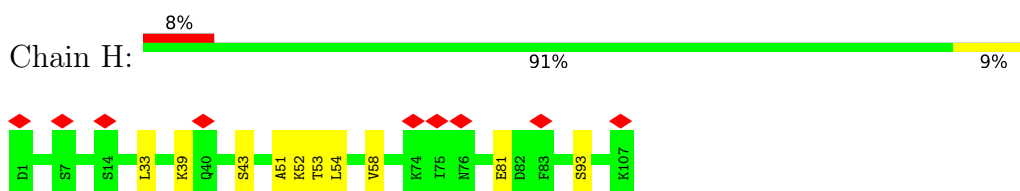
- Molecule 1: 4G5 light chain



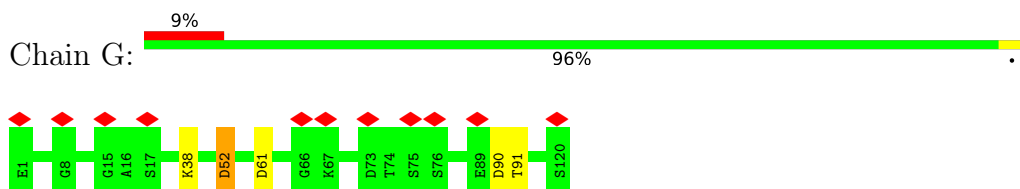
- Molecule 1: 4G5 light chain



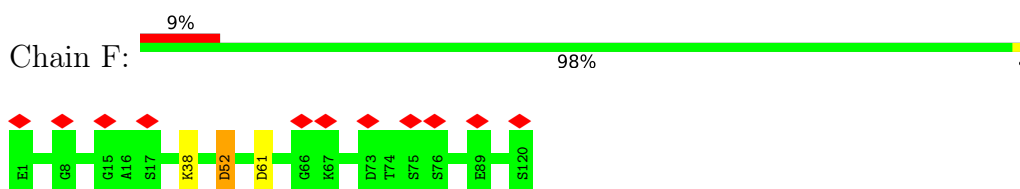
- Molecule 1: 4G5 light chain



- Molecule 2: 4G5 heavy chain



- Molecule 2: 4G5 heavy chain



[illegible][illegible]

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 ($\text{\AA}$)	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 ($\text{\AA}$)	0.98350006, 0.98350006, 0.98350006	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	D	0.71	0/760	1.05	5/1039 (0.5%)
1	E	0.70	0/760	1.05	5/1039 (0.5%)
1	H	0.71	0/760	1.05	5/1039 (0.5%)
2	F	0.67	0/890	1.09	4/1219 (0.3%)
2	G	0.66	0/890	1.09	4/1219 (0.3%)
2	I	0.67	0/890	1.09	4/1219 (0.3%)
3	A	0.68	0/626	0.78	2/848 (0.2%)
3	B	0.68	0/626	0.78	2/848 (0.2%)
3	C	0.68	0/626	0.78	2/848 (0.2%)
All	All	0.68	0/6828	1.00	33/9318 (0.4%)

There are no bond length outliers.

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	I	52	ASP	CA-C-N	7.79	127.51	119.56
2	I	52	ASP	C-N-CA	7.79	127.51	119.56
2	G	52	ASP	CA-C-N	7.76	127.48	119.56
2	G	52	ASP	C-N-CA	7.76	127.48	119.56
2	F	52	ASP	CA-C-N	7.72	127.43	119.56

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	740	0	613	6	0
1	E	740	0	613	6	0
1	H	740	0	613	6	0
2	F	870	0	781	1	0
2	G	870	0	781	2	0
2	I	870	0	781	1	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	22	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.

The worst 5 of 22 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

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	105/107 (98%)	101 (96%)	3 (3%)	1 (1%)	12	45
1	E	105/107 (98%)	101 (96%)	3 (3%)	1 (1%)	12	45
1	H	105/107 (98%)	101 (96%)	3 (3%)	1 (1%)	12	45
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%)	37	65

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
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%)	76 (99%)	1 (1%)	61	72
2	G	77/102 (76%)	76 (99%)	1 (1%)	61	72
2	I	77/102 (76%)	76 (99%)	1 (1%)	61	72
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

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	576/1956 (29%)	573 (100%)	3 (0%)	78	80

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	38	LYS
2	F	38	LYS
2	I	38	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	157	GLN
3	C	148	ASN
3	C	464	ASN
3	C	157	GLN
3	A	148	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

The worst 5 of 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

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.

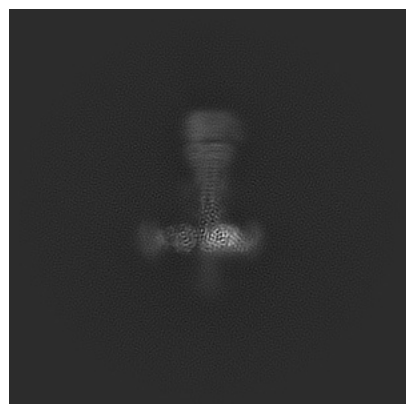
6 Map visualisation [i](#)

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.

