



## wwPDB EM Validation Summary Report ⓘ

Nov 14, 2022 – 02:46 AM EST

PDB ID : 6WXB  
EMDB ID : EMD-21954  
Title : Cryo-EM Structure of Influenza Hemagglutinin (HA) Trimer Vitrified Using Back-it-up  
Authors : Tan, Y.Z.; Rubinstein, J.L.  
Deposited on : 2020-05-10  
Resolution : 2.90 Å(reported)  
Based on initial model : 3WHE

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

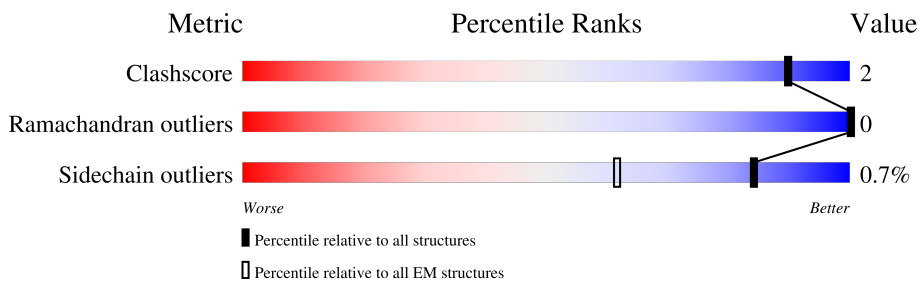
# 1 Overall quality at a glance i

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	562	
1	B	562	
1	C	562	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 22896 atoms, of which 11247 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	485	7499	2379	3683	671	747	19	0	0
1	B	485	7499	2379	3683	671	747	19	0	0
1	C	485	7499	2379	3683	671	747	19	0	0

There are 153 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	512	ASP	-	expression tag	UNP Q91MA7
A	513	GLY	-	expression tag	UNP Q91MA7
A	514	GLY	-	expression tag	UNP Q91MA7
A	515	GLY	-	expression tag	UNP Q91MA7
A	516	GLY	-	expression tag	UNP Q91MA7
A	517	THR	-	expression tag	UNP Q91MA7
A	518	GLY	-	expression tag	UNP Q91MA7
A	519	GLY	-	expression tag	UNP Q91MA7
A	520	GLY	-	expression tag	UNP Q91MA7
A	521	GLY	-	expression tag	UNP Q91MA7
A	522	THR	-	expression tag	UNP Q91MA7
A	523	GLY	-	expression tag	UNP Q91MA7
A	524	ARG	-	expression tag	UNP Q91MA7
A	525	MET	-	expression tag	UNP Q91MA7
A	526	LYS	-	expression tag	UNP Q91MA7
A	527	GLN	-	expression tag	UNP Q91MA7
A	528	ILE	-	expression tag	UNP Q91MA7
A	529	GLU	-	expression tag	UNP Q91MA7
A	530	ASP	-	expression tag	UNP Q91MA7
A	531	LYS	-	expression tag	UNP Q91MA7
A	532	ILE	-	expression tag	UNP Q91MA7
A	533	GLU	-	expression tag	UNP Q91MA7
A	534	GLU	-	expression tag	UNP Q91MA7
A	535	ILE	-	expression tag	UNP Q91MA7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	536	LEU	-	expression tag	UNP Q91MA7
A	537	SER	-	expression tag	UNP Q91MA7
A	538	LYS	-	expression tag	UNP Q91MA7
A	539	ILE	-	expression tag	UNP Q91MA7
A	540	TYR	-	expression tag	UNP Q91MA7
A	541	HIS	-	expression tag	UNP Q91MA7
A	542	ILE	-	expression tag	UNP Q91MA7
A	543	GLU	-	expression tag	UNP Q91MA7
A	544	ASN	-	expression tag	UNP Q91MA7
A	545	GLU	-	expression tag	UNP Q91MA7
A	546	ILE	-	expression tag	UNP Q91MA7
A	547	ALA	-	expression tag	UNP Q91MA7
A	548	ARG	-	expression tag	UNP Q91MA7
A	549	ILE	-	expression tag	UNP Q91MA7
A	550	LYS	-	expression tag	UNP Q91MA7
A	551	LYS	-	expression tag	UNP Q91MA7
A	552	LEU	-	expression tag	UNP Q91MA7
A	553	ILE	-	expression tag	UNP Q91MA7
A	554	GLY	-	expression tag	UNP Q91MA7
A	555	GLU	-	expression tag	UNP Q91MA7
A	556	ARG	-	expression tag	UNP Q91MA7
A	557	HIS	-	expression tag	UNP Q91MA7
A	558	HIS	-	expression tag	UNP Q91MA7
A	559	HIS	-	expression tag	UNP Q91MA7
A	560	HIS	-	expression tag	UNP Q91MA7
A	561	HIS	-	expression tag	UNP Q91MA7
A	562	HIS	-	expression tag	UNP Q91MA7
B	512	ASP	-	expression tag	UNP Q91MA7
B	513	GLY	-	expression tag	UNP Q91MA7
B	514	GLY	-	expression tag	UNP Q91MA7
B	515	GLY	-	expression tag	UNP Q91MA7
B	516	GLY	-	expression tag	UNP Q91MA7
B	517	THR	-	expression tag	UNP Q91MA7
B	518	GLY	-	expression tag	UNP Q91MA7
B	519	GLY	-	expression tag	UNP Q91MA7
B	520	GLY	-	expression tag	UNP Q91MA7
B	521	GLY	-	expression tag	UNP Q91MA7
B	522	THR	-	expression tag	UNP Q91MA7
B	523	GLY	-	expression tag	UNP Q91MA7
B	524	ARG	-	expression tag	UNP Q91MA7
B	525	MET	-	expression tag	UNP Q91MA7
B	526	LYS	-	expression tag	UNP Q91MA7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	527	GLN	-	expression tag	UNP Q91MA7
B	528	ILE	-	expression tag	UNP Q91MA7
B	529	GLU	-	expression tag	UNP Q91MA7
B	530	ASP	-	expression tag	UNP Q91MA7
B	531	LYS	-	expression tag	UNP Q91MA7
B	532	ILE	-	expression tag	UNP Q91MA7
B	533	GLU	-	expression tag	UNP Q91MA7
B	534	GLU	-	expression tag	UNP Q91MA7
B	535	ILE	-	expression tag	UNP Q91MA7
B	536	LEU	-	expression tag	UNP Q91MA7
B	537	SER	-	expression tag	UNP Q91MA7
B	538	LYS	-	expression tag	UNP Q91MA7
B	539	ILE	-	expression tag	UNP Q91MA7
B	540	TYR	-	expression tag	UNP Q91MA7
B	541	HIS	-	expression tag	UNP Q91MA7
B	542	ILE	-	expression tag	UNP Q91MA7
B	543	GLU	-	expression tag	UNP Q91MA7
B	544	ASN	-	expression tag	UNP Q91MA7
B	545	GLU	-	expression tag	UNP Q91MA7
B	546	ILE	-	expression tag	UNP Q91MA7
B	547	ALA	-	expression tag	UNP Q91MA7
B	548	ARG	-	expression tag	UNP Q91MA7
B	549	ILE	-	expression tag	UNP Q91MA7
B	550	LYS	-	expression tag	UNP Q91MA7
B	551	LYS	-	expression tag	UNP Q91MA7
B	552	LEU	-	expression tag	UNP Q91MA7
B	553	ILE	-	expression tag	UNP Q91MA7
B	554	GLY	-	expression tag	UNP Q91MA7
B	555	GLU	-	expression tag	UNP Q91MA7
B	556	ARG	-	expression tag	UNP Q91MA7
B	557	HIS	-	expression tag	UNP Q91MA7
B	558	HIS	-	expression tag	UNP Q91MA7
B	559	HIS	-	expression tag	UNP Q91MA7
B	560	HIS	-	expression tag	UNP Q91MA7
B	561	HIS	-	expression tag	UNP Q91MA7
B	562	HIS	-	expression tag	UNP Q91MA7
C	512	ASP	-	expression tag	UNP Q91MA7
C	513	GLY	-	expression tag	UNP Q91MA7
C	514	GLY	-	expression tag	UNP Q91MA7
C	515	GLY	-	expression tag	UNP Q91MA7
C	516	GLY	-	expression tag	UNP Q91MA7
C	517	THR	-	expression tag	UNP Q91MA7

