



## wwPDB EM Validation Summary Report ⓘ

Nov 3, 2024 – 09:40 pm GMT

PDB ID : 6Z9M  
EMDB ID : EMD-11123  
Title : Pseudoatomic model of the pre-fusion conformation of glycoprotein B of Herpes simplex virus 1  
Authors : Vollmer, B.; Prazak, V.; Vasishtan, D.; Jefferys, E.E.; Hernandez-Duran, A.; Vallbracht, M.; Klupp, B.; Mettenleiter, T.C.; Backovic, M.; Rey, F.A.; Topf, M.; Gruenewald, K.  
Deposited on : 2020-06-04  
Resolution : 9.10 Å(reported)  
Based on initial model : 5V2S

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

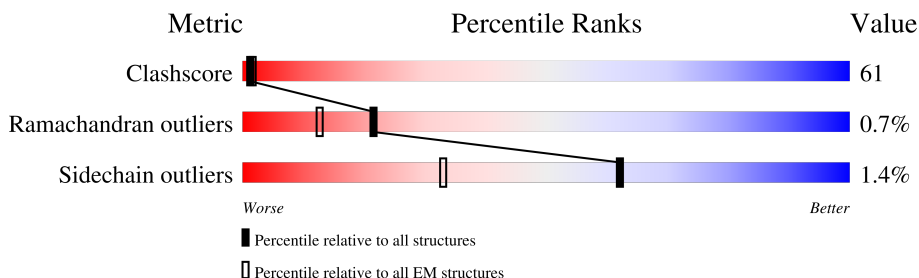
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 9.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	904	<div> <div>20%</div> <div>15%</div> <div>50%</div> <div>33%</div> </div>
1	B	904	<div> <div>20%</div> <div>15%</div> <div>50%</div> <div>33%</div> </div>
1	C	904	<div> <div>22%</div> <div>16%</div> <div>50%</div> <div>33%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14694 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.

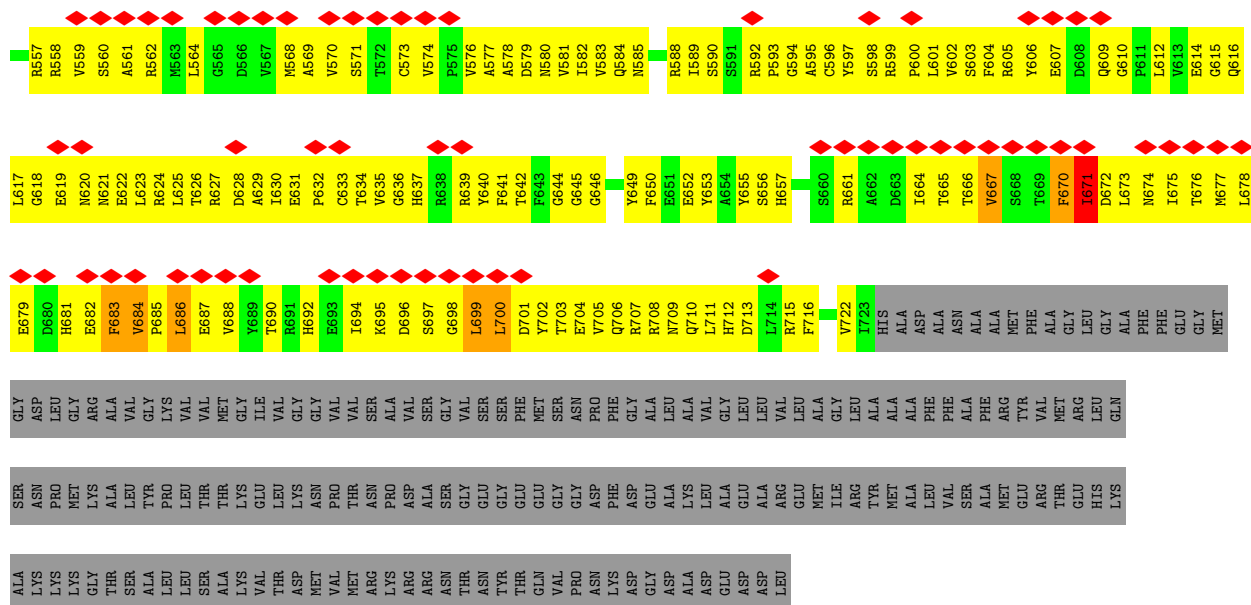
- Molecule 1 is a protein called Envelope glycoprotein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	606	Total	C	N	O	S	0	0
			4898	3089	863	924	22		
1	B	606	Total	C	N	O	S	0	0
			4898	3089	863	924	22		
1	C	606	Total	C	N	O	S	0	0
			4898	3089	863	924	22		

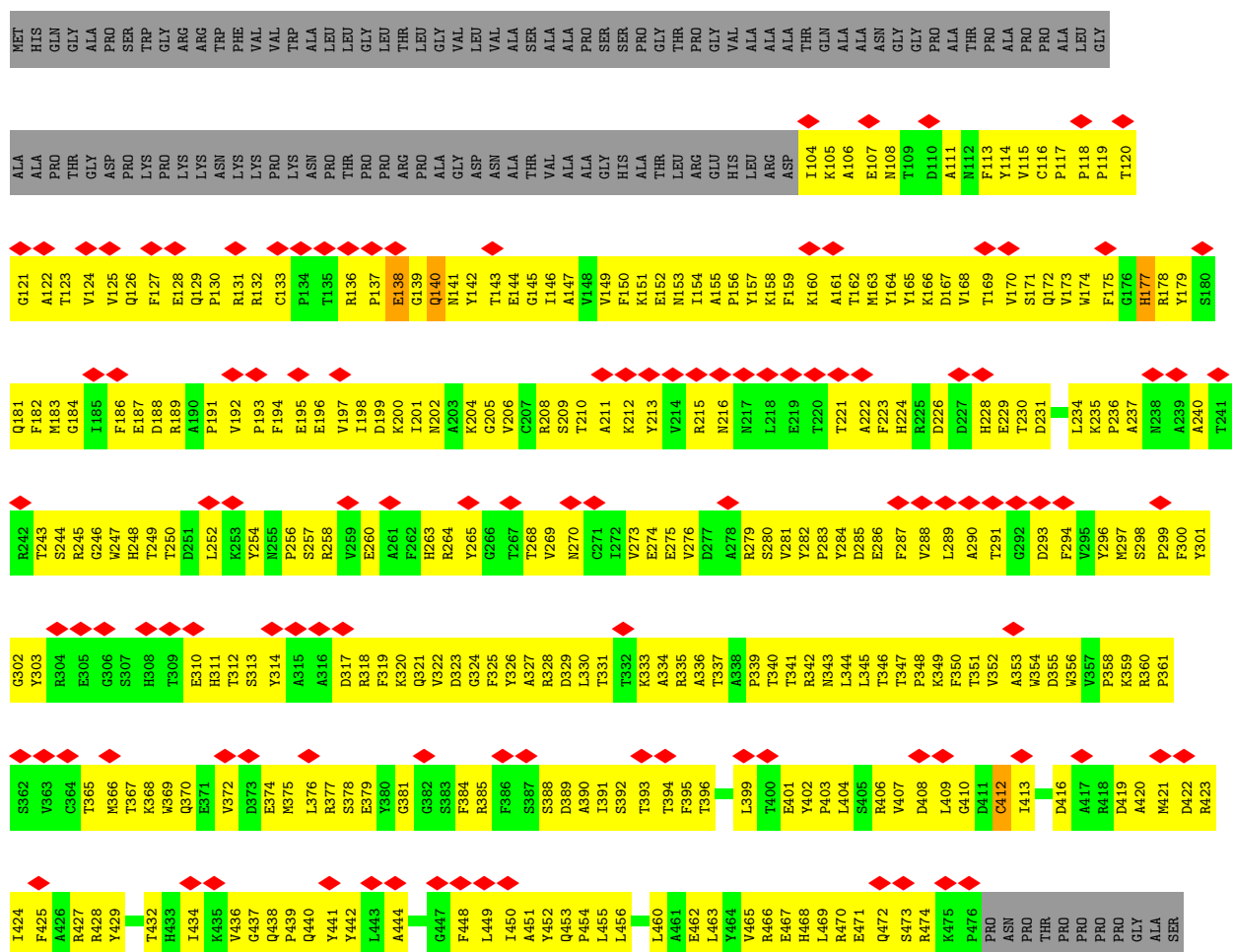
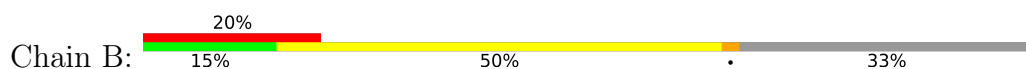
There are 3 discrepancies between the modelled and reference sequences:

