



## Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 05:03 AM EST

PDB ID : 7T7V  
EMDB ID : EMD-25739  
Title : Munc13-1 C1-C2B-MUN-C2C Lateral conformation on lipid bilayer surface  
Authors : Grushin, K.; Sindelar, C.V.  
Deposited on : 2021-12-15  
Resolution : 10.00 Å(reported)

This is a Full wwPDB EM Validation 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  
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) : 2.31.3

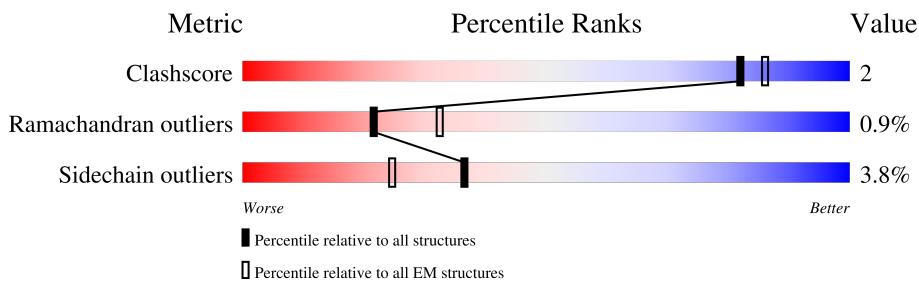
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 10.00 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	1154	<div> <div>10%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18010 atoms, of which 8976 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 Protein unc-13 homolog A.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1132	Total	C	H	N	O	S	0	0
			18010	5715	8976	1545	1719	55		

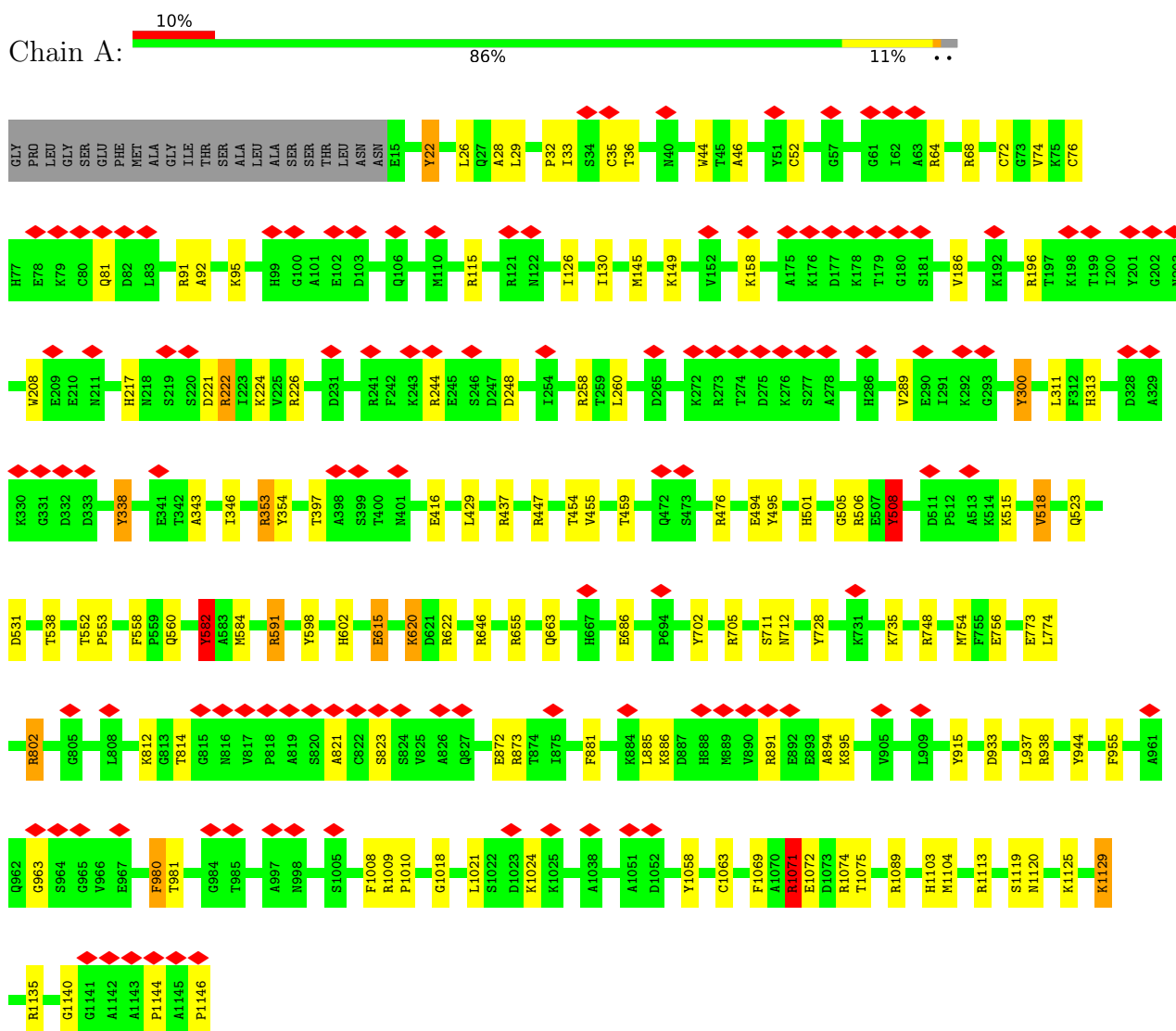
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP Q4KUS2
A	-6	PRO	-	expression tag	UNP Q4KUS2
A	-5	LEU	-	expression tag	UNP Q4KUS2
A	-4	GLY	-	expression tag	UNP Q4KUS2
A	-3	SER	-	expression tag	UNP Q4KUS2
A	-2	GLU	-	expression tag	UNP Q4KUS2
A	-1	PHE	-	expression tag	UNP Q4KUS2
A	0	MET	-	expression tag	UNP Q4KUS2
A	133	VAL	ILE	conflict	UNP Q4KUS2
A	873	ARG	LYS	conflict	UNP Q4KUS2
A	880	GLU	-	linker	UNP Q4KUS2
A	881	PHE	-	linker	UNP Q4KUS2