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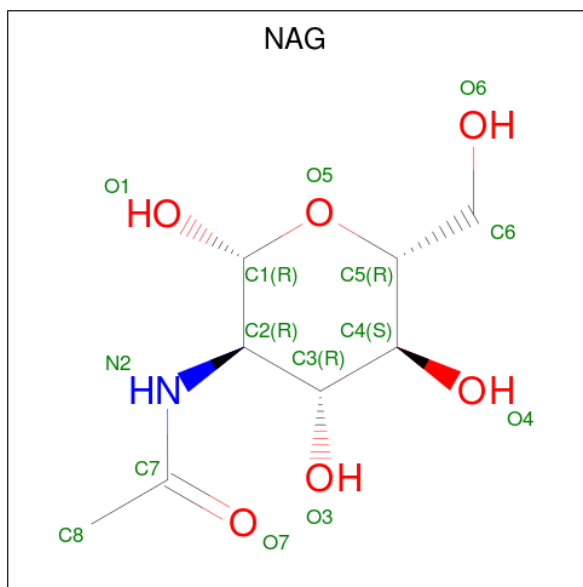
Chain	Residue	Modelled	Actual	Comment	Reference
C	518	GLY	-	expression tag	UNP Q91MA7
C	519	GLY	-	expression tag	UNP Q91MA7
C	520	GLY	-	expression tag	UNP Q91MA7
C	521	GLY	-	expression tag	UNP Q91MA7
C	522	THR	-	expression tag	UNP Q91MA7
C	523	GLY	-	expression tag	UNP Q91MA7
C	524	ARG	-	expression tag	UNP Q91MA7
C	525	MET	-	expression tag	UNP Q91MA7
C	526	LYS	-	expression tag	UNP Q91MA7
C	527	GLN	-	expression tag	UNP Q91MA7
C	528	ILE	-	expression tag	UNP Q91MA7
C	529	GLU	-	expression tag	UNP Q91MA7
C	530	ASP	-	expression tag	UNP Q91MA7
C	531	LYS	-	expression tag	UNP Q91MA7
C	532	ILE	-	expression tag	UNP Q91MA7
C	533	GLU	-	expression tag	UNP Q91MA7
C	534	GLU	-	expression tag	UNP Q91MA7
C	535	ILE	-	expression tag	UNP Q91MA7
C	536	LEU	-	expression tag	UNP Q91MA7
C	537	SER	-	expression tag	UNP Q91MA7
C	538	LYS	-	expression tag	UNP Q91MA7
C	539	ILE	-	expression tag	UNP Q91MA7
C	540	TYR	-	expression tag	UNP Q91MA7
C	541	HIS	-	expression tag	UNP Q91MA7
C	542	ILE	-	expression tag	UNP Q91MA7
C	543	GLU	-	expression tag	UNP Q91MA7
C	544	ASN	-	expression tag	UNP Q91MA7
C	545	GLU	-	expression tag	UNP Q91MA7
C	546	ILE	-	expression tag	UNP Q91MA7
C	547	ALA	-	expression tag	UNP Q91MA7
C	548	ARG	-	expression tag	UNP Q91MA7
C	549	ILE	-	expression tag	UNP Q91MA7
C	550	LYS	-	expression tag	UNP Q91MA7
C	551	LYS	-	expression tag	UNP Q91MA7
C	552	LEU	-	expression tag	UNP Q91MA7
C	553	ILE	-	expression tag	UNP Q91MA7
C	554	GLY	-	expression tag	UNP Q91MA7
C	555	GLU	-	expression tag	UNP Q91MA7
C	556	ARG	-	expression tag	UNP Q91MA7
C	557	HIS	-	expression tag	UNP Q91MA7
C	558	HIS	-	expression tag	UNP Q91MA7
C	559	HIS	-	expression tag	UNP Q91MA7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	560	HIS	-	expression tag	UNP Q91MA7
C	561	HIS	-	expression tag	UNP Q91MA7
C	562	HIS	-	expression tag	UNP Q91MA7

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



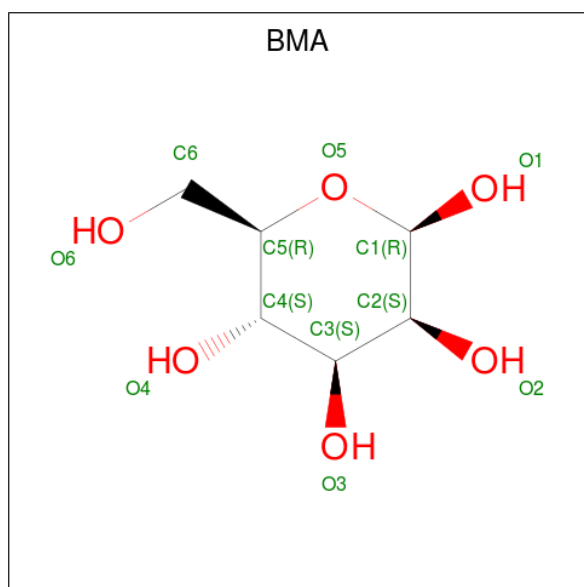
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	H	N		O
2	A	1	Total	C	H	N	O	0
			112	32	56	4	20	
2	A	1	Total	C	H	N	O	0
			112	32	56	4	20	
2	A	1	Total	C	H	N	O	0
			112	32	56	4	20	
2	A	1	Total	C	H	N	O	0
			112	32	56	4	20	
2	B	1	Total	C	H	N	O	0
			112	32	56	4	20	
2	B	1	Total	C	H	N	O	0
			112	32	56	4	20	
2	B	1	Total	C	H	N	O	0
			112	32	56	4	20	
2	B	1	Total	C	H	N	O	0
			112	32	56	4	20	
2	C	1	Total	C	H	N	O	0
			112	32	56	4	20	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
2	C	1	Total	C	H	N	O	0
			112	32	56	4	20	
2	C	1	Total	C	H	N	O	0
			112	32	56	4	20	
2	C	1	Total	C	H	N	O	0
			112	32	56	4	20	

- Molecule 3 is beta-D-mannopyranose (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



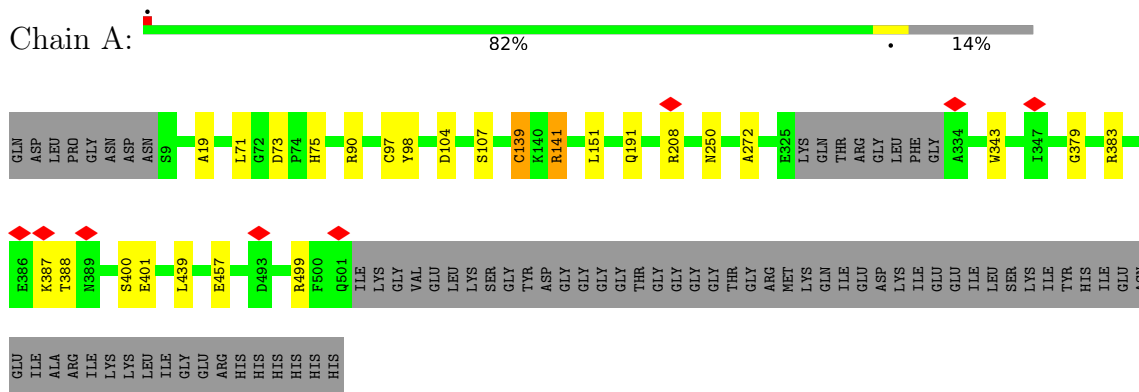
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
3	A	1	Total	C	H	O	0
			21	6	10	5	
3	B	1	Total	C	H	O	0
			21	6	10	5	
3	C	1	Total	C	H	O	0
			21	6	10	5	



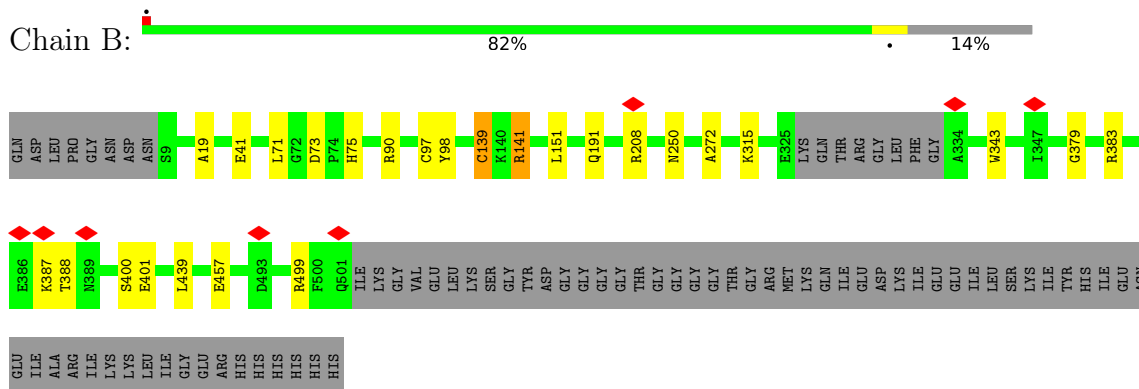
### 3 Residue-property plots [i](#)

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.