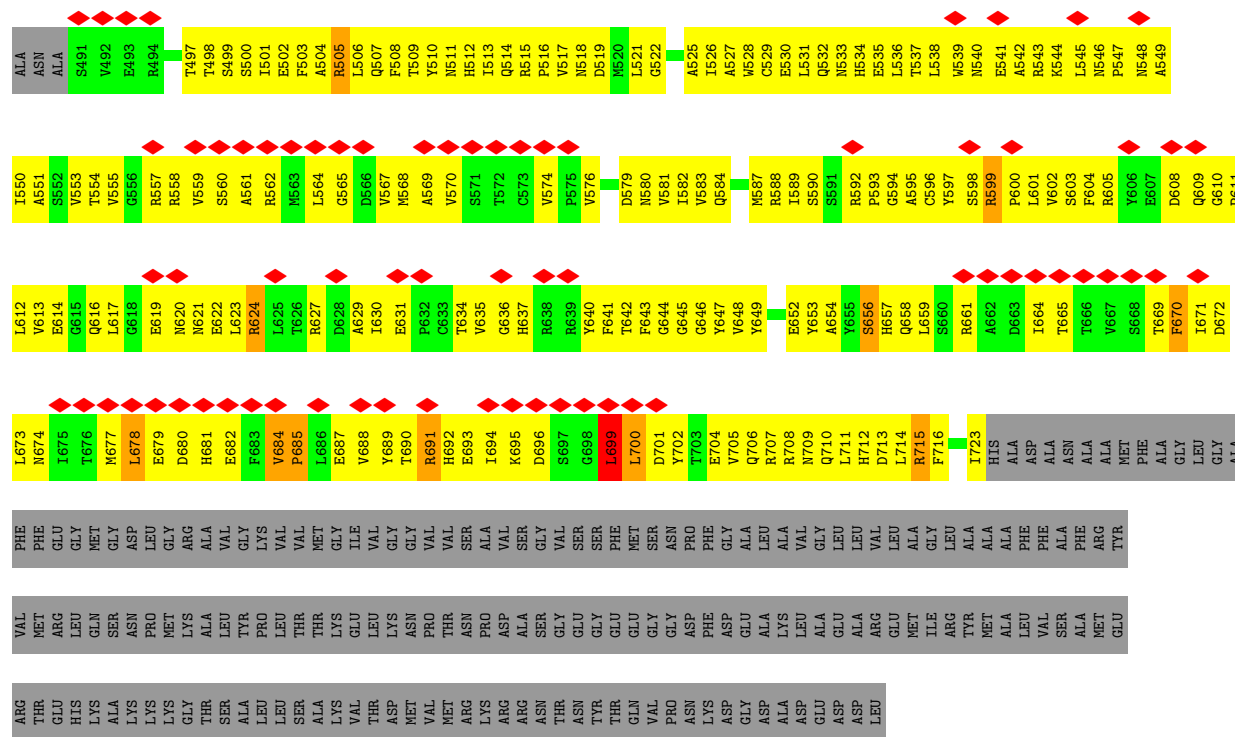
Chain	Residue	Modelled	Actual	Comment	Reference
A	516	PRO	HIS	engineered mutation	UNP A1Z0P7
B	516	PRO	HIS	engineered mutation	UNP A1Z0P7
C	516	PRO	HIS	engineered mutation	UNP A1Z0P7



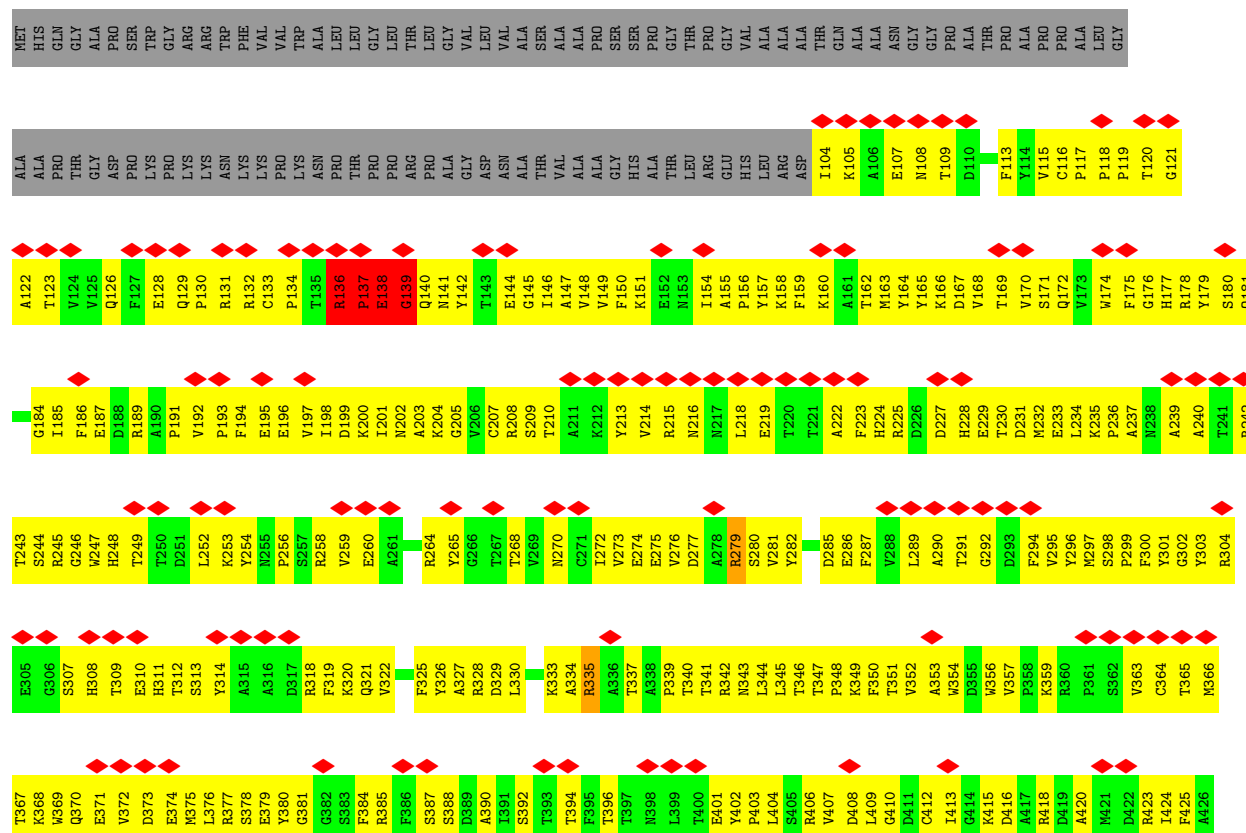
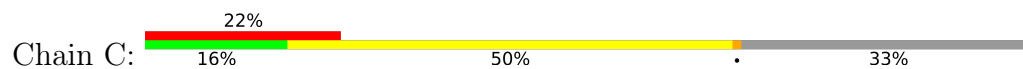


