



## wwPDB EM Validation Summary Report ⓘ

Feb 6, 2025 – 04:12 PM EST

PDB ID : 9CR3  
EMDB ID : EMD-45831  
Title : CryoEM Structure of the human full length NAD Kinase  
Authors : Li, Y.; Chen, Z.; Labesse, G.; Hoxhaj, G.  
Deposited on : 2024-07-20  
Resolution : 3.18 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](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) : 2.40

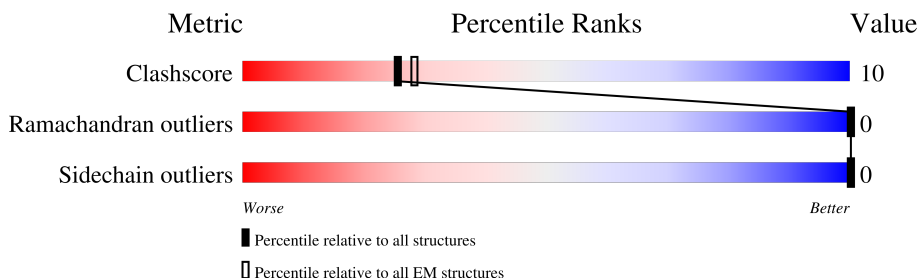
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.18 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	477	
1	B	477	
1	C	477	
1	D	477	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9299 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 NAD kinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	299	Total	C	N	O	S	0	0
			2315	1482	393	425	15		
1	D	299	Total	C	N	O	S	0	0
			2314	1482	392	425	15		
1	C	301	Total	C	N	O	S	0	0
			2335	1493	398	429	15		
1	B	301	Total	C	N	O	S	0	0
			2335	1493	398	429	15		

There are 124 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	447	THR	-	expression tag	UNP O95544
A	448	ARG	-	expression tag	UNP O95544
A	449	THR	-	expression tag	UNP O95544
A	450	ARG	-	expression tag	UNP O95544
A	451	PRO	-	expression tag	UNP O95544
A	452	LEU	-	expression tag	UNP O95544
A	453	GLU	-	expression tag	UNP O95544
A	454	GLN	-	expression tag	UNP O95544
A	455	LYS	-	expression tag	UNP O95544
A	456	LEU	-	expression tag	UNP O95544
A	457	ILE	-	expression tag	UNP O95544
A	458	SER	-	expression tag	UNP O95544
A	459	GLU	-	expression tag	UNP O95544
A	460	GLU	-	expression tag	UNP O95544
A	461	ASP	-	expression tag	UNP O95544
A	462	LEU	-	expression tag	UNP O95544
A	463	ALA	-	expression tag	UNP O95544
A	464	ALA	-	expression tag	UNP O95544
A	465	ASN	-	expression tag	UNP O95544
A	466	ASP	-	expression tag	UNP O95544
A	467	ILE	-	expression tag	UNP O95544
A	468	LEU	-	expression tag	UNP O95544

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Chain	Residue	Modelled	Actual	Comment	Reference
A	469	ASP	-	expression tag	UNP O95544
A	470	TYR	-	expression tag	UNP O95544
A	471	LYS	-	expression tag	UNP O95544
A	472	ASP	-	expression tag	UNP O95544
A	473	ASP	-	expression tag	UNP O95544
A	474	ASP	-	expression tag	UNP O95544
A	475	ASP	-	expression tag	UNP O95544
A	476	LYS	-	expression tag	UNP O95544
A	477	VAL	-	expression tag	UNP O95544
D	447	THR	-	expression tag	UNP O95544
D	448	ARG	-	expression tag	UNP O95544
D	449	THR	-	expression tag	UNP O95544
D	450	ARG	-	expression tag	UNP O95544
D	451	PRO	-	expression tag	UNP O95544
D	452	LEU	-	expression tag	UNP O95544
D	453	GLU	-	expression tag	UNP O95544
D	454	GLN	-	expression tag	UNP O95544
D	455	LYS	-	expression tag	UNP O95544
D	456	LEU	-	expression tag	UNP O95544
D	457	ILE	-	expression tag	UNP O95544
D	458	SER	-	expression tag	UNP O95544
D	459	GLU	-	expression tag	UNP O95544
D	460	GLU	-	expression tag	UNP O95544
D	461	ASP	-	expression tag	UNP O95544
D	462	LEU	-	expression tag	UNP O95544
D	463	ALA	-	expression tag	UNP O95544
D	464	ALA	-	expression tag	UNP O95544
D	465	ASN	-	expression tag	UNP O95544
D	466	ASP	-	expression tag	UNP O95544
D	467	ILE	-	expression tag	UNP O95544
D	468	LEU	-	expression tag	UNP O95544
D	469	ASP	-	expression tag	UNP O95544
D	470	TYR	-	expression tag	UNP O95544
D	471	LYS	-	expression tag	UNP O95544
D	472	ASP	-	expression tag	UNP O95544
D	473	ASP	-	expression tag	UNP O95544
D	474	ASP	-	expression tag	UNP O95544
D	475	ASP	-	expression tag	UNP O95544
D	476	LYS	-	expression tag	UNP O95544
D	477	VAL	-	expression tag	UNP O95544
C	447	THR	-	expression tag	UNP O95544
C	448	ARG	-	expression tag	UNP O95544

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Chain	Residue	Modelled	Actual	Comment	Reference
C	449	THR	-	expression tag	UNP O95544
C	450	ARG	-	expression tag	UNP O95544
C	451	PRO	-	expression tag	UNP O95544
C	452	LEU	-	expression tag	UNP O95544
C	453	GLU	-	expression tag	UNP O95544
C	454	GLN	-	expression tag	UNP O95544
C	455	LYS	-	expression tag	UNP O95544
C	456	LEU	-	expression tag	UNP O95544
C	457	ILE	-	expression tag	UNP O95544
C	458	SER	-	expression tag	UNP O95544
C	459	GLU	-	expression tag	UNP O95544
C	460	GLU	-	expression tag	UNP O95544
C	461	ASP	-	expression tag	UNP O95544
C	462	LEU	-	expression tag	UNP O95544
C	463	ALA	-	expression tag	UNP O95544
C	464	ALA	-	expression tag	UNP O95544
C	465	ASN	-	expression tag	UNP O95544
C	466	ASP	-	expression tag	UNP O95544
C	467	ILE	-	expression tag	UNP O95544
C	468	LEU	-	expression tag	UNP O95544
C	469	ASP	-	expression tag	UNP O95544
C	470	TYR	-	expression tag	UNP O95544
C	471	LYS	-	expression tag	UNP O95544
C	472	ASP	-	expression tag	UNP O95544
C	473	ASP	-	expression tag	UNP O95544
C	474	ASP	-	expression tag	UNP O95544
C	475	ASP	-	expression tag	UNP O95544
C	476	LYS	-	expression tag	UNP O95544
C	477	VAL	-	expression tag	UNP O95544
B	447	THR	-	expression tag	UNP O95544
B	448	ARG	-	expression tag	UNP O95544
B	449	THR	-	expression tag	UNP O95544
B	450	ARG	-	expression tag	UNP O95544
B	451	PRO	-	expression tag	UNP O95544
B	452	LEU	-	expression tag	UNP O95544
B	453	GLU	-	expression tag	UNP O95544
B	454	GLN	-	expression tag	UNP O95544
B	455	LYS	-	expression tag	UNP O95544
B	456	LEU	-	expression tag	UNP O95544
B	457	ILE	-	expression tag	UNP O95544
B	458	SER	-	expression tag	UNP O95544
B	459	GLU	-	expression tag	UNP O95544

