



## wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 03:50 AM EDT

PDB ID : 8SL1  
EMDB ID : EMD-40571  
Title : Cryo-EM structure of PAPP-A2  
Authors : Judge, R.A.; Stoll, V.S.; Eaton, D.; Hao, Q.; Bratkowski, M.A.  
Deposited on : 2023-04-20  
Resolution : 3.13 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  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

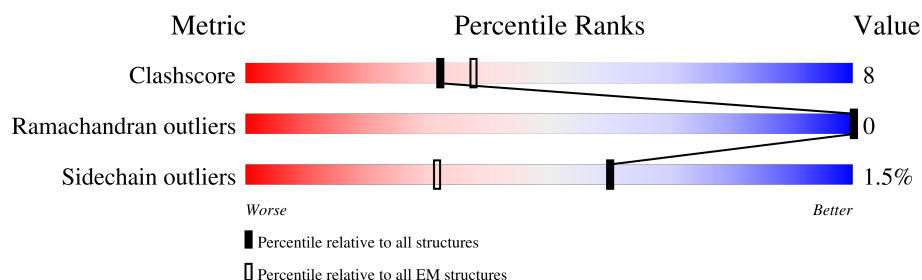
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.13 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	1570	
2	B	2	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6608 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.

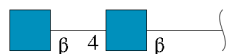
- Molecule 1 is a protein called Pappalysin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	843	6562	4133	1115	1269	45	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	500	GLN	GLU	conflict	UNP Q9BXP8
A	1558	THR	-	expression tag	UNP Q9BXP8
A	1559	ARG	-	expression tag	UNP Q9BXP8
A	1560	THR	-	expression tag	UNP Q9BXP8
A	1561	GLY	-	expression tag	UNP Q9BXP8
A	1562	GLY	-	expression tag	UNP Q9BXP8
A	1563	ASP	-	expression tag	UNP Q9BXP8
A	1564	TYR	-	expression tag	UNP Q9BXP8
A	1565	LYS	-	expression tag	UNP Q9BXP8
A	1566	ASP	-	expression tag	UNP Q9BXP8
A	1567	ASP	-	expression tag	UNP Q9BXP8
A	1568	ASP	-	expression tag	UNP Q9BXP8
A	1569	ASP	-	expression tag	UNP Q9BXP8
A	1570	LYS	-	expression tag	UNP Q9BXP8

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	2	28	16	2	10	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
5	A	2	Total	Ca	0
			2	2	

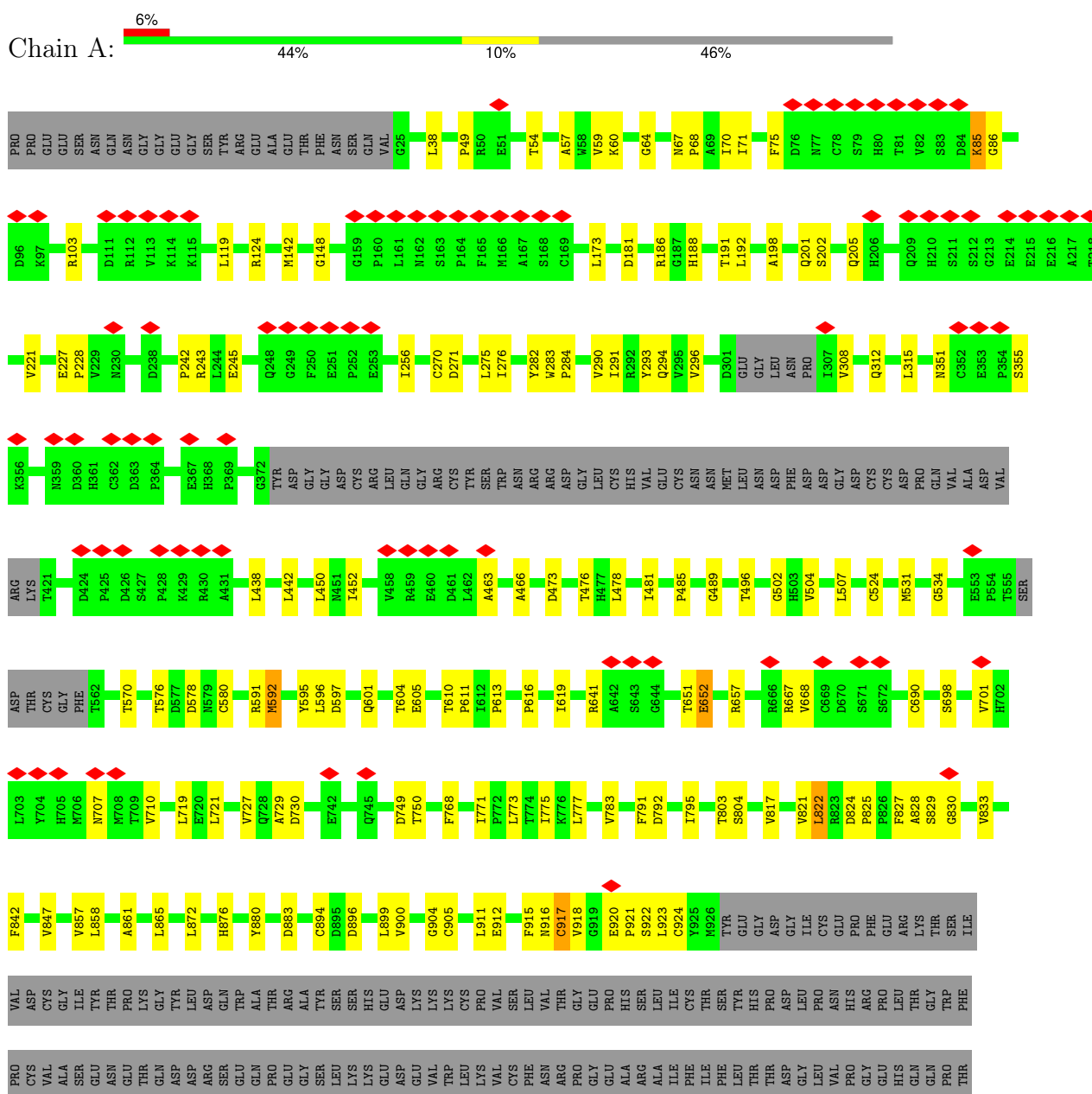
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	O	0
			1	1	

