



wwPDB EM Validation Summary Report ⓘ

Oct 21, 2024 – 01:57 PM JST

PDB ID : 7VGQ
EMDB ID : EMD-31975
Title : Cryo-EM structure of Machupo virus polymerase L in complex with matrix protein Z
Authors : Zhang, X.; Ma, J.; Zhang, S.
Deposited on : 2021-09-18
Resolution : 4.00 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

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>.

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

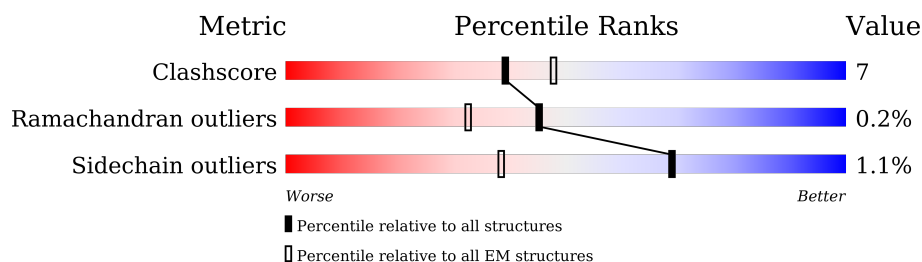
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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	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 ≥ 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	2238	<div> <div>19%</div> <div>60%</div> <div>11%</div> <div>28%</div> </div>
2	B	496	<div> <div>8%</div> <div>90%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13156 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 RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1612	Total	C	N	O	S	0	0
			12749	8144	2129	2389	87		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2210	TRP	-	expression tag	UNP Q6IUF8
A	2211	SER	-	expression tag	UNP Q6IUF8
A	2212	HIS	-	expression tag	UNP Q6IUF8
A	2213	PRO	-	expression tag	UNP Q6IUF8
A	2214	GLN	-	expression tag	UNP Q6IUF8
A	2215	PHE	-	expression tag	UNP Q6IUF8
A	2216	GLU	-	expression tag	UNP Q6IUF8
A	2217	LYS	-	expression tag	UNP Q6IUF8
A	2218	GLY	-	expression tag	UNP Q6IUF8
A	2219	GLY	-	expression tag	UNP Q6IUF8
A	2220	GLY	-	expression tag	UNP Q6IUF8
A	2221	SER	-	expression tag	UNP Q6IUF8
A	2222	GLY	-	expression tag	UNP Q6IUF8
A	2223	GLY	-	expression tag	UNP Q6IUF8
A	2224	GLY	-	expression tag	UNP Q6IUF8
A	2225	SER	-	expression tag	UNP Q6IUF8
A	2226	GLY	-	expression tag	UNP Q6IUF8
A	2227	GLY	-	expression tag	UNP Q6IUF8
A	2228	SER	-	expression tag	UNP Q6IUF8
A	2229	SER	-	expression tag	UNP Q6IUF8
A	2230	ALA	-	expression tag	UNP Q6IUF8
A	2231	TRP	-	expression tag	UNP Q6IUF8
A	2232	SER	-	expression tag	UNP Q6IUF8
A	2233	HIS	-	expression tag	UNP Q6IUF8
A	2234	PRO	-	expression tag	UNP Q6IUF8
A	2235	GLN	-	expression tag	UNP Q6IUF8
A	2236	PHE	-	expression tag	UNP Q6IUF8
A	2237	GLU	-	expression tag	UNP Q6IUF8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2238	LYS	-	expression tag	UNP Q6IUF8