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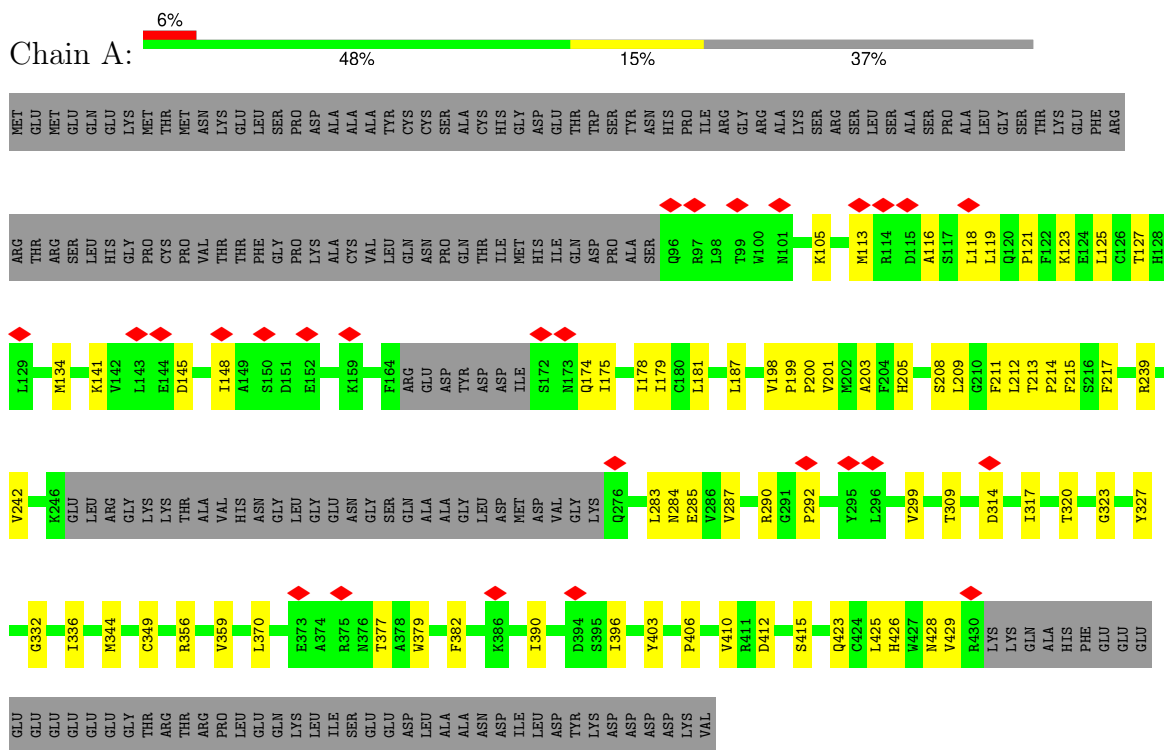
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Chain	Residue	Modelled	Actual	Comment	Reference
B	460	GLU	-	expression tag	UNP O95544
B	461	ASP	-	expression tag	UNP O95544
B	462	LEU	-	expression tag	UNP O95544
B	463	ALA	-	expression tag	UNP O95544
B	464	ALA	-	expression tag	UNP O95544
B	465	ASN	-	expression tag	UNP O95544
B	466	ASP	-	expression tag	UNP O95544
B	467	ILE	-	expression tag	UNP O95544
B	468	LEU	-	expression tag	UNP O95544
B	469	ASP	-	expression tag	UNP O95544
B	470	TYR	-	expression tag	UNP O95544
B	471	LYS	-	expression tag	UNP O95544
B	472	ASP	-	expression tag	UNP O95544
B	473	ASP	-	expression tag	UNP O95544
B	474	ASP	-	expression tag	UNP O95544
B	475	ASP	-	expression tag	UNP O95544
B	476	LYS	-	expression tag	UNP O95544
B	477	VAL	-	expression tag	UNP O95544

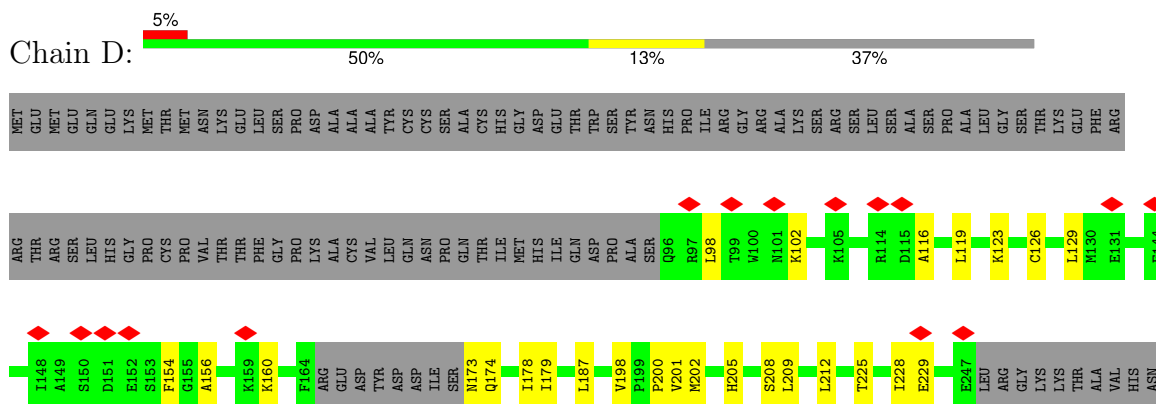
### 3 Residue-property plots

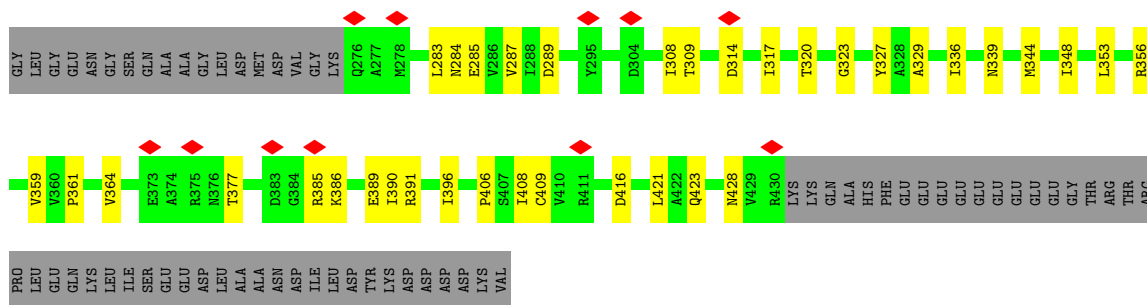
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: NAD kinase

