



wwPDB EM Validation Summary Report ⓘ

Oct 1, 2024 – 12:18 AM JST

PDB ID : 5H64
EMDB ID : EMD-6668
Title : Cryo-EM structure of mTORC1
Authors : Yang, H.; Wang, J.; Liu, M.; Chen, X.; Huang, M.; Tan, D.; Dong, M.; Wong, C.C.L.; Wang, J.; Xu, Y.; Wang, H.
Deposited on : 2016-11-10
Resolution : 4.40 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
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The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

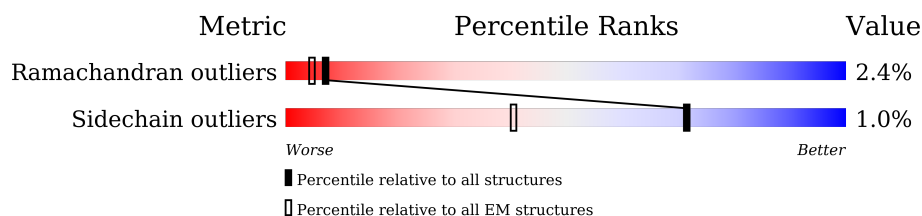
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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)
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 ≥ 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	2549	 13% 77% 5% 18%
1	a	2549	 13% 77% 5% 18%
2	B	1335	 5% 55% 40%
2	b	1335	 5% 55% 40%
3	C	326	 6% 95%
3	c	326	 7% 95%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 45252 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 Serine/threonine-protein kinase mTOR.

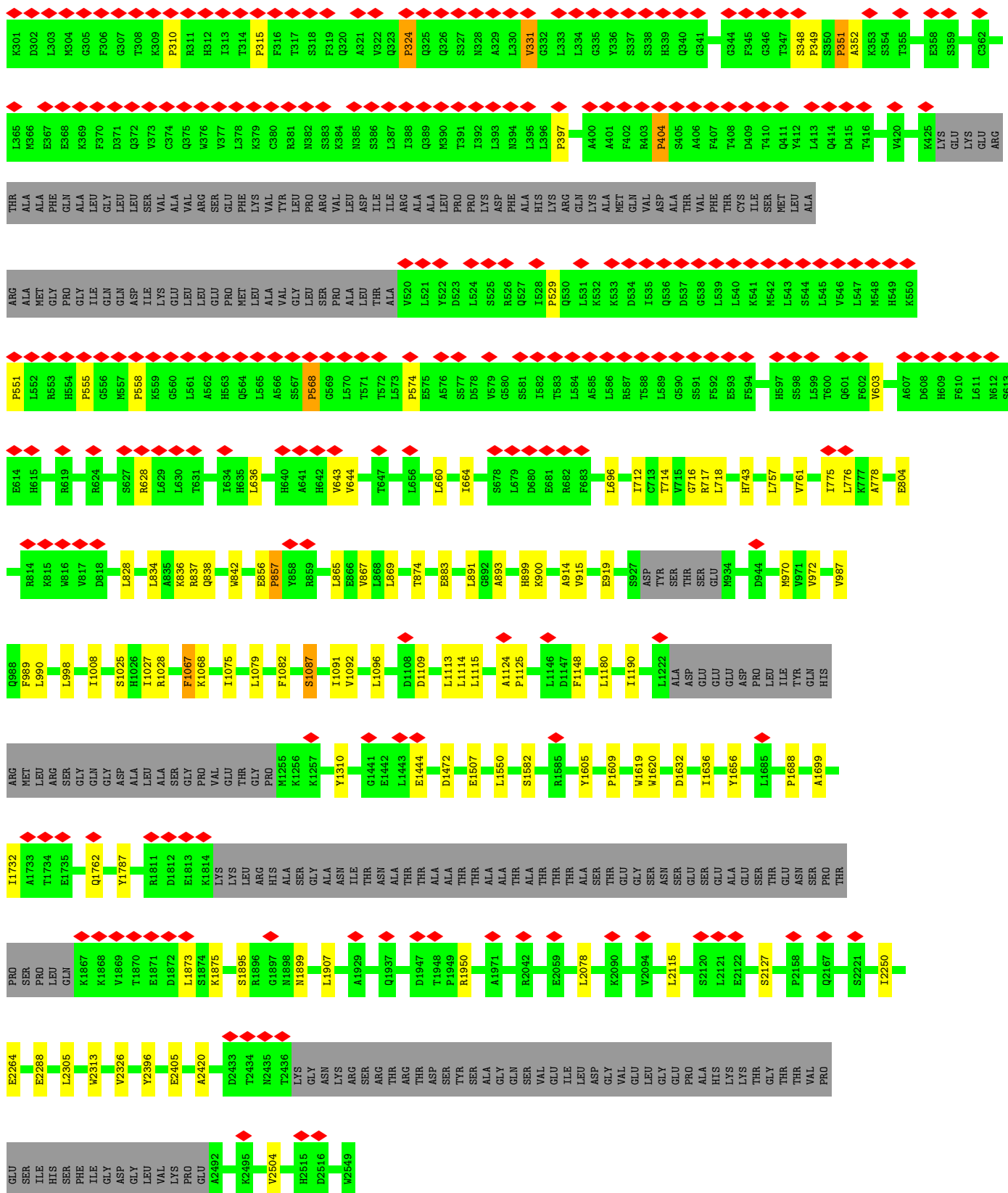
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2101	Total	C	N	O	S	0	0
			15617	9886	2788	2849	94		
1	a	2101	Total	C	N	O	S	0	0
			15617	9886	2788	2849	94		