- Molecule 2 is a protein called Maltose/maltodextrin-binding periplasmic protein,RING finger protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	49	Total	C	N	O	S	0	0
			405	254	73	69	9		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-401	MET	-	expression tag	UNP P0AEX9
B	-400	HIS	-	expression tag	UNP P0AEX9
B	-399	HIS	-	expression tag	UNP P0AEX9
B	-398	HIS	-	expression tag	UNP P0AEX9
B	-397	HIS	-	expression tag	UNP P0AEX9
B	-396	HIS	-	expression tag	UNP P0AEX9
B	-395	HIS	-	expression tag	UNP P0AEX9
B	-394	HIS	-	expression tag	UNP P0AEX9
B	-393	HIS	-	expression tag	UNP P0AEX9
B	-26	ASN	-	linker	UNP P0AEX9
B	-25	SER	-	linker	UNP P0AEX9
B	-24	SER	-	linker	UNP P0AEX9
B	-23	SER	-	linker	UNP P0AEX9
B	-22	ASN	-	linker	UNP P0AEX9
B	-21	ASN	-	linker	UNP P0AEX9
B	-20	ASN	-	linker	UNP P0AEX9
B	-19	ASN	-	linker	UNP P0AEX9
B	-18	ASN	-	linker	UNP P0AEX9
B	-17	ASN	-	linker	UNP P0AEX9
B	-16	ASN	-	linker	UNP P0AEX9
B	-15	ASN	-	linker	UNP P0AEX9
B	-14	ASN	-	linker	UNP P0AEX9
B	-13	ASN	-	linker	UNP P0AEX9
B	-12	LEU	-	linker	UNP P0AEX9
B	-11	GLY	-	linker	UNP P0AEX9
B	-10	ILE	-	linker	UNP P0AEX9
B	-9	GLU	-	linker	UNP P0AEX9
B	-8	LEU	-	linker	UNP P0AEX9
B	-7	GLU	-	linker	UNP P0AEX9
B	-6	VAL	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	LEU	-	linker	UNP P0AEX9
B	-4	PHE	-	linker	UNP P0AEX9
B	-3	GLN	-	linker	UNP P0AEX9
B	-2	GLY	-	linker	UNP P0AEX9
B	-1	PRO	-	linker	UNP P0AEX9
B	0	GLY	-	linker	UNP P0AEX9
B	1	SER	-	linker	UNP P0AEX9

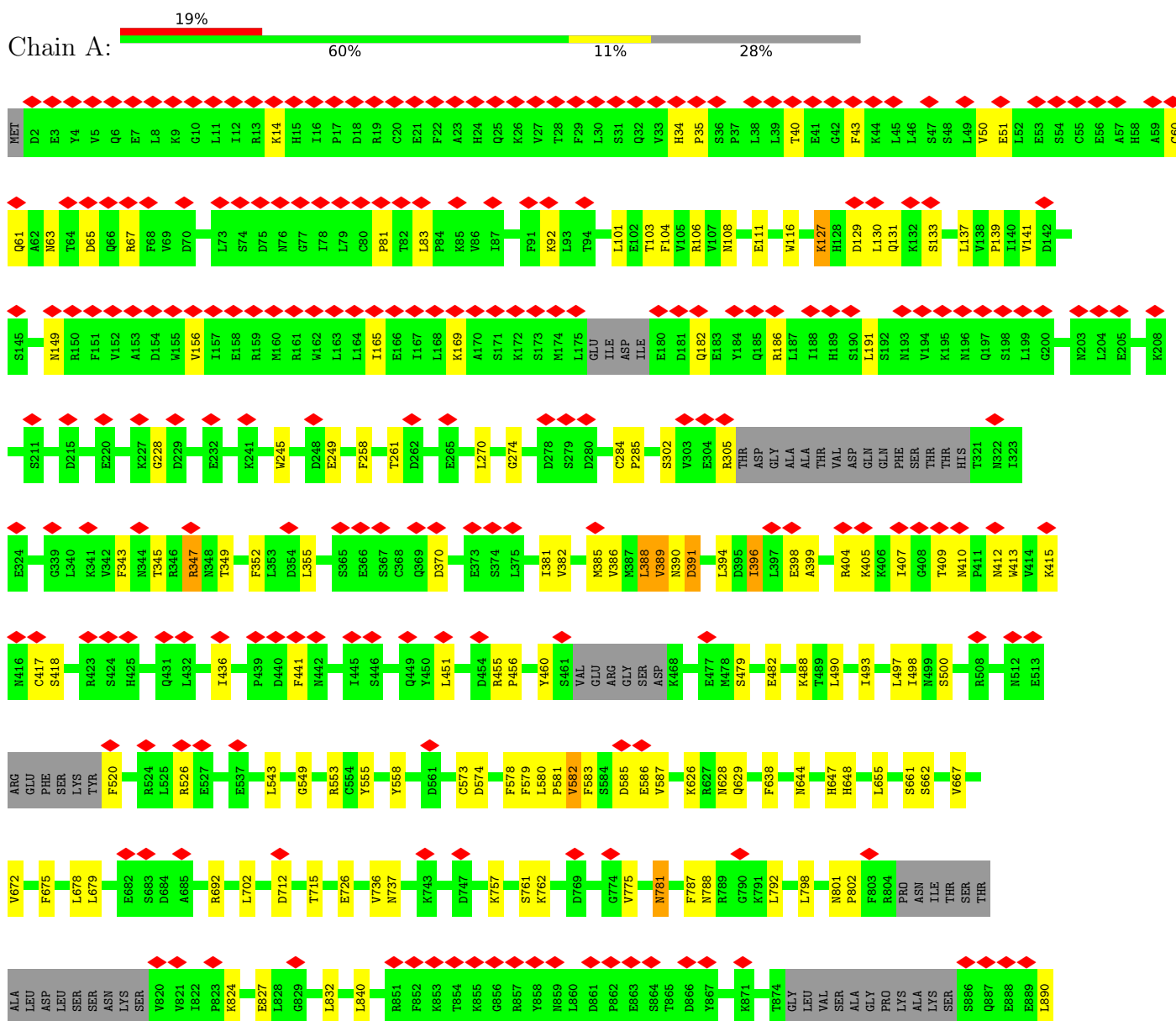
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	B	2	Total 2	Zn 2	0