### • Molecule 1: Envelope glycoprotein B





### • Molecule 1: Envelope glycoprotein B



Lys	ASP	H681	N621	V559	L495	R427
Lys	LEU	E682	E622	S660	S500	R428
Lys	GLY	F683	L623	A561	T501	Y429
GLY	ARG	F684	R624	R562	E502	I434
THR	ALA	P685	L625	R563	F503	K435
SER	VAL	P686	T626	L564	A504	V436
ALA	GLY	L687	R627	R565	R505	G437
LEU	LYS	E687	D628	G565	L506	Q438
LEU	VAL	V688	A629	D566	Q507	P439
LEU	VAL	V688	L630	V567	F508	Q440
SER	THR	V689	E631	N568	T509	Y441
ALA	GLY	T690	P632	A569	Y510	Y442
ALA	GLY	E691	O633	N511	H512	L443
THR	VAL	H692	T634	V570	L513	A444
ASP	GLY	E693	V635	S571	Q514	R445
ASN	GLY	L694	G636	T572	R515	G446
THR	VAL	V695	H637	V574	P516	G447
ARG	SER	D696	R638	R575	N518	F448
ASN	ALA	S697	R639	V576	D519	L449
THR	VAL	G698	V640	A577	N520	I450
ALA	SER	L699	F641	A578	L521	A451
ASN	GLY	L700	T642	D579	G522	Y452
THR	VAL	V701	F643	N580	R523	Q453
GLY	SER	T702	G644	V581	V524	P454
GLY	SER	PHE	G645	V582	A525	L455
GLY	THR	T703	G646	V583	T526	L456
GLN	MET	E704	V647	Q584	A527	L463
VAL	SER	V705	V648	N585	N528	Y464
PRO	ASN	Q706	V649	R588	C529	V465
GLY	PRO	R707	F650	L589	E530	R466
ASN	PHE	R708	E651		L531	E467
ASN	GLY	N709	E652		Q532	R468
Lys	GLY	Q710	V653		H534	L469
ASP	ALA	LEU	H711	R592	G594	R470
ALA	ALA	ALA	L712	F693	E535	E471
LEU	VAL	D713	V655	R593	L536	Q472
ASP	GLY	L714	S656	A595	T537	S473
ASP	LEU	R715	Q658	C596	L538	R474
ASP	ALA	F716	L659	V597	N539	K475
LEU	ARG	A717	R660	R598	N540	P476
LEU	MET	D718	R661	R599	E541	PRO
ALA	ALA	GLY	A662	P600	R542	ASN
THR	LEU	T723	D663	L601	R543	PRO
ARG	ALA	ALA	L664	V602	K544	THR
THR	ALA	ASP	T665	S603	L545	PRO
ALA	PHE	ALA	T666	F604	N546	PRO
VAL	PHE	ASN	V667	R605	P547	PRO
SER	ALA	ALA	V667	Y606	N548	PRO
ALA	PHE	ALA	S668	E607	A549	PRO
THR	ARG	MET	T669	D608	T550	GLY
GLY	THR	PHE	F670	Q609	A551	ALA
ARG	VAL	ALA	O670	G610	S552	SER
MET	VAL	ALA	D672	P611		ALA
THR	MET	LEU	L673	L612		ASN
THR	ARG	GLY	L673	V613		ALA
GLY	ARG	GLY	L674	E614		ASN
THR	THR	ALA	R674	G615		ALA
HIS	LEU	PHE	L675	Q616		ALA
Lys	LEU	PHE	T676	L617		S491
ALA	SER	GLY	T676	G618		V492
		GLY	N677	E619		E493
			L678	N620		R494
			E679			
			D680			

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of subtomograms used	46067	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	2.3	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.311	Depositor
Minimum map value	-0.336	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.056	Depositor
Map size ( $\text{\AA}$ )	160.0, 160.0, 160.0	wwPDB
Map dimensions	100, 100, 100	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.6, 1.6, 1.6	Depositor



## 5 Model quality

### 5.1 Standard geometry

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	0.36	0/5018	0.58	1/6817 (0.0%)
1	B	0.35	0/5018	0.57	2/6817 (0.0%)
1	C	0.36	0/5018	0.58	2/6817 (0.0%)
All	All	0.36	0/15054	0.58	5/20451 (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	10
1	B	0	6
1	C	0	8
All	All	0	24

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	699	LEU	CA-CB-CG	6.85	131.06	115.30
1	C	137	PRO	C-N-CA	5.86	136.36	121.70
1	C	139	GLY	N-CA-C	5.35	126.47	113.10
1	B	678	LEU	CA-CB-CG	5.18	127.21	115.30
1	B	699	LEU	C-N-CA	5.11	134.48	121.70

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	136	ARG	Peptide
1	A	137	PRO	Peptide

*Continued on next page...*

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Mol	Chain	Res	Type	Group
1	A	138	GLU	Peptide
1	A	139	GLY	Peptide
1	A	670	PHE	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	4898	0	4726	645	0
1	B	4898	0	4726	639	0
1	C	4898	0	4726	571	0
All	All	14694	0	14178	1757	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 61.