- Molecule 2 is a protein called Regulatory-associated protein of mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	797	Total	C	N	O	S	0	0
			4553	2817	832	894	10		
2	b	797	Total	C	N	O	S	0	0
			4553	2817	832	894	10		

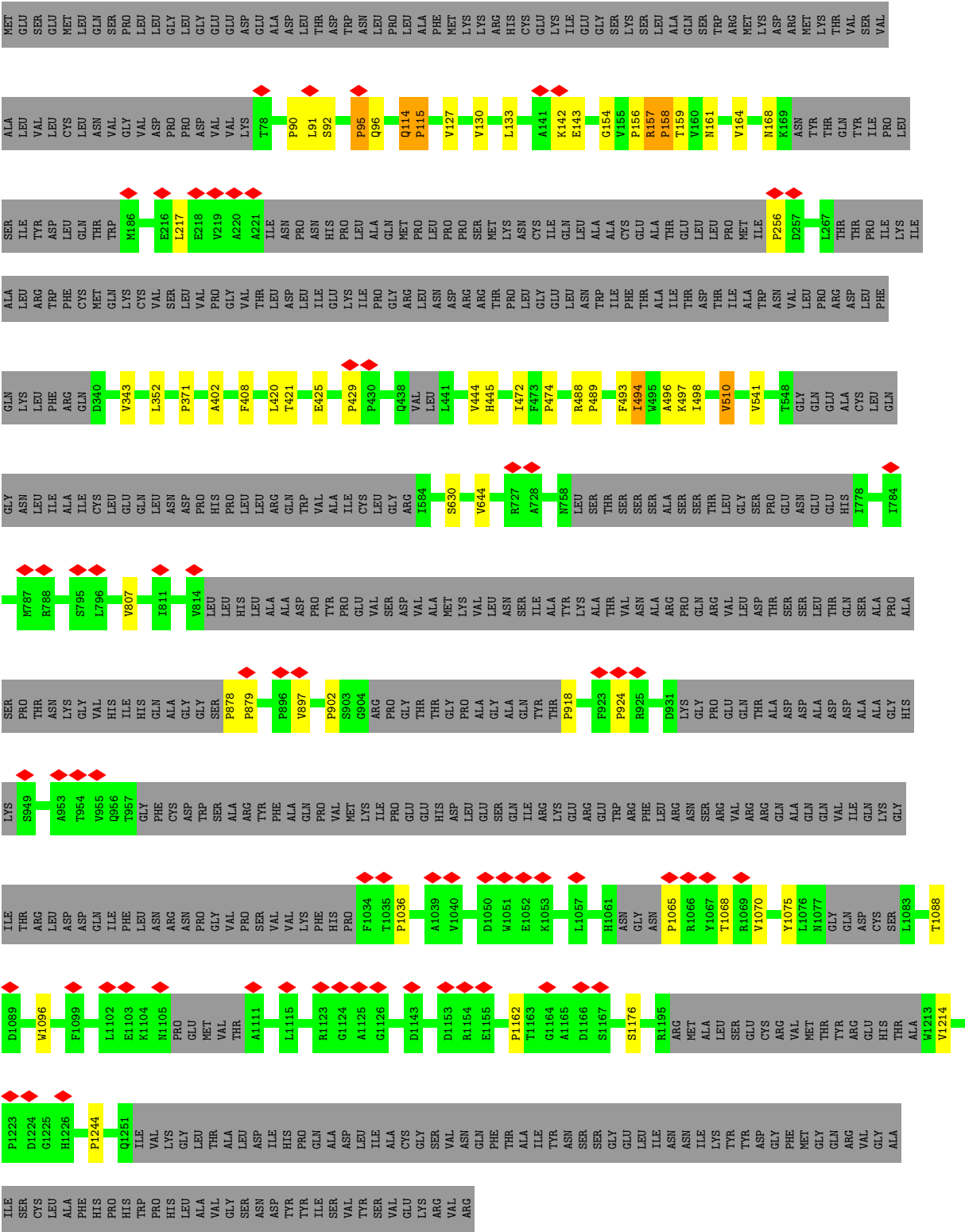
- Molecule 3 is a protein called Target of rapamycin complex subunit LST8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	317	Total	C	N	O	S	0	0
			2456	1526	436	476	18		
3	c	317	Total	C	N	O	S	0	0
			2456	1526	436	476	18		



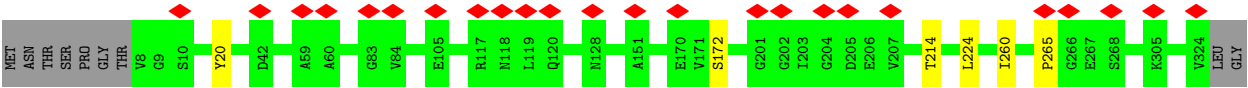
- Molecule 2: Regulatory-associated protein of mTOR







• Molecule 3: Target of rapamycin complex subunit LST8



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	115039	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 ($e^-/\text{\AA}^2$)	8.25	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0142	Depositor
Map size (Å)	391.962, 391.962, 391.962	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.30654, 1.30654, 1.30654	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.56	4/15910 (0.0%)	0.78	38/21634 (0.2%)
1	a	0.56	4/15910 (0.0%)	0.78	38/21634 (0.2%)
2	B	0.40	1/4567 (0.0%)	0.73	13/6217 (0.2%)
2	b	0.40	1/4567 (0.0%)	0.73	13/6217 (0.2%)
3	C	0.49	0/2514	0.68	1/3426 (0.0%)
3	c	0.49	0/2514	0.68	1/3426 (0.0%)
All	All	0.53	10/45982 (0.0%)	0.76	104/62554 (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	47
1	a	0	46
2	B	0	14
2	b	0	14
3	C	0	4
3	c	0	4
All	All	0	129

