



## Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 02:22 AM EST

PDB ID : 6O7T  
EMDB ID : EMD-0644  
Title : Saccharomyces cerevisiae V-ATPase Vph1-VO  
Authors : Vasanthakumar, T.; Bueler, S.A.; Wu, D.; Beilsten-Edmands, V.; Robinson, C.V.; Rubinstein, J.L.  
Deposited on : 2019-03-08  
Resolution : 3.20 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) : 2.31.2

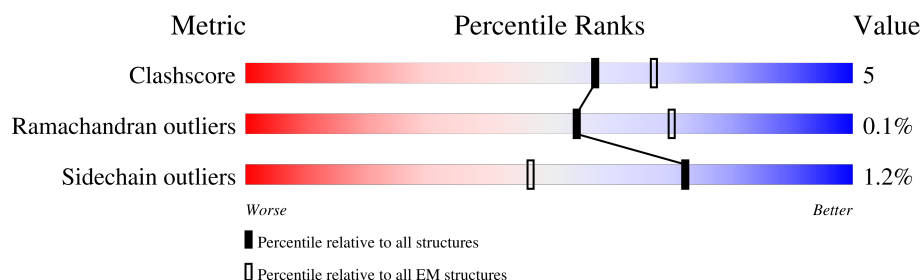
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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	862	
2	b	265	
3	c	213	
4	d	345	
5	f	85	
6	g	160	
6	h	160	
6	i	160	

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Mol	Chain	Length	Quality of chain
6	j	160	<div><div></div><div>12%</div><div>97%</div><div></div><div>..</div></div>
6	k	160	<div><div></div><div>12%</div><div>98%</div><div></div><div>..</div></div>
6	l	160	<div><div></div><div>6%</div><div>95%</div><div></div><div>..</div></div>
6	m	160	<div><div></div><div>6%</div><div>98%</div><div></div><div>..</div></div>
6	n	160	<div><div></div><div>13%</div><div>98%</div><div></div><div>..</div></div>
7	o	164	<div><div></div><div></div><div>95%</div><div>5%</div><div></div></div>
8	e	73	<div><div></div><div>88%</div><div>12%</div><div></div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 19730 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 V-type proton ATPase subunit a, vacuolar isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	734	Total	C	N	O	S	0	0
			5358	3484	888	956	30		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	841	ASP	-	SEE REMARK 999	UNP P32563
a	842	TYR	-	SEE REMARK 999	UNP P32563
a	843	LYS	-	SEE REMARK 999	UNP P32563
a	844	ASP	-	SEE REMARK 999	UNP P32563
a	845	HIS	-	SEE REMARK 999	UNP P32563
a	846	ASP	-	SEE REMARK 999	UNP P32563
a	847	GLY	-	SEE REMARK 999	UNP P32563
a	848	ASP	-	SEE REMARK 999	UNP P32563
a	849	TYR	-	SEE REMARK 999	UNP P32563
a	850	LYS	-	SEE REMARK 999	UNP P32563
a	851	ASP	-	SEE REMARK 999	UNP P32563
a	852	HIS	-	SEE REMARK 999	UNP P32563
a	853	ASP	-	SEE REMARK 999	UNP P32563
a	854	ILE	-	SEE REMARK 999	UNP P32563
a	855	ASP	-	SEE REMARK 999	UNP P32563
a	856	TYR	-	SEE REMARK 999	UNP P32563
a	857	LYS	-	SEE REMARK 999	UNP P32563
a	858	ASP	-	SEE REMARK 999	UNP P32563
a	859	ASP	-	SEE REMARK 999	UNP P32563
a	860	ASP	-	SEE REMARK 999	UNP P32563
a	861	ASP	-	SEE REMARK 999	UNP P32563
a	862	LYS	-	SEE REMARK 999	UNP P32563

- Molecule 2 is a protein called V0 assembly protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	38	Total	C	N	O	S	0	0
			279	190	41	46	2		

- Molecule 3 is a protein called V-type proton ATPase subunit c''.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	195	Total	C	N	O	S	0	0
			1414	938	220	249	7		

- Molecule 4 is a protein called V-type proton ATPase subunit d.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	314	Total	C	N	O	S	0	0
			2181	1388	367	418	8		

- Molecule 5 is a protein called Putative protein YPR170W-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	f	63	Total	C	N	O	S	0	0
			467	308	73	83	3		

- Molecule 6 is a protein called V-type proton ATPase subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	g	155	Total	C	N	O	S	0	0
			1080	709	174	190	7		
6	h	159	Total	C	N	O	S	0	0
			1085	716	173	191	5		
6	i	158	Total	C	N	O	S	0	0
			1071	705	171	188	7		
6	j	158	Total	C	N	O	S	0	0
			1035	672	168	190	5		
6	k	158	Total	C	N	O	S	0	0
			1049	685	168	191	5		
6	l	156	Total	C	N	O	S	0	0
			1025	665	169	187	4		
6	m	158	Total	C	N	O	S	0	0
			1050	690	167	188	5		
6	n	158	Total	C	N	O	S	0	0
			1034	678	166	185	5		

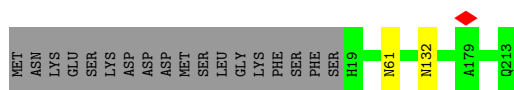
- Molecule 7 is a protein called V-type proton ATPase subunit c'.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	o	156	Total	C	N	O	S	0	0
			1096	725	171	189	11		