The worst 5 of 1757 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:439:PRO:HA	1:B:452:TYR:O	1.36	1.20
1:B:604:PHE:O	1:B:612:LEU:HA	1.42	1.15
1:C:604:PHE:O	1:C:612:LEU:HA	1.48	1.13
1:C:149:VAL:HA	1:C:449:LEU:O	1.56	1.06
1:B:174:TRP:HB2	1:B:183:MET:HG2	1.40	1.02

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	602/904 (67%)	513 (85%)	85 (14%)	4 (1%)	19	57
1	B	602/904 (67%)	484 (80%)	115 (19%)	3 (0%)	25	64
1	C	602/904 (67%)	494 (82%)	102 (17%)	6 (1%)	13	49
All	All	1806/2712 (67%)	1491 (83%)	302 (17%)	13 (1%)	21	57

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	PRO
1	A	671	ILE
1	C	137	PRO
1	C	687	GLU
1	C	688	VAL

### 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	A	529/746 (71%)	522 (99%)	7 (1%)	65	77
1	B	529/746 (71%)	520 (98%)	9 (2%)	56	72
1	C	529/746 (71%)	523 (99%)	6 (1%)	70	80
All	All	1587/2238 (71%)	1565 (99%)	22 (1%)	62	75

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	691	ARG
1	C	279	ARG
1	C	136	ARG
1	C	335	ARG
1	A	667	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28

such sidechains are listed below:

Mol	Chain	Res	Type
1	C	153	ASN
1	C	692	HIS
1	C	181	GLN
1	C	511	ASN
1	C	177	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](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

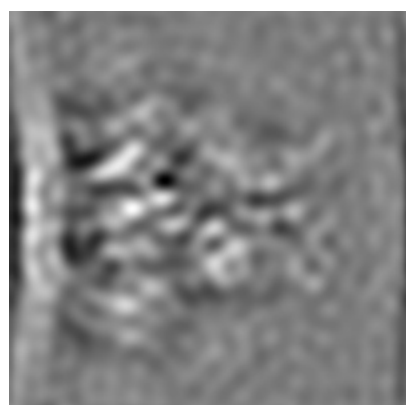
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11123. These allow visual inspection of the internal detail of the map and identification of artifacts.

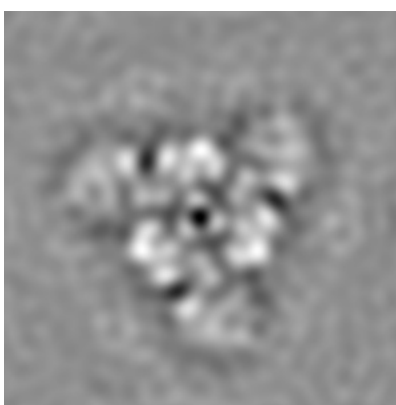
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

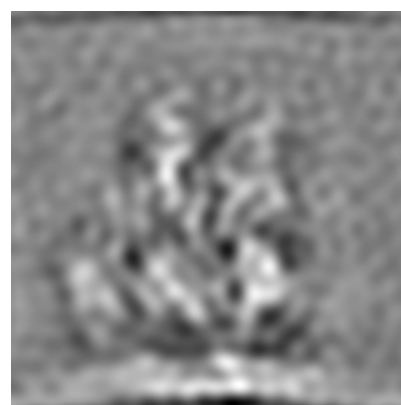
#### 6.1.1 Primary map



X



Y

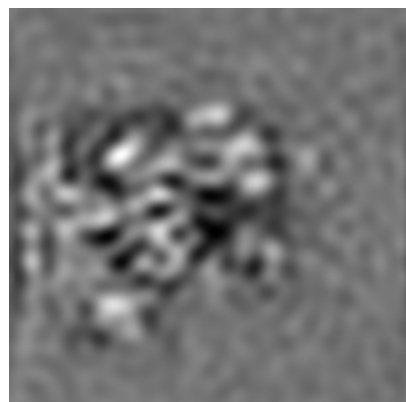


Z

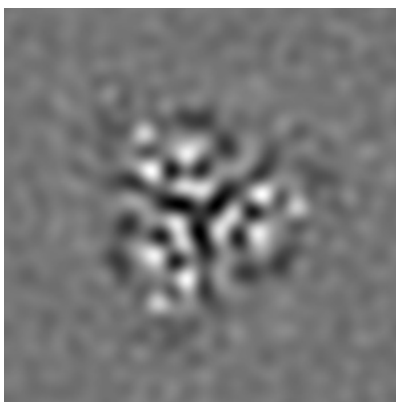
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

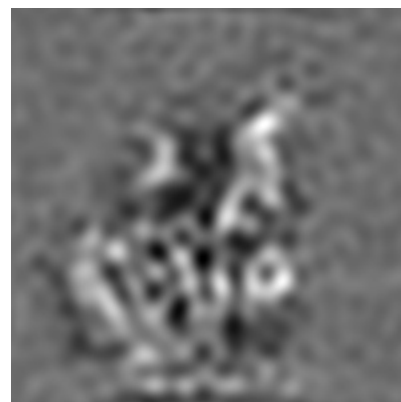
#### 6.2.1 Primary map



X Index: 50



Y Index: 50

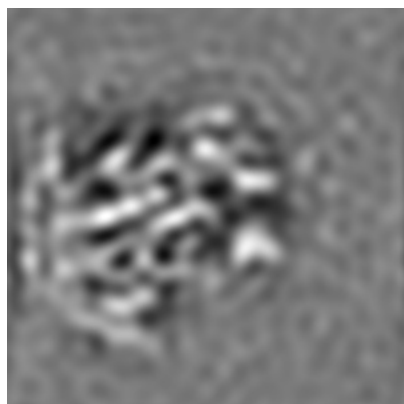


Z Index: 50

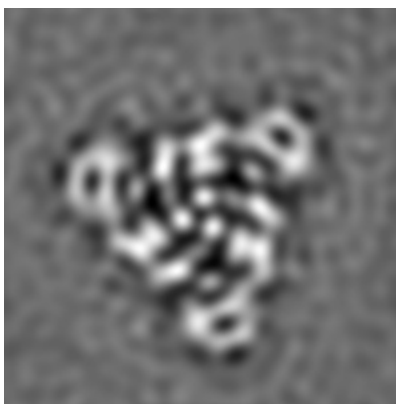
The images above show central slices of the map in three orthogonal directions.

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

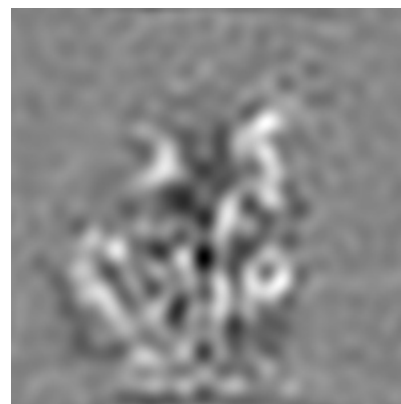
### 6.3.1 Primary map



X Index: 52



Y Index: 29

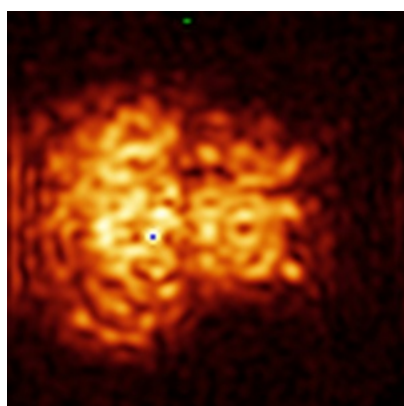


Z Index: 49

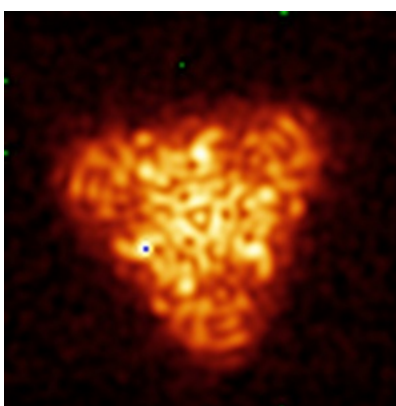
The images above show the largest variance slices of the map in three orthogonal directions.