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2313	TRP	CB-CG	-7.38	1.36	1.50
1	a	2313	TRP	CB-CG	-7.37	1.36	1.50
1	A	1619	TRP	CB-CG	-6.24	1.39	1.50
1	a	1619	TRP	CB-CG	-6.22	1.39	1.50
1	a	842	TRP	CB-CG	-5.75	1.40	1.50

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	114	GLN	C-N-CD	-17.81	81.41	120.60
2	B	114	GLN	C-N-CD	-17.81	81.41	120.60
1	a	1113	LEU	CA-CB-CG	-10.98	90.05	115.30
1	A	1113	LEU	CA-CB-CG	-10.97	90.06	115.30
2	b	115	PRO	CA-N-CD	-10.09	97.38	111.50

There are no chirality outliers.

5 of 129 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	226	LYS	Peptide
1	A	257	ARG	Peptide
1	A	260	ARG	Peptide
1	A	261	ILE	Peptide
1	A	275	SER	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	2089/2549 (82%)	1654 (79%)	386 (18%)	49 (2%)	5	29
1	a	2089/2549 (82%)	1656 (79%)	384 (18%)	49 (2%)	5	29
2	B	767/1335 (58%)	608 (79%)	132 (17%)	27 (4%)	3	21
2	b	767/1335 (58%)	609 (79%)	131 (17%)	27 (4%)	3	21
3	C	315/326 (97%)	281 (89%)	33 (10%)	1 (0%)	37	72
3	c	315/326 (97%)	281 (89%)	33 (10%)	1 (0%)	37	72
All	All	6342/8420 (75%)	5089 (80%)	1099 (17%)	154 (2%)	7	28

5 of 154 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	PRO
1	A	351	PRO
1	A	404	PRO
1	A	568	PRO
1	A	664	ILE

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	1487/2220 (67%)	1485 (100%)	2 (0%)	92	95
1	a	1487/2220 (67%)	1485 (100%)	2 (0%)	92	95
2	B	185/1163 (16%)	167 (90%)	18 (10%)	6	22
2	b	177/1163 (15%)	160 (90%)	17 (10%)	7	22
3	C	269/276 (98%)	269 (100%)	0	100	100
3	c	269/276 (98%)	269 (100%)	0	100	100
All	All	3874/7318 (53%)	3835 (99%)	39 (1%)	71	81

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	897	VAL
2	b	1088	THR
2	b	902	PRO
2	b	1036	PRO
2	b	1214	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	722	ASN
1	a	1604	GLN

Continued on next page...

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Mol	Chain	Res	Type
3	c	251	ASN
1	a	829	GLN
1	a	1206	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

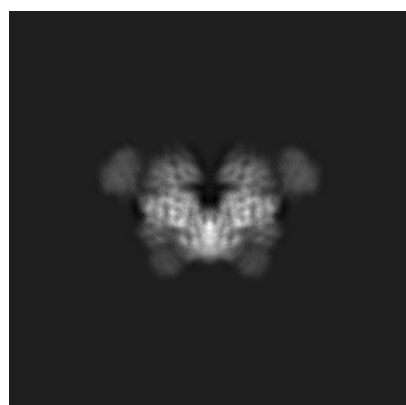
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6668. These allow visual inspection of the internal detail of the map and identification of artifacts.

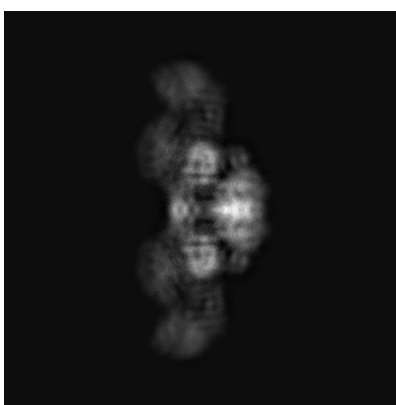
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

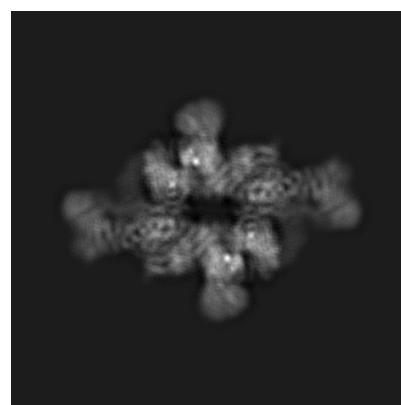
6.1.1 Primary map



X



Y

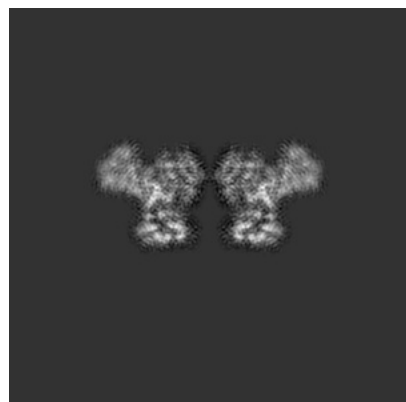


Z

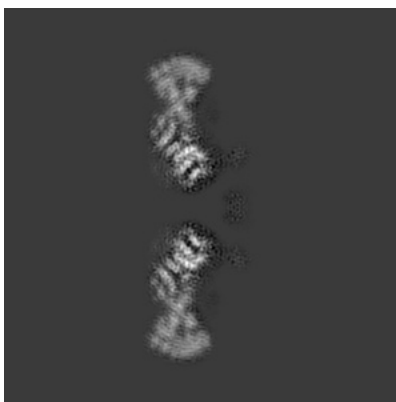
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