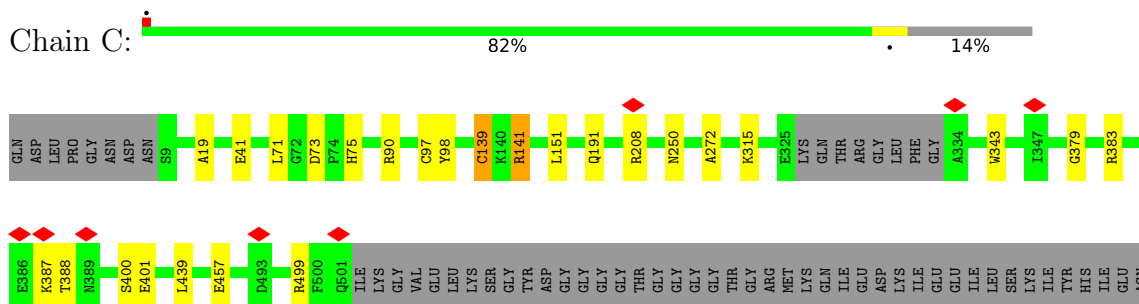
- Molecule 1: Hemagglutinin



- Molecule 1: Hemagglutinin



- Molecule 1: Hemagglutinin



GLU  
ILE  
ALA  
ARG  
ILE  
LYS  
LYS  
LEU  
ILE  
GLY  
GLU  
ARG  
HIS  
HIS  
HIS  
HIS  
HIS

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	128305	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 ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	11.195	Depositor
Minimum map value	-7.251	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.298	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	263.68, 263.68, 263.68	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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, BMA

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	0.33	0/3895	0.56	1/5283 (0.0%)
1	B	0.33	0/3895	0.56	1/5283 (0.0%)
1	C	0.33	0/3895	0.56	1/5283 (0.0%)
All	All	0.33	0/11685	0.56	3/15849 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	439	LEU	CA-CB-CG	5.18	127.22	115.30
1	C	439	LEU	CA-CB-CG	5.18	127.21	115.30
1	B	439	LEU	CA-CB-CG	5.17	127.19	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	B	141	ARG	Peptide
1	C	141	ARG	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3816	3683	3684	13	0
1	B	3816	3683	3684	13	0
1	C	3816	3683	3684	13	0
2	A	56	56	52	1	0
2	B	56	56	52	1	0
2	C	56	56	52	1	0
3	A	11	10	10	0	0
3	B	11	10	10	0	0
3	C	11	10	10	0	0
All	All	11649	11247	11238	39	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 39 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ASP:OD2	1:B:75:HIS:NE2	2.31	0.64
1:C:73:ASP:OD2	1:C:75:HIS:NE2	2.31	0.64
1:A:73:ASP:OD2	1:A:75:HIS:NE2	2.31	0.63
1:B:401:GLU:OE2	1:C:208:ARG:NH1	2.37	0.58
1:A:401:GLU:OE2	1:B:208:ARG:NH1	2.37	0.57

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	A	481/562 (86%)	454 (94%)	27 (6%)	0	100	100
1	B	481/562 (86%)	454 (94%)	27 (6%)	0	100	100
1	C	481/562 (86%)	454 (94%)	27 (6%)	0	100	100
All	All	1443/1686 (86%)	1362 (94%)	81 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	424/485 (87%)	421 (99%)	3 (1%)	84	95
1	B	424/485 (87%)	421 (99%)	3 (1%)	84	95
1	C	424/485 (87%)	421 (99%)	3 (1%)	84	95
All	All	1272/1455 (87%)	1263 (99%)	9 (1%)	84	95

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	141	ARG
1	C	400	SER
1	B	139	CYS
1	B	141	ARG
1	B	400	SER

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

15 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	A	603	1	14,14,15	1.67	1 (7%)	17,19,21	2.65	1 (5%)
2	NAG	B	601	1	14,14,15	0.28	0	17,19,21	0.37	0
2	NAG	C	603	1	14,14,15	0.28	0	17,19,21	0.37	0
2	NAG	B	602	1	14,14,15	1.49	1 (7%)	17,19,21	1.01	1 (5%)
2	NAG	B	603	1	14,14,15	1.67	1 (7%)	17,19,21	2.66	1 (5%)
2	NAG	A	604	-	14,14,15	1.39	2 (14%)	17,19,21	0.97	1 (5%)
2	NAG	C	601	-	14,14,15	1.39	2 (14%)	17,19,21	0.97	1 (5%)
3	BMA	C	602	-	11,11,12	1.33	1 (9%)	15,15,17	1.20	1 (6%)
2	NAG	C	605	1	14,14,15	1.67	2 (14%)	17,19,21	2.66	1 (5%)
3	BMA	B	605	-	11,11,12	1.33	1 (9%)	15,15,17	1.20	1 (6%)
3	BMA	A	605	-	11,11,12	1.33	1 (9%)	15,15,17	1.20	1 (6%)
2	NAG	C	604	1	14,14,15	1.51	1 (7%)	17,19,21	1.01	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	A	601	1	14,14,15	0.28	0	17,19,21	0.37	0
2	NAG	B	604	-	14,14,15	1.39	2 (14%)	17,19,21	0.97	1 (5%)
2	NAG	A	602	1	14,14,15	1.50	1 (7%)	17,19,21	1.00	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
2	NAG	A	603	1	-	2/6/23/26	0/1/1/1
2	NAG	B	601	1	-	2/6/23/26	0/1/1/1
2	NAG	C	603	1	-	2/6/23/26	0/1/1/1
2	NAG	B	602	1	-	2/6/23/26	0/1/1/1
2	NAG	B	603	1	-	2/6/23/26	0/1/1/1
2	NAG	A	604	-	-	2/6/23/26	0/1/1/1
2	NAG	C	601	-	-	2/6/23/26	0/1/1/1
3	BMA	C	602	-	-	0/2/19/22	0/1/1/1
2	NAG	C	605	1	-	2/6/23/26	0/1/1/1
3	BMA	B	605	-	-	0/2/19/22	0/1/1/1
3	BMA	A	605	-	-	0/2/19/22	0/1/1/1
2	NAG	C	604	1	-	2/6/23/26	0/1/1/1
2	NAG	A	601	1	-	2/6/23/26	0/1/1/1
2	NAG	B	604	-	-	2/6/23/26	0/1/1/1
2	NAG	A	602	1	-	2/6/23/26	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	603	NAG	O5-C1	5.86	1.53	1.43
2	B	603	NAG	O5-C1	5.85	1.53	1.43
2	C	605	NAG	O5-C1	5.84	1.53	1.43
2	C	604	NAG	O5-C1	-5.40	1.35	1.43
2	A	602	NAG	O5-C1	-5.39	1.35	1.43

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	603	NAG	C1-O5-C5	10.41	126.29	112.19

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	605	NAG	C1-O5-C5	10.39	126.27	112.19
2	A	603	NAG	C1-O5-C5	10.38	126.25	112.19
2	C	604	NAG	C3-C4-C5	3.38	116.28	110.24
2	B	602	NAG	C3-C4-C5	3.37	116.26	110.24

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	604	NAG	C1-C2-N2-C7
2	B	604	NAG	C1-C2-N2-C7
2	C	601	NAG	C1-C2-N2-C7
2	A	602	NAG	O5-C5-C6-O6
2	B	602	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	604	NAG	1	0
2	C	601	NAG	1	0
2	B	604	NAG	1	0