### 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: Pappalysin-2



LEU	ARG	PRO	PRO	LEU	PHE	MET	LEU	VAL
ASP	ARG	SER	GLU	LEU	SER	LYS	ARG	THR
GLU	GLN	GLU	PRO	PRO	CYS	PRO	THR	LEU
THR	TRP	LEU	HIS	HIS	SER	ALA	SER	THR
CYS	HIS	ASN	VAL	CYS	GLU	ILE	SER	LEU
PRO	PRO	SER	PHE	LEU	GLY	THR	ARG	THR
ASP	ASP	VAL	GLU	GLN	THR	CYS	ILE	ASP
PRO	PRO	GLU	GLY	ASP	LYS	GLN	GLY	VAL
LYS	LEU	TYR	MET	ASN	PHE	ARG	LEU	ARG
ALA	VAL	LYS	TYR	HIS	LEU	GLY	SER	GLY
GLU	HIS	CYS	GLU	ASP	LYS	PHE	ALA	SER
GLU	CYS	GLN	CYS	VAL	ARG	ALA	PRO	ASN
ASN	ILE	GLY	THR	GLY	CYS	LEU	SER	HIS
GLN	GLN	TYR	ASN	THR	ILE	GLN	CYS	LEU
THR	SER	GLY	PHE	CYS	SER	SER	ILE	THR
ARG	CYS	ILE	SER	LYS	CYS	SER	SER	GLY
THR	GLU	GLY	LEU	TYR	VAL	GLY	GLU	TYR
GLY	PRO	ALA	ASP	GLU	PRO	GLN	ASP	GLY
GLY	PHE	VAL	SER	ASP	PRO	GLN	GLU	LEU
ASP	GLN	CYS	GLN	LYS	ALA	ILE	GLY	LEU
ASP	ALA	SER	CYS	PRO	LYS	ARG	GLN	CYS
LYS	ASP	PRO	VAL	GLY	LEU	PRO	ASN	GLN
ASP	GLY	LEU	LEU	TYR	GLN	MET	HIS	ASN
ASP	TRP	CYS	ASN	TYR	GLY	GLN	ASN	ASN
ASP	CYS	VAL	VAL	VAL	LEU	LYS	GLY	PRO
LYS	ASP	PRO	THR	GLU	SER	ILE	GLN	LEU
	ILE	PRO	GLU	GLU	TRP	ILE	CYS	ILE
	ASN	SER	ARG	ALA	LEU	LEU	ILE	ASN
	ASN	ASP	GLU	GLU	THR	THR	HIS	THR
	ARG	PRO	LYS	GLY	CYS	CYS	ARG	THR
	ALA	VAL	LEU	GLY	GLU	TRP	VAL	THR
	TYR	MET	ILE	ASN	ASP	GLY	LYS	ASN
	THR	PRO	LEU	ASN	GLY	HIS	CYS	ASN
	GLY	LEU	ILE	LYS	ASN	VAL	ASP	THR
	GLY	GLU	GLY	ILE	GLY	VAL	HIS	ASN
	ASP	THR	GLU	GLY	GLU	ASP	LEU	THR
	THR	GLU	THR	GLY	VAL	CYS	LEU	THR
	GLY	GLU	GLN	GLY	THR	PRO	LEU	VAL
	GLY	HIS	GLU	GLY	LYS	VAL	ASP	VAL
	THR	TRP	PHE	ILE	ASP	CYS	HIS	ASN
	SER	MET	LYS	ILE	GLY	THR	ALA	LEU
	SER	GLU	LEU	TRP	GLU	GLY	ASP	ASN
	SER	GLU	LEU	TRP	GLY	ASP	ALA	ASP
	SER	GLU	LEU	TRP	GLY	GLY	ALA	PHE
	LYS	PRO	CYS	GLU	CYS	GLY	VAL	SER
	LYS	VAL	VAL	GLN	PRO	VAL	VAL	SER
	VAL	LYS	ASN	GLY	ASP	ASP	ASN	ARG
	ILE	VAL	VAL	SER	PRO	SER	CYS	PRO
	PRO	GLN	GLN	CYS	ILE	SER	THR	VAL
	PHE	SER	GLY	ILE	THR	LEU	SER	GLY
	ALA	ILE	GLY	PRO	ILE	VAL	ILE	THR
	ALA	VAL	CYS	VAL	ASN	ASN	GLY	SER
	ASP	CYS	THR	VAL	ALA	TYR	PRO	ALA
	CYS	THR	GLY	CYS	ASN	ASN	GLY	VAL
	ASP	GLY	PRO	CYS	THR	ALA	GLY	ALA

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:



100%

NAG1  
NAG2

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	105000	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)	1400	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.791	Depositor
Minimum map value	-1.930	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.265	Depositor
Map size (Å)	240.84001, 240.84001, 240.84001	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.669, 0.669, 0.669	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: CA, ZN, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.26	0/6744	0.49	0/9201

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	6562	0	6217	108	0
2	B	28	0	25	0	0
3	A	1	0	0	0	0
4	A	14	0	13	0	0
5	A	2	0	0	0	0
6	A	1	0	0	0	0
All	All	6608	0	6255	108	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 8.

The worst 5 of 108 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:A:821:VAL:HG22	1:A:857:VAL:HG12	1.58	0.86
1:A:894:CYS:SG	1:A:911:LEU:HD12	2.19	0.82
1:A:822:LEU:HD11	1:A:858:LEU:HD11	1.63	0.80
1:A:894:CYS:HB2	1:A:905:CYS:CB	2.15	0.75
1:A:119:LEU:HD11	1:A:142:MET:HG3	1.69	0.75

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	835/1570 (53%)	793 (95%)	42 (5%)	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	734/1383 (53%)	723 (98%)	11 (2%)	60	78

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	652	GLU
1	A	791	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	917	CYS
1	A	822	LEU
1	A	351	ASN

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](#)

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	B	1	1,2	14,14,15	0.20	0	17,19,21	0.43	0
2	NAG	B	2	2	14,14,15	0.22	0	17,19,21	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

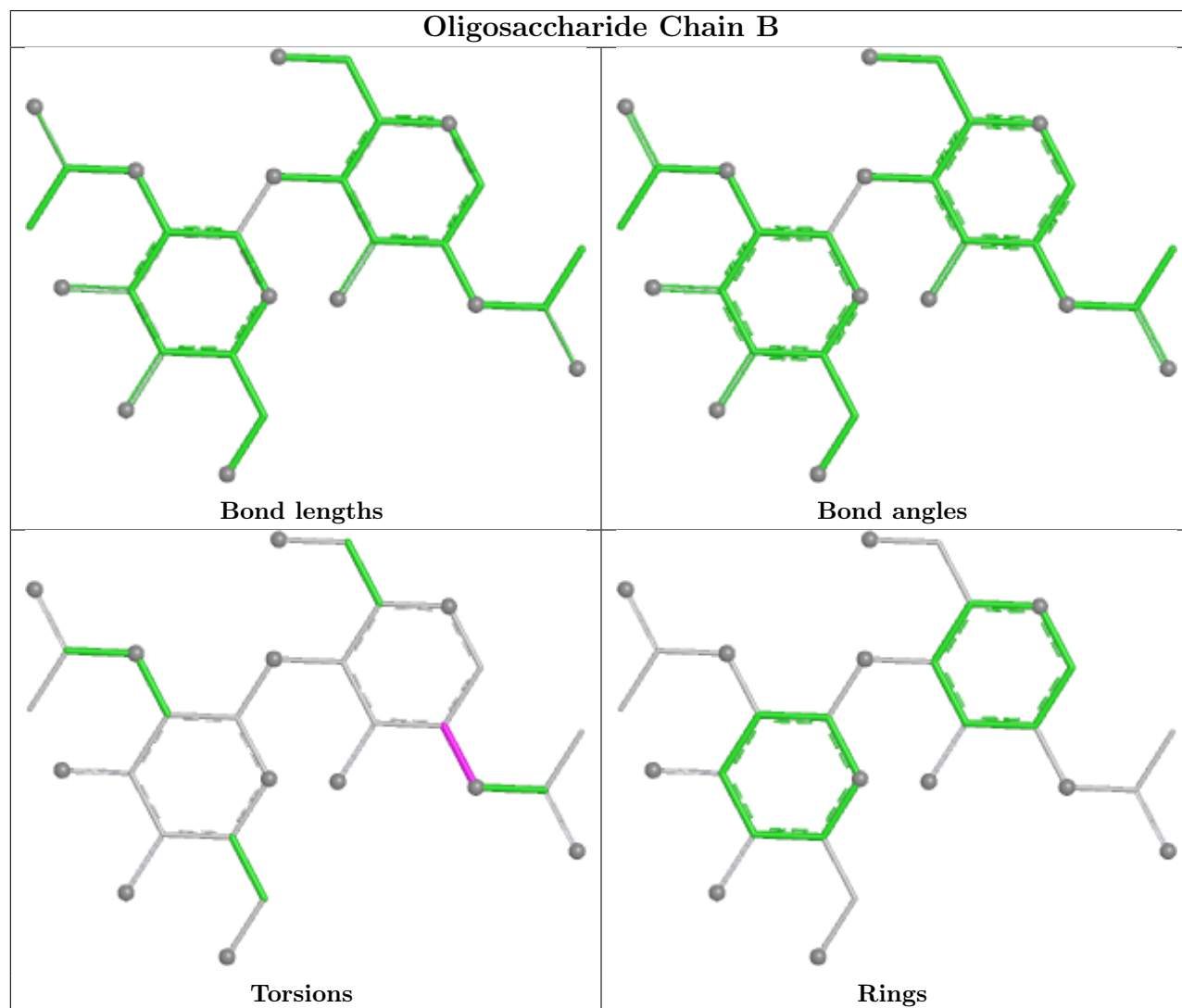
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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	1802	1	14,14,15	0.22	0	17,19,21	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1802	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1802	NAG	C4-C5-C6-O6
4	A	1802	NAG	O5-C5-C6-O6
4	A	1802	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