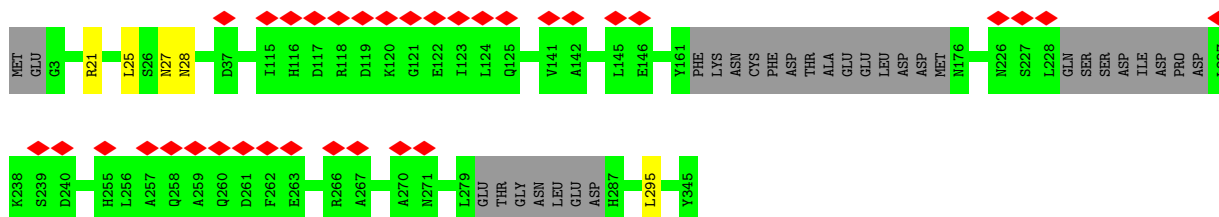
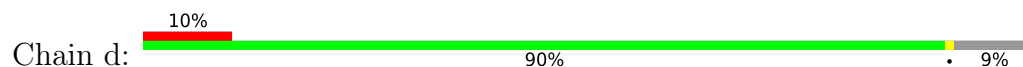
- Molecule 8 is a protein called V-type proton ATPase subunit e.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	e	64	Total	C	N	O	S	0	0
			506	340	82	79	5		

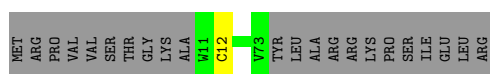




- Molecule 4: V-type proton ATPase subunit d



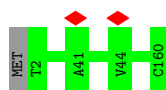
- Molecule 5: Putative protein YPR170W-B



- Molecule 6: V-type proton ATPase subunit c



- Molecule 6: V-type proton ATPase subunit c



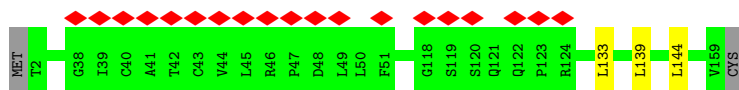
- Molecule 6: V-type proton ATPase subunit c



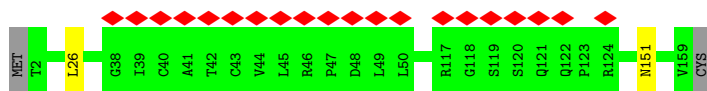
- Molecule 6: V-type proton ATPase subunit c







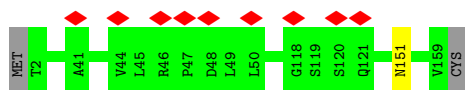
- Molecule 6: V-type proton ATPase subunit c



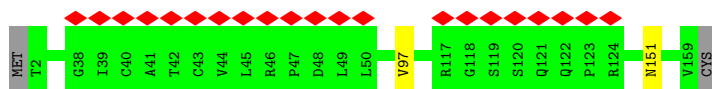
- Molecule 6: V-type proton ATPase subunit c



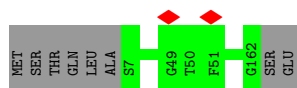
- Molecule 6: V-type proton ATPase subunit c



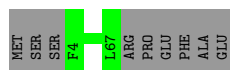
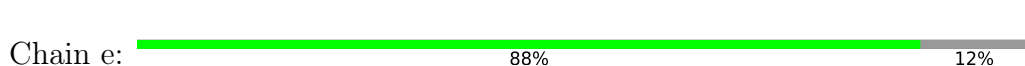
- Molecule 6: V-type proton ATPase subunit c



- Molecule 7: V-type proton ATPase subunit c'



- Molecule 8: V-type proton ATPase subunit e



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	296105	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 ( $e^-/\text{\AA}^2$ )	42.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	6.381	Depositor
Minimum map value	-4.939	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.180	Depositor
Recommended contour level	0.6	Depositor
Map size ( $\text{\AA}$ )	271.36, 271.36, 271.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.06, 1.06, 1.06	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	0.42	0/5480	0.67	3/7477 (0.0%)
2	b	0.42	0/283	0.67	0/388
3	c	0.49	0/1442	0.67	0/1965
4	d	0.34	0/2220	0.59	2/3041 (0.1%)
5	f	0.35	0/481	0.58	0/661
6	g	0.49	0/1096	0.80	3/1491 (0.2%)
6	h	0.49	0/1101	0.74	0/1502
6	i	0.46	0/1086	0.71	1/1481 (0.1%)
6	j	0.46	0/1048	0.78	3/1431 (0.2%)
6	k	0.44	0/1063	0.68	0/1453
6	l	0.44	0/1039	0.78	2/1420 (0.1%)
6	m	0.44	0/1065	0.68	0/1456
6	n	0.47	1/1048 (0.1%)	0.72	1/1433 (0.1%)
7	o	0.47	0/1117	0.69	0/1519
8	e	0.43	0/521	0.55	0/714
All	All	0.44	1/20090 (0.0%)	0.69	15/27432 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	n	97	VAL	CB-CG2	-6.65	1.38	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	800	LEU	CB-CG-CD2	-7.94	97.50	111.00
6	n	97	VAL	CG1-CB-CG2	-7.14	99.47	110.90
6	j	139	LEU	CA-CB-CG	6.57	130.41	115.30
6	g	99	LEU	CA-CB-CG	6.04	129.18	115.30
6	j	133	LEU	CA-CB-CG	6.00	129.10	115.30
6	g	139	LEU	CB-CG-CD2	-5.98	100.83	111.00
6	j	144	LEU	CA-CB-CG	5.86	128.78	115.30
1	a	349	LEU	CA-CB-CG	-5.62	102.38	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	25	LEU	CA-CB-CG	5.58	128.13	115.30
6	l	91	LEU	CA-CB-CG	5.56	128.08	115.30
6	i	144	LEU	CA-CB-CG	5.43	127.79	115.30
6	g	102	LEU	CA-CB-CG	5.26	127.39	115.30
1	a	649	LEU	CA-CB-CG	5.20	127.27	115.30
6	l	150	LEU	CA-CB-CG	5.20	127.26	115.30
4	d	295	LEU	CA-CB-CG	5.18	127.21	115.30

There are no chirality outliers.