## 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.

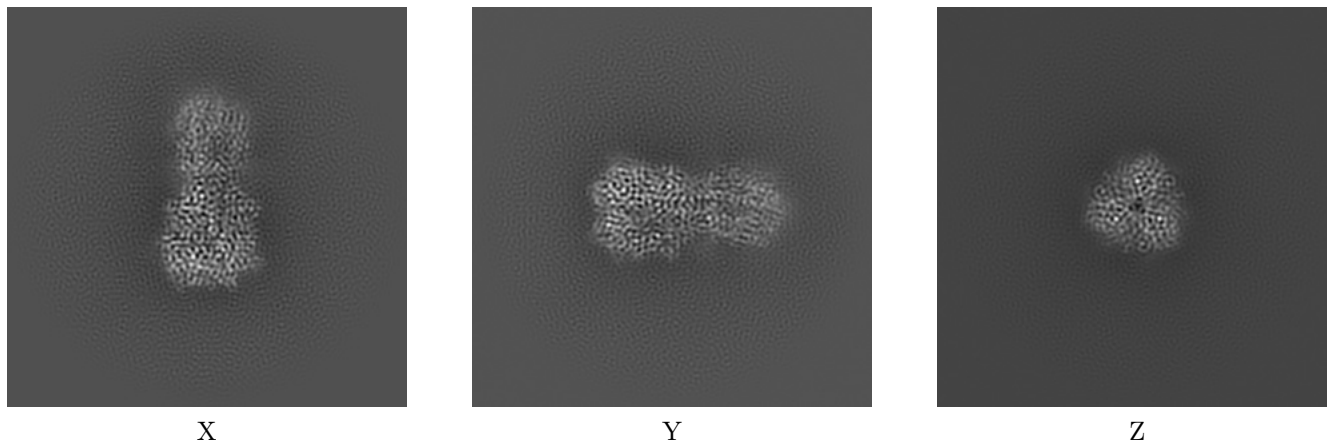
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21954. These allow visual inspection of the internal detail of the map and identification of artifacts.

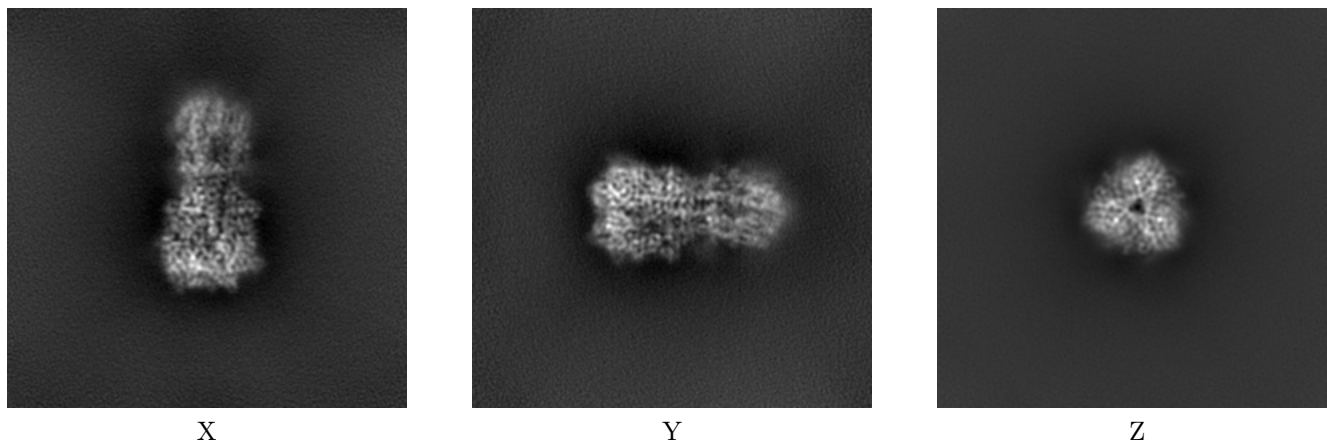
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



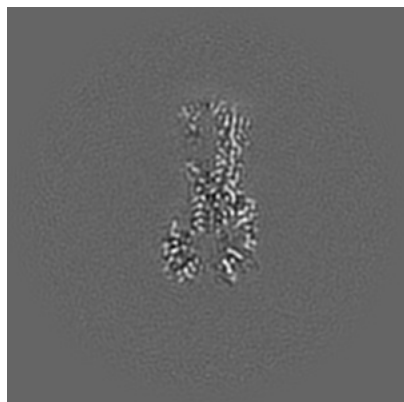
#### 6.1.2 Raw map



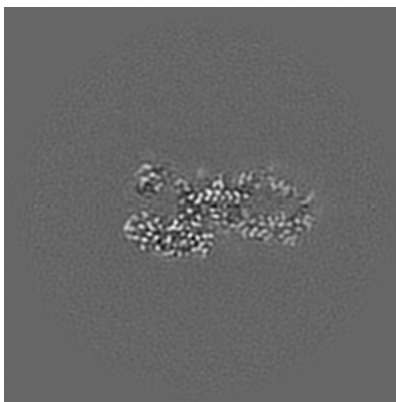
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

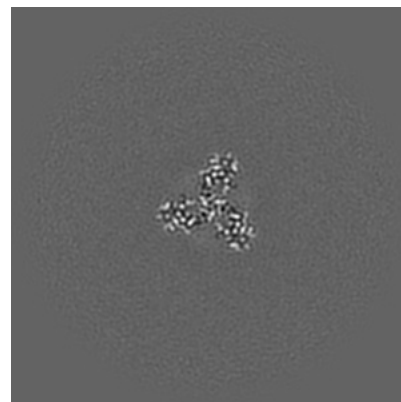
### 6.2.1 Primary map



X Index: 128

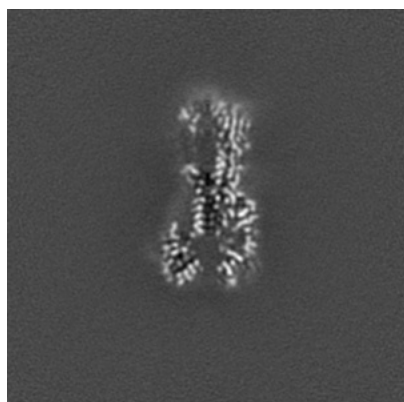


Y Index: 128

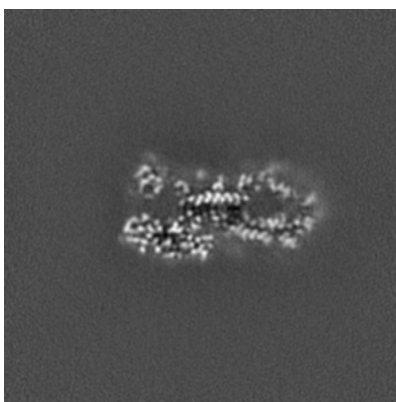


Z Index: 128

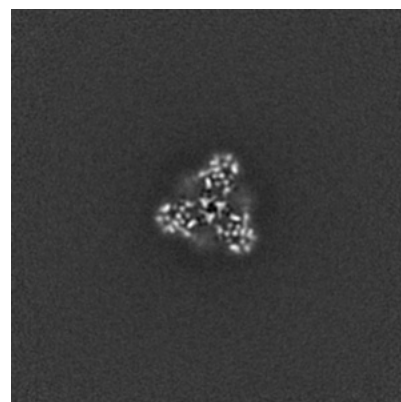
### 6.2.2 Raw map



X Index: 128



Y Index: 128

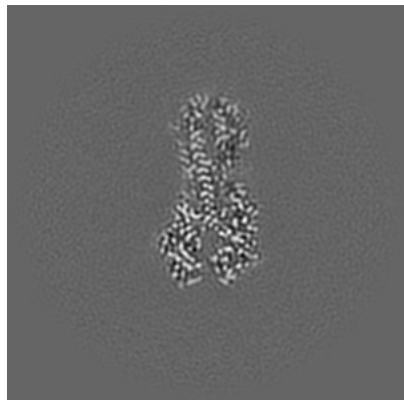


Z Index: 128

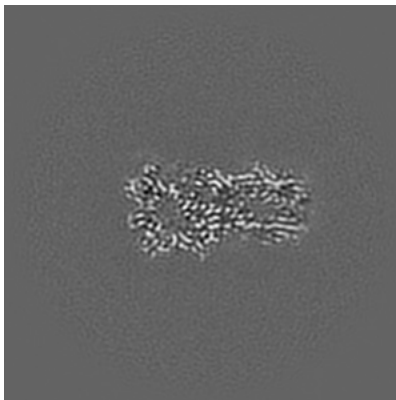
The images above show central slices of the map in three orthogonal directions.