### 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: Protein unc-13 homolog A



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	72894	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF correction was performed during 3D reconstruction in RELION 3.1	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	110	Depositor
Minimum defocus (nm)	3500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.085	Depositor
Minimum map value	0.000	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.31	Depositor
Map size ( $\text{\AA}$ )	411.59998, 411.59998, 411.59998	wwPDB
Map dimensions	196, 196, 196	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	2.1, 2.1, 2.1	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	0.67	0/9220	1.04	31/12466 (0.2%)

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	9

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	591	ARG	NE-CZ-NH1	11.03	125.82	120.30
1	A	1071	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	A	196	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	A	437	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	A	938	ARG	NE-CZ-NH1	7.51	124.05	120.30
1	A	1009	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	A	1135	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	A	705	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	A	91	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	655	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	A	873	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	A	22	TYR	CB-CG-CD1	-6.07	117.36	121.00
1	A	980	PHE	CB-CG-CD2	5.90	124.93	120.80
1	A	622	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	A	748	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	523	GLN	C-N-CA	5.76	134.40	122.30
1	A	226	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	338	TYR	CB-CG-CD2	-5.49	117.71	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	598	TYR	CB-CG-CD2	-5.41	117.76	121.00
1	A	980	PHE	CB-CG-CD1	-5.37	117.04	120.80
1	A	476	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	353	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	A	506	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	258	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	702	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	A	518	VAL	CA-CB-CG1	5.12	118.58	110.90
1	A	447	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	591	ARG	NH1-CZ-NH2	-5.07	113.83	119.40
1	A	508	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	A	1089	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1071	ARG	Sidechain
1	A	244	ARG	Sidechain
1	A	300	TYR	Sidechain
1	A	495	TYR	Sidechain
1	A	582	TYR	Sidechain
1	A	591	ARG	Sidechain
1	A	728	TYR	Sidechain
1	A	802	ARG	Sidechain
1	A	944	TYR	Sidechain

## 5.2 Too-close contacts

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	9034	8976	8973	45	0
All	All	9034	8976	8973	45	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.