There are no planarity outliers.

## 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	5358	0	4883	0	0
2	b	279	0	289	0	0
3	c	1414	0	1442	0	0
4	d	2181	0	1802	0	0
5	f	467	0	431	0	0
6	g	1080	0	1124	0	0
6	h	1085	0	1082	0	0
6	i	1071	0	1076	0	0
6	j	1035	0	978	0	0
6	k	1049	0	1015	0	0
6	l	1025	0	970	0	0
6	m	1050	0	1021	0	0
6	n	1034	0	994	0	0
7	o	1096	0	1115	0	0
8	e	506	0	514	0	0
All	All	19730	0	18736	0	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 5.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	728/862 (84%)	688 (94%)	39 (5%)	1 (0%)	51	83
2	b	36/265 (14%)	36 (100%)	0	0	100	100
3	c	193/213 (91%)	187 (97%)	6 (3%)	0	100	100
4	d	306/345 (89%)	293 (96%)	13 (4%)	0	100	100
5	f	61/85 (72%)	58 (95%)	3 (5%)	0	100	100
6	g	153/160 (96%)	148 (97%)	5 (3%)	0	100	100
6	h	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
6	i	156/160 (98%)	151 (97%)	5 (3%)	0	100	100
6	j	156/160 (98%)	147 (94%)	9 (6%)	0	100	100
6	k	156/160 (98%)	153 (98%)	3 (2%)	0	100	100
6	l	154/160 (96%)	148 (96%)	4 (3%)	2 (1%)	12	47
6	m	156/160 (98%)	152 (97%)	4 (3%)	0	100	100
6	n	156/160 (98%)	147 (94%)	9 (6%)	0	100	100
7	o	154/164 (94%)	148 (96%)	6 (4%)	0	100	100
8	e	62/73 (85%)	61 (98%)	1 (2%)	0	100	100
All	All	2784/3287 (85%)	2672 (96%)	109 (4%)	3 (0%)	54	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	l	154	ALA
6	l	119	SER
1	a	483	PHE

### 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	486/749 (65%)	477 (98%)	9 (2%)	57	81
2	b	29/244 (12%)	29 (100%)	0	100	100
3	c	141/168 (84%)	139 (99%)	2 (1%)	67	86
4	d	175/309 (57%)	172 (98%)	3 (2%)	60	83
5	f	48/72 (67%)	47 (98%)	1 (2%)	53	79
6	g	106/119 (89%)	106 (100%)	0	100	100
6	h	98/119 (82%)	98 (100%)	0	100	100
6	i	98/119 (82%)	95 (97%)	3 (3%)	40	72
6	j	86/119 (72%)	86 (100%)	0	100	100
6	k	91/119 (76%)	89 (98%)	2 (2%)	52	79
6	l	85/119 (71%)	85 (100%)	0	100	100
6	m	91/119 (76%)	90 (99%)	1 (1%)	73	88
6	n	86/119 (72%)	85 (99%)	1 (1%)	71	88
7	o	108/125 (86%)	108 (100%)	0	100	100
8	e	54/65 (83%)	54 (100%)	0	100	100
All	All	1782/2684 (66%)	1760 (99%)	22 (1%)	72	88

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	47	LYS
1	a	418	MET
1	a	448	LYS
1	a	480	ASN
1	a	535	TYR
1	a	565	MET
1	a	648	LEU
1	a	649	LEU
1	a	650	LEU
3	c	61	ASN

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Mol	Chain	Res	Type
3	c	132	ASN
4	d	21	ARG
4	d	27	ASN
4	d	28	ASN
5	f	12	CYS
6	i	37	VAL
6	i	139	LEU
6	i	151	ASN
6	k	26	LEU
6	k	151	ASN
6	m	151	ASN
6	n	151	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	18	GLN
1	a	68	GLN
1	a	311	GLN
1	a	381	HIS
1	a	480	ASN
3	c	132	ASN
3	c	138	ASN
3	c	156	ASN
4	d	27	ASN
4	d	28	ASN
4	d	29	GLN
4	d	106	ASN
4	d	222	ASN
5	f	35	HIS
6	g	90	GLN
6	i	90	GLN
6	j	151	ASN
6	k	53	ASN
6	k	82	GLN
6	k	90	GLN
6	k	151	ASN
6	m	151	ASN
6	n	151	ASN
7	o	159	ASN
8	e	55	GLN

### 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.



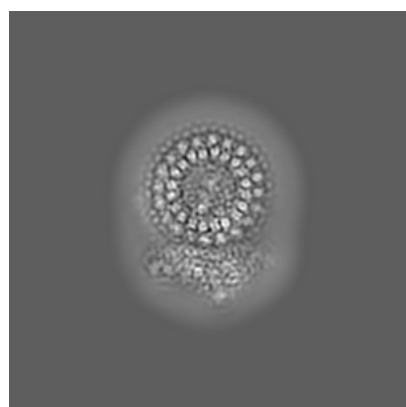
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0644. These allow visual inspection of the internal detail of the map and identification of artifacts.