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

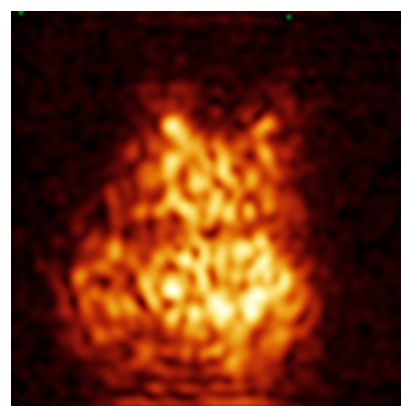
### 6.4.1 Primary map



X



Y

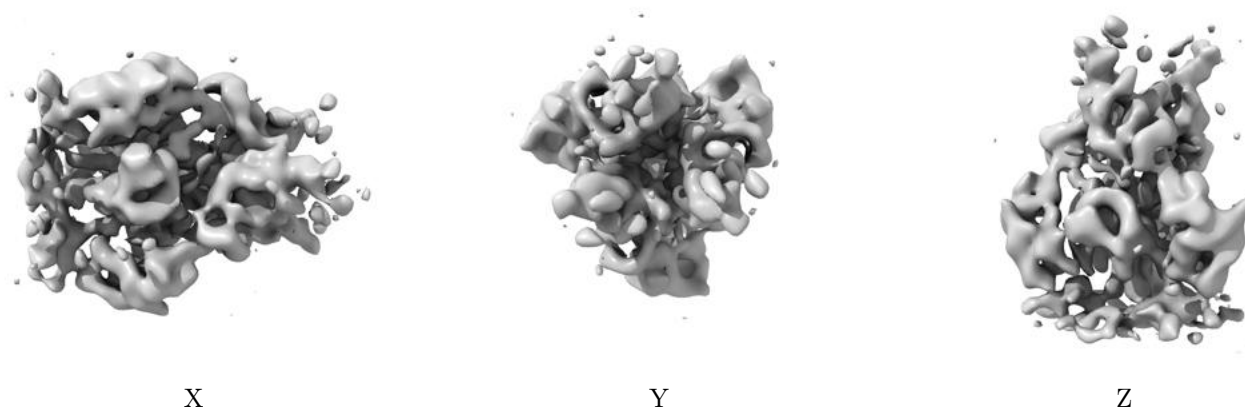


Z

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 0.056. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

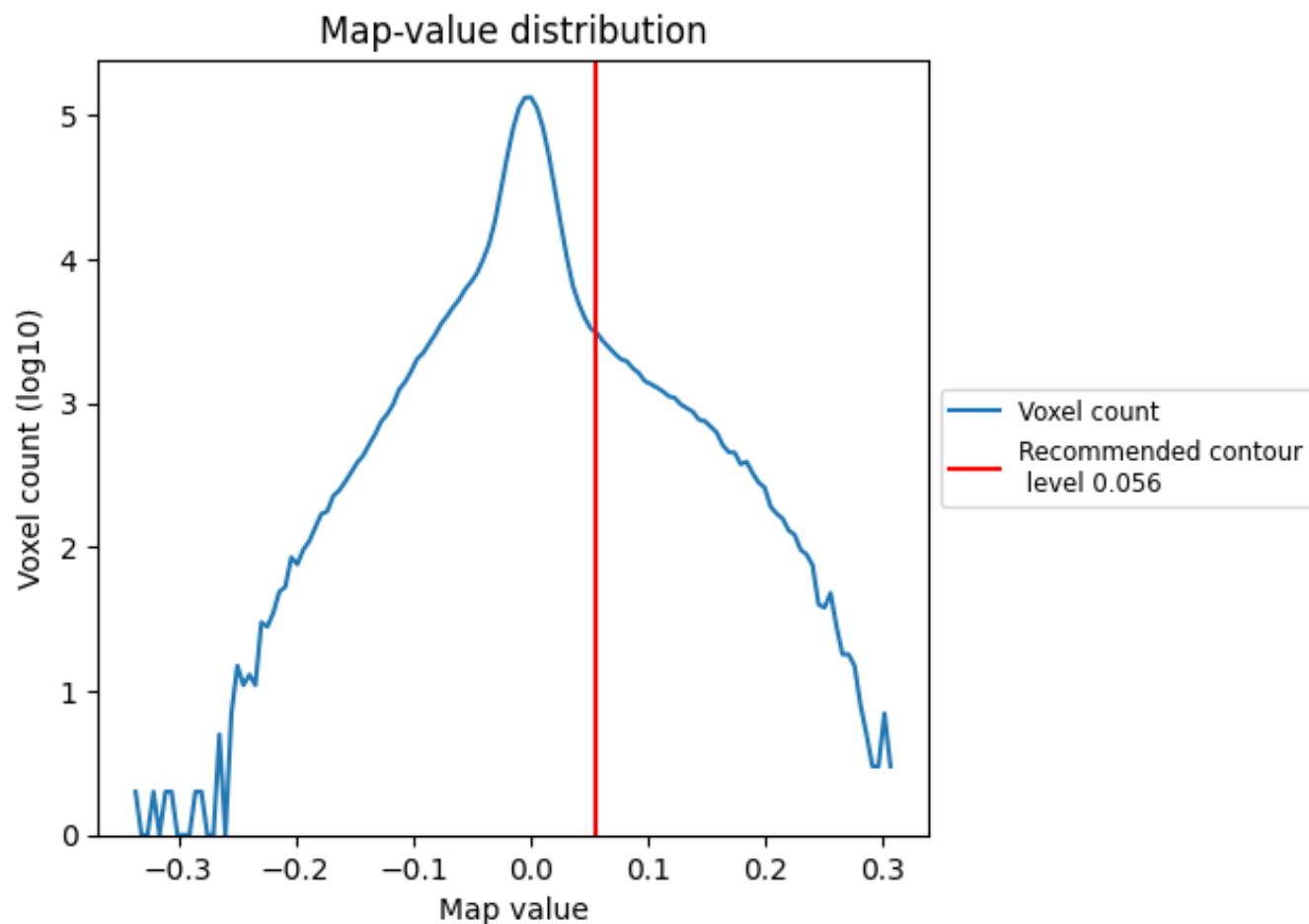
## 6.6 Mask visualisation [i](#)

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.