All (45) 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:29:LEU:HD21	1:A:346:ILE:HA	1.57	0.86
1:A:311:LEU:HD21	1:A:343:ALA:HB1	1.75	0.68
1:A:260:LEU:HB3	1:A:289:VAL:HG21	1.80	0.62
1:A:29:LEU:HD22	1:A:130:ILE:HD11	1.80	0.61
1:A:1103:HIS:CG	1:A:1146:PRO:HA	2.40	0.56
1:A:582:TYR:CD2	1:A:582:TYR:C	2.81	0.54
1:A:1021:LEU:HD23	1:A:1024:LYS:HE2	1.88	0.54
1:A:735:LYS:H	1:A:735:LYS:HD2	1.74	0.53
1:A:501:HIS:CG	1:A:518:VAL:HB	2.45	0.51
1:A:812:LYS:O	1:A:814:THR:HG23	2.12	0.50
1:A:1129:LYS:HE3	1:A:1129:LYS:HA	1.95	0.48
1:A:1063:CYS:SG	1:A:1075:THR:HG23	2.54	0.48
1:A:32:PRO:HG2	1:A:35:CYS:SG	2.54	0.47
1:A:615:GLU:H	1:A:615:GLU:CD	2.17	0.47
1:A:29:LEU:HD23	1:A:126:ILE:CG2	2.45	0.47
1:A:814:THR:HG21	1:A:821:ALA:O	2.15	0.47
1:A:33:ILE:HA	1:A:36:THR:HG23	1.97	0.46
1:A:300:TYR:CG	1:A:354:TYR:HB3	2.51	0.46
1:A:1018:GLY:HA3	1:A:1058:TYR:CD1	2.52	0.45
1:A:22:TYR:CE2	1:A:26:LEU:HD11	2.51	0.45
1:A:881:PHE:CE2	1:A:1113:ARG:HG3	2.51	0.45
1:A:72:CYS:HA	1:A:92:ALA:CB	2.46	0.44
1:A:505:GLY:HA3	1:A:515:LYS:HA	1.99	0.44
1:A:221:ASP:HA	1:A:222:ARG:HH21	1.82	0.44
1:A:145:MET:SD	1:A:149:LYS:HE3	2.58	0.43
1:A:881:PHE:CZ	1:A:1113:ARG:HG3	2.53	0.43
1:A:429:LEU:HD22	1:A:454:THR:HG23	2.00	0.43
1:A:711:SER:HA	1:A:774:LEU:HD22	2.00	0.43
1:A:72:CYS:SG	1:A:74:VAL:HG12	2.58	0.43
1:A:508:TYR:CZ	1:A:538:THR:HG22	2.54	0.43
1:A:552:THR:HB	1:A:553:PRO:HD3	2.00	0.43
1:A:72:CYS:HA	1:A:92:ALA:HA	1.99	0.43
1:A:1071:ARG:HB3	1:A:1071:ARG:CZ	2.49	0.43
1:A:455:VAL:O	1:A:459:THR:HG23	2.19	0.43
1:A:72:CYS:HA	1:A:92:ALA:HB2	2.01	0.42
1:A:1120:ASN:HA	1:A:1125:LYS:HE3	2.02	0.42
1:A:620:LYS:HE3	1:A:620:LYS:HA	2.02	0.41
1:A:955:PHE:CZ	1:A:1104:MET:SD	3.13	0.41
1:A:1008:PHE:CD2	1:A:1010:PRO:HD3	2.55	0.41
1:A:44:TRP:CH2	1:A:46:ALA:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ALA:HA	1:A:353:ARG:CD	2.51	0.41
1:A:646:ARG:CZ	1:A:712:ASN:HB3	2.51	0.41
1:A:52:CYS:SG	1:A:76:CYS:HA	2.61	0.40
1:A:186:VAL:HG23	1:A:208:TRP:CZ2	2.56	0.40
1:A:872:GLU:HA	1:A:937:LEU:HD13	2.03	0.40

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	1130/1154 (98%)	1060 (94%)	60 (5%)	10 (1%)	17 57

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	894	ALA
1	A	397	THR
1	A	895	LYS
1	A	1071	ARG
1	A	885	LEU
1	A	1119	SER
1	A	1140	GLY
1	A	981	THR
1	A	1144	PRO
1	A	963	GLY

### 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	1006/1022 (98%)	968 (96%)	38 (4%)	33 57

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ARG
1	A	81	GLN
1	A	95	LYS
1	A	115	ARG
1	A	158	LYS
1	A	217	HIS
1	A	222	ARG
1	A	224	LYS
1	A	248	ASP
1	A	313	HIS
1	A	338	TYR
1	A	416	GLU
1	A	494	GLU
1	A	508	TYR
1	A	531	ASP
1	A	558	PHE
1	A	560	GLN
1	A	582	TYR
1	A	584	MET
1	A	602	HIS
1	A	615	GLU
1	A	620	LYS
1	A	663	GLN
1	A	686	GLU
1	A	754	MET
1	A	756	GLU
1	A	773	GLU
1	A	802	ARG
1	A	823	SER
1	A	886	LYS
1	A	891	ARG
1	A	915	TYR
1	A	933	ASP
1	A	980	PHE

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Mol	Chain	Res	Type
1	A	1069	PHE
1	A	1072	GLU
1	A	1074	ARG
1	A	1129	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	A	395	HIS
1	A	587	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 monosaccharides 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.

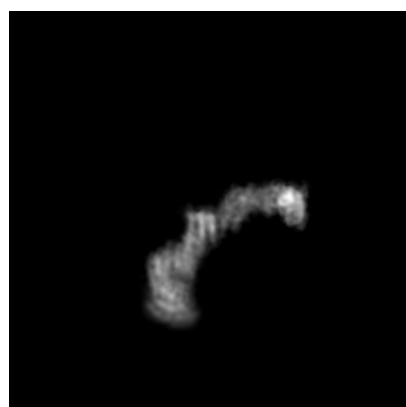
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25739. These allow visual inspection of the internal detail of the map and identification of artifacts.