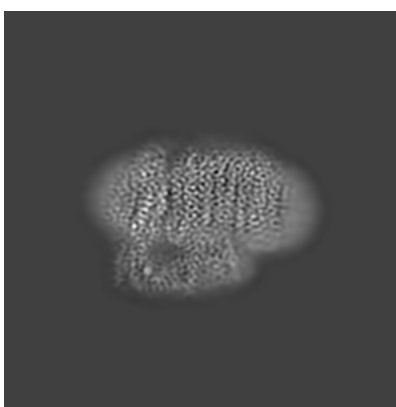
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

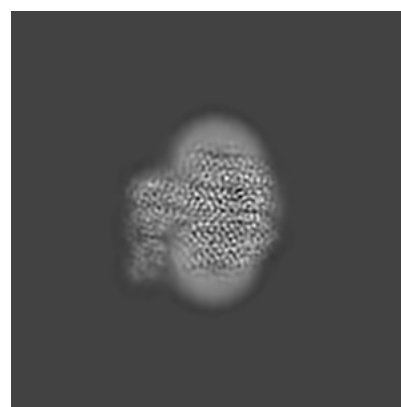
#### 6.1.1 Primary map



X



Y

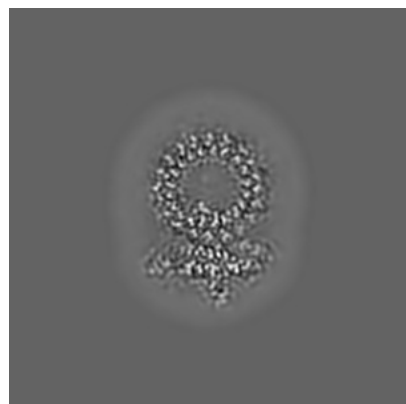


Z

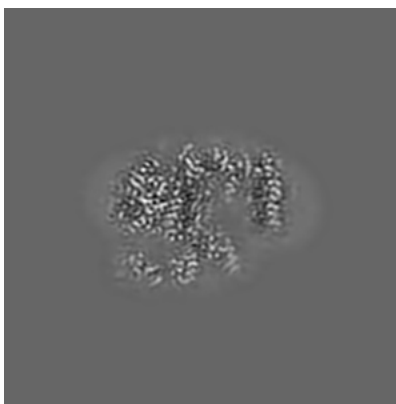
The images above show the map projected in three orthogonal directions.

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

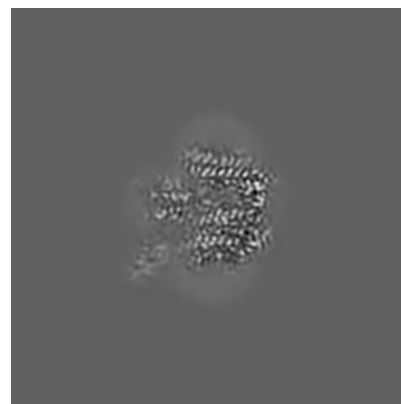
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

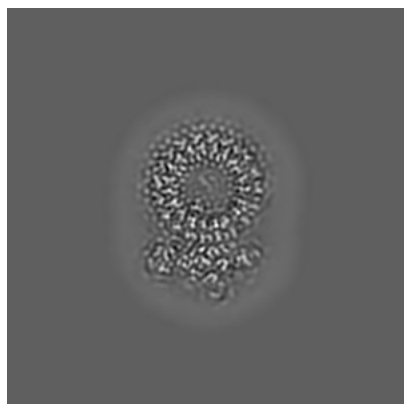


Z Index: 128

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

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

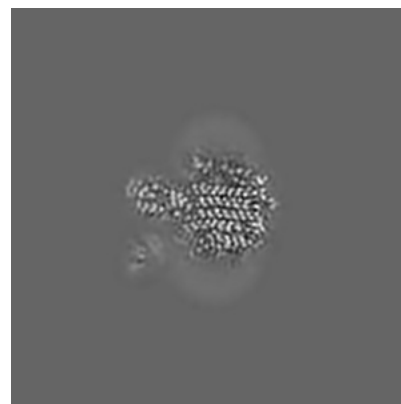
### 6.3.1 Primary map



X Index: 136



Y Index: 133

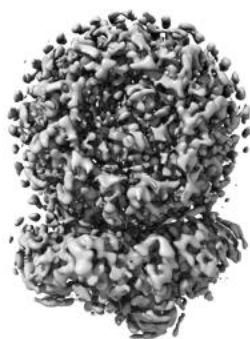


Z Index: 118

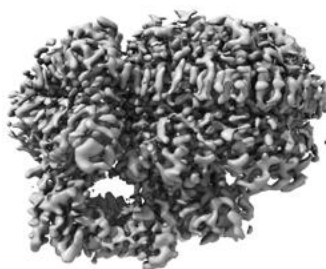
The images above show the largest variance slices of the map in three orthogonal directions.