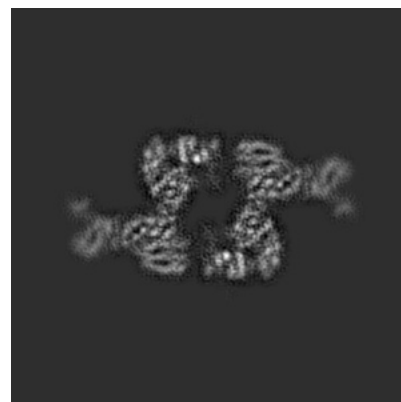
6.2.1 Primary map



X Index: 150



Y Index: 150

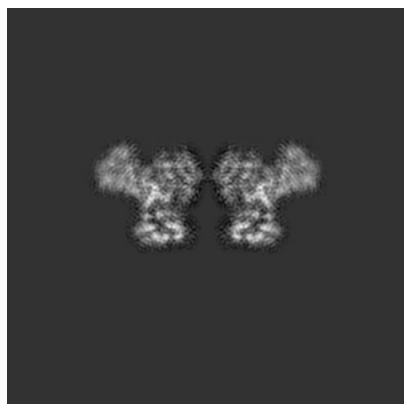


Z Index: 150

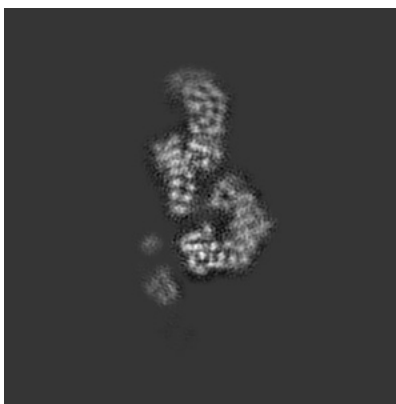
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

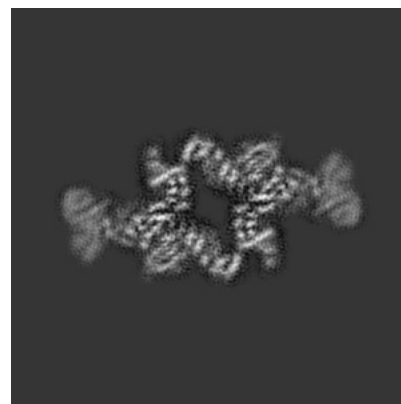
6.3.1 Primary map



X Index: 150



Y Index: 170

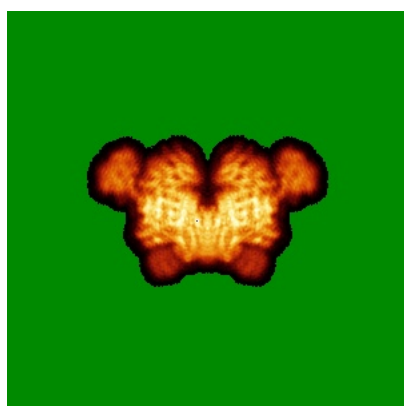


Z Index: 141

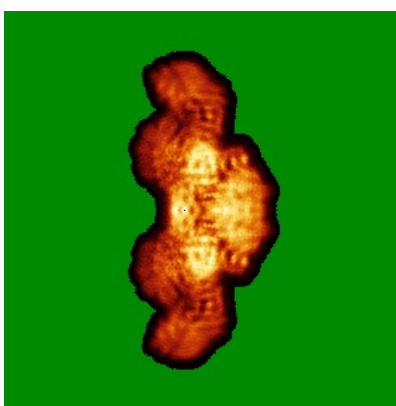
The images above show the largest variance slices of the map in three orthogonal directions.

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

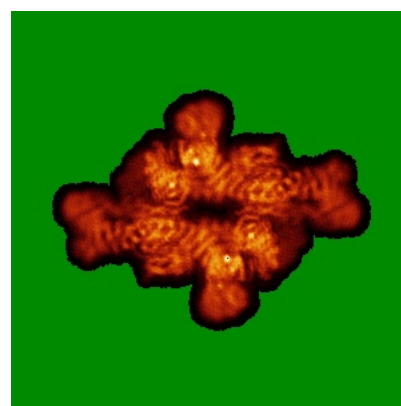
6.4.1 Primary map



X



Y

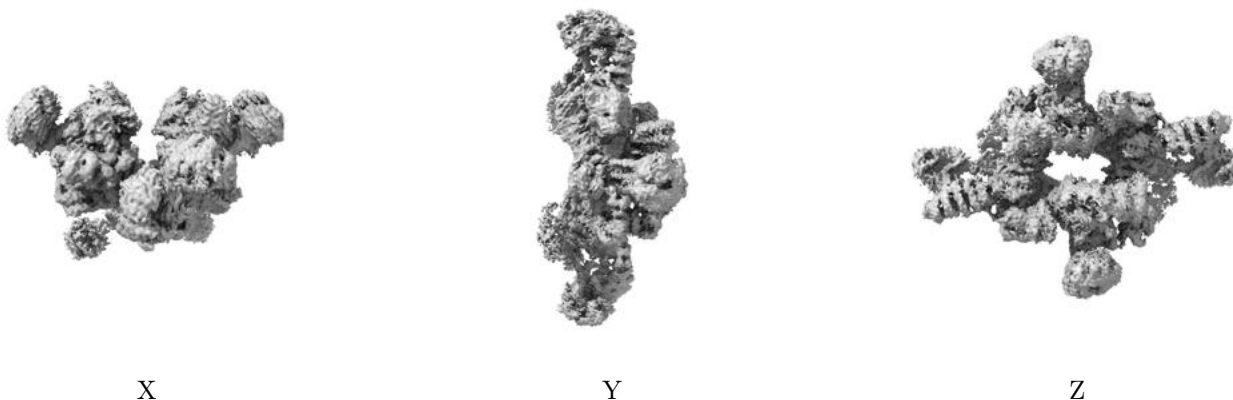


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0142. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