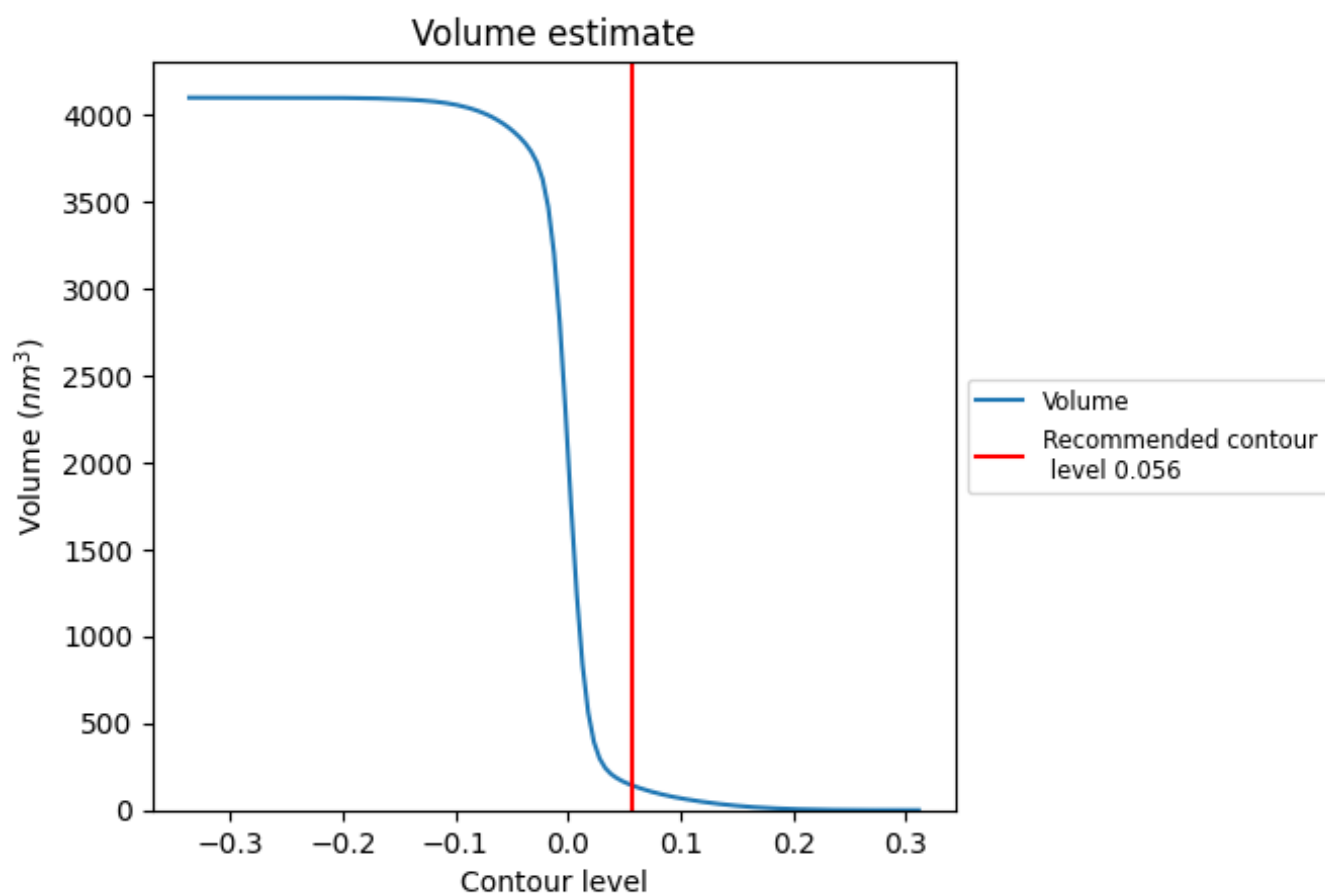
### 7.1 Map-value distribution [i](#)



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.



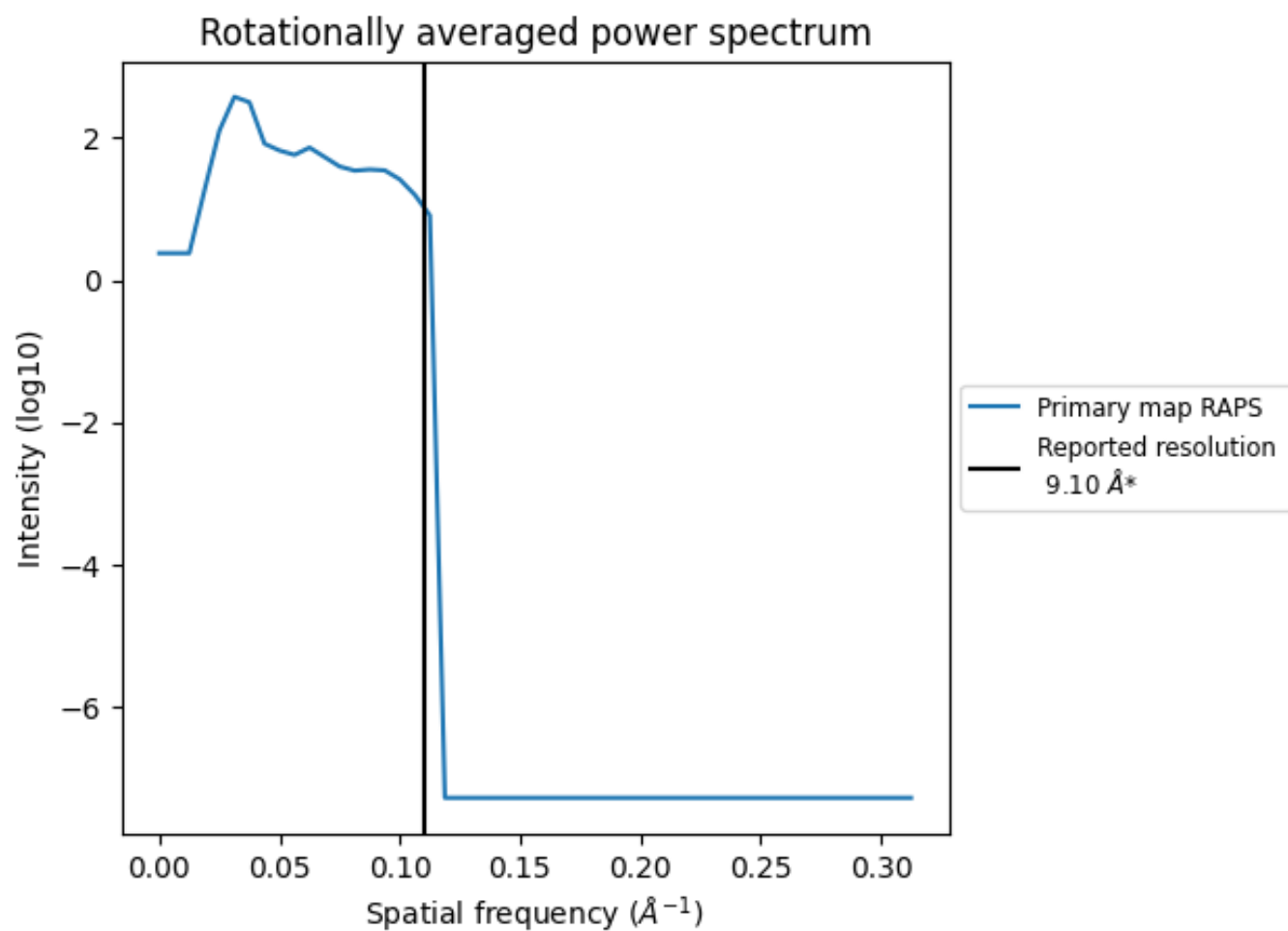
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 145 nm<sup>3</sup>; this corresponds to an approximate mass of 131 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](#)