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

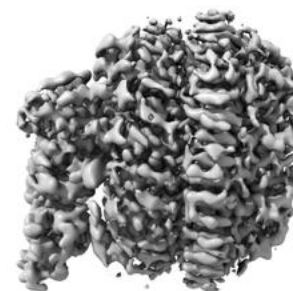
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

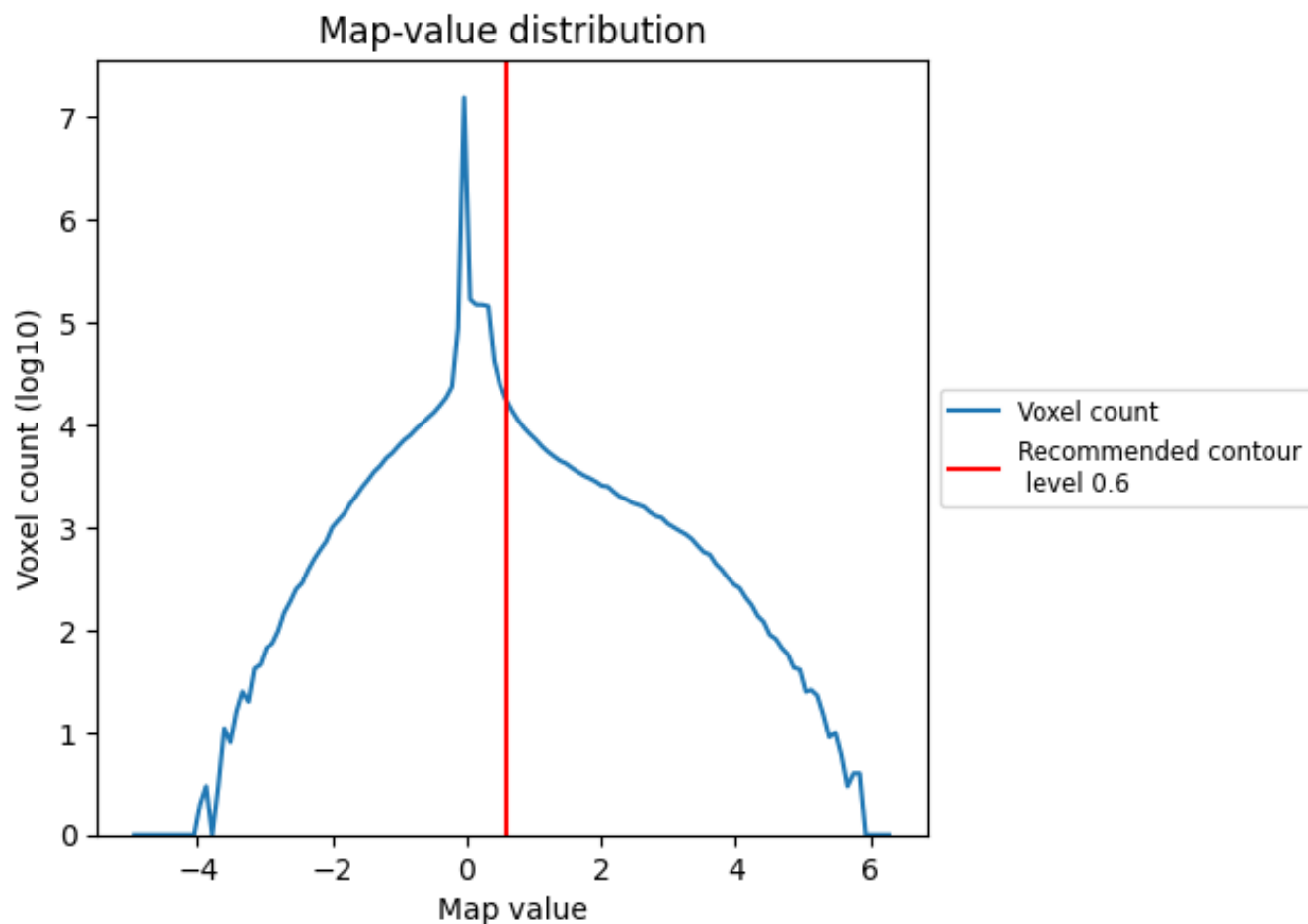
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