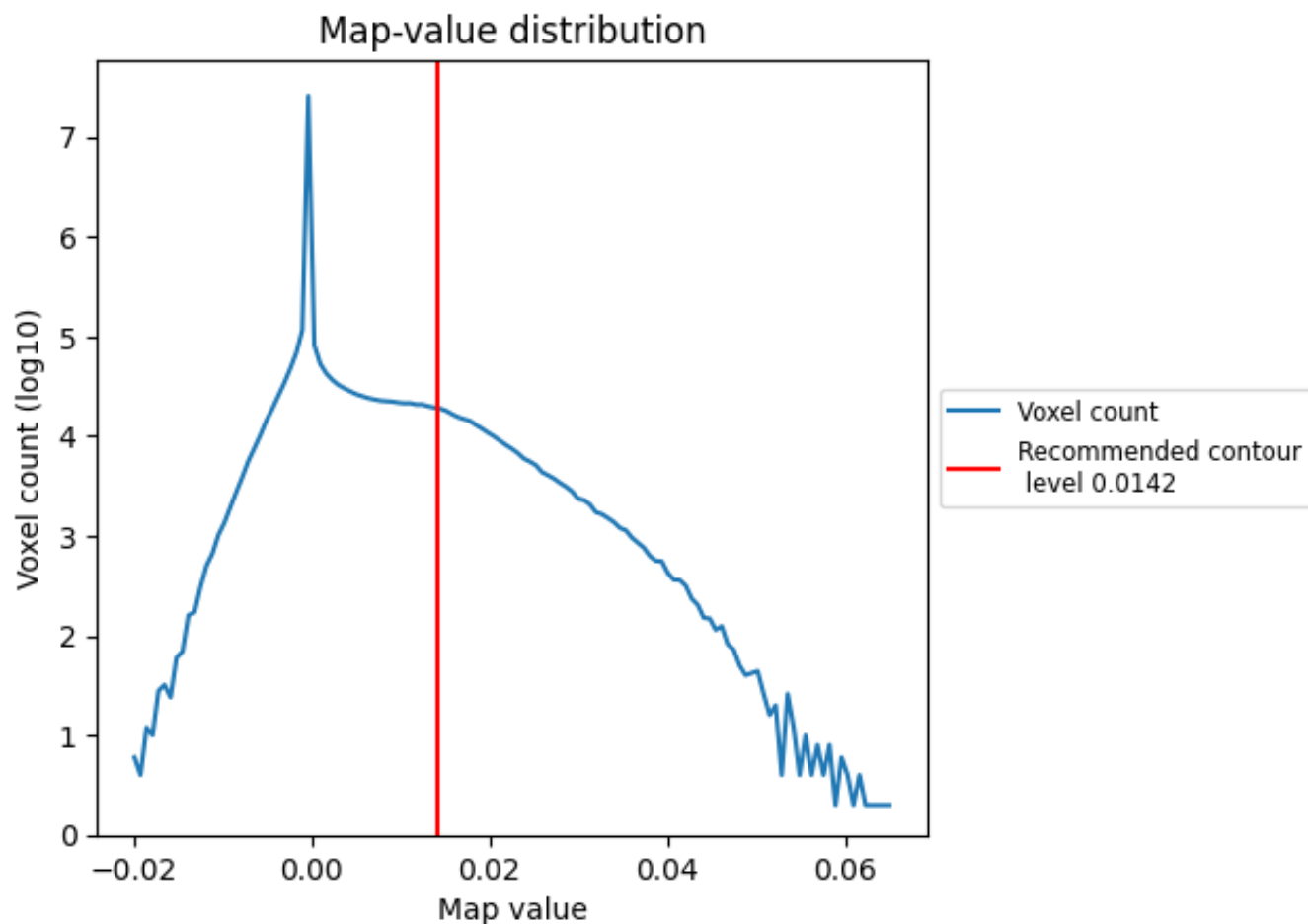
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