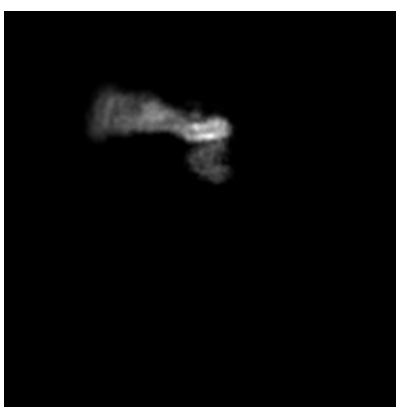
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

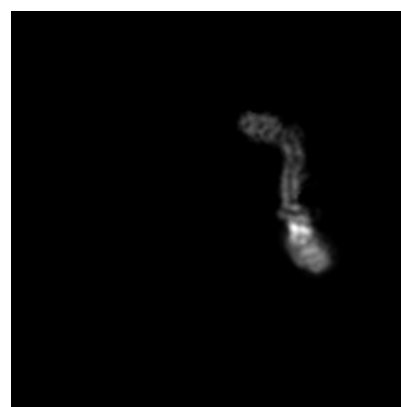
#### 6.1.1 Primary map



X



Y

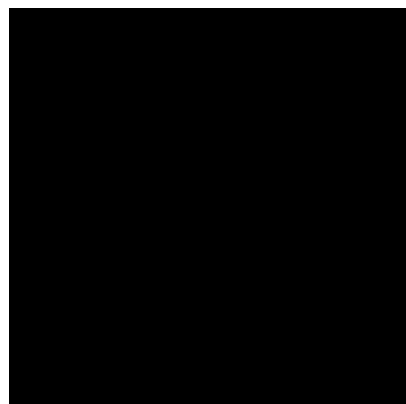


Z

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

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

#### 6.2.1 Primary map



X Index: 98



Y Index: 98



Z Index: 98

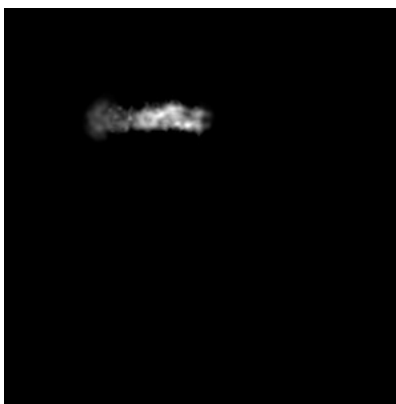
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 139



Y Index: 88

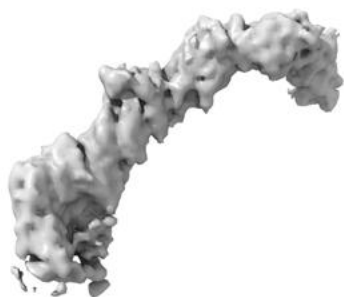


Z Index: 101

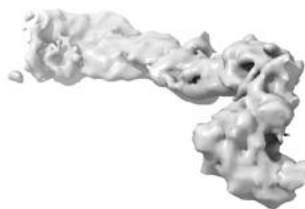
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.31. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

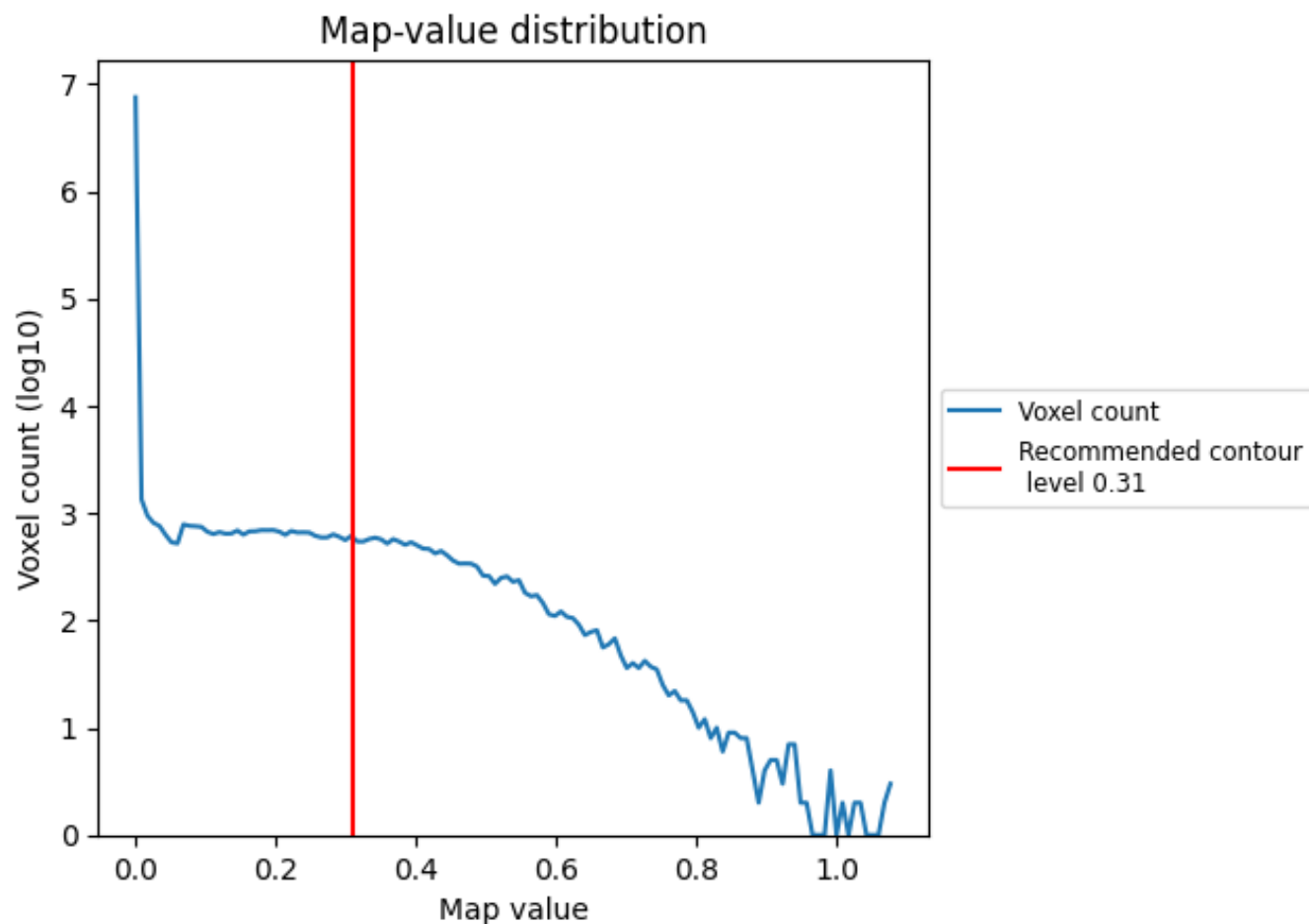
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