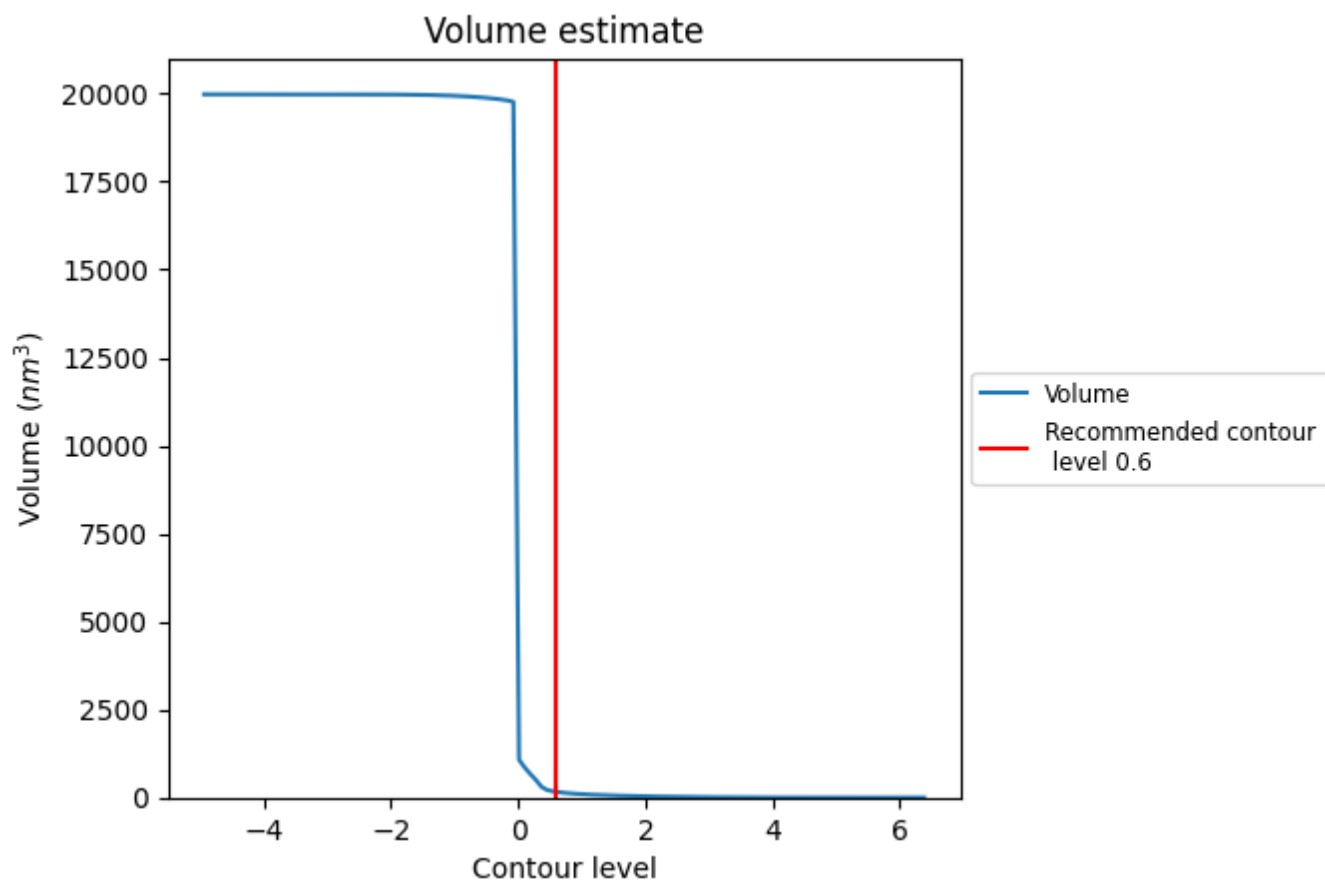
This section contains the results of statistical analysis of the map.

### 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.

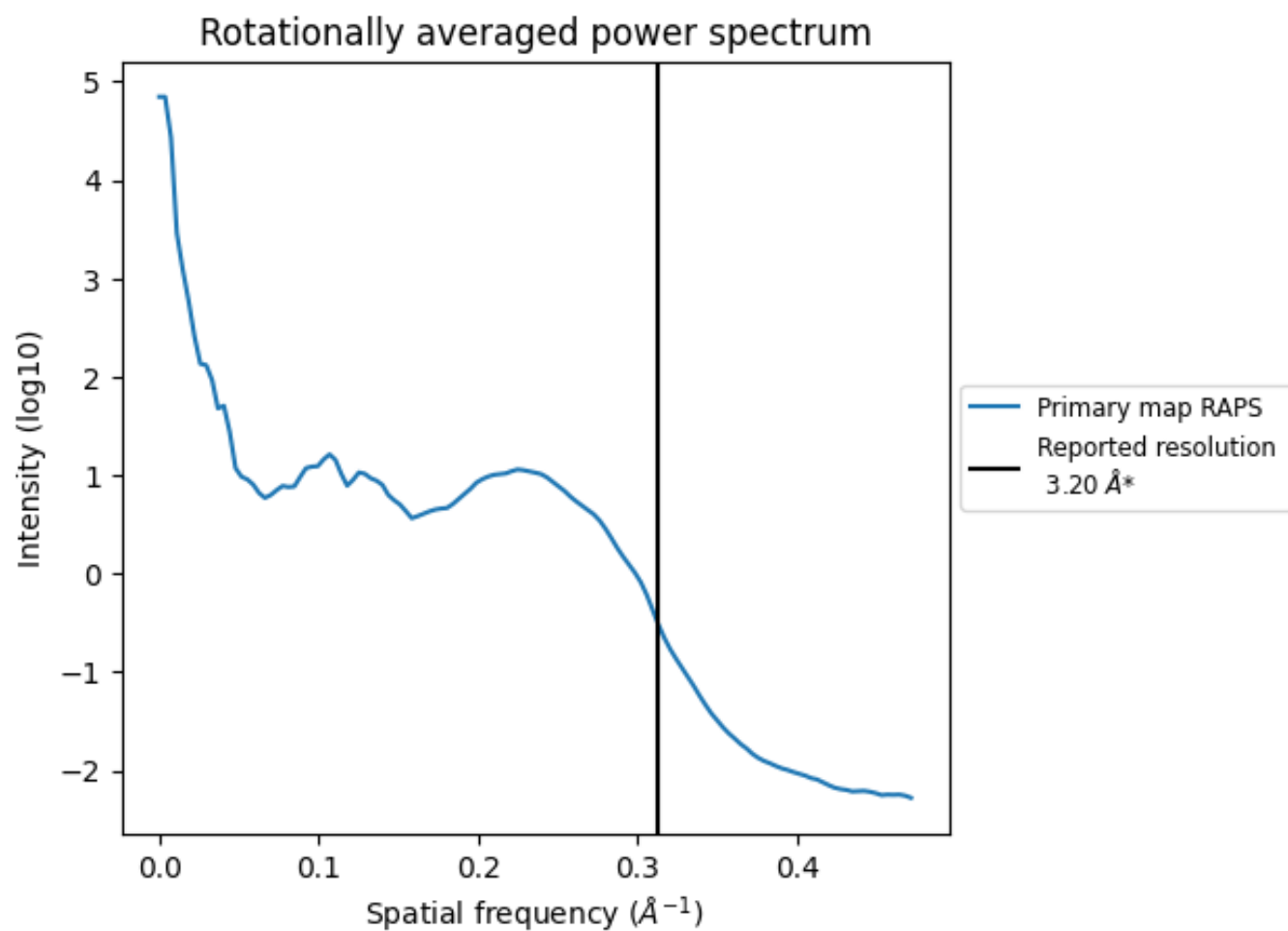
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 163 nm<sup>3</sup>; this corresponds to an approximate mass of 147 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 0.312 Å<sup>-1</sup>