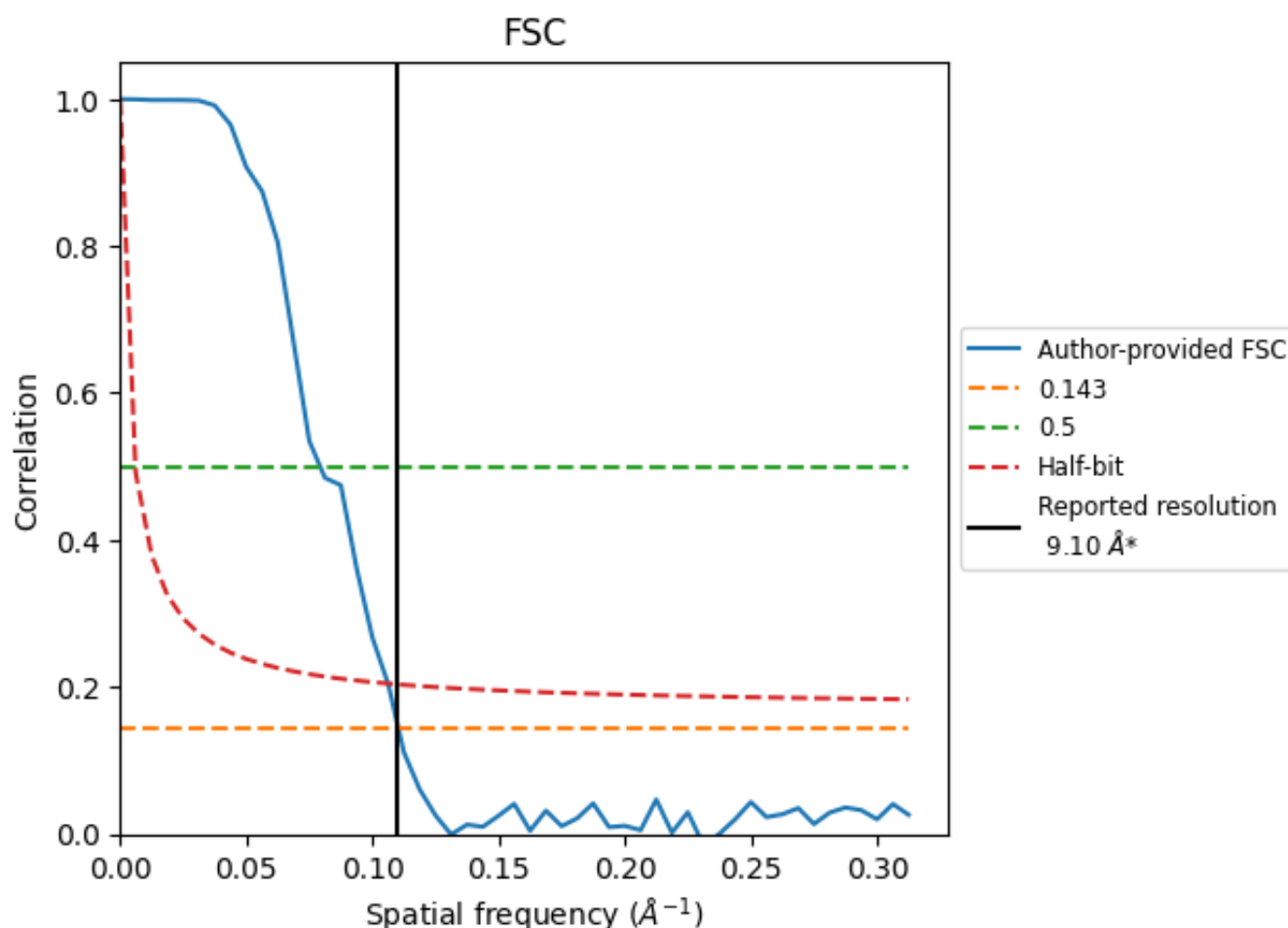


\*Reported resolution corresponds to spatial frequency of 0.110 Å<sup>-1</sup>

## 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 0.110 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

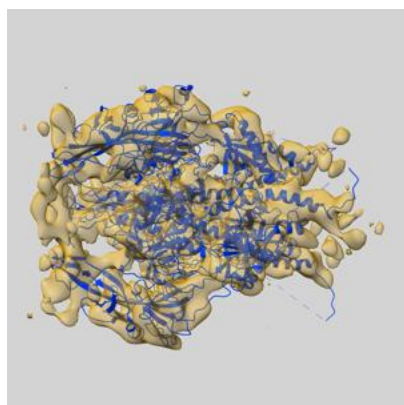
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.10	-	-
Author-provided FSC curve	9.07	12.61	9.43
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

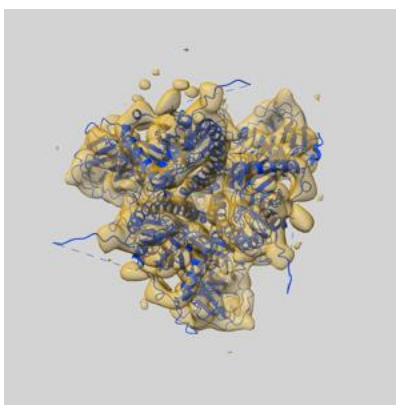
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11123 and PDB model 6Z9M. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

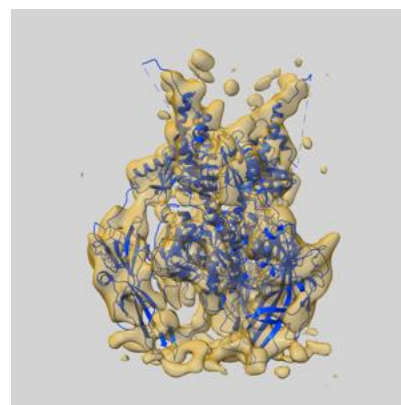
### 9.1 Map-model overlay [i](#)