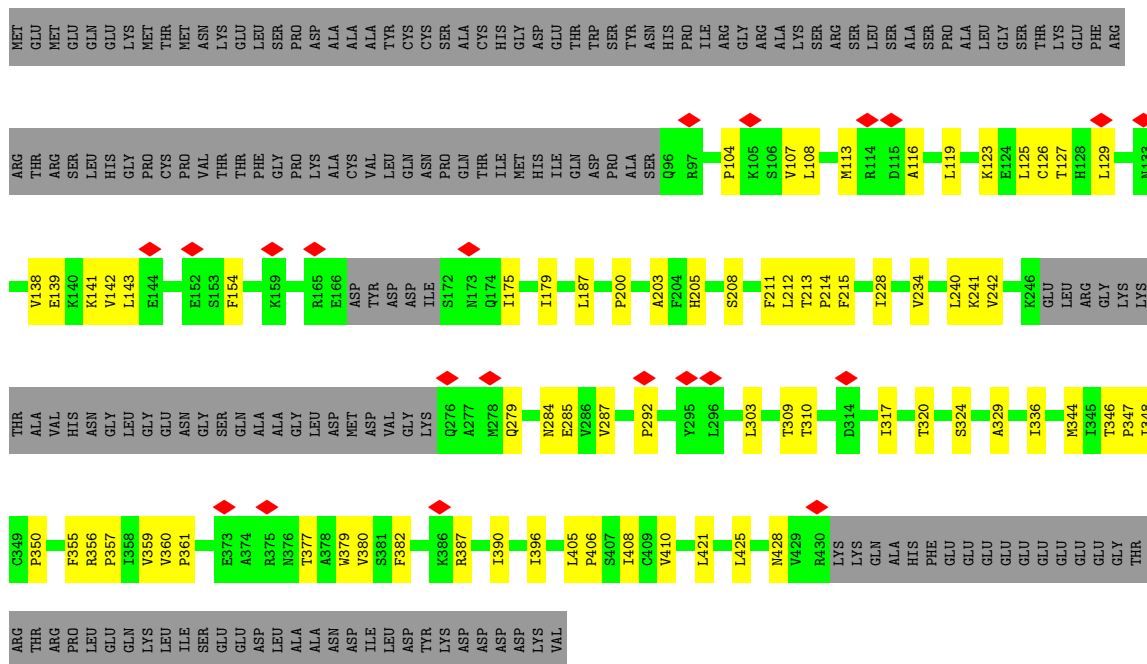


#### • Molecule 1: NAD kinase

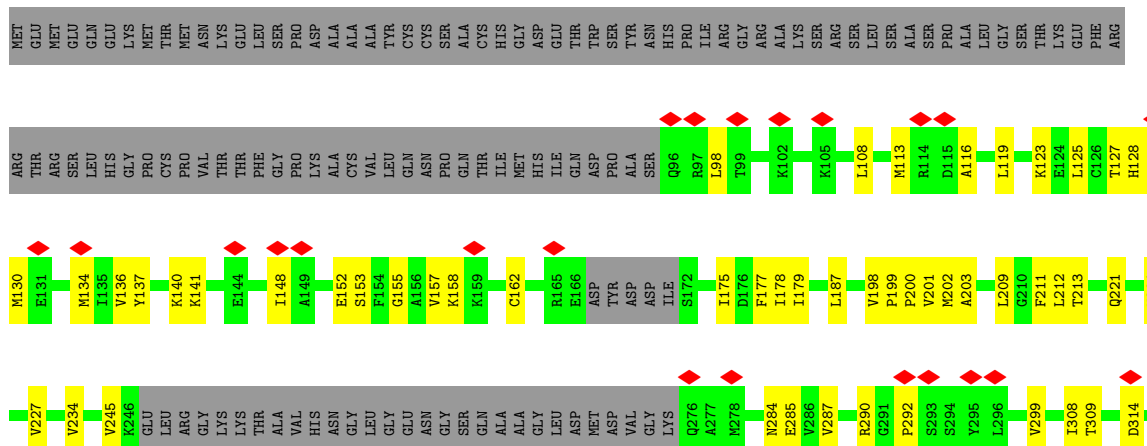




- Molecule 1: NAD kinase



- Molecule 1: NAD kinase



I317	I318	S324	T325	A329	I336	H337	M344	R356	P357	I358	V359	V360	P361	V364	K367	L370	E373	A374	R375	W379	R385	K386	E389	I390	D394	S395	I396	S397	P406	S407	I408	D412	P413	V414	S415	L421	A422	Q423	M428	V429	R430	LYS
LYS	GLN	ALA	HIS	PHE	GLU	GLU	GLU	GLU	GLU	GLU	THR	ARG	ARG	PRO	LEU	GLN	LYS	LEU	TLE	SER	GLU	GLU	GLU	ASP	LEU	ALA	ALA	ASN	ASP	TLE	LEU	ASP	TYR	LYS	ASP	ASP	ASP	ASP	LYS	VAL		

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D2	Depositor
Number of particles used	77606	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.744	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	249.0, 249.0, 249.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.27	0/2366	0.50	0/3214
1	B	0.27	0/2386	0.52	0/3240
1	C	0.27	0/2386	0.50	0/3240
1	D	0.27	0/2365	0.51	0/3213
All	All	0.27	0/9503	0.51	0/12907

There are no bond length outliers.

There are no bond angle outliers.

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	A	2315	0	2339	48	0
1	B	2335	0	2358	63	0
1	C	2335	0	2358	54	0
1	D	2314	0	2334	46	0
All	All	9299	0	9389	188	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 10.

The worst 5 of 188 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:385:ARG:HG3	1:B:386:LYS:H	1.50	0.75
1:A:412:ASP:OD1	1:A:415:SER:OG	2.04	0.74
1:D:385:ARG:HG2	1:D:386:LYS:H	1.59	0.68
1:D:389:GLU:OE2	1:D:391:ARG:NH2	2.27	0.67
1:B:123:LYS:HE2	1:B:148:ILE:HD13	1.74	0.67

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	293/477 (61%)	278 (95%)	15 (5%)	0	100	100
1	B	295/477 (62%)	276 (94%)	19 (6%)	0	100	100
1	C	295/477 (62%)	278 (94%)	17 (6%)	0	100	100
1	D	293/477 (61%)	273 (93%)	20 (7%)	0	100	100
All	All	1176/1908 (62%)	1105 (94%)	71 (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	262/413 (63%)	262 (100%)	0	100	100
1	B	264/413 (64%)	264 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	264/413 (64%)	264 (100%)	0	100	100
1	D	261/413 (63%)	261 (100%)	0	100	100
All	All	1051/1652 (64%)	1051 (100%)	0	100	100

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

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

### 5.3.3 RNA ⓘ

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 ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

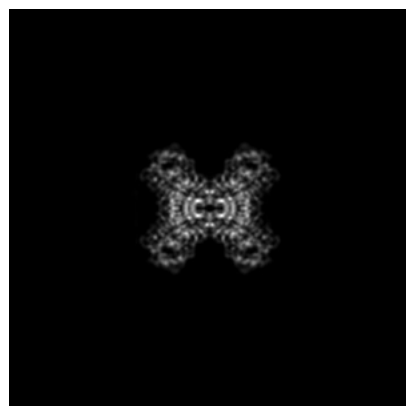
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45831. These allow visual inspection of the internal detail of the map and identification of artifacts.

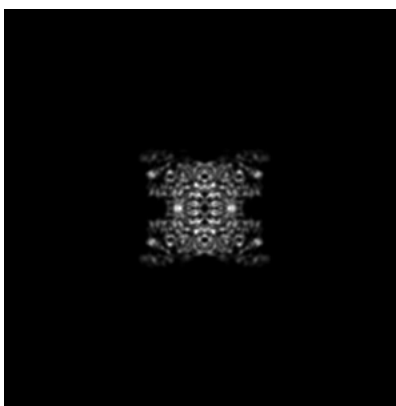
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