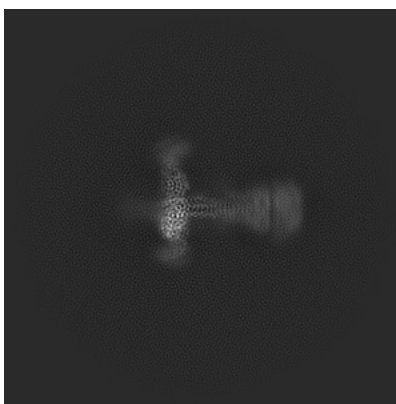
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

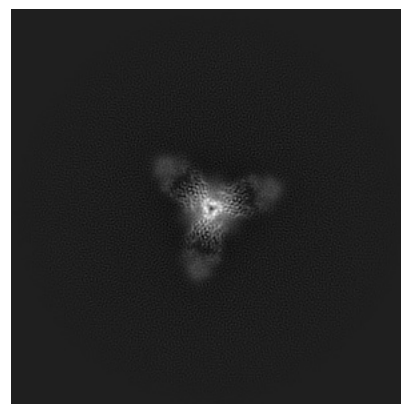
6.1.1 Primary map



X

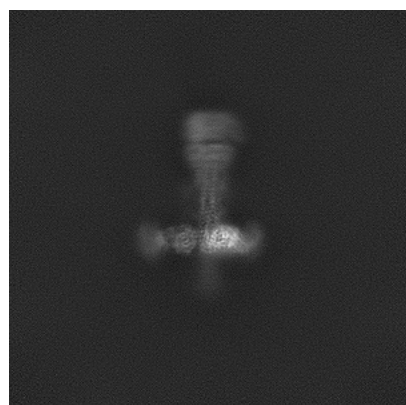


Y

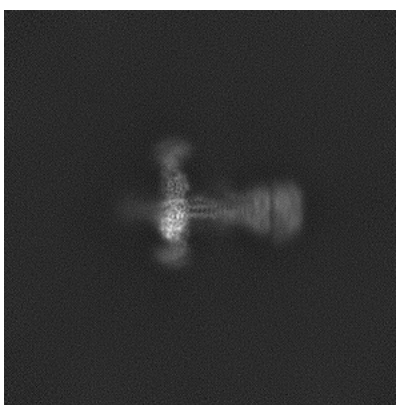


Z

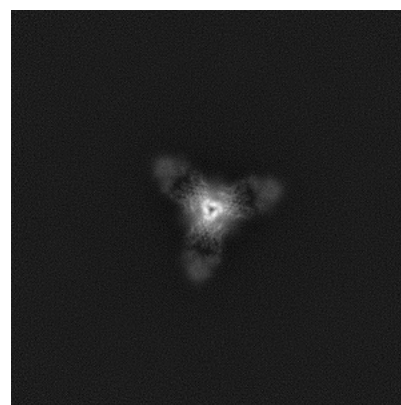
6.1.2 Raw map



X



Y



Z

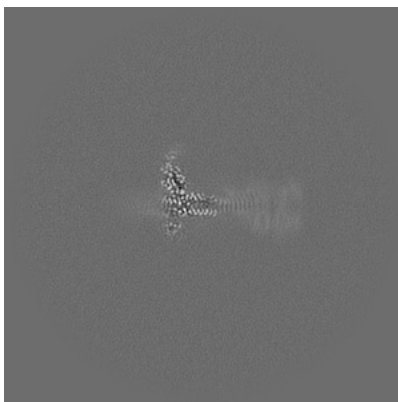
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

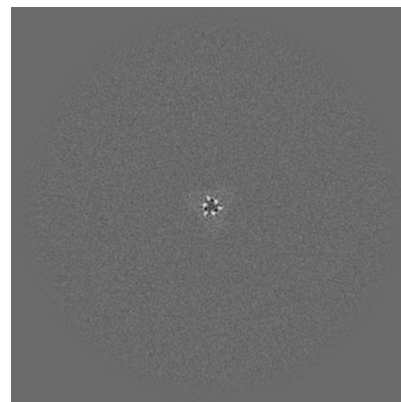
6.2.1 Primary map



X Index: 240



Y Index: 240



Z Index: 240

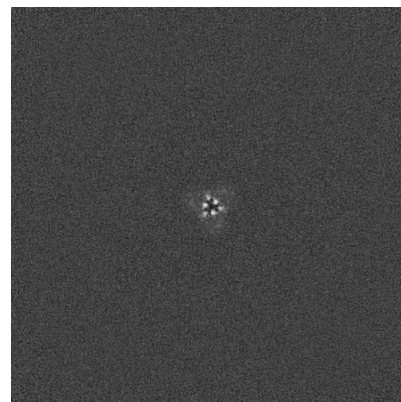
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

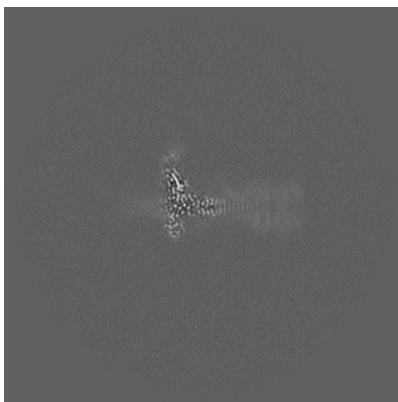
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