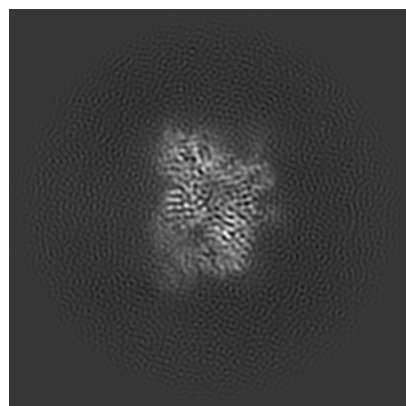
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40571. These allow visual inspection of the internal detail of the map and identification of artifacts.

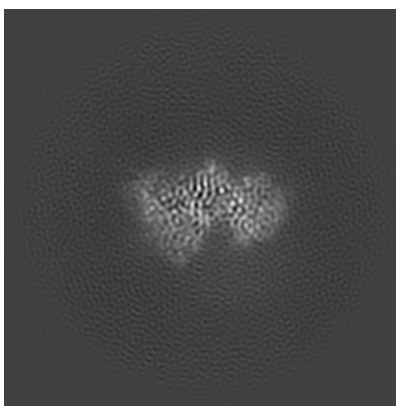
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

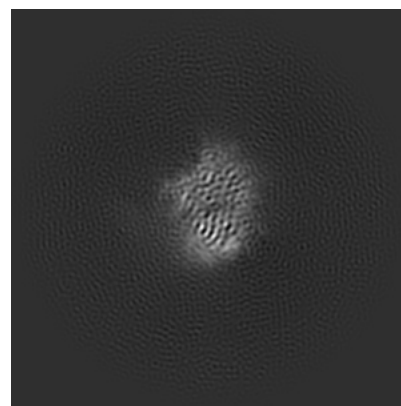
#### 6.1.1 Primary map



X

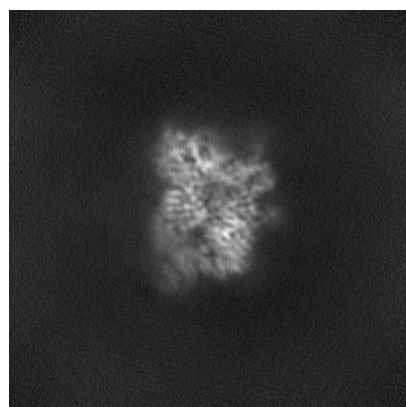


Y

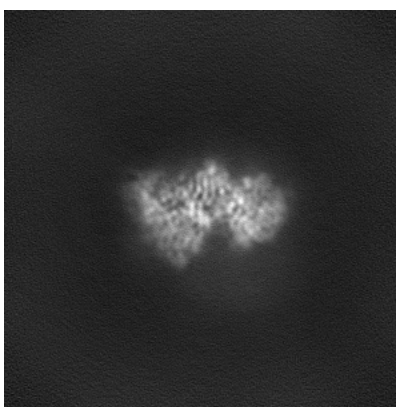


Z

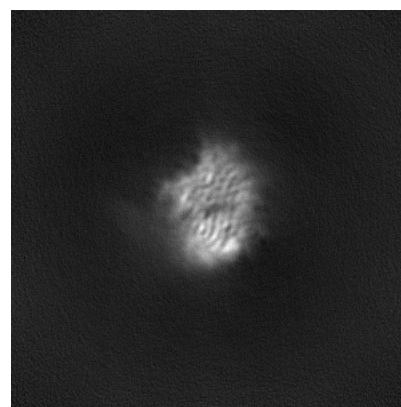
#### 6.1.2 Raw map



X



Y

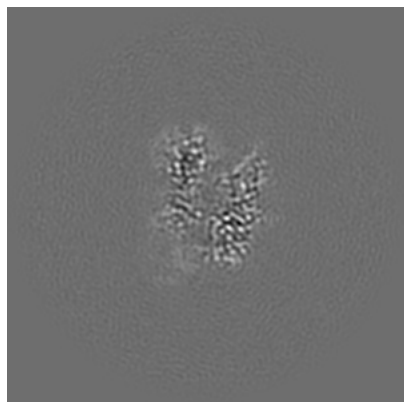


Z

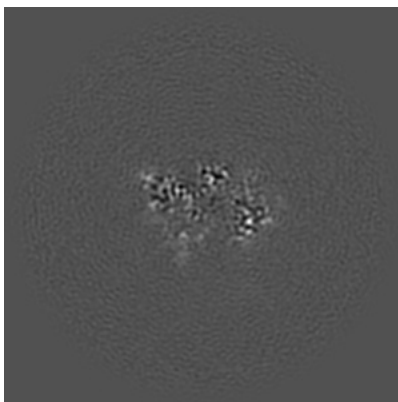
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