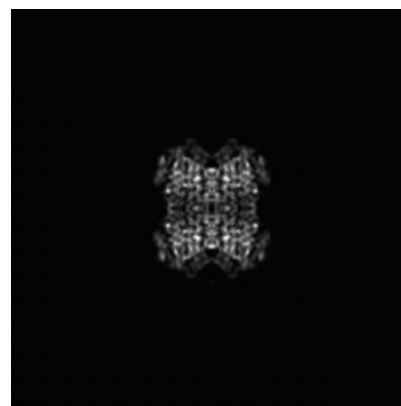
#### 6.1.1 Primary map



X

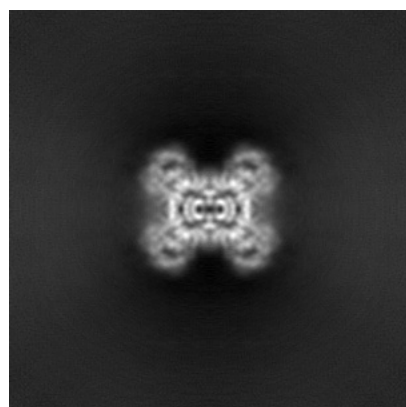


Y

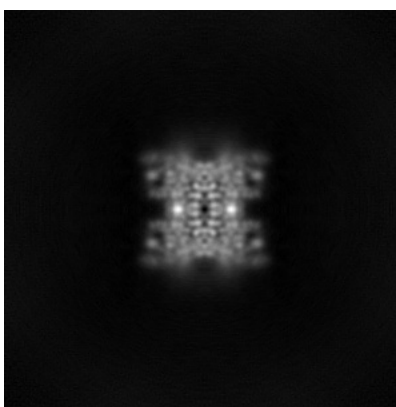


Z

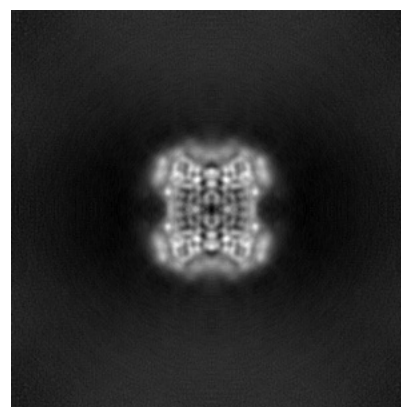
#### 6.1.2 Raw map



X



Y

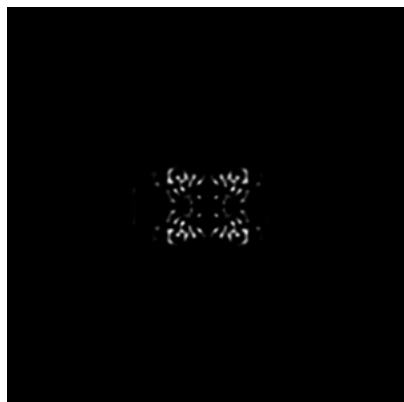


Z

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

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 150

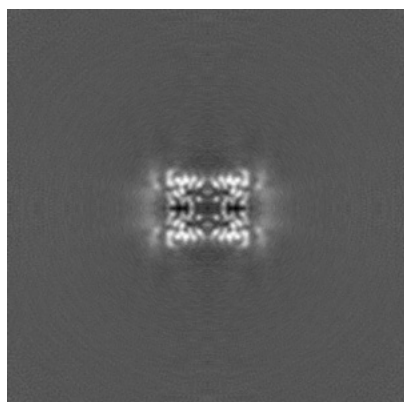


Y Index: 150

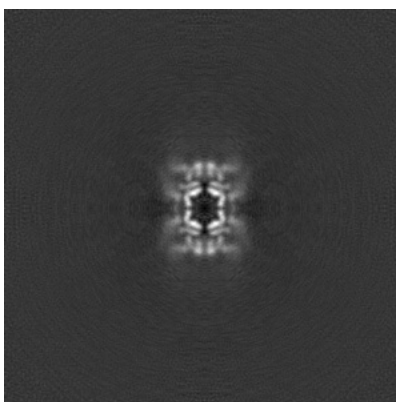


Z Index: 150

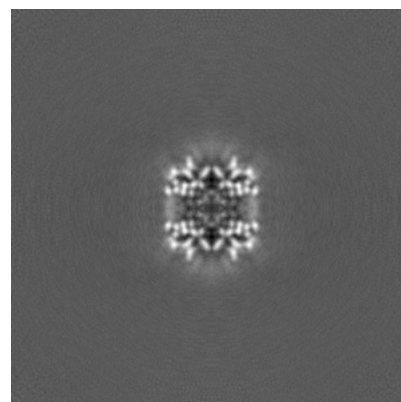
### 6.2.2 Raw map



X Index: 150



Y Index: 150



Z Index: 150

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: 161

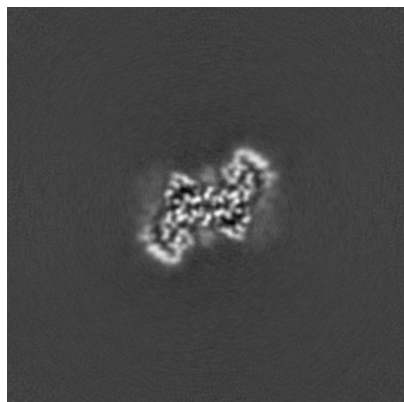


Y Index: 127

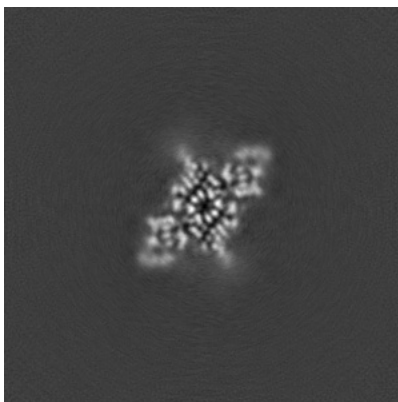


Z Index: 157

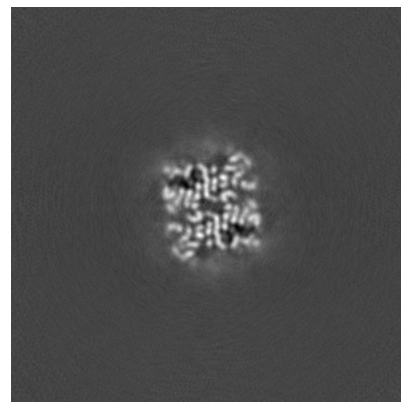
### 6.3.2 Raw map



X Index: 139



Y Index: 127

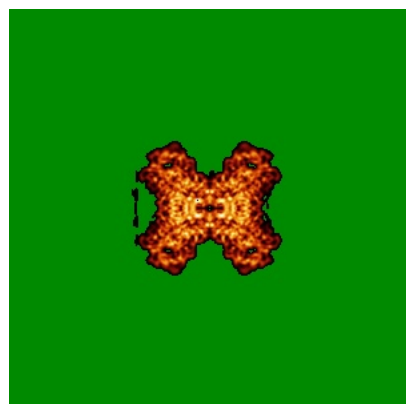


Z Index: 144

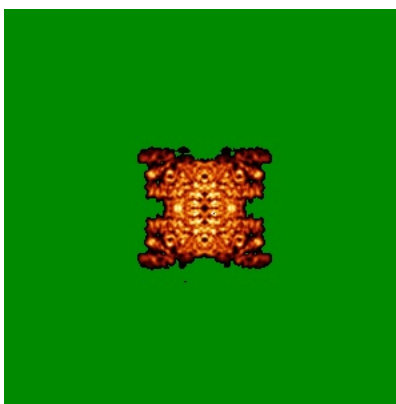
The images above show the largest variance slices of the map in three orthogonal directions.