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: RNA-directed RNA polymerase L





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	492364	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.541	Depositor
Minimum map value	-0.375	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.067	Depositor
Map size (Å)	192.0, 192.0, 192.0	wwPDB
Map dimensions	120, 120, 120	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.6, 1.6, 1.6	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: ZN

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	0.46	0/12967	0.69	5/17487 (0.0%)
2	B	0.43	0/417	0.58	0/566
All	All	0.46	0/13384	0.69	5/18053 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	ILE	N-CA-C	8.23	133.23	111.00
1	A	451	LEU	CA-CB-CG	6.45	130.14	115.30
1	A	1693	LEU	CA-CB-CG	5.21	127.27	115.30
1	A	1319	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	1558	LEU	CA-CB-CG	5.01	126.83	115.30

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	12749	0	12784	179	0
2	B	405	0	378	6	0
3	B	2	0	0	0	0
All	All	13156	0	13162	184	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 7.

The worst 5 of 184 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:975:LEU:HD12	1:A:976:PRO:CD	1.69	1.23
1:A:394:LEU:CD1	1:A:399:ALA:HB2	1.67	1.23
1:A:975:LEU:HD12	1:A:976:PRO:HD2	1.24	1.13
1:A:389:VAL:HG12	1:A:390:ASN:H	1.07	1.12
1:A:975:LEU:CD1	1:A:976:PRO:HD2	1.83	1.08

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	1582/2238 (71%)	1364 (86%)	215 (14%)	3 (0%)	44	76
2	B	47/496 (10%)	36 (77%)	11 (23%)	0	100	100
All	All	1629/2734 (60%)	1400 (86%)	226 (14%)	3 (0%)	45	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	391	ASP
1	A	959	ARG
1	A	389	VAL

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	1441/2026 (71%)	1425 (99%)	16 (1%)	70	80
2	B	47/412 (11%)	47 (100%)	0	100	100
All	All	1488/2438 (61%)	1472 (99%)	16 (1%)	69	80

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1114	ASN
1	A	1111	ASN
1	A	757	LYS
1	A	1026	MET
1	A	702	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1297	ASN
1	A	1689	ASN
1	A	1785	ASN
1	A	1586	GLN
1	A	644	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

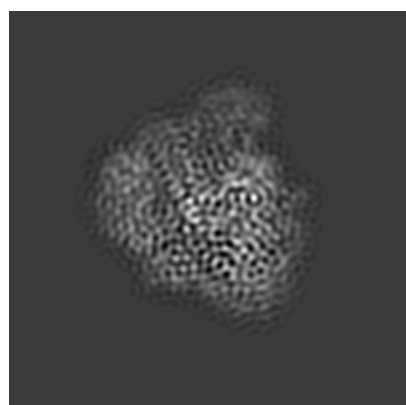
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31975. These allow visual inspection of the internal detail of the map and identification of artifacts.