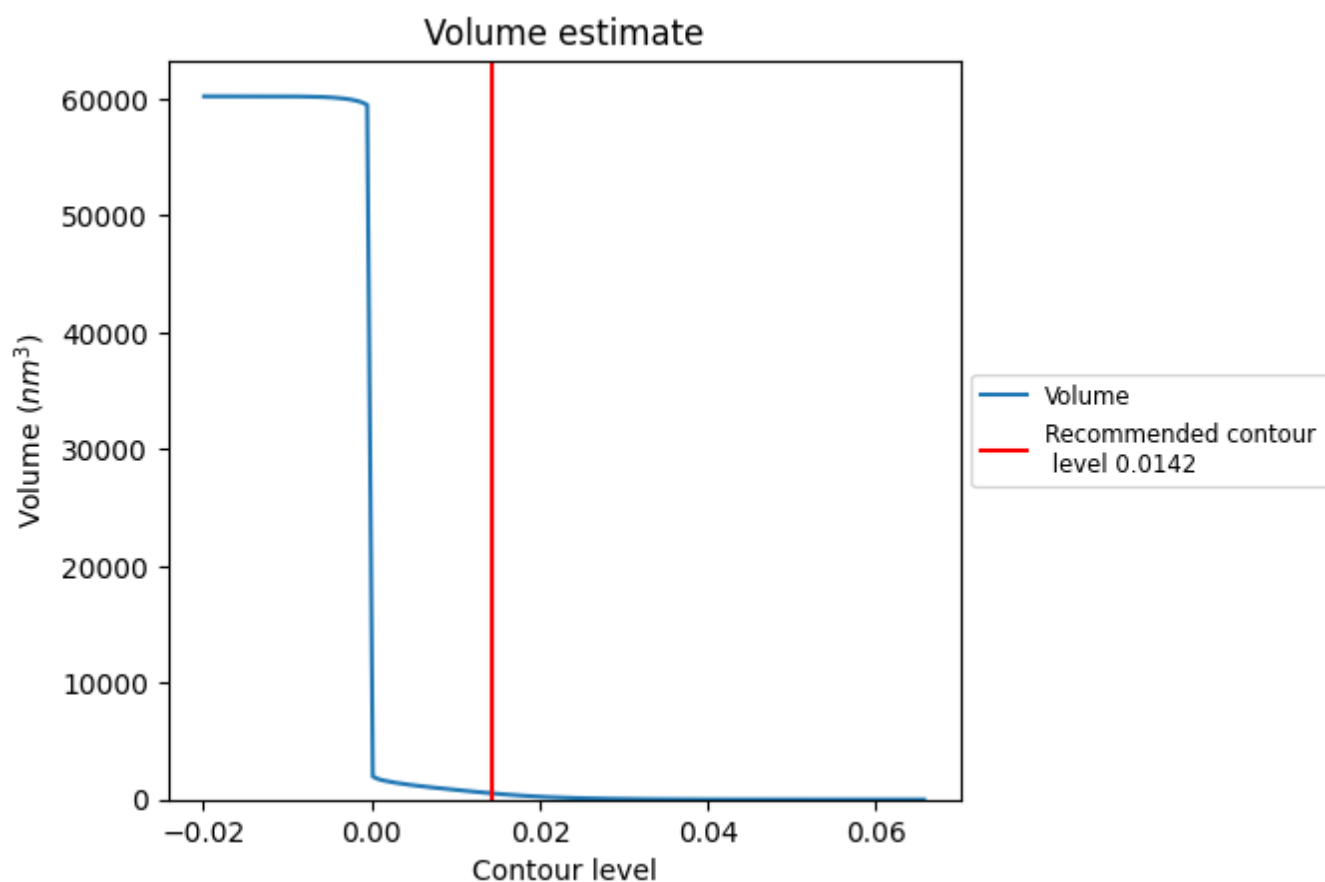
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

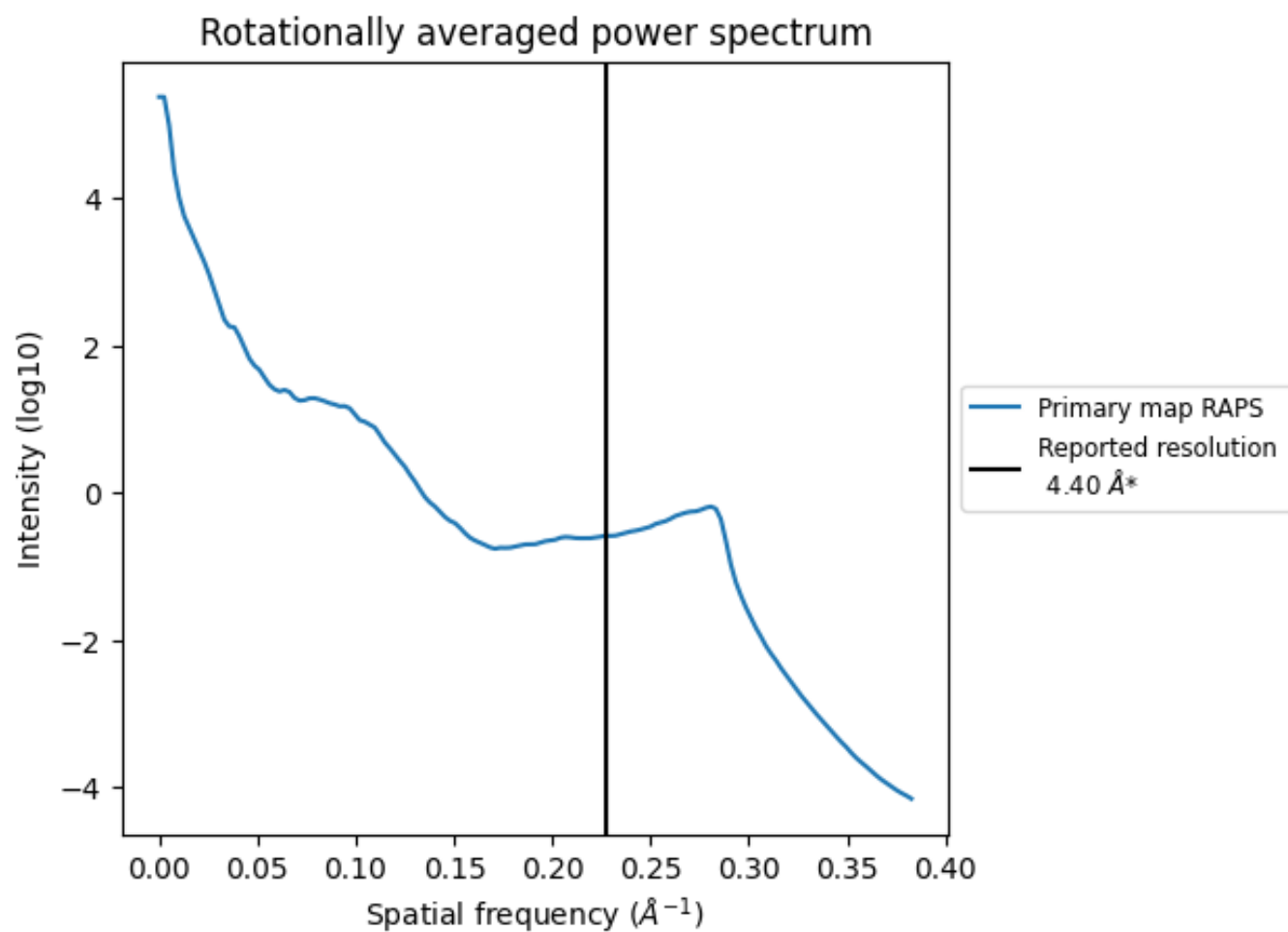
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 541 nm³; this corresponds to an approximate mass of 489 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 0.227 Å⁻¹