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

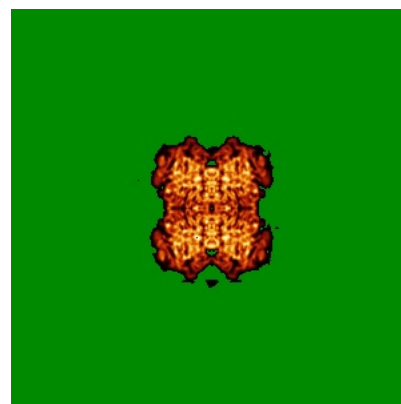
### 6.4.1 Primary map



X

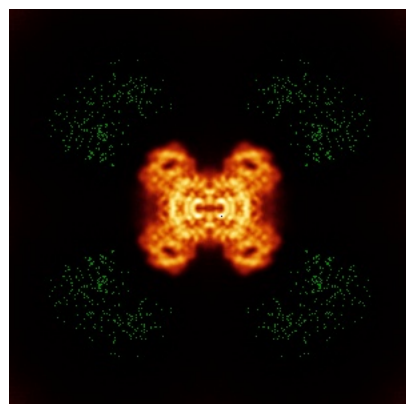


Y

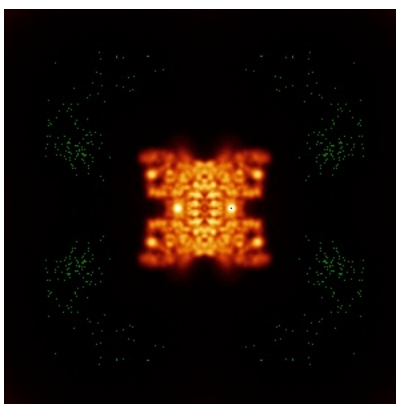


Z

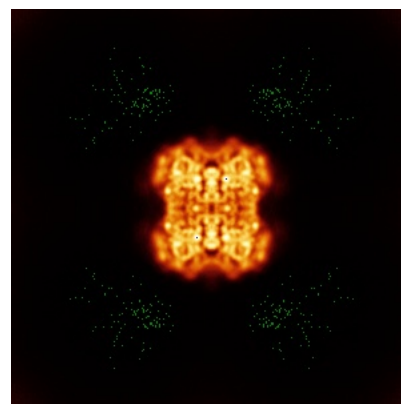
### 6.4.2 Raw map



X



Y

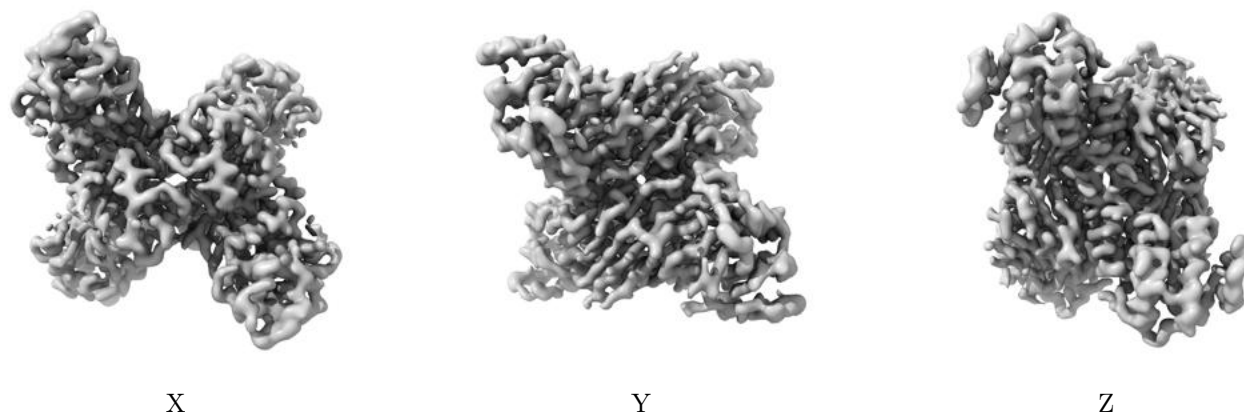


Z

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.

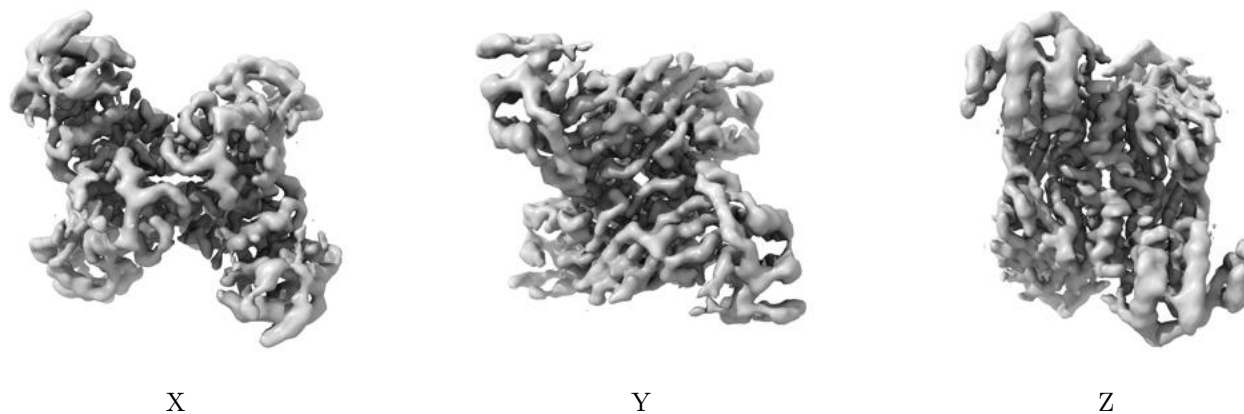
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

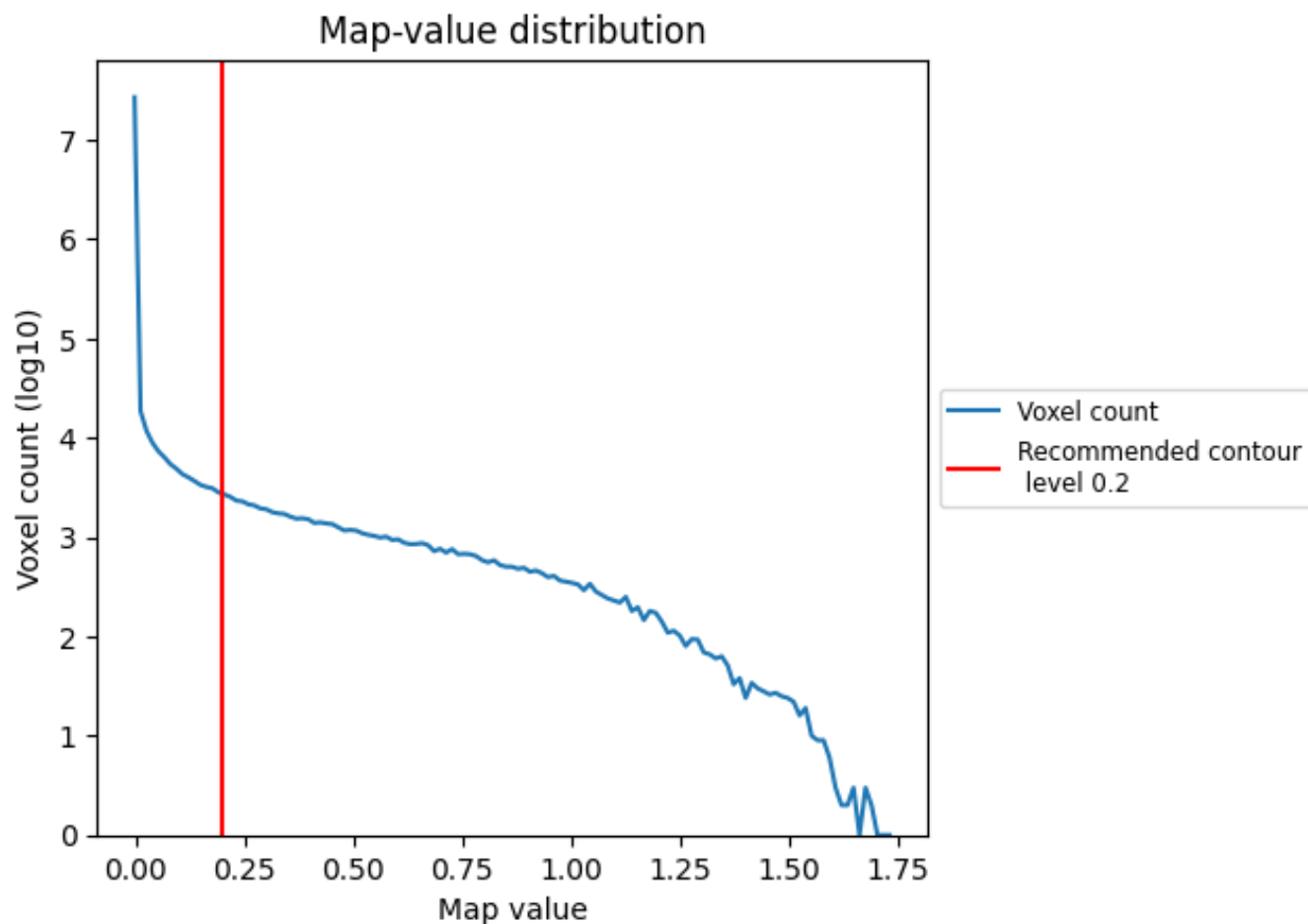
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