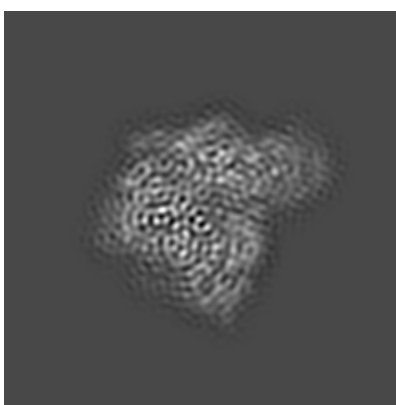
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

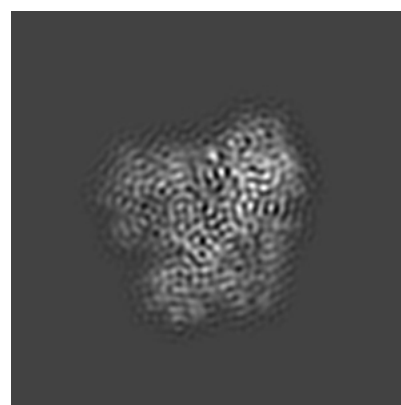
6.1.1 Primary map



X



Y

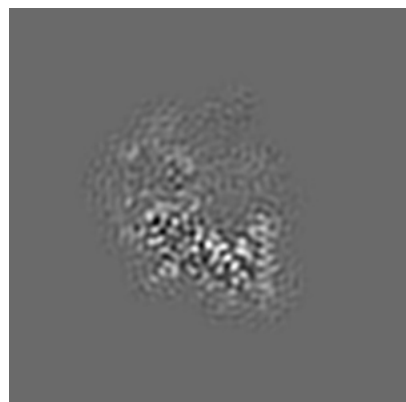


Z

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

6.2 Central slices [i](#)

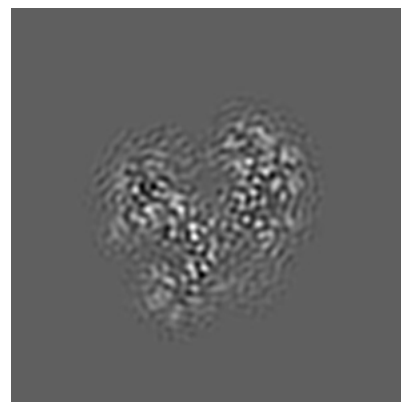
6.2.1 Primary map



X Index: 60



Y Index: 60

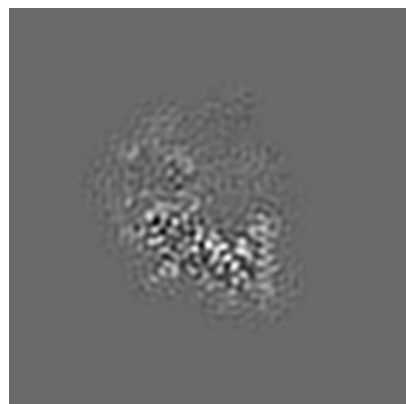


Z Index: 60

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: 60



Y Index: 61

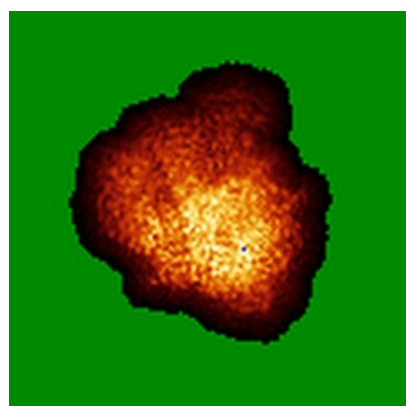


Z Index: 56

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

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

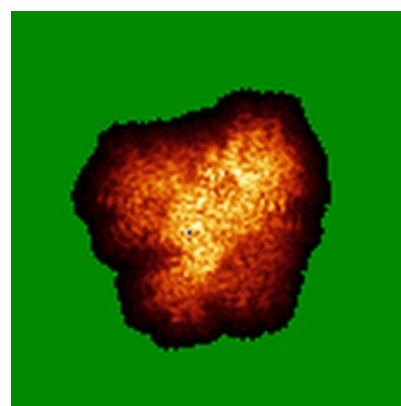
6.4.1 Primary map



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 0.067. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