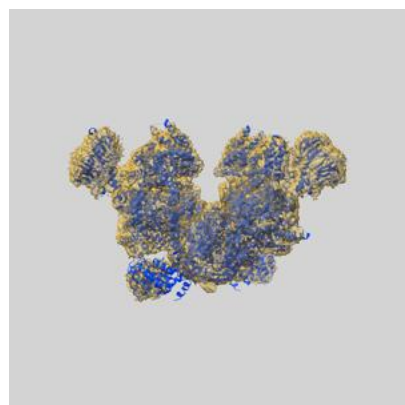
8 Fourier-Shell correlation ⓘ

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

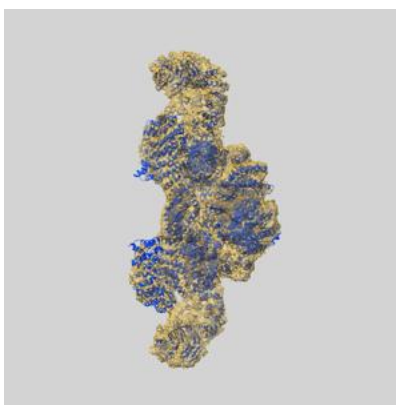
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6668 and PDB model 5H64. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

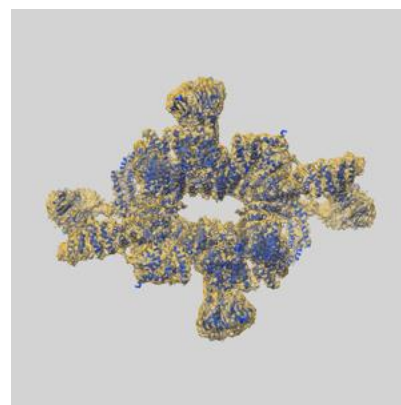
9.1 Map-model overlay [i](#)