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

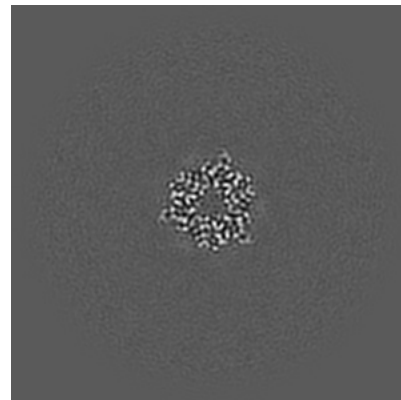
### 6.3.1 Primary map



X Index: 134

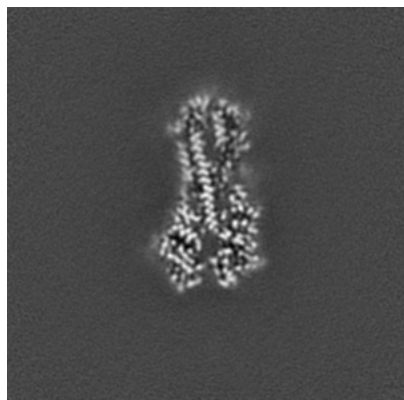


Y Index: 120

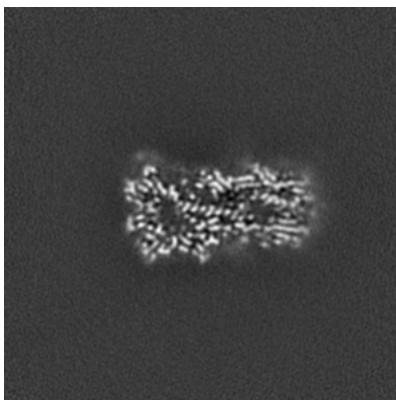


Z Index: 96

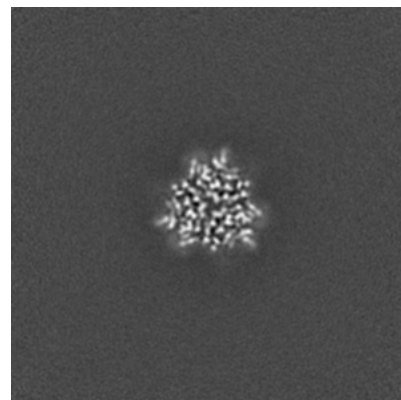
### 6.3.2 Raw map



X Index: 134



Y Index: 120

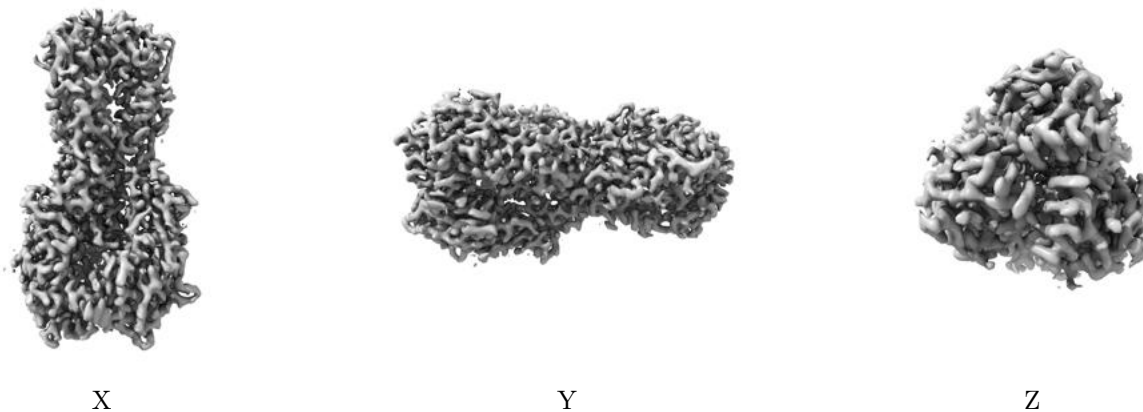


Z Index: 90

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

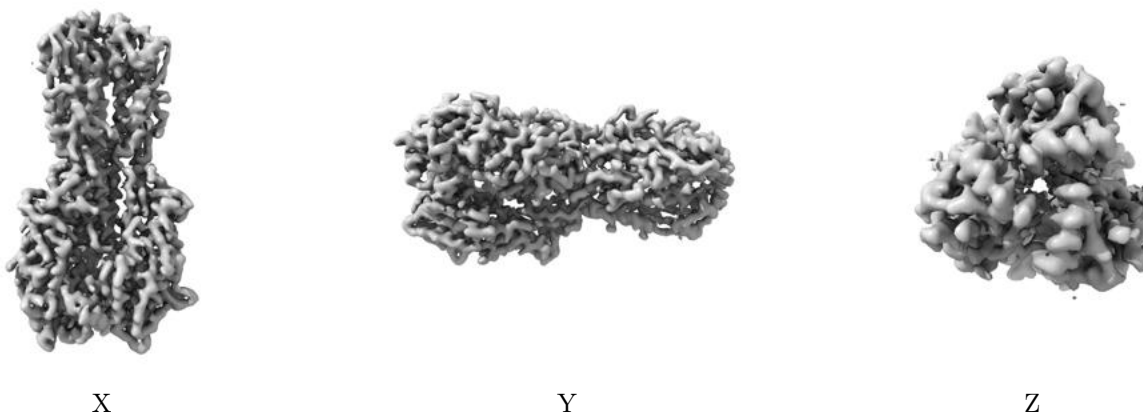
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

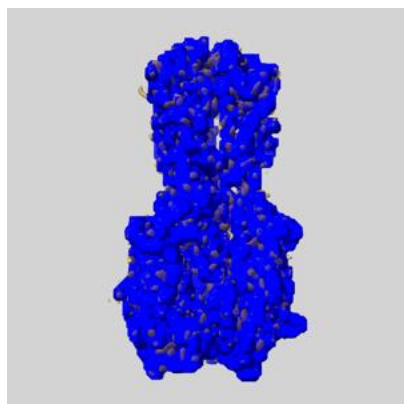
## 6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

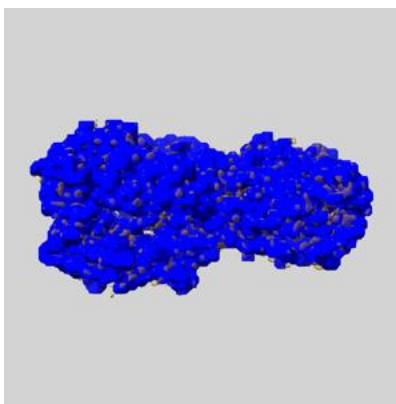
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

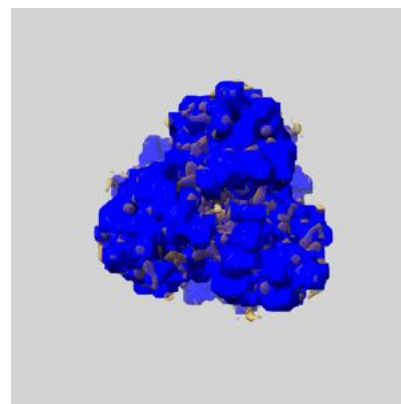
### 6.5.1 emd\_21954\_msk\_1.map [i](#)