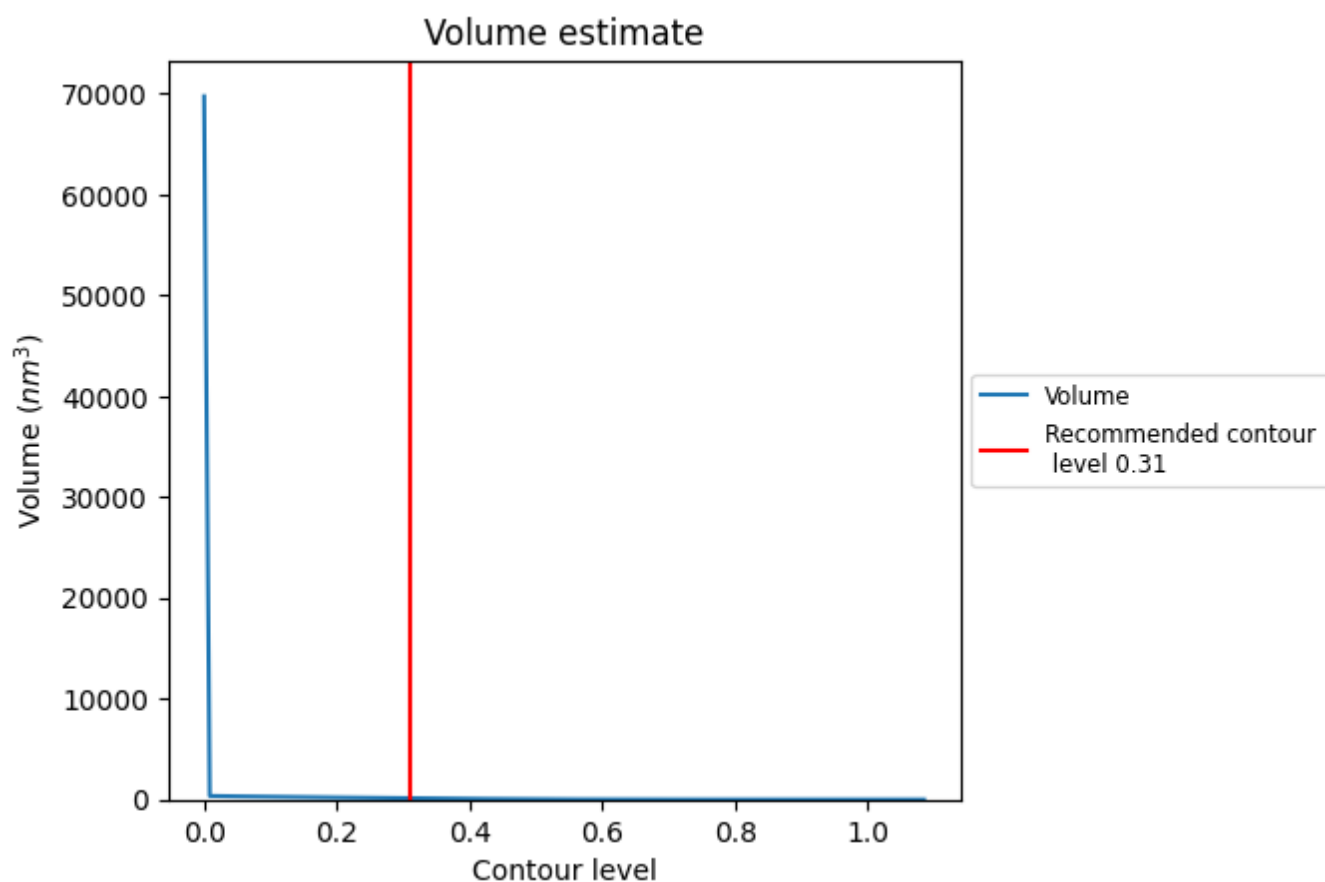
This section contains the results of statistical analysis of the map.