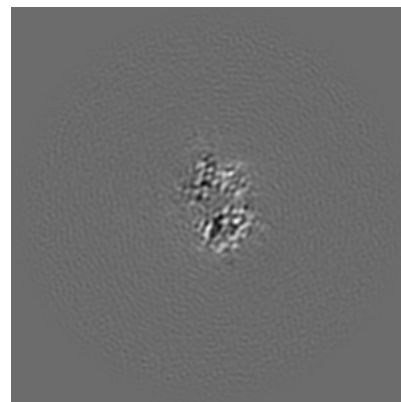
### 6.2.1 Primary map



X Index: 180

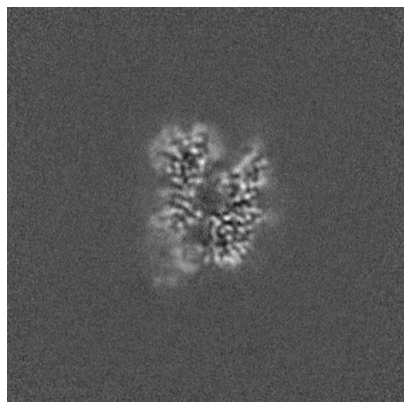


Y Index: 180

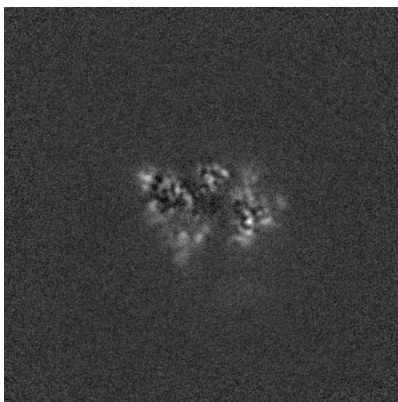


Z Index: 180

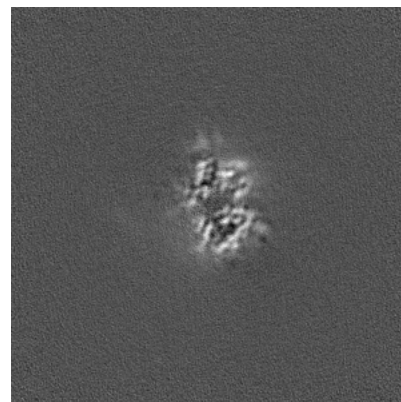
### 6.2.2 Raw map



X Index: 180



Y Index: 180



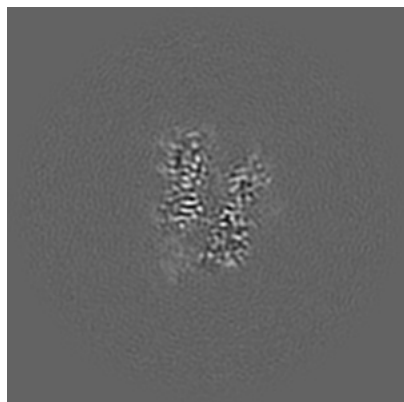
Z Index: 180

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

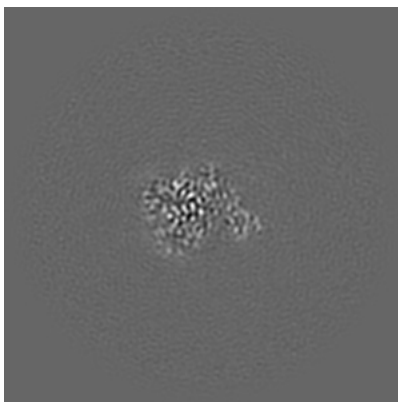


## 6.3 Largest variance slices [i](#)

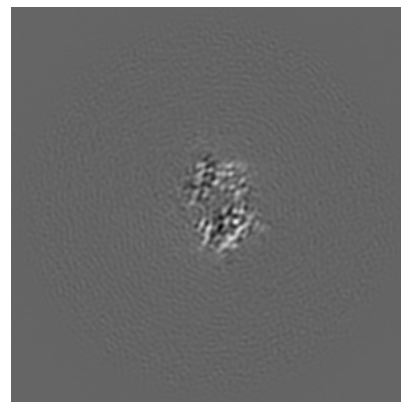
### 6.3.1 Primary map



X Index: 185

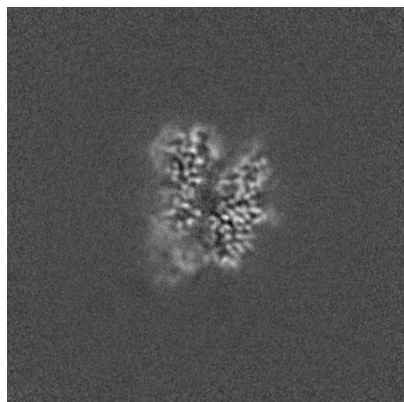


Y Index: 198

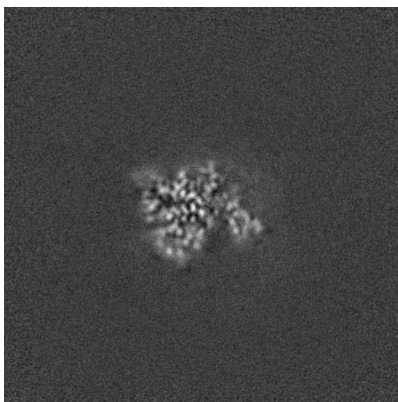


Z Index: 181

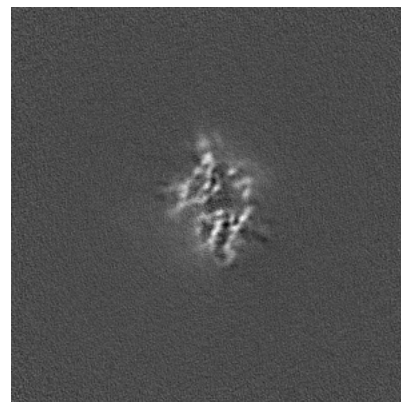
### 6.3.2 Raw map



X Index: 178



Y Index: 197



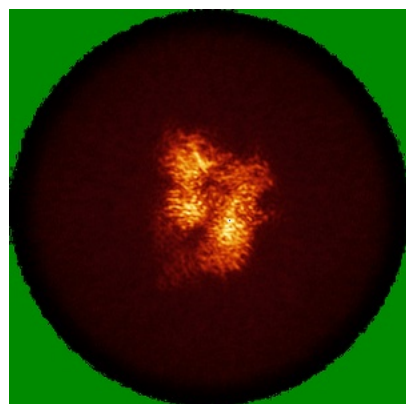
Z Index: 176

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

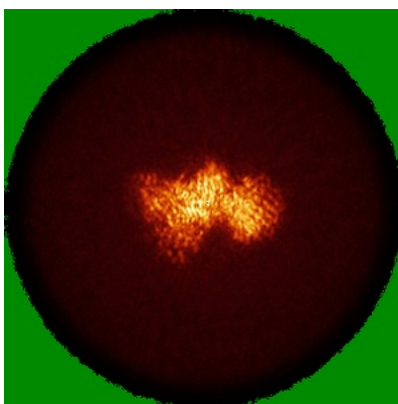