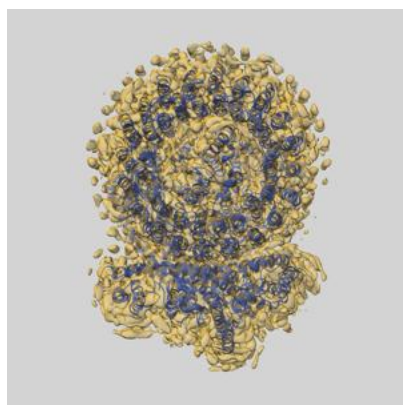
## 8 Fourier-Shell correlation

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

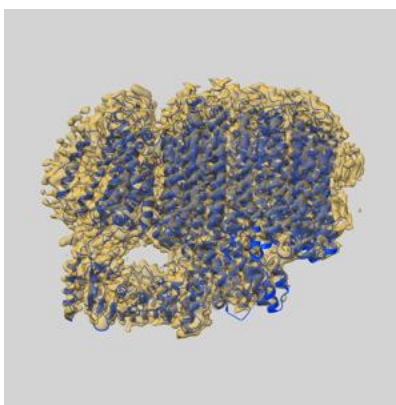
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0644 and PDB model 6O7T. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

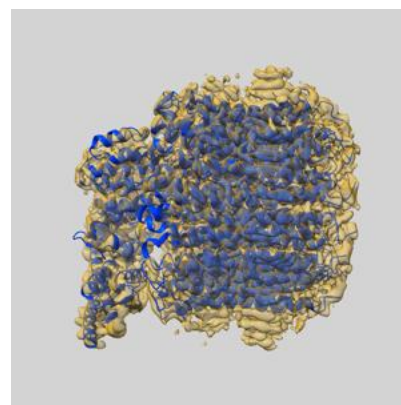
### 9.1 Map-model overlay [i](#)



X



Y

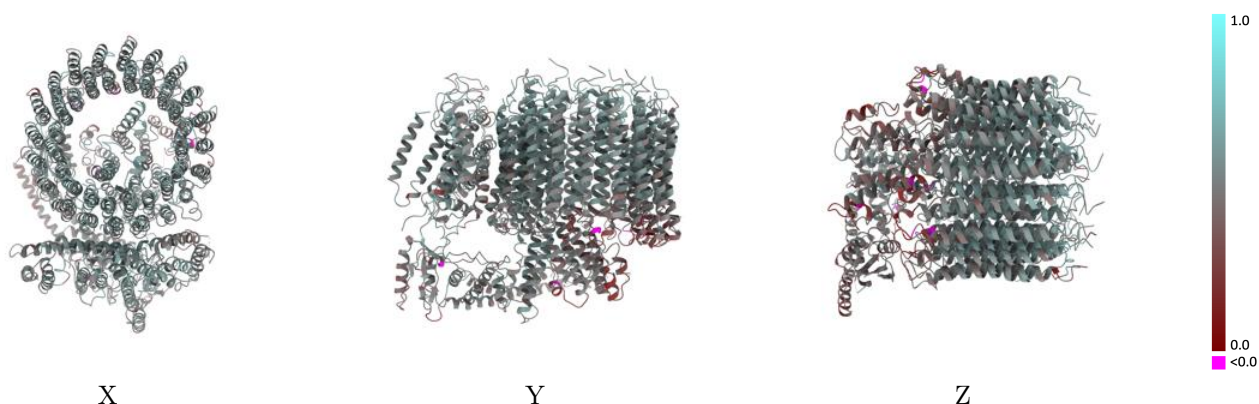


Z

The images above show the 3D surface view of the map at the recommended contour level 0.6 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.