X



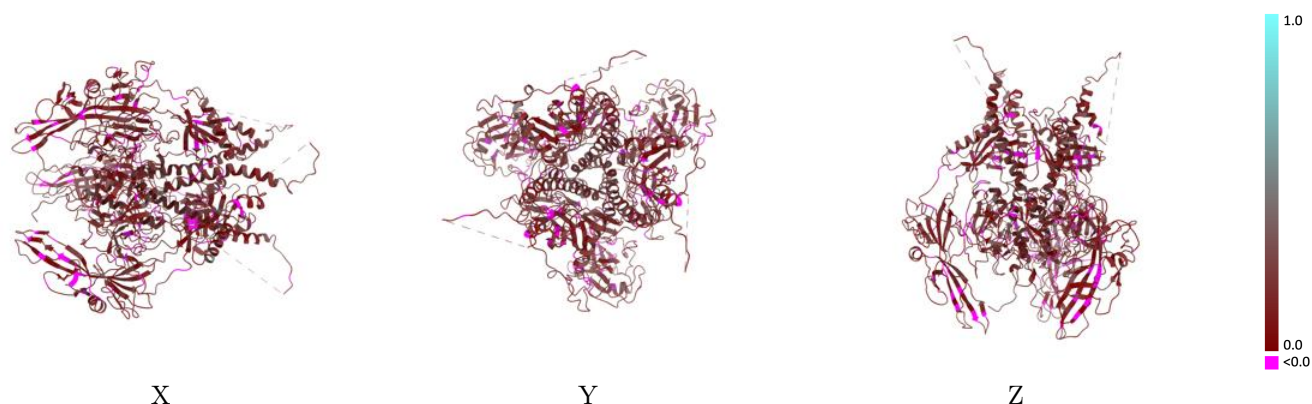
Y



Z

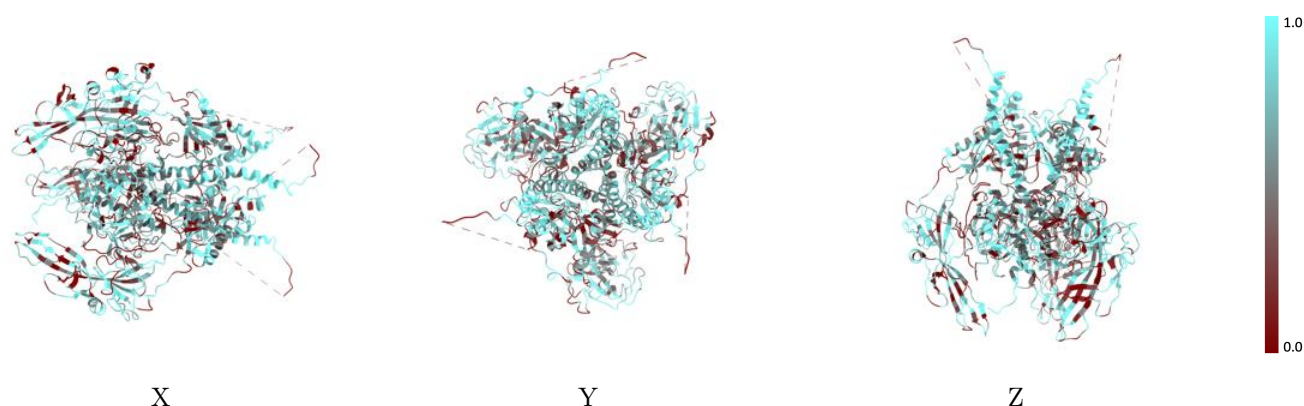
The images above show the 3D surface view of the map at the recommended contour level 0.056 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



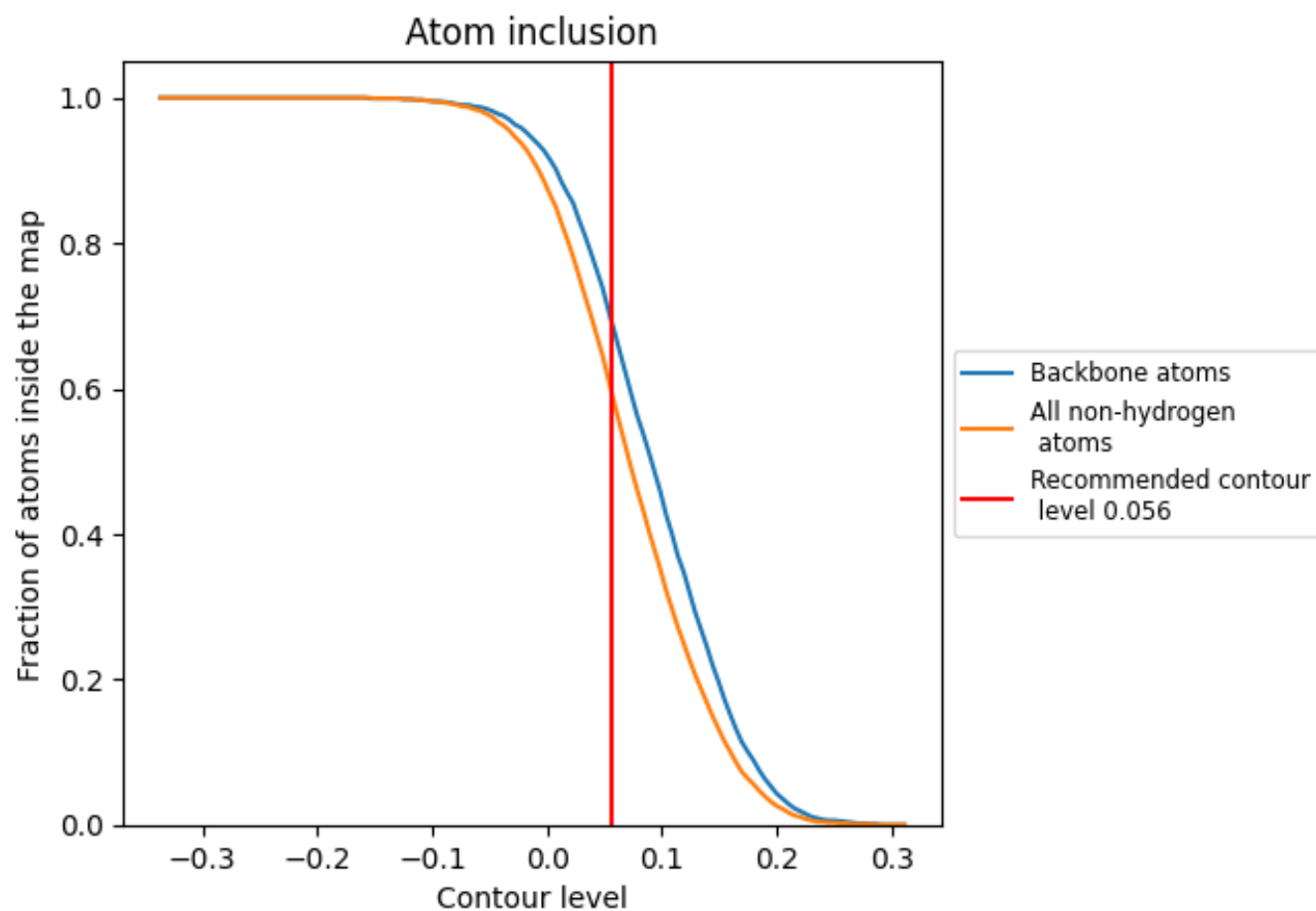
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.056).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 60% 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 (0.056) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5970	<div></div> 0.1550
A	<div></div> 0.6000	<div></div> 0.1540
B	<div></div> 0.6020	<div></div> 0.1540
C	<div></div> 0.5900	<div></div> 0.1580