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

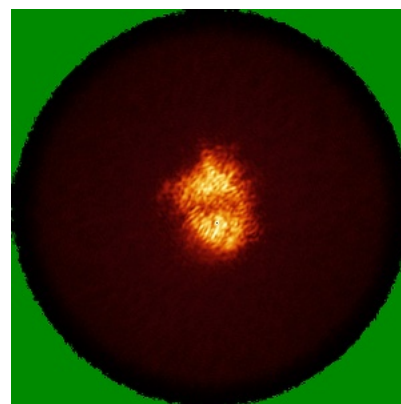
### 6.4.1 Primary map



X

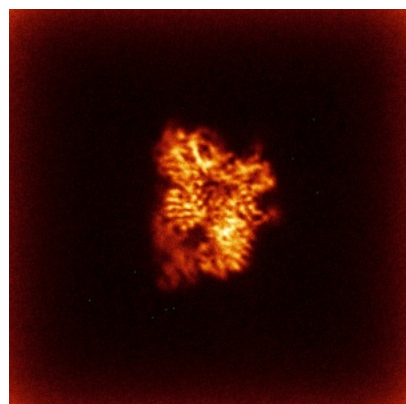


Y

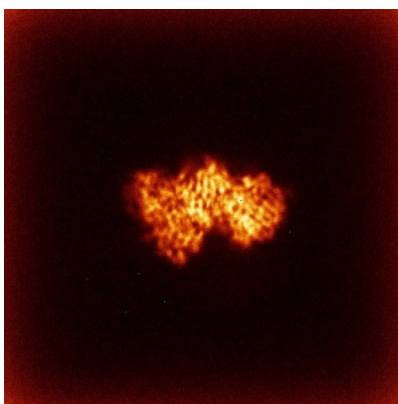


Z

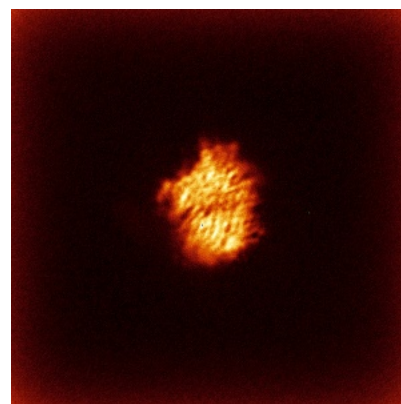
### 6.4.2 Raw map



X



Y

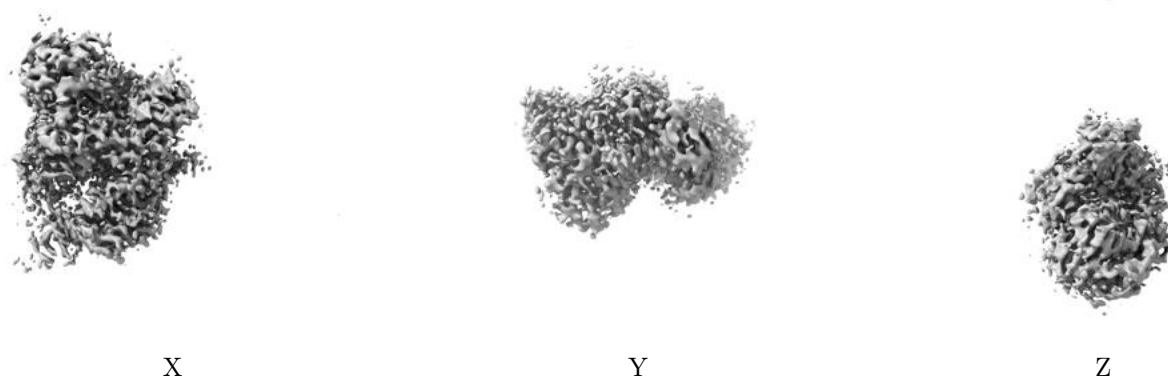


Z

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.

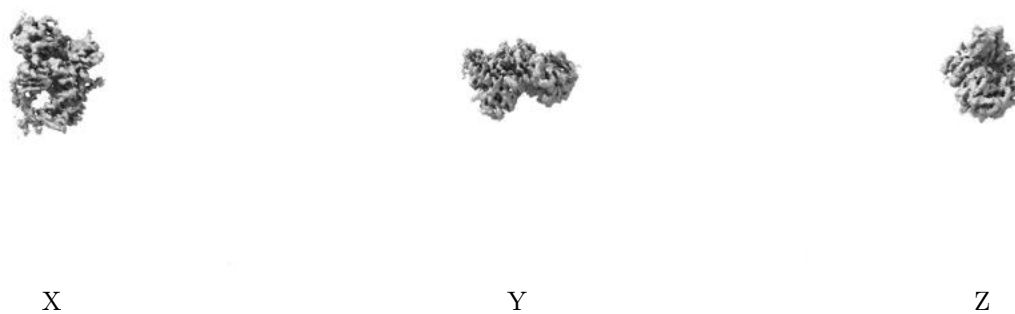
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.265. 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.

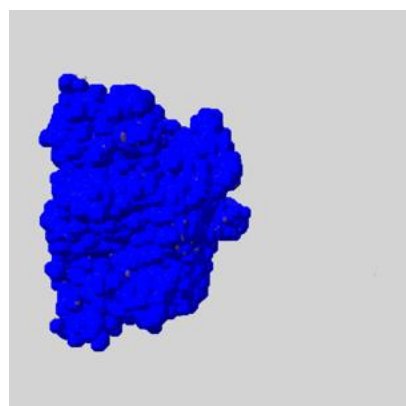
## 6.6 Mask visualisation [i](#)

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

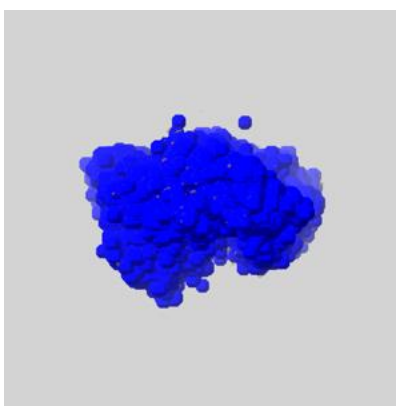
A mask typically either:

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

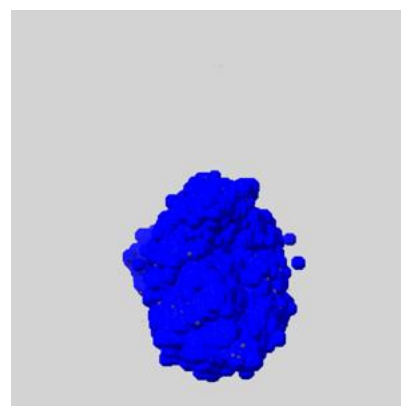
### 6.6.1 emd\_40571\_msk\_1.map [i](#)