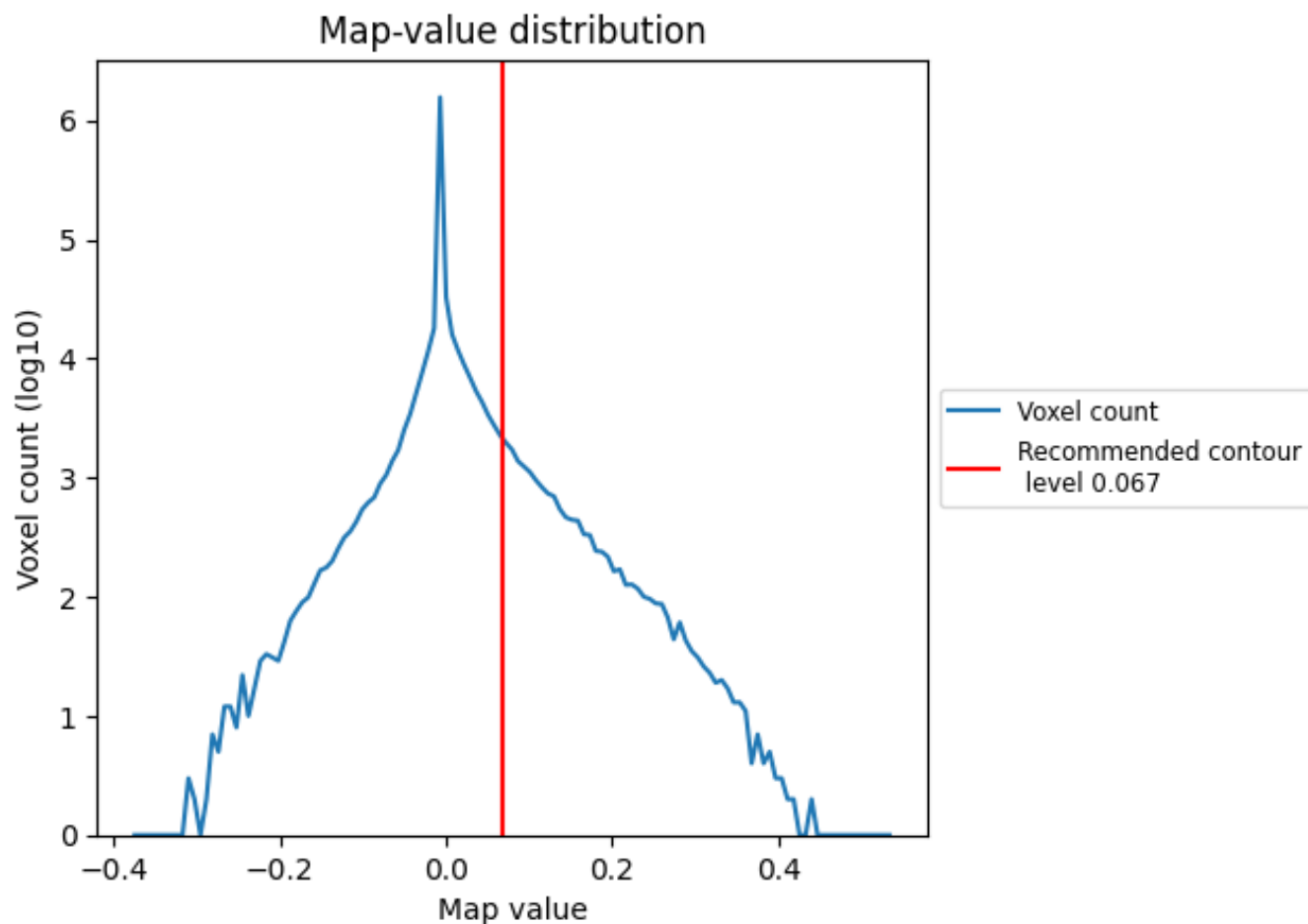
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