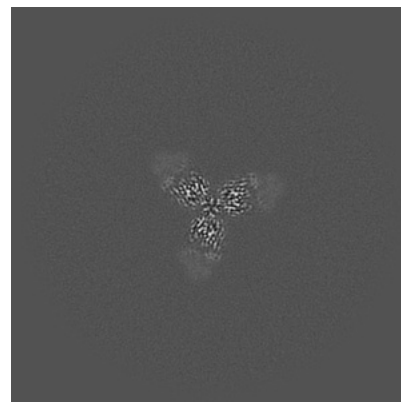
6.3.1 Primary map



X Index: 233



Y Index: 243



Z Index: 207

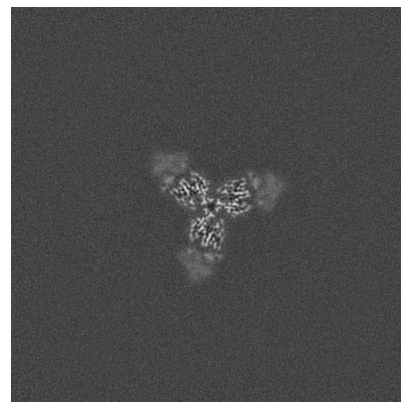
6.3.2 Raw map



X Index: 233



Y Index: 246

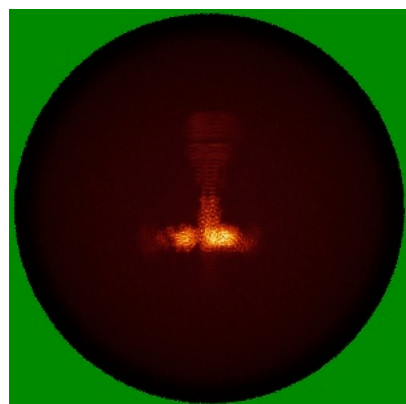


Z Index: 208

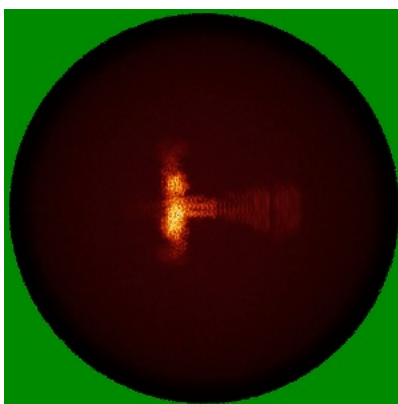
The images above show the largest variance slices of the map in three orthogonal directions.