### 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](#)

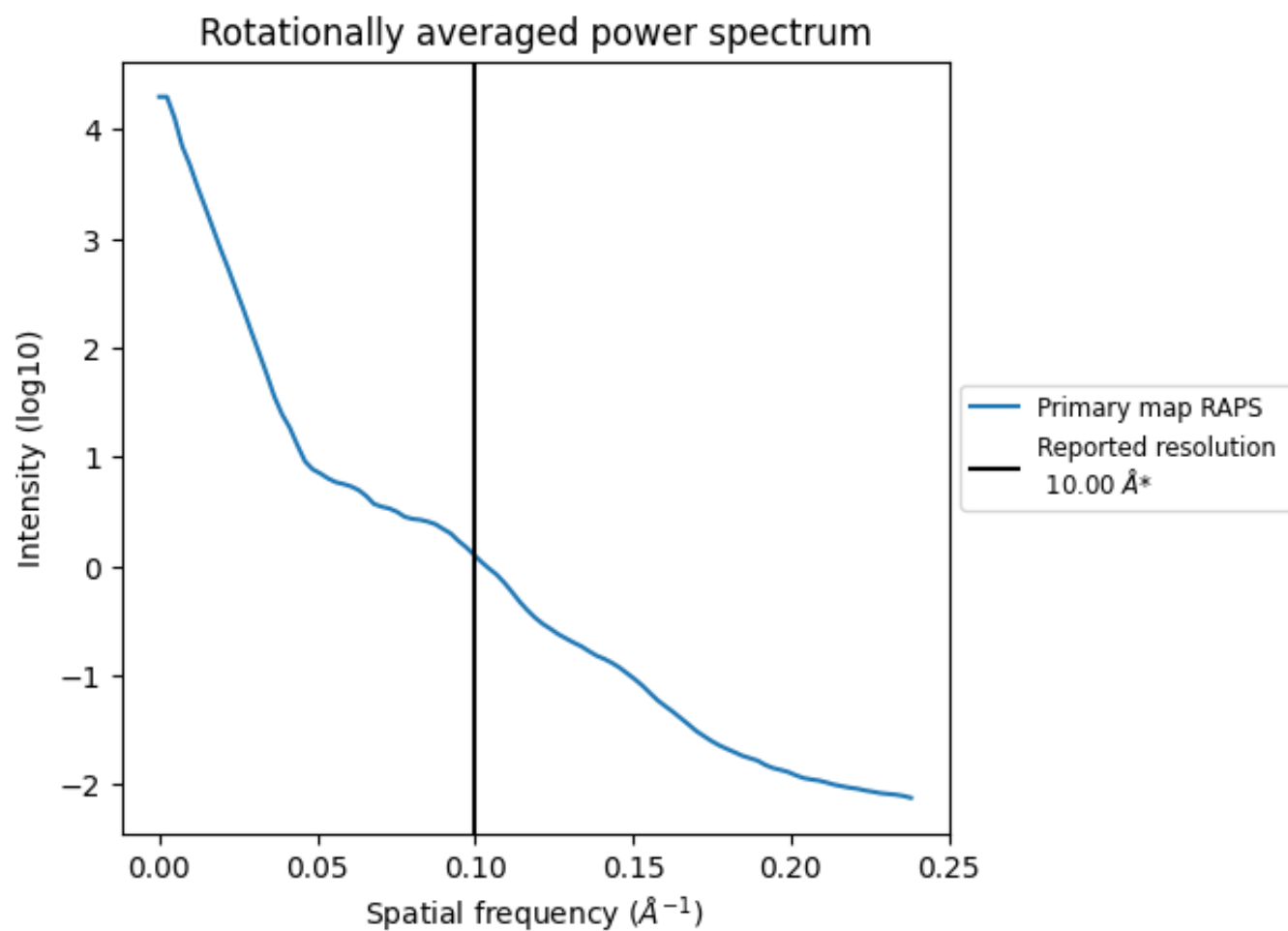


The volume at the recommended contour level is 132 nm<sup>3</sup>; this corresponds to an approximate mass of 119 kDa.