X



Y

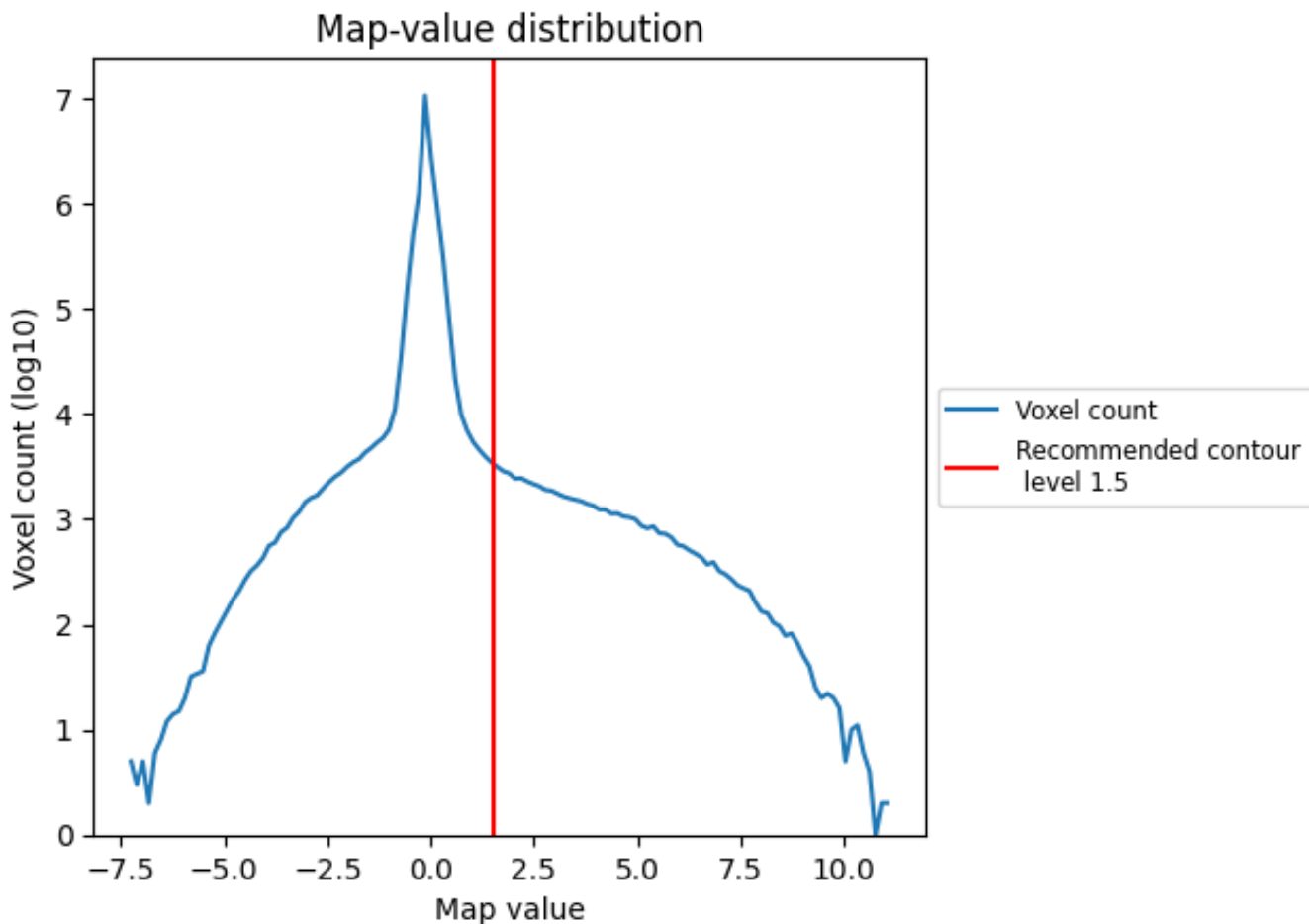


Z

## 7 Map analysis [i](#)

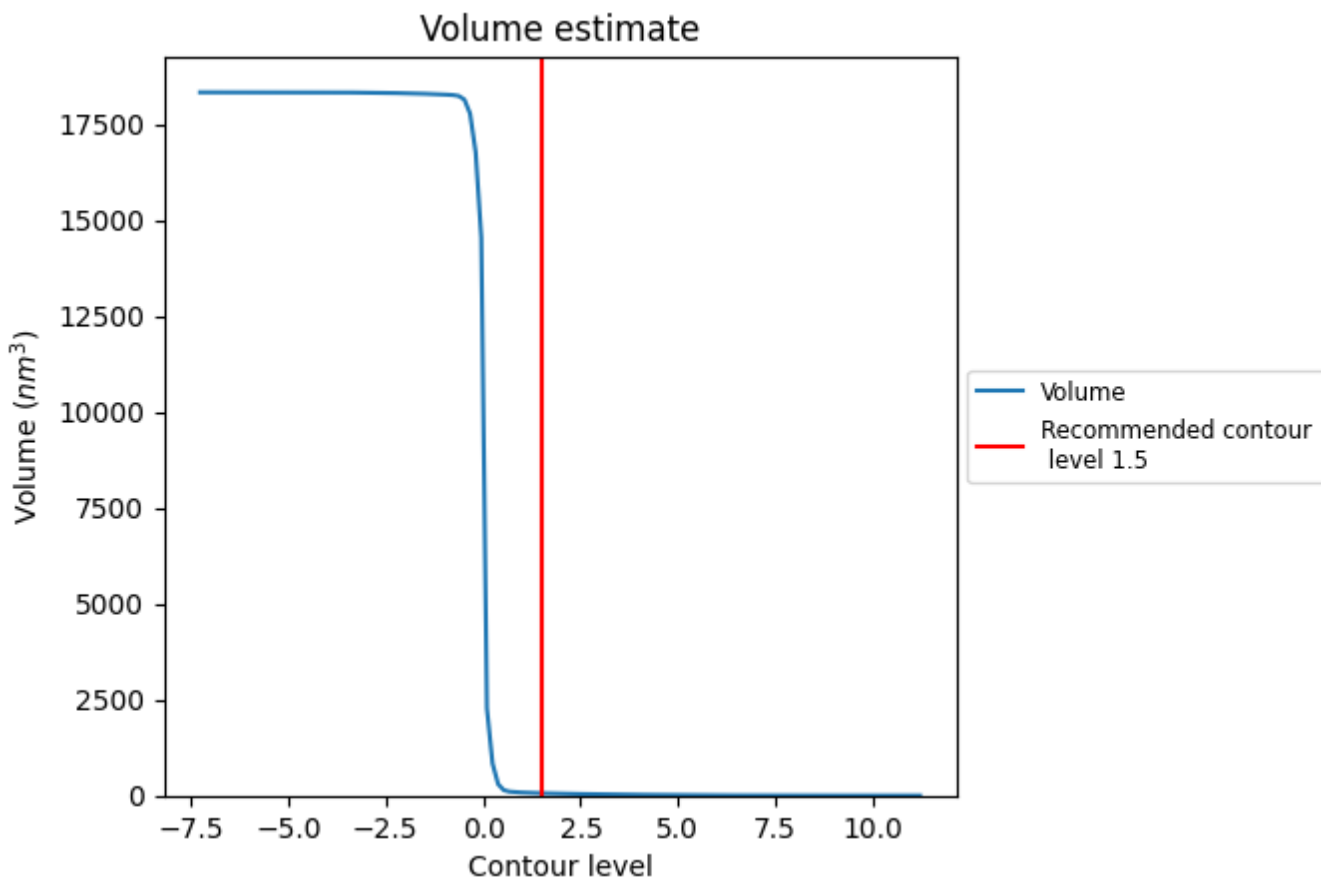
This section contains the results of statistical analysis of the map.