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

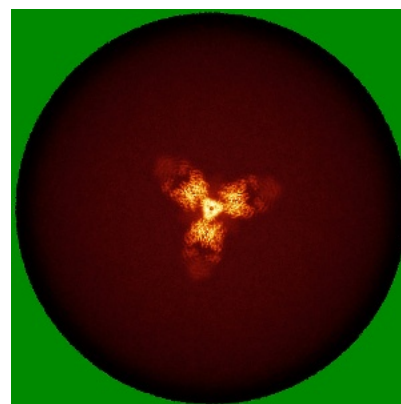
6.4.1 Primary map



X

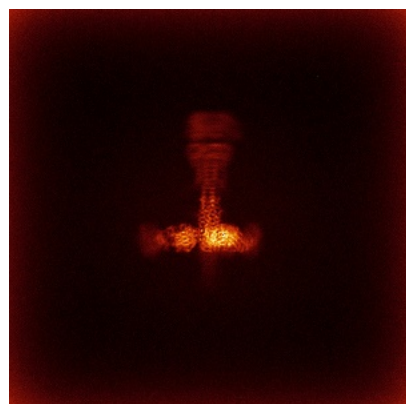


Y

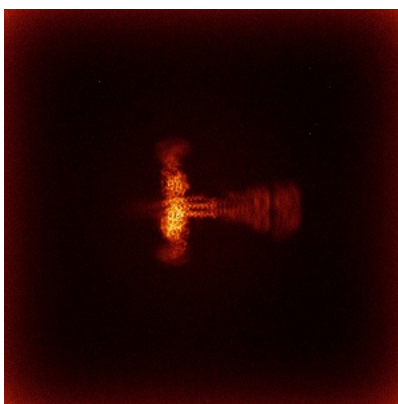


Z

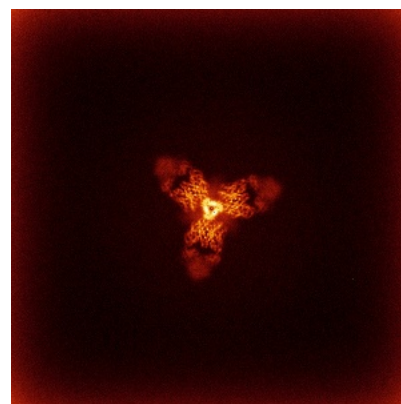
6.4.2 Raw map



X



Y

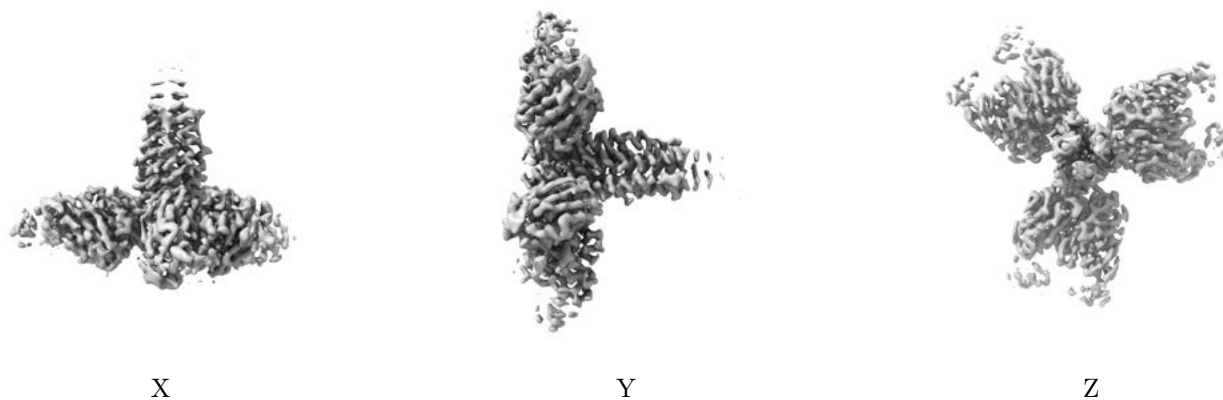


Z

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.

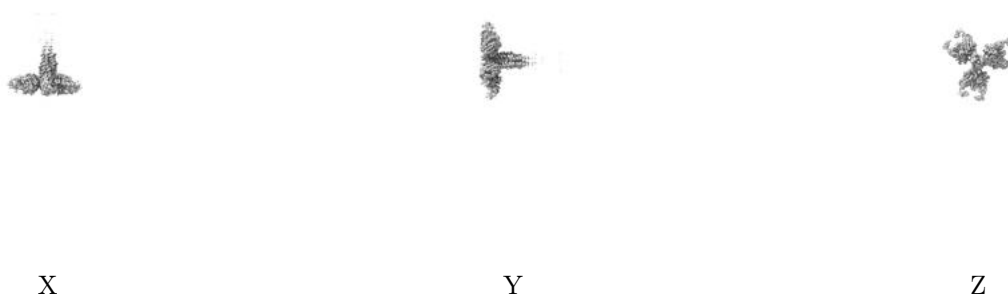
6.5 Orthogonal surface views [i](#)

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.

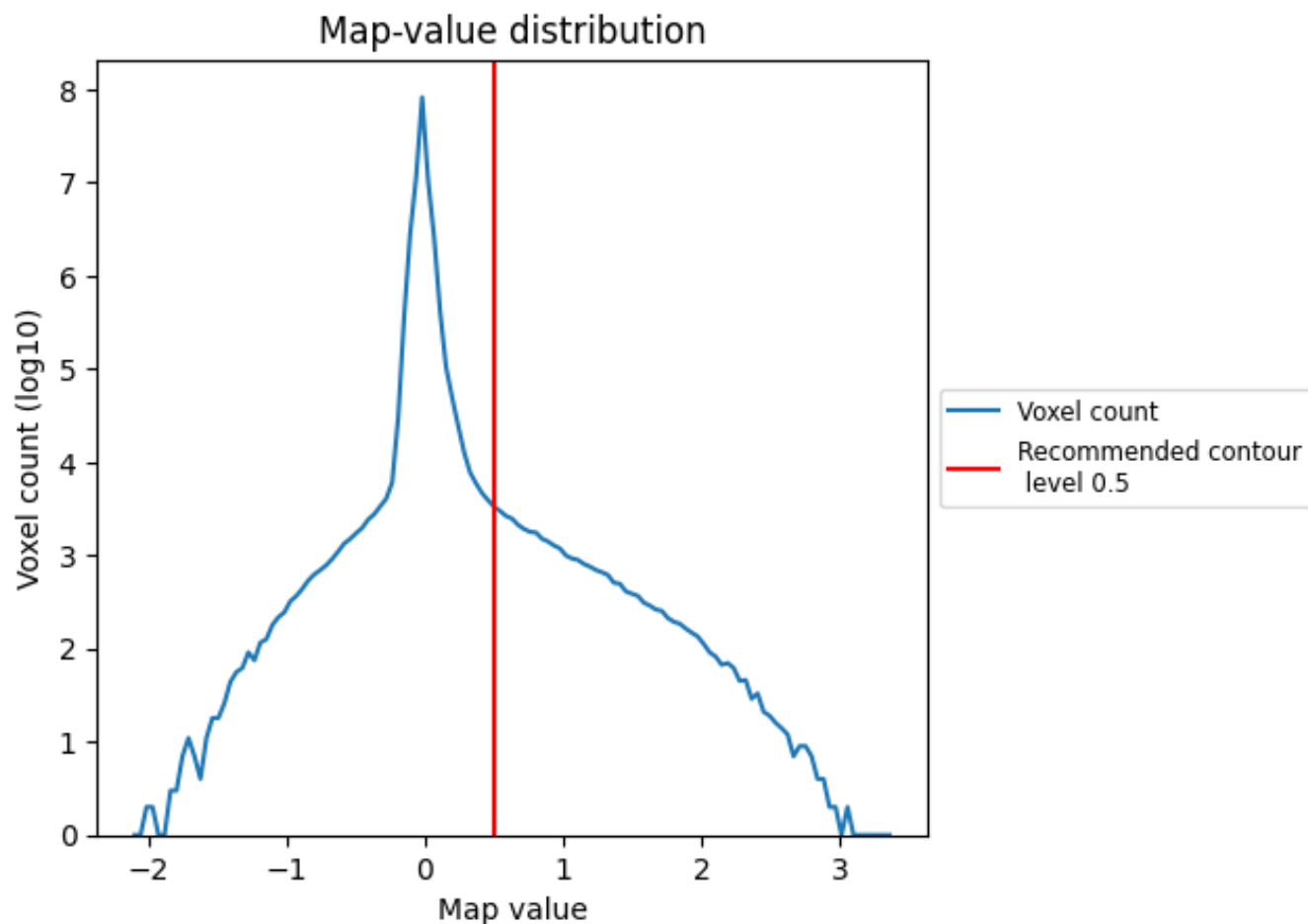
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