X



Y

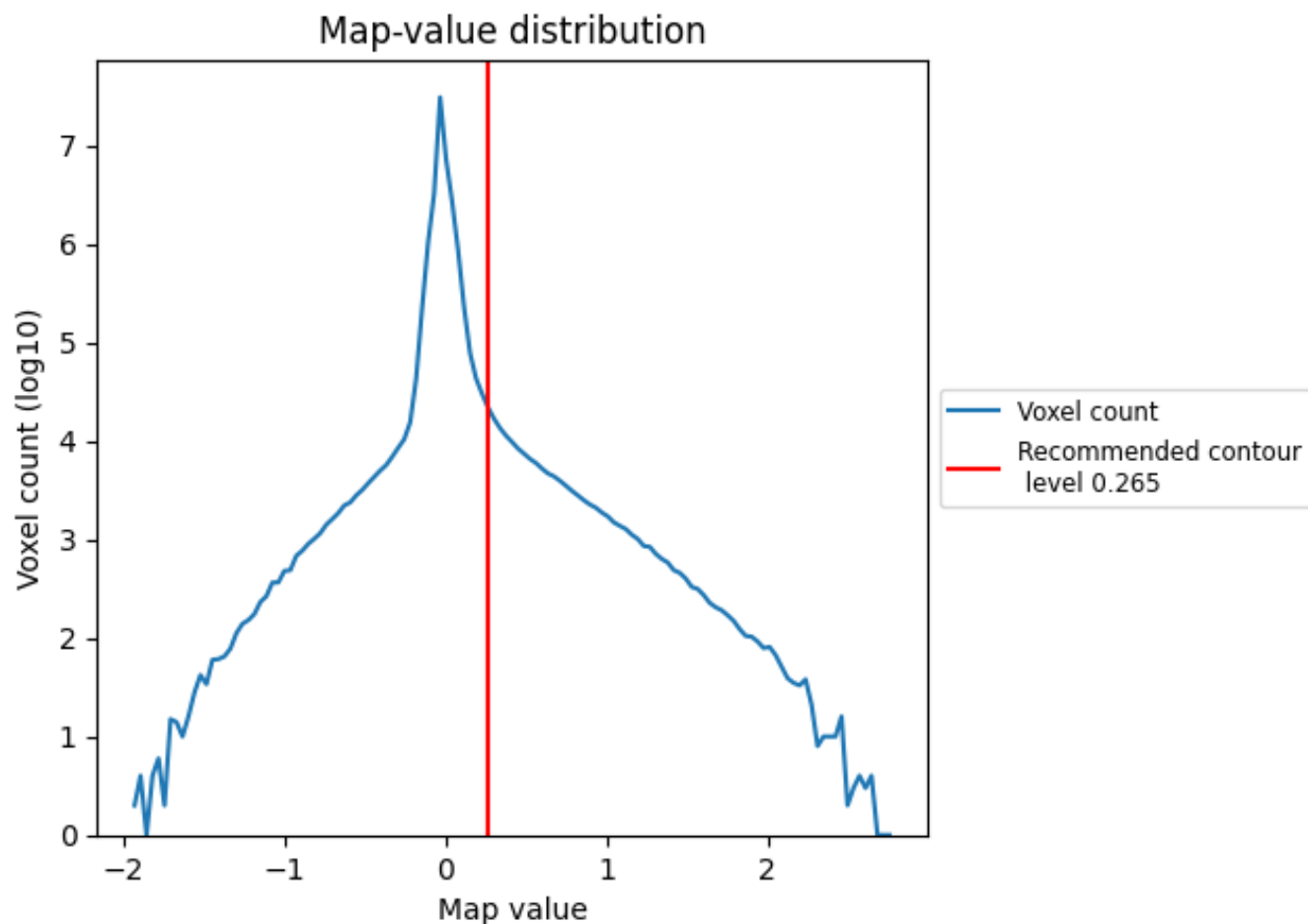


Z

## 7 Map analysis [i](#)

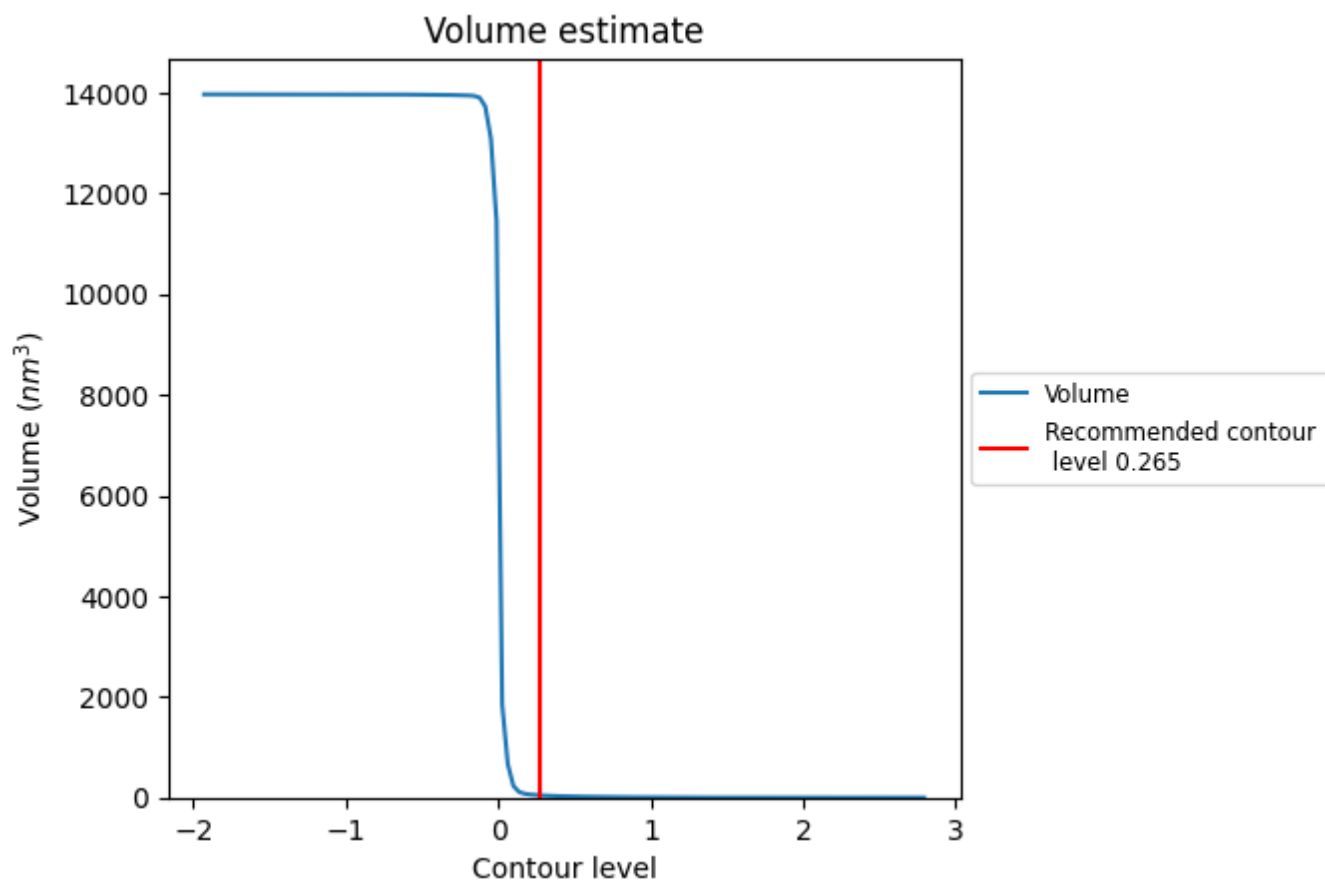
This section contains the results of statistical analysis of the map.

### 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.

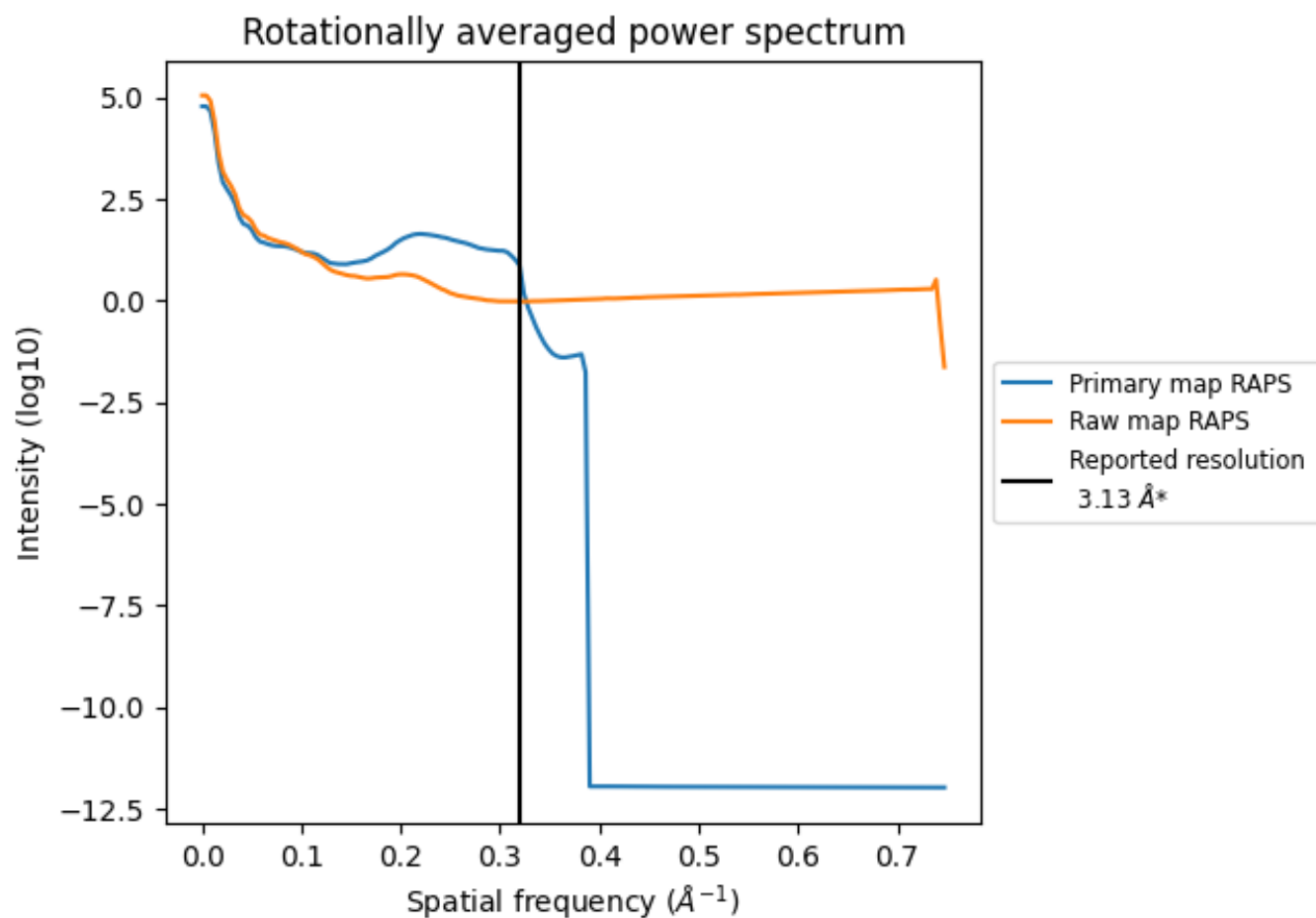
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 46 nm<sup>3</sup>; this corresponds to an approximate mass of 42 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 ⓘ