### 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](#)

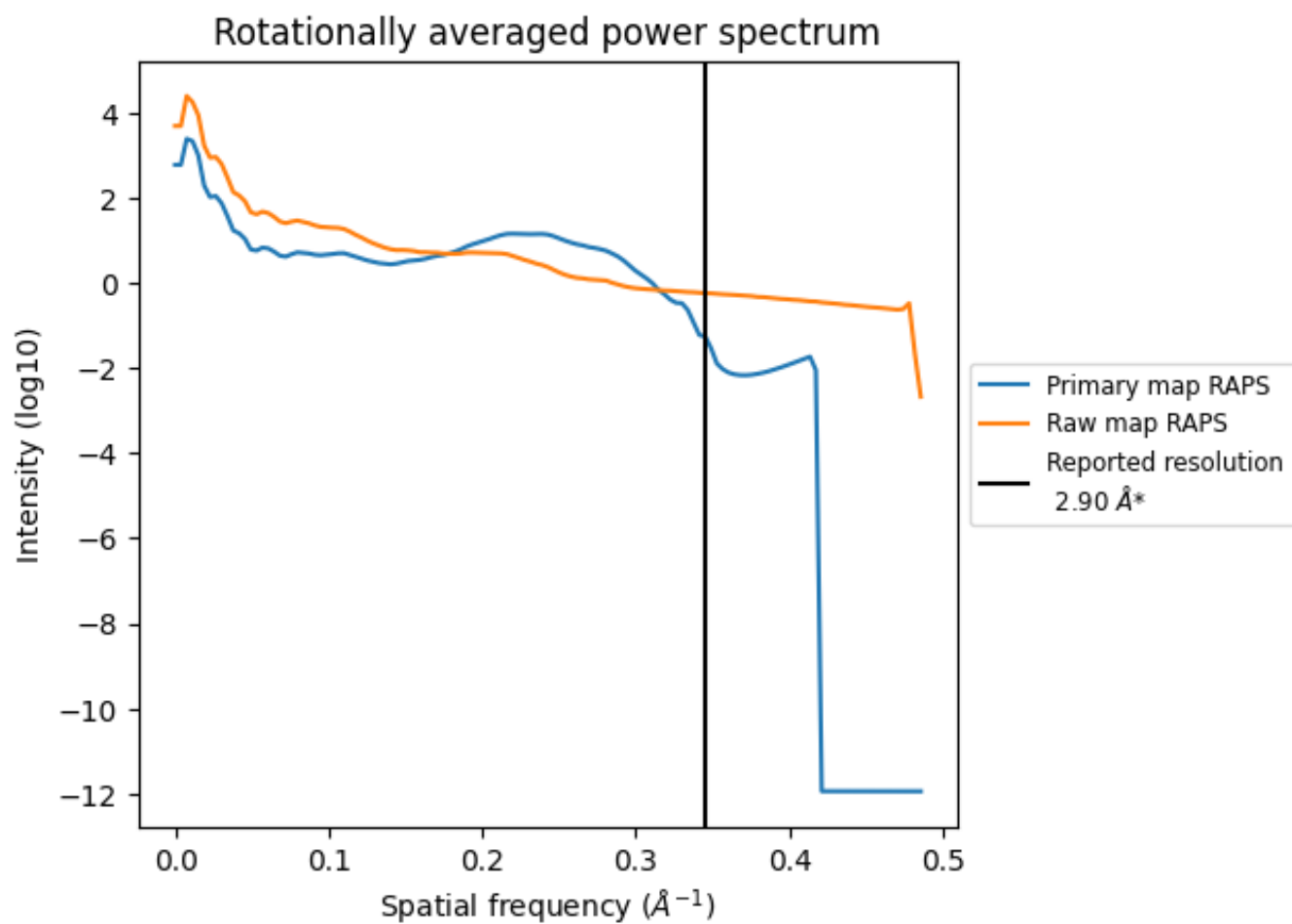


The volume at the recommended contour level is 61  $\text{nm}^3$ ; this corresponds to an approximate mass of 55 kDa.

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 [i](#)

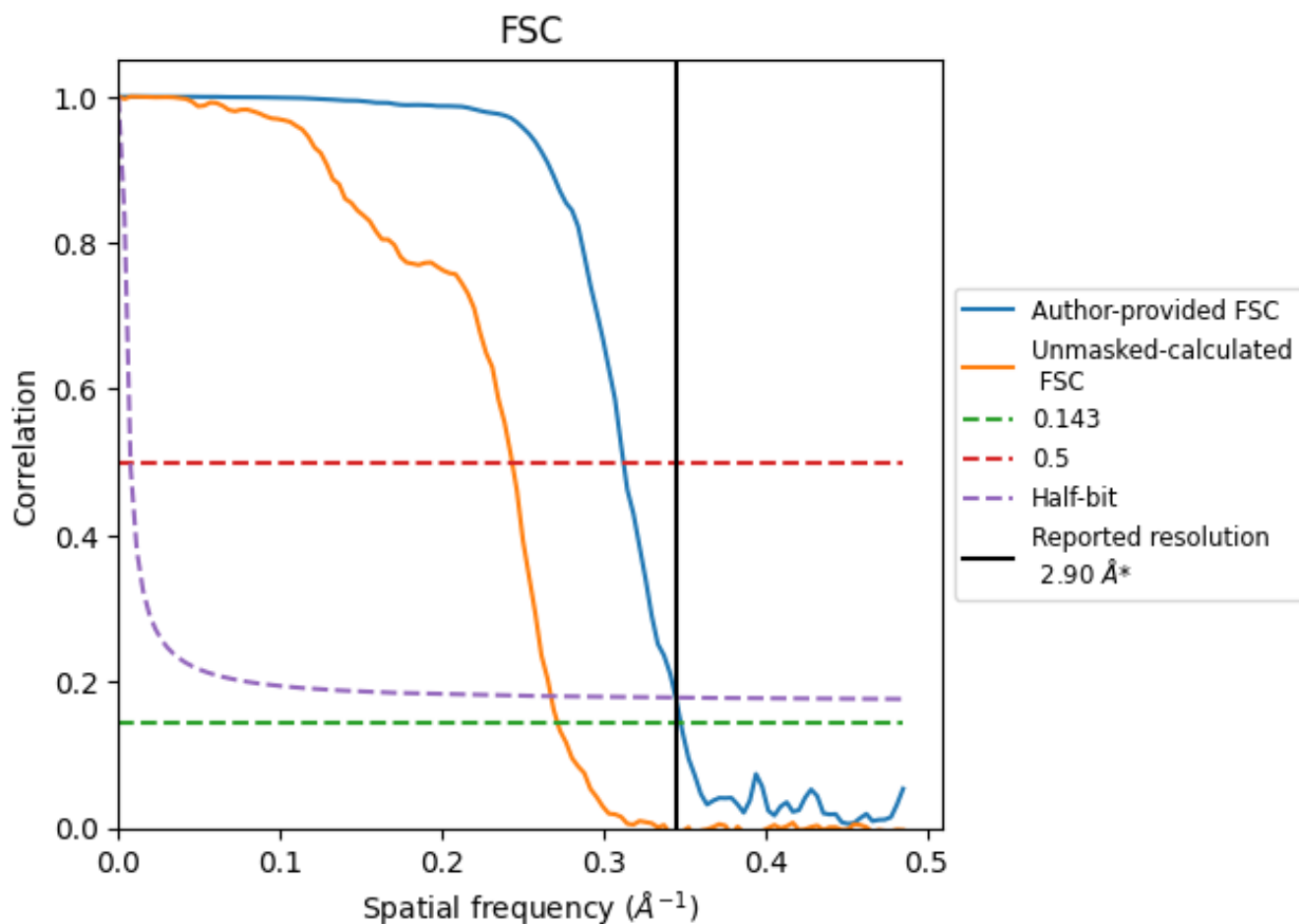


\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>

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

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

### 8.1 FSC [\(i\)](#)



\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

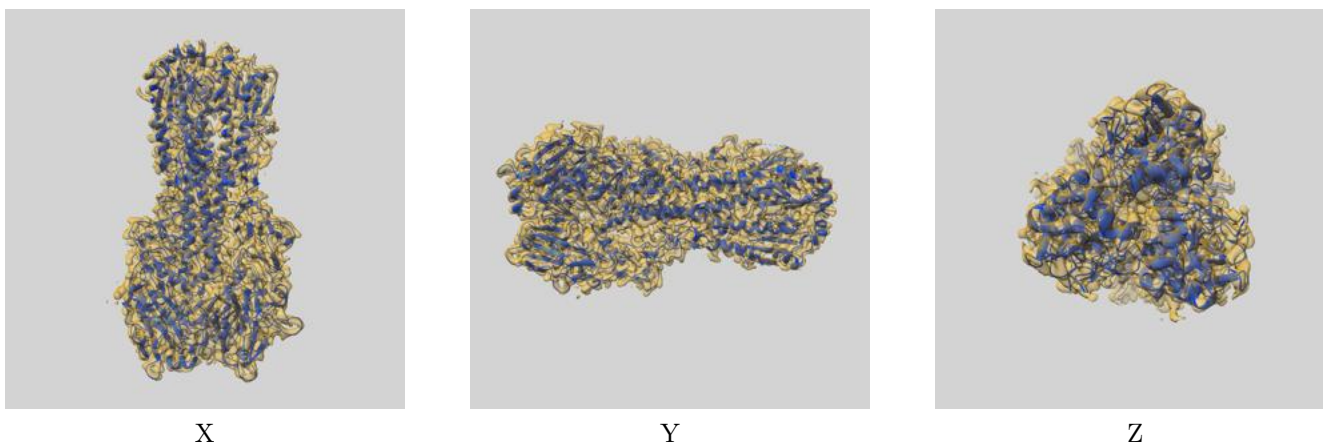
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.87	3.20	2.90
Unmasked-calculated*	3.68	4.11	3.74