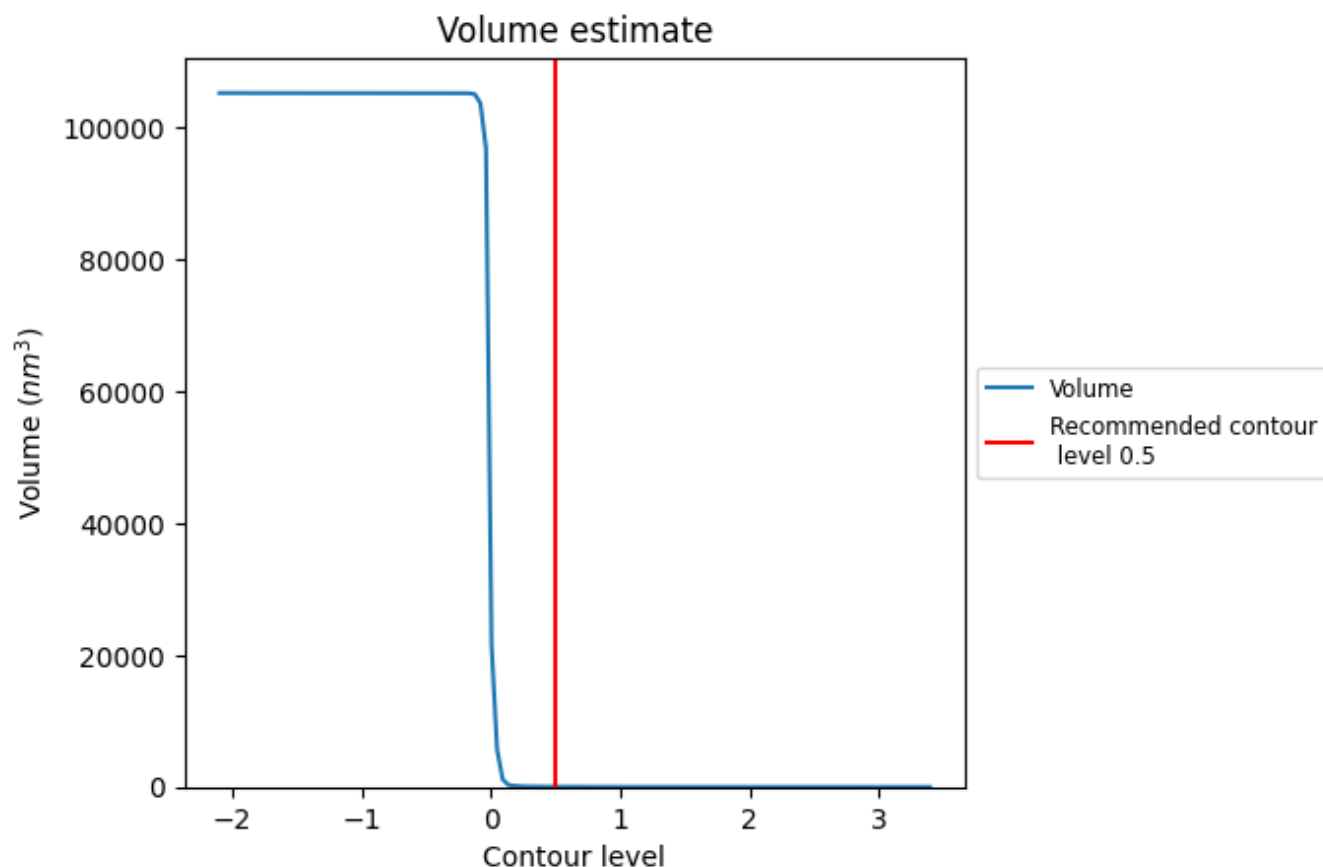
This section contains the results of statistical analysis of the map.

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.