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 0.100 Å<sup>-1</sup>

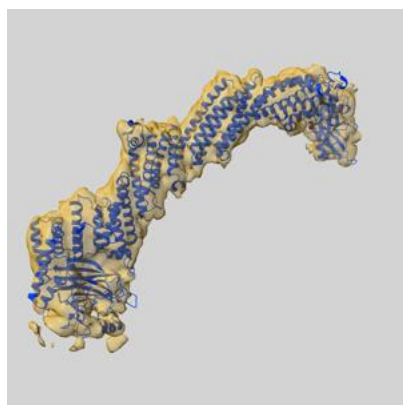
## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

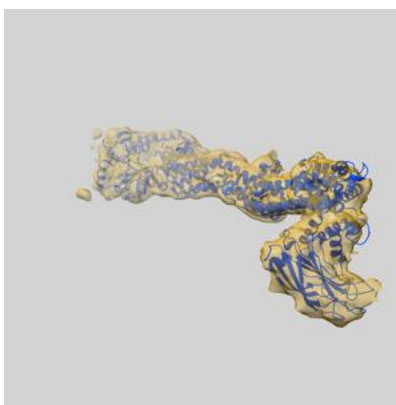
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25739 and PDB model 7T7V. Per-residue inclusion information can be found in section [3](#) on page [4](#).

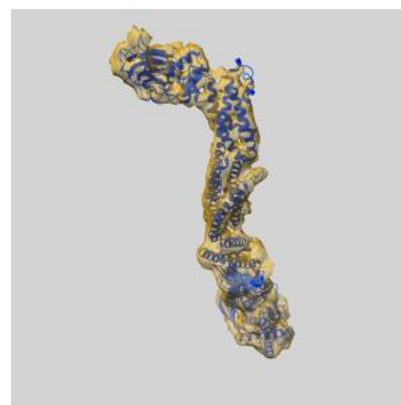
### 9.1 Map-model overlay [i](#)



X



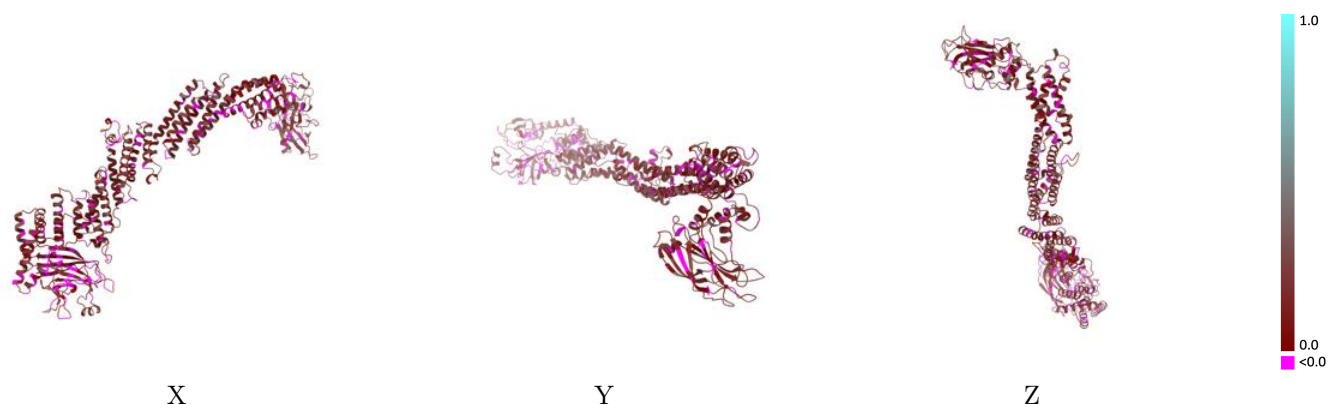
Y



Z

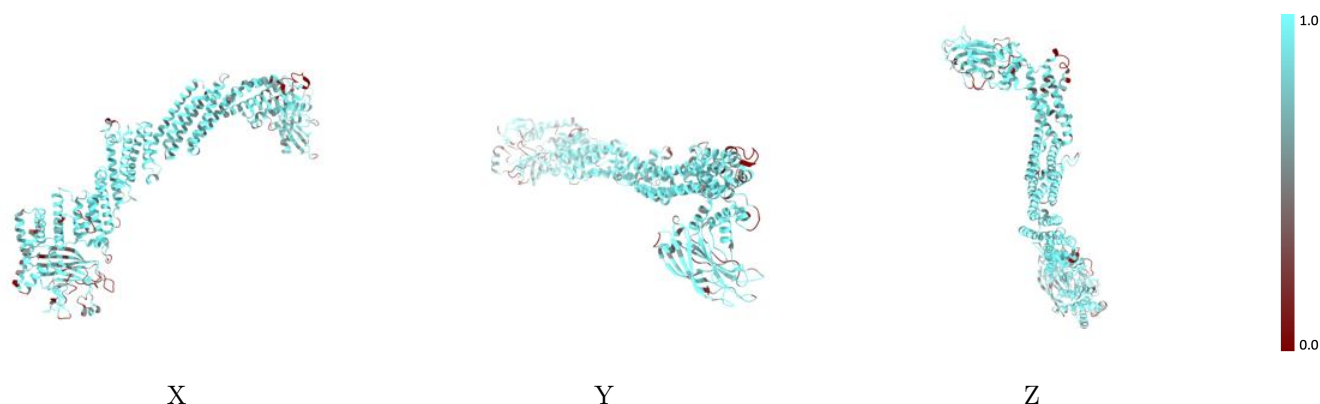
The images above show the 3D surface view of the map at the recommended contour level 0.31 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