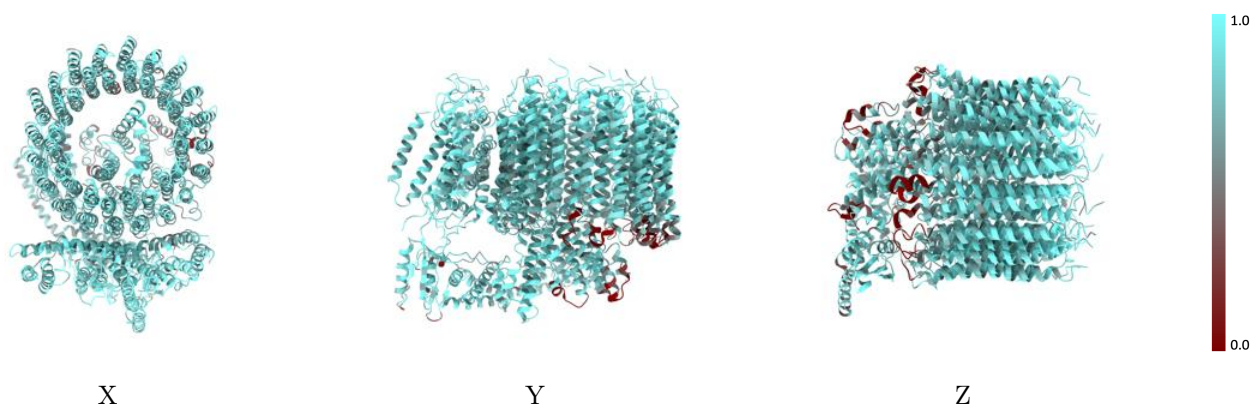


## 9.2 Q-score mapped to coordinate model [i](#)



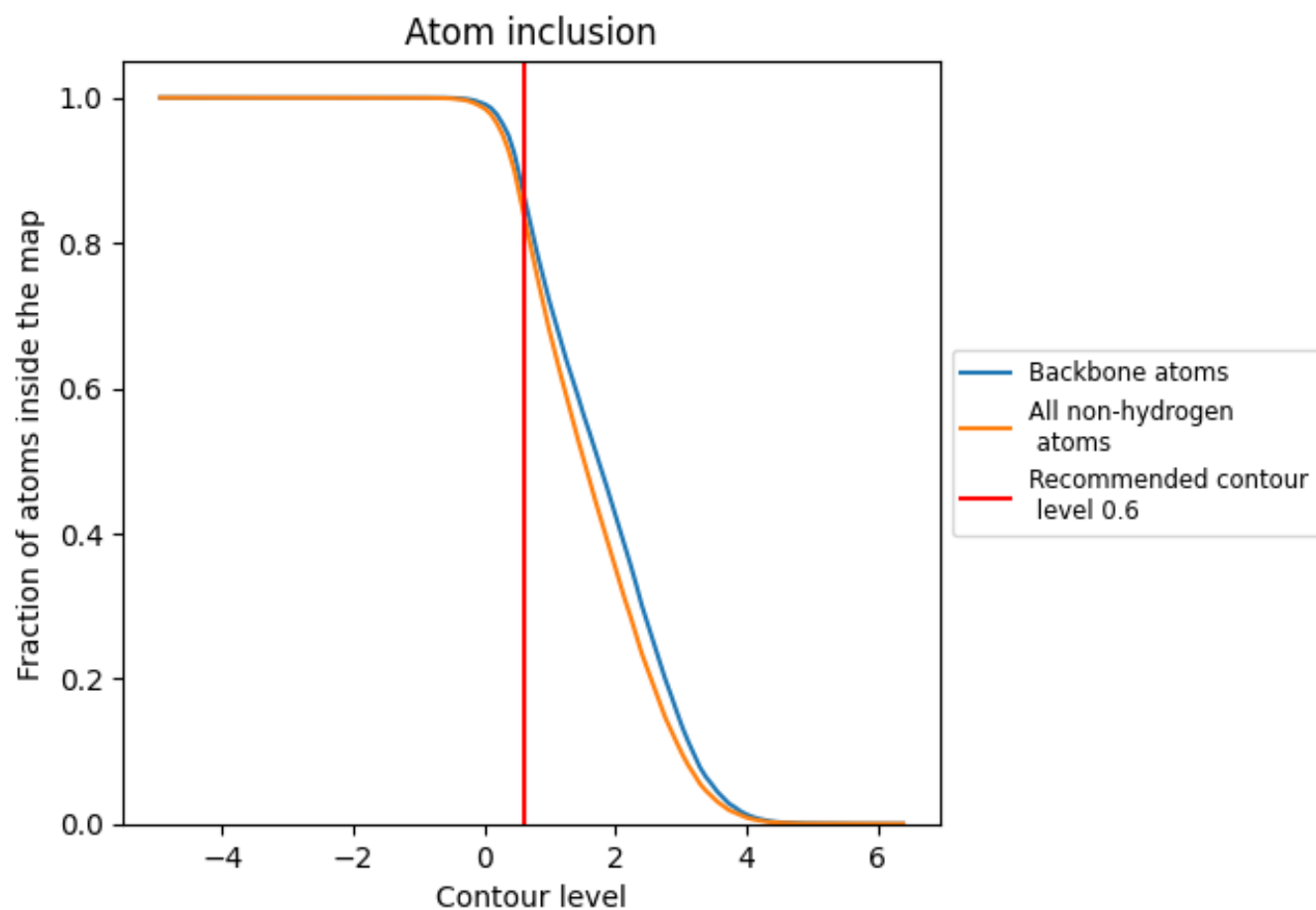
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).

































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 84% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8404	 0.5080
a	 0.8510	 0.4940
b	 0.8845	 0.5560
c	 0.8820	 0.5480
d	 0.7950	 0.4740
e	 0.8710	 0.5150
f	 0.8362	 0.4830
g	 0.9045	 0.5620
h	 0.8567	 0.5300
i	 0.8775	 0.5320
j	 0.8014	 0.4950
k	 0.7829	 0.4830
l	 0.8335	 0.5070
m	 0.8426	 0.5100
n	 0.7758	 0.4940
o	 0.8436	 0.5290