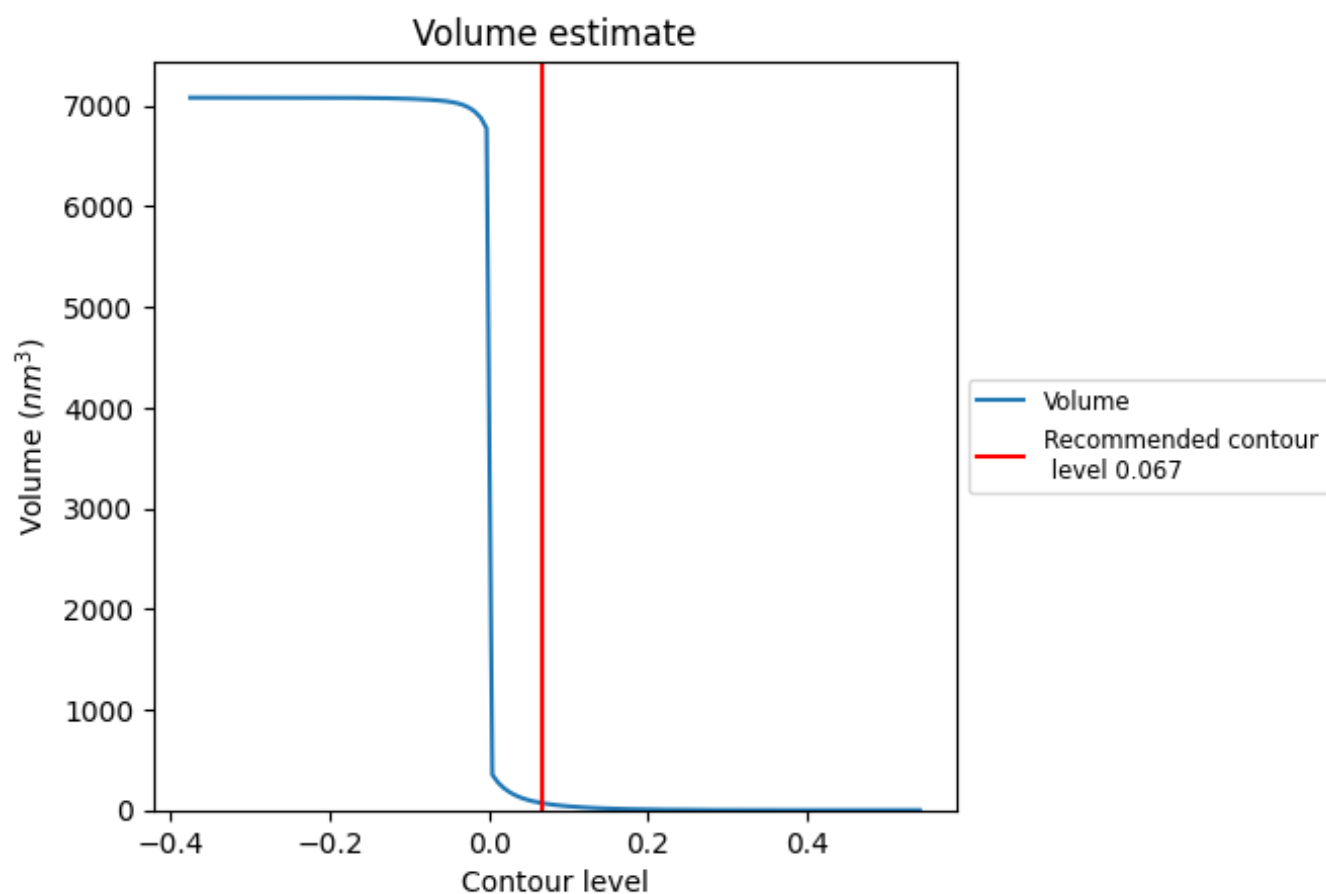
This section contains the results of statistical analysis of the map.

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.