X



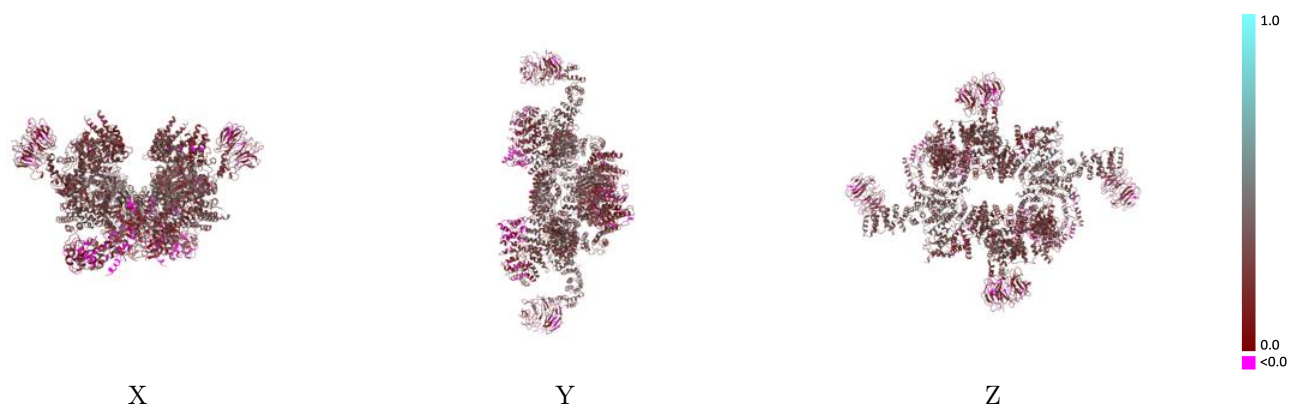
Y



Z

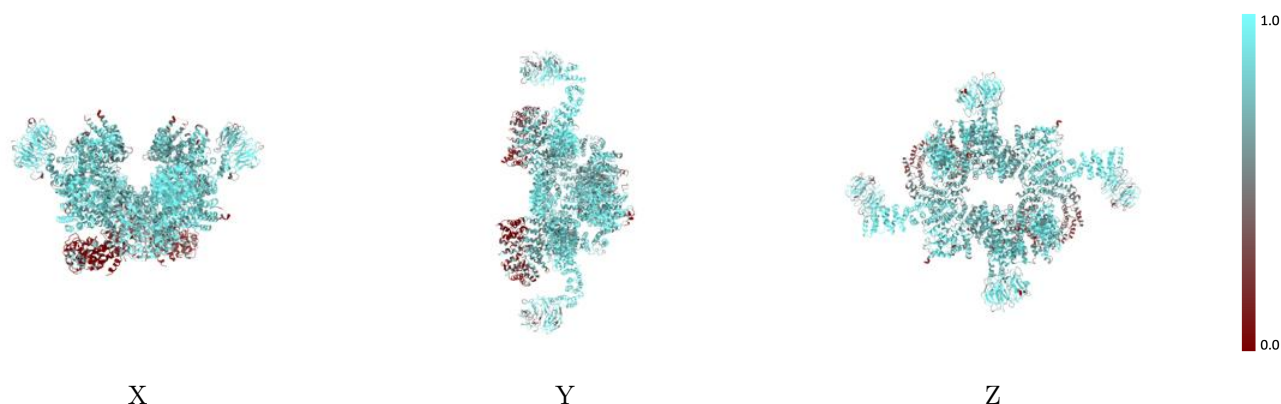
The images above show the 3D surface view of the map at the recommended contour level 0.0142 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



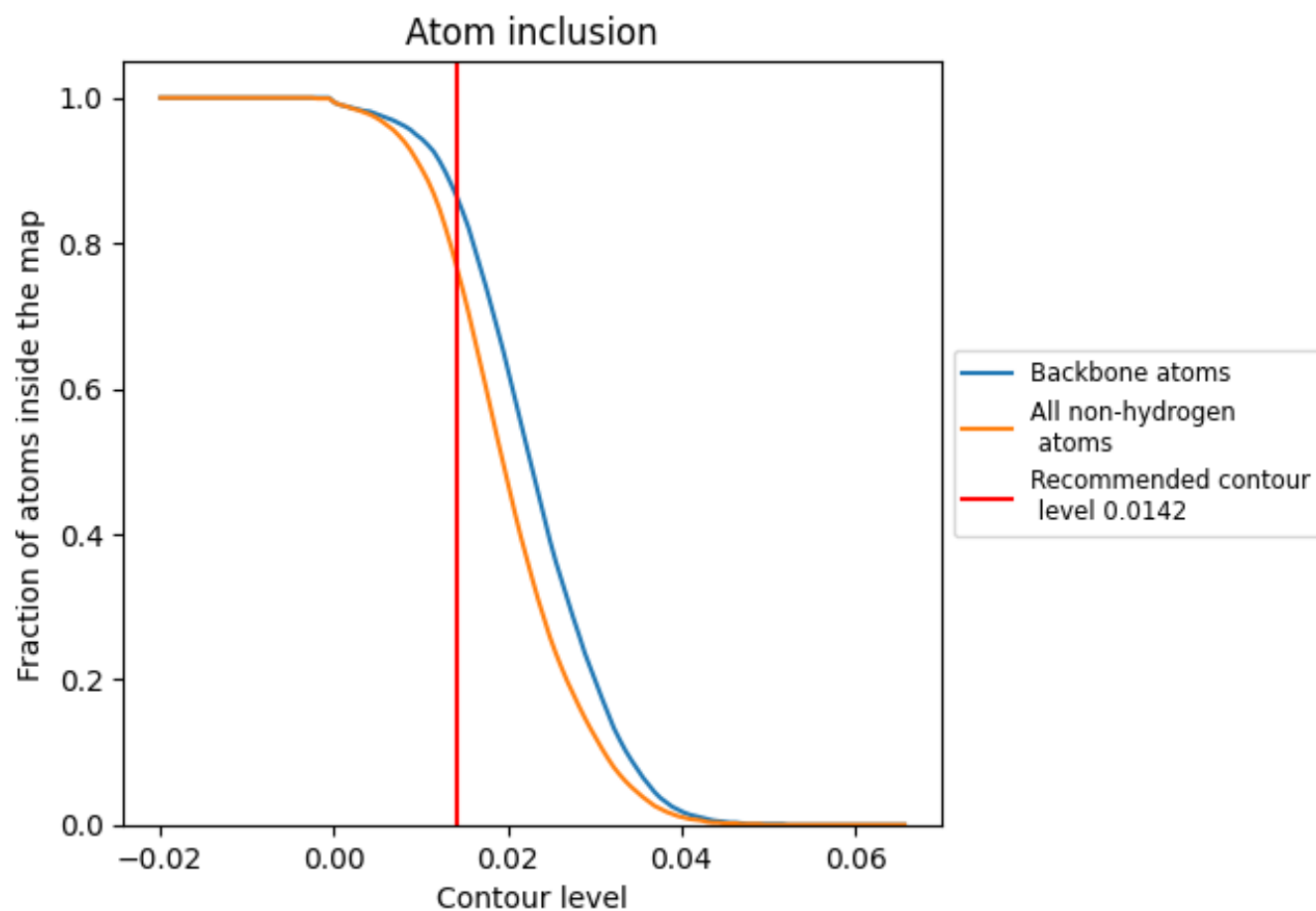
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0142).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 76% 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 (0.0142) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7650	<div><div></div></div> 0.2490
A	<div><div></div></div> 0.7330	<div><div></div></div> 0.2560
B	<div><div></div></div> 0.8370	<div><div></div></div> 0.2700
C	<div><div></div></div> 0.8400	<div><div></div></div> 0.1710
a	<div><div></div></div> 0.7330	<div><div></div></div> 0.2550
b	<div><div></div></div> 0.8360	<div><div></div></div> 0.2700
c	<div><div></div></div> 0.8370	<div><div></div></div> 0.1680

1.0

0.0

<0.0