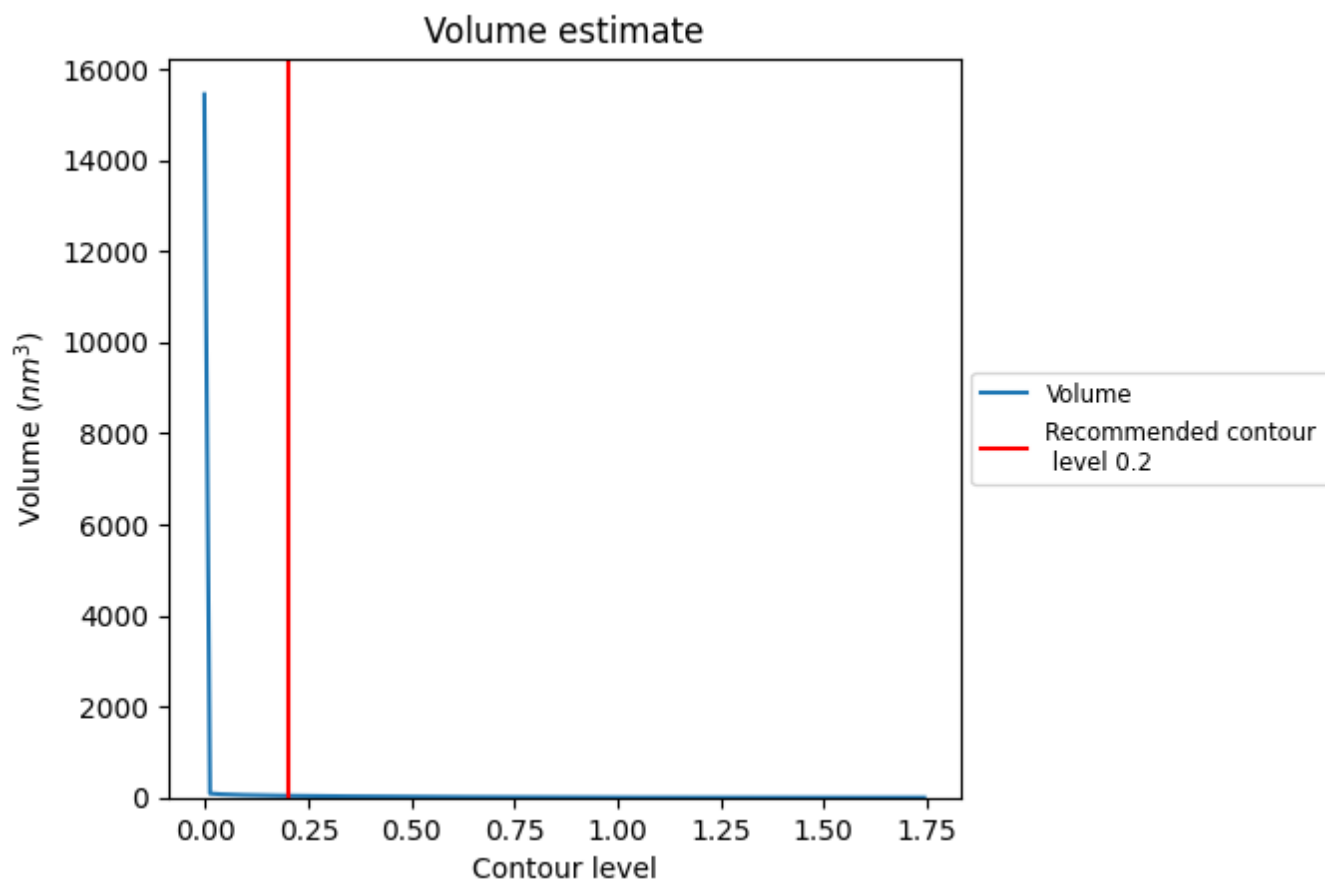
This section contains the results of statistical analysis of the map.

### 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.

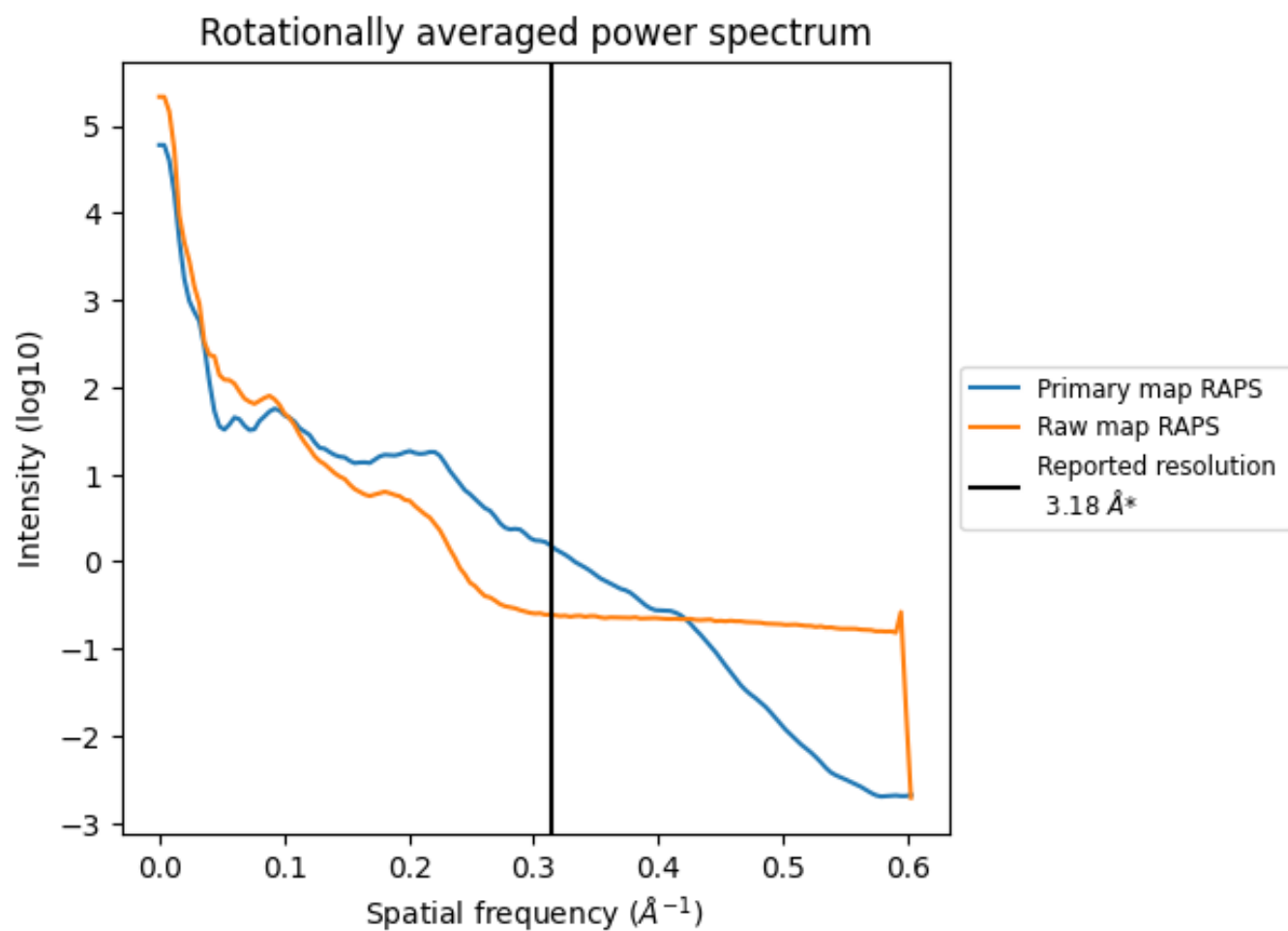
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 40  $\text{nm}^3$ ; this corresponds to an approximate mass of 36 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 ⓘ