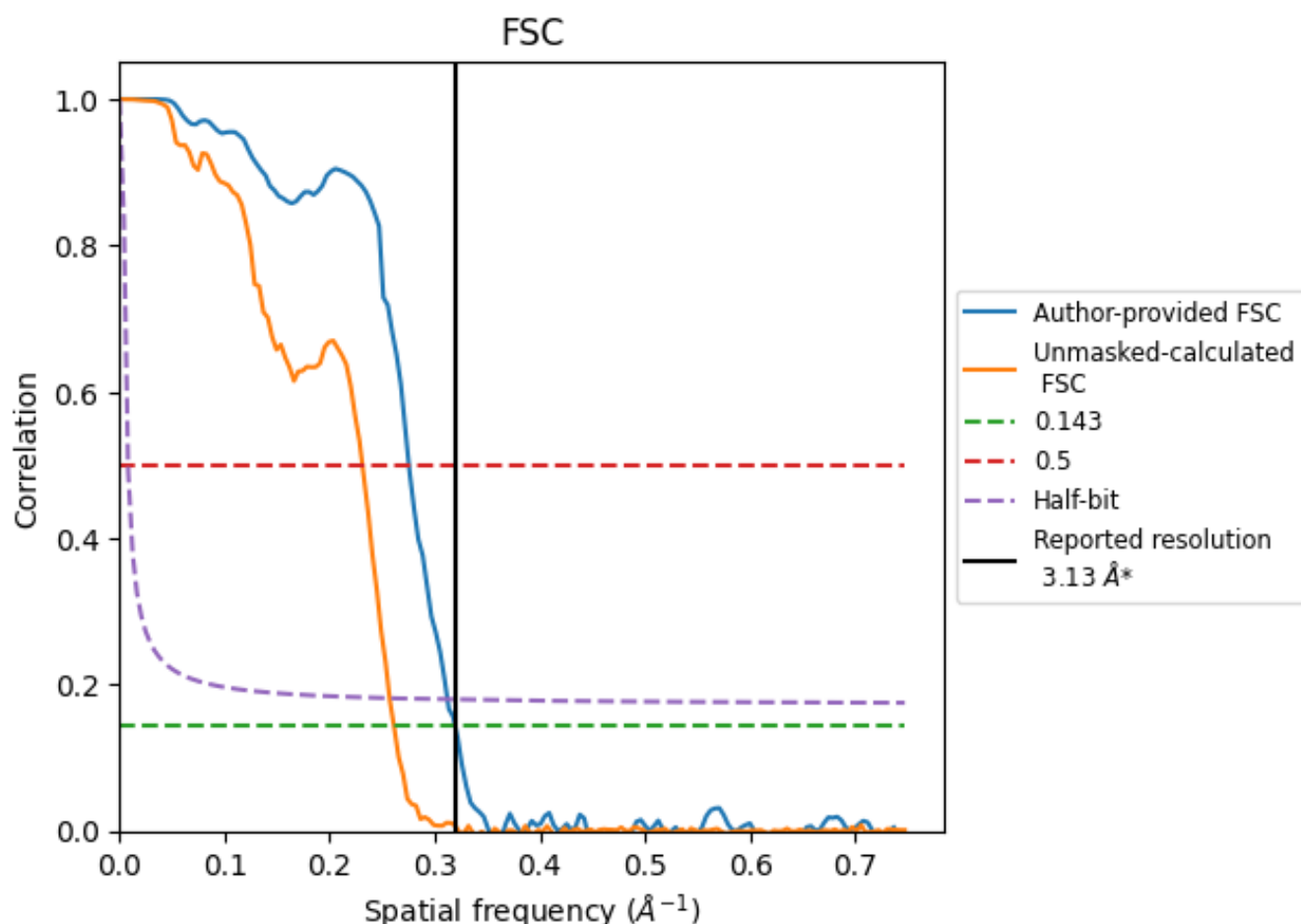


\*Reported resolution corresponds to spatial frequency of 0.319 Å<sup>-1</sup>

## 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 0.319 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	3.13	-	-
Author-provided FSC curve	3.13	3.63	3.20
Unmasked-calculated*	3.83	4.33	3.89

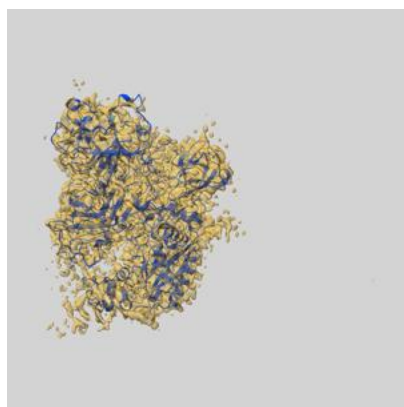
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.83 differs from the reported value 3.13 by more than 10 %



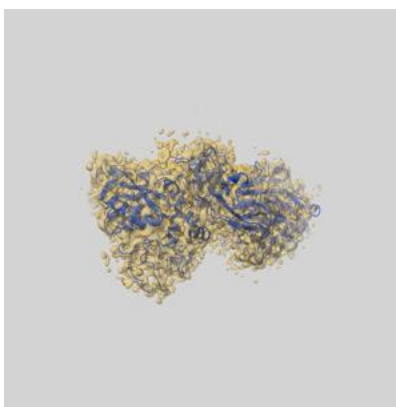
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40571 and PDB model 8SL1. Per-residue inclusion information can be found in section [3](#) on page [5](#).