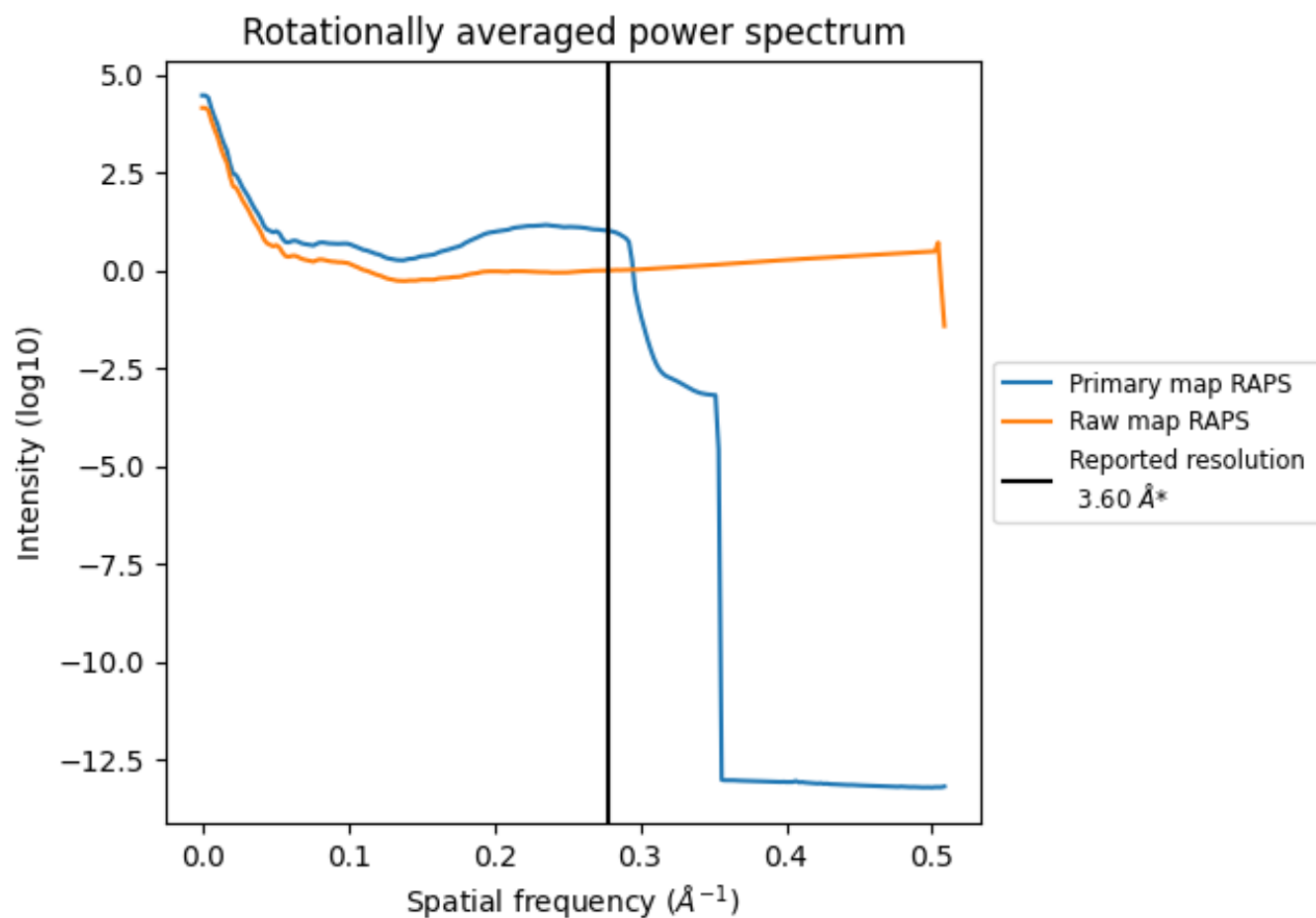
7.2 Volume estimate [i](#)