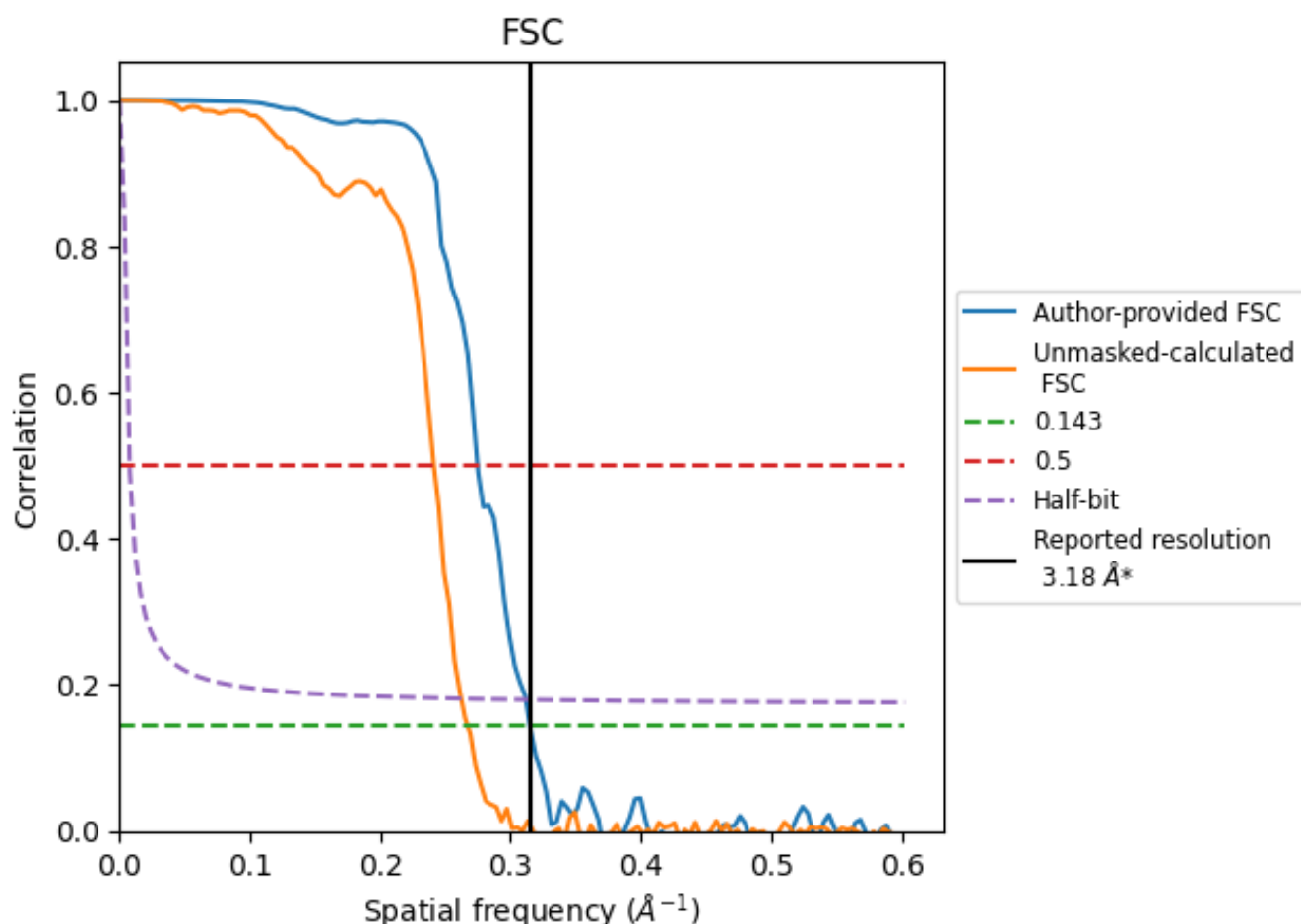


\*Reported resolution corresponds to spatial frequency of 0.314 Å<sup>-1</sup>

## 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 0.314 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

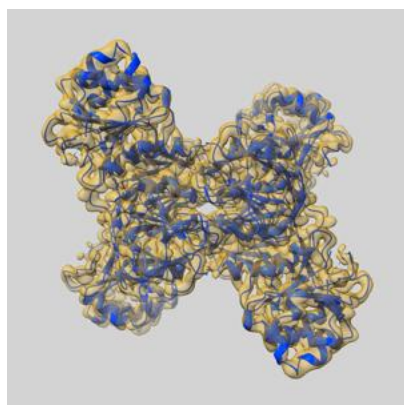
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.18	-	-
Author-provided FSC curve	3.18	3.64	3.21
Unmasked-calculated*	3.74	4.15	3.81

\*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 3.74 differs from the reported value 3.18 by more than 10 %

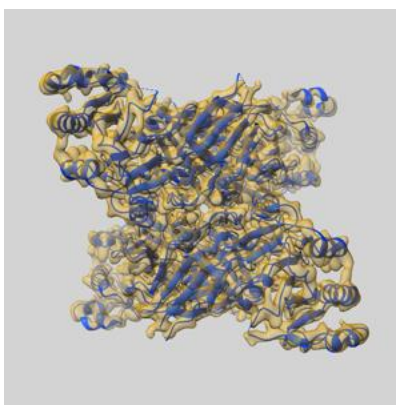
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45831 and PDB model 9CR3. Per-residue inclusion information can be found in section [3](#) on page [7](#).