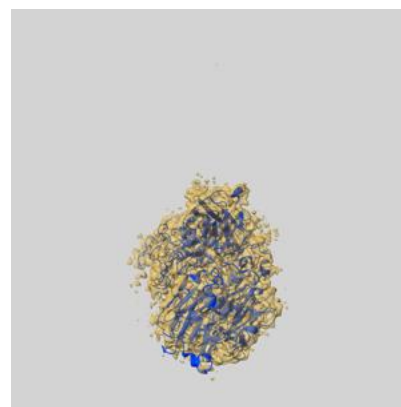
### 9.1 Map-model overlay [i](#)



X



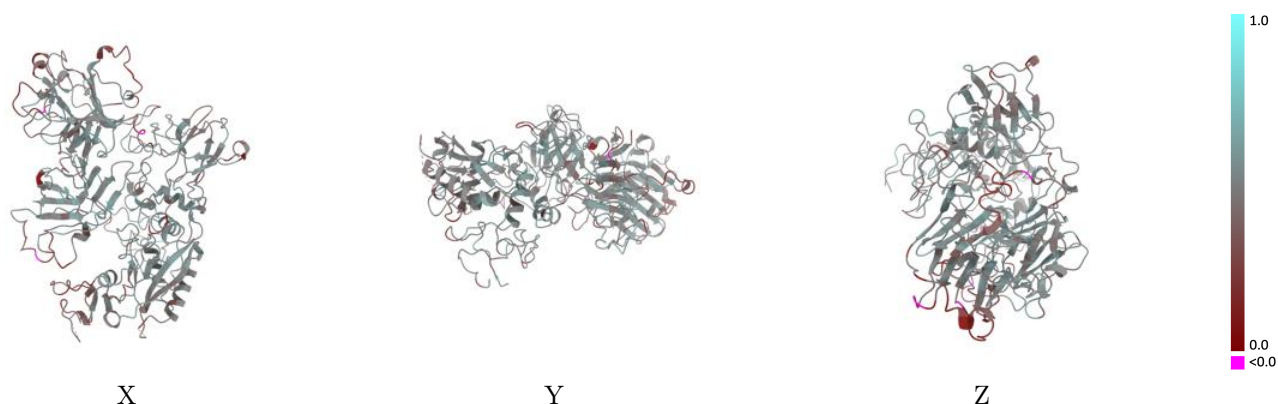
Y



Z

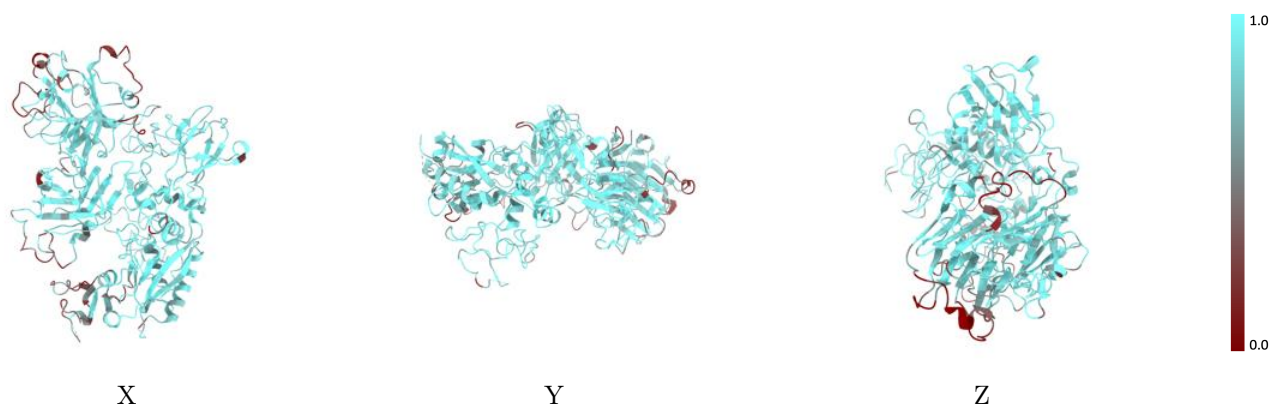
The images above show the 3D surface view of the map at the recommended contour level 0.265 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



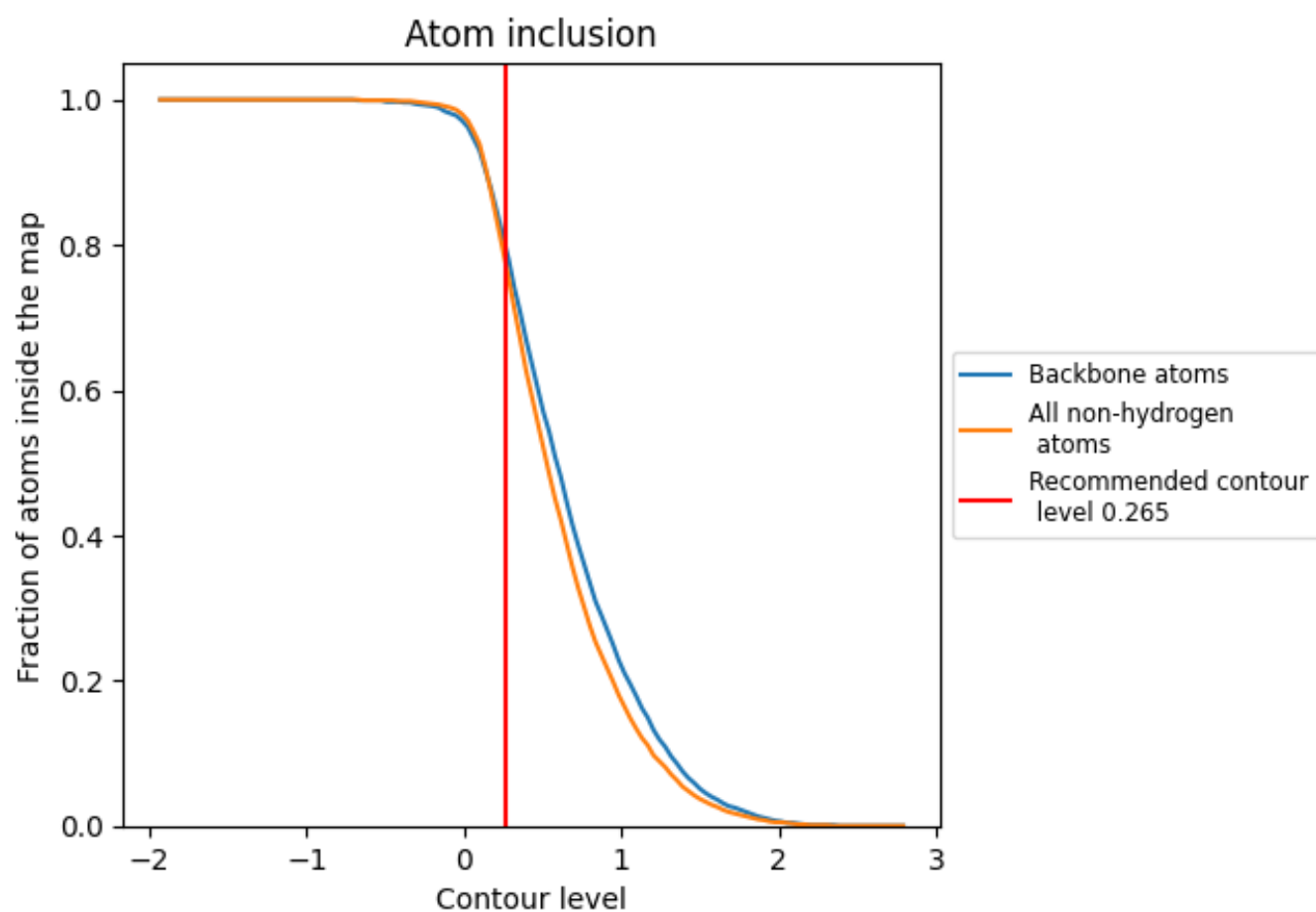
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.265).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 77% 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 (0.265) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7740	<div></div> 0.4660
A	<div></div> 0.7730	<div></div> 0.4650
B	<div></div> 1.0000	<div></div> 0.5930