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 ⓘ

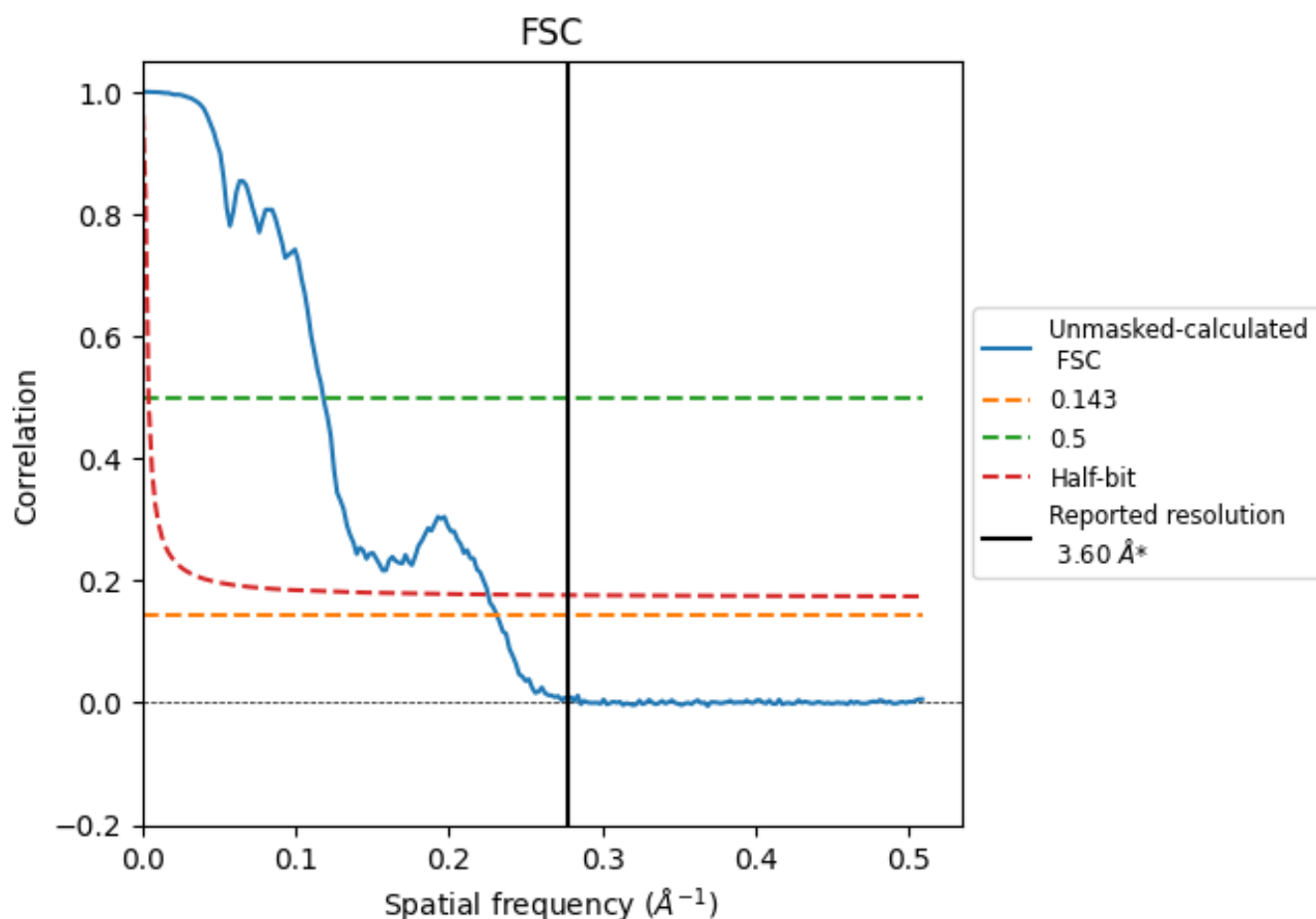


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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

8.2 Resolution estimates [i](#)

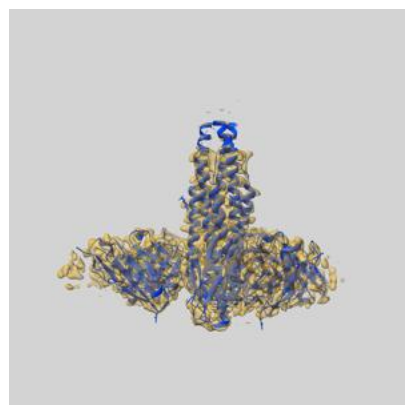
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.33	8.47	4.43

*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 %

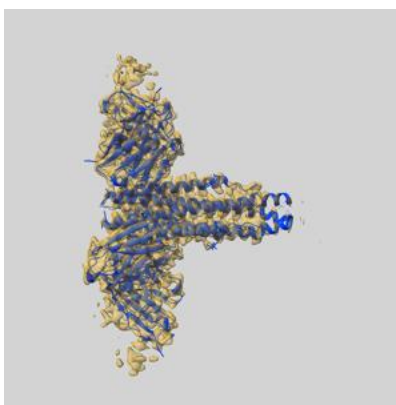
9 Map-model fit [i](#)

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](#).

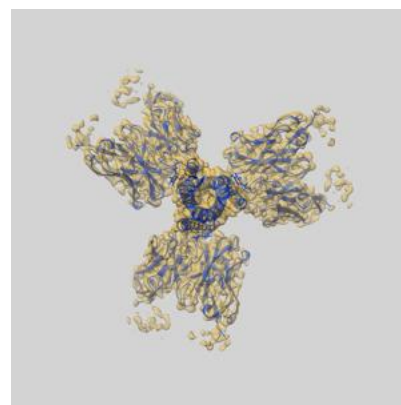
9.1 Map-model overlay [i](#)