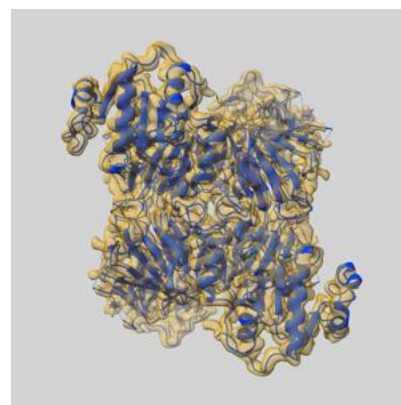
### 9.1 Map-model overlay [i](#)



X



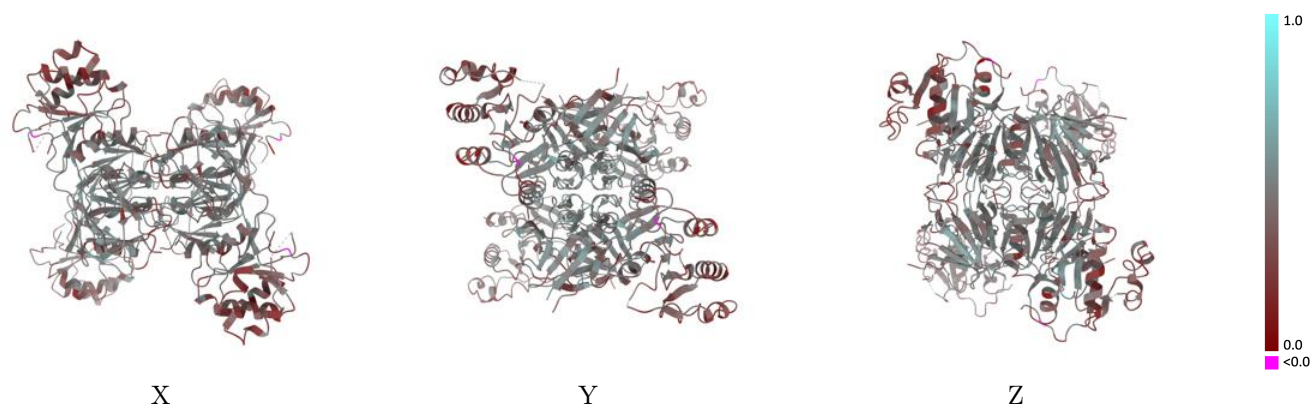
Y



Z

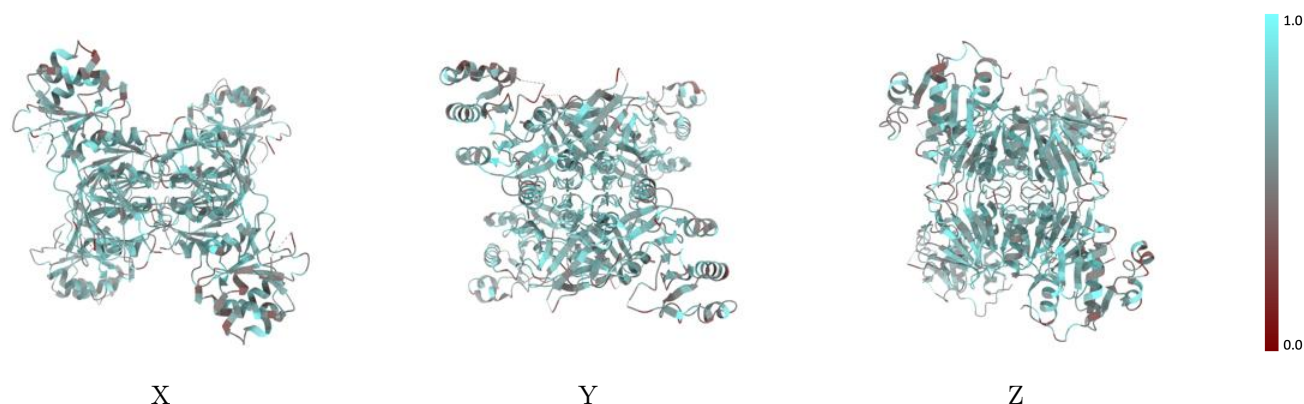
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



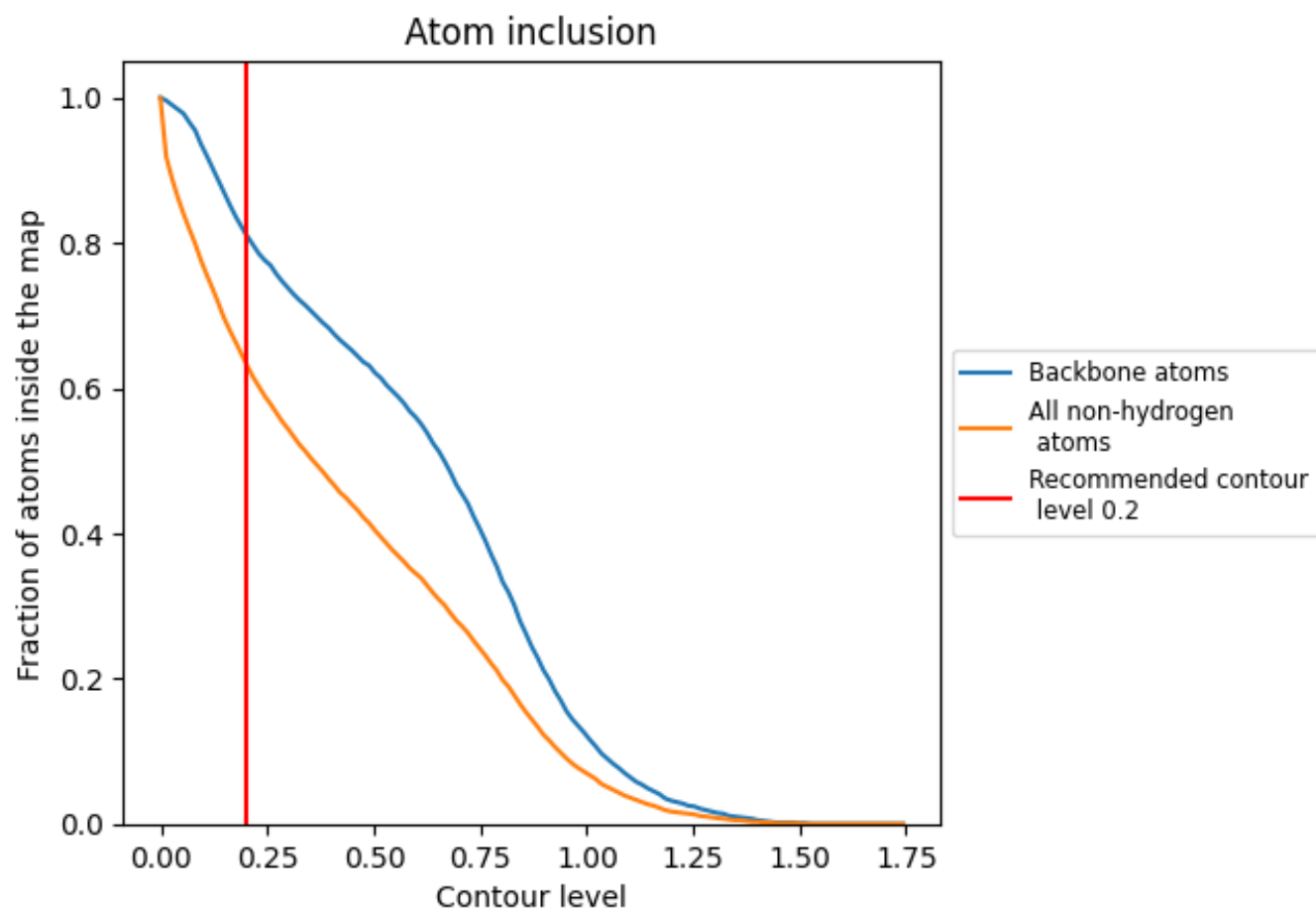
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 63% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6330	<div></div> 0.4100
A	<div></div> 0.6310	<div></div> 0.4090
B	<div></div> 0.6280	<div></div> 0.4080
C	<div></div> 0.6380	<div></div> 0.4150
D	<div></div> 0.6330	<div></div> 0.4090