\*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 3.68 differs from the reported value 2.9 by more than 10 %

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

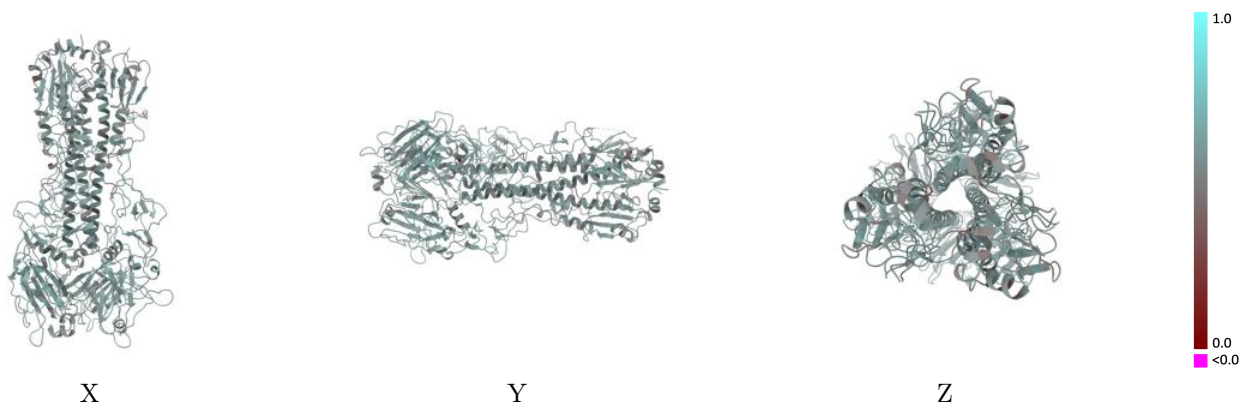
This section contains information regarding the fit between EMDB map EMD-21954 and PDB model 6WXB. Per-residue inclusion information can be found in section [3](#) on page [9](#).

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



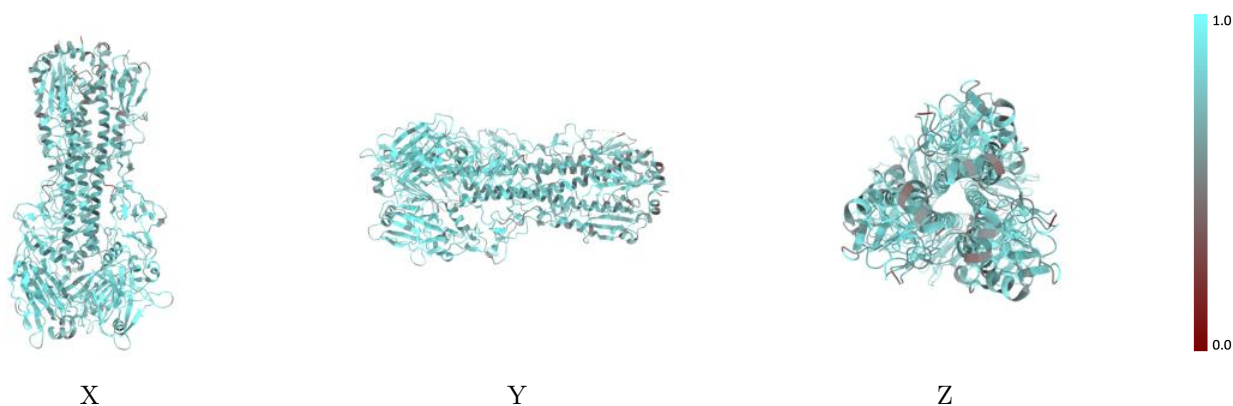
The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



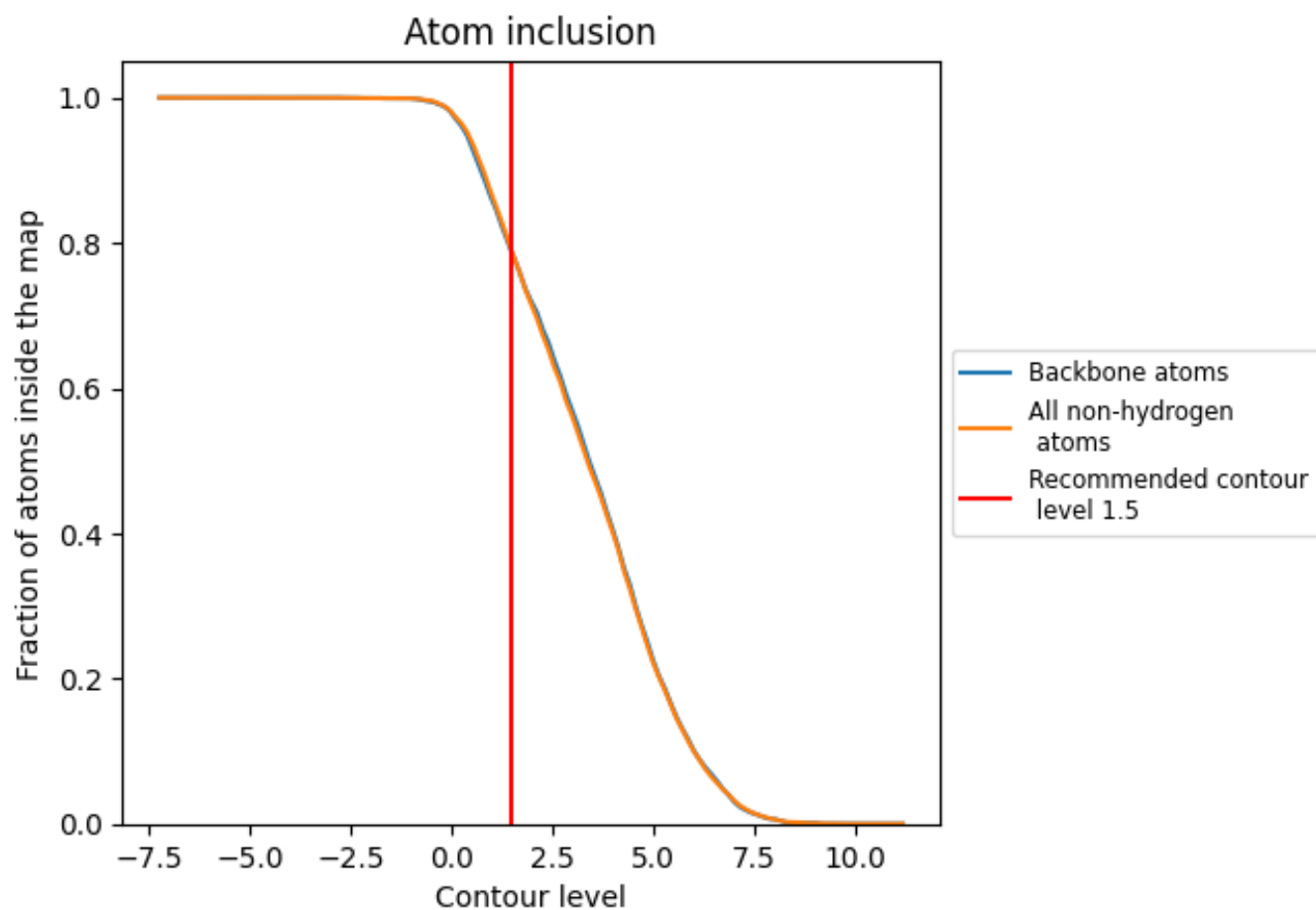
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.5).









## 9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7867	 0.5510
A	 0.7879	 0.5510
B	 0.7887	 0.5510
C	 0.7856	 0.5520