X



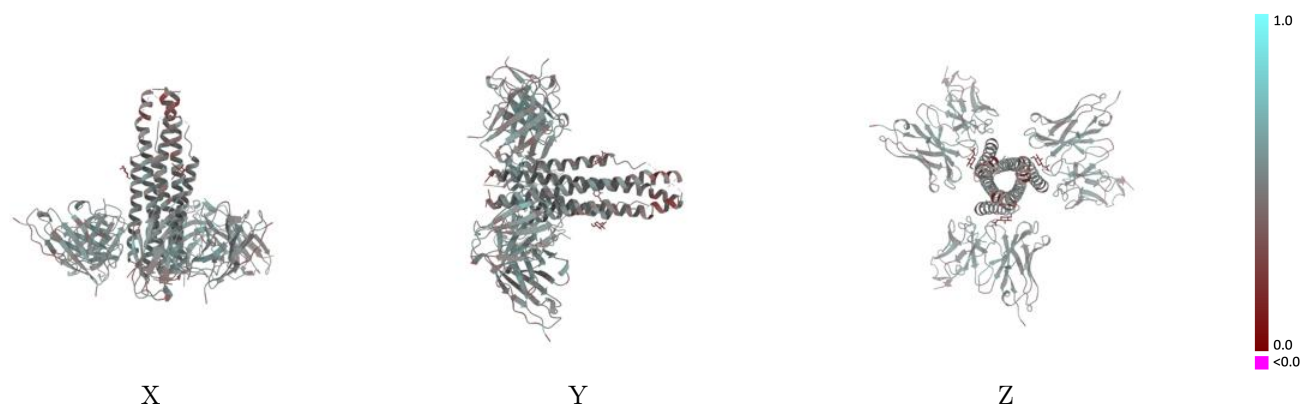
Y



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](#)

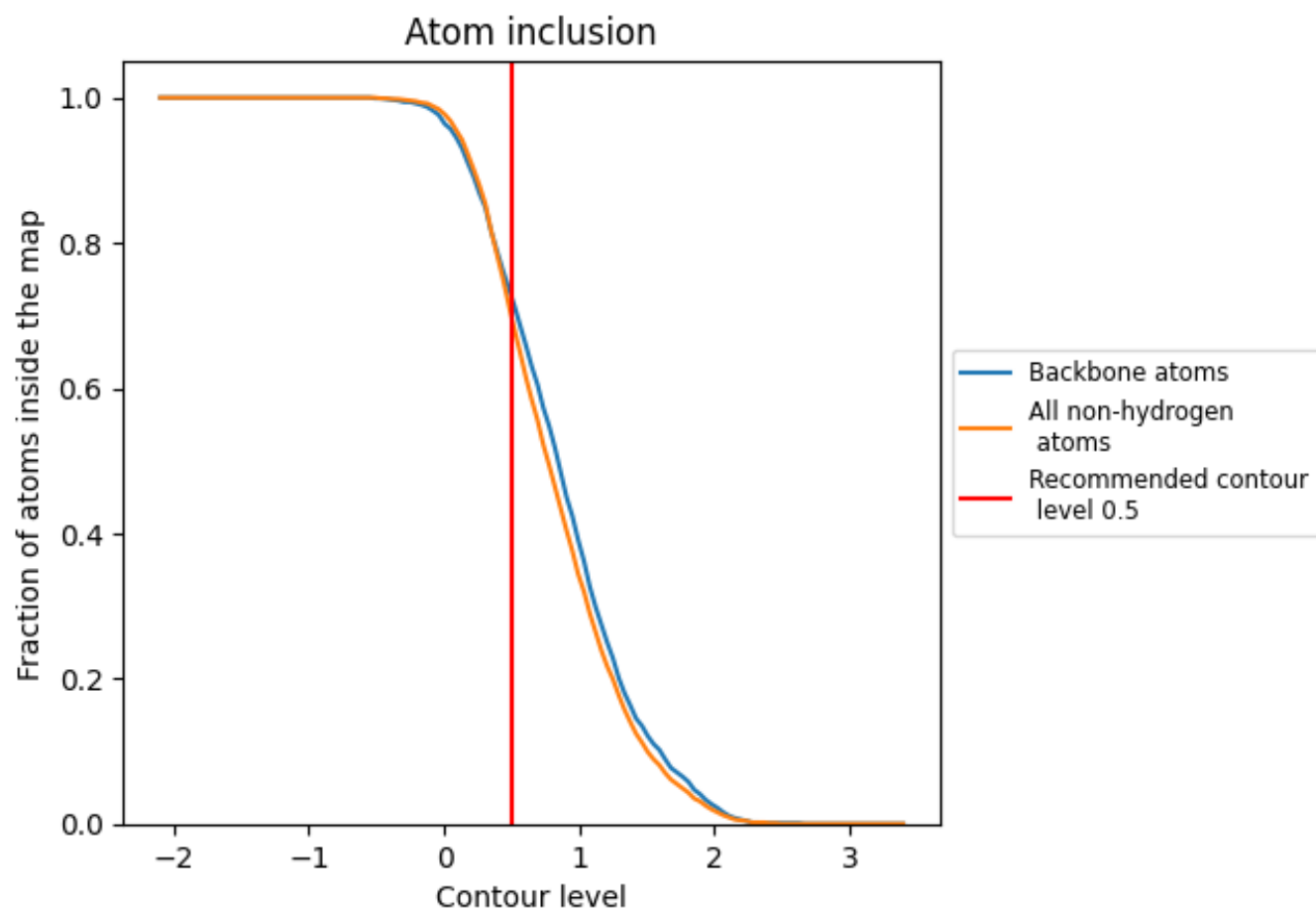


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

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	0.6980	0.4980
A	0.6460	0.4720
B	0.6470	0.4720
C	0.6490	0.4740
D	0.7430	0.5090
E	0.7490	0.5070
F	0.6970	0.5070
G	0.7010	0.5060
H	0.7360	0.5090
I	0.6970	0.5110