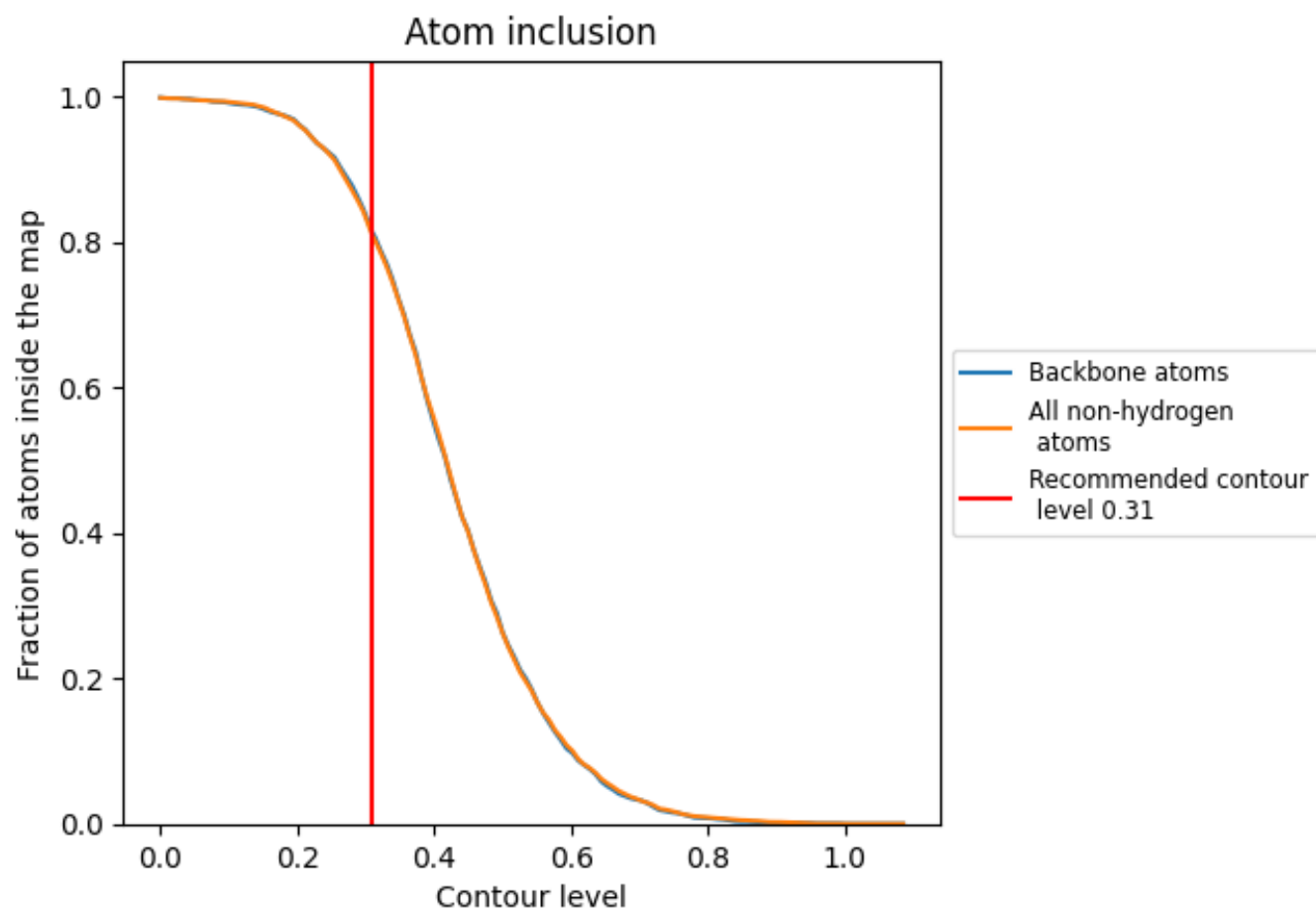
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.31).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 81% 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 (0.31) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8077	<div></div> 0.1330
A	<div></div> 0.8070	<div></div> 0.1330