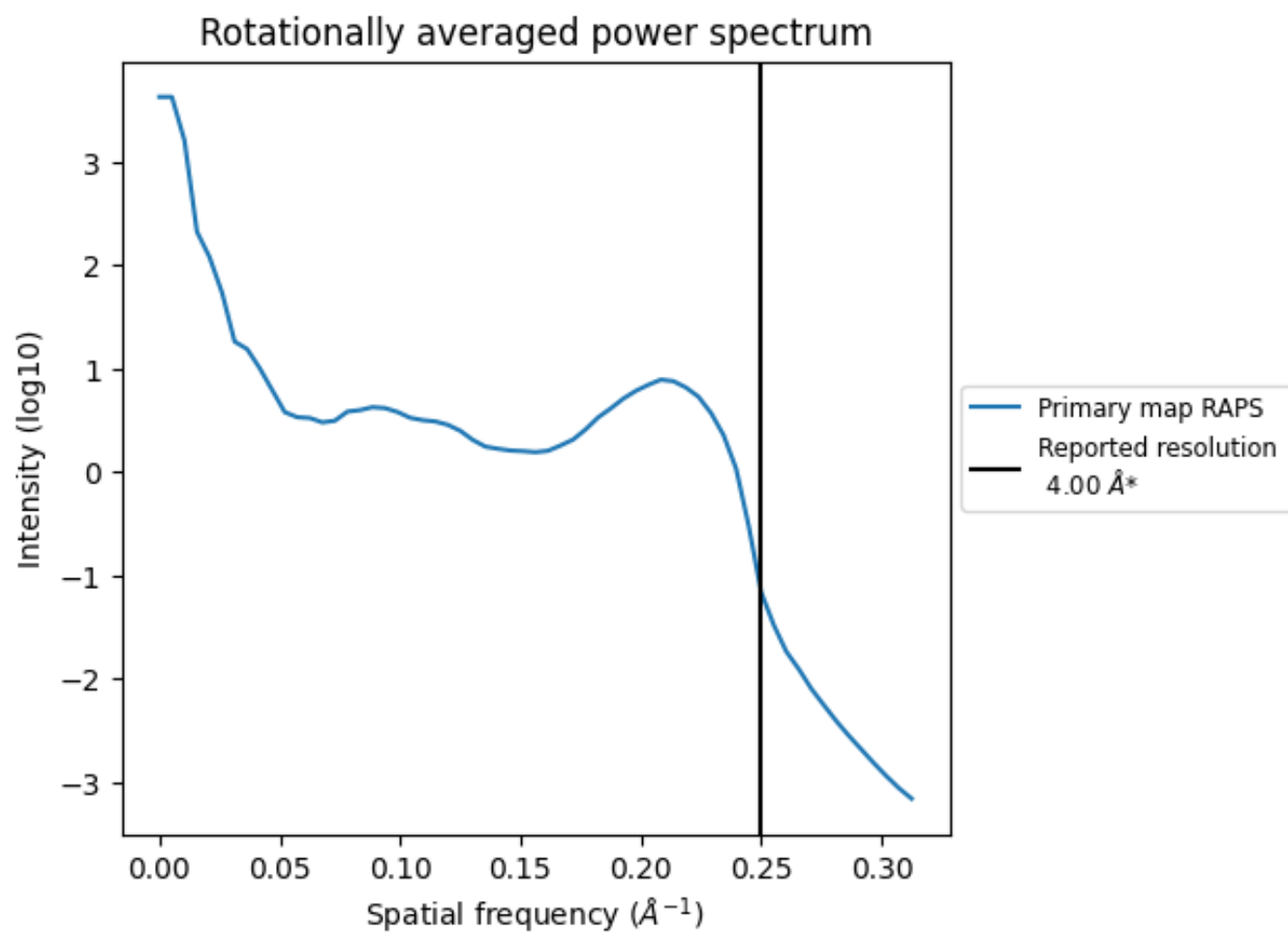
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 70 nm³; this corresponds to an approximate mass of 63 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 0.250 Å⁻¹

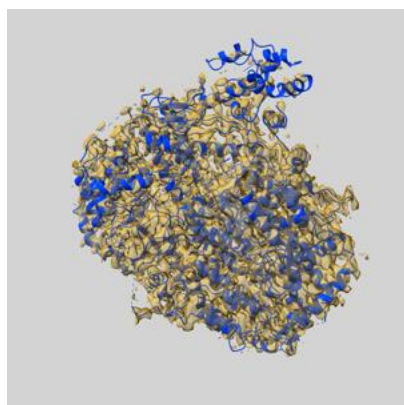
8 Fourier-Shell correlation ⓘ

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

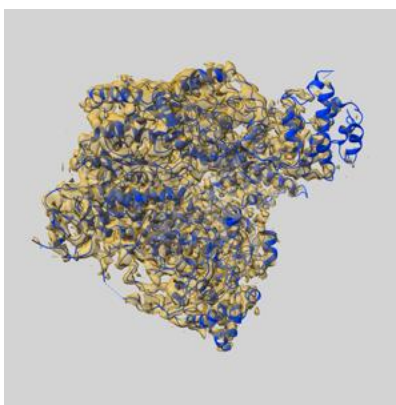
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31975 and PDB model 7VGQ. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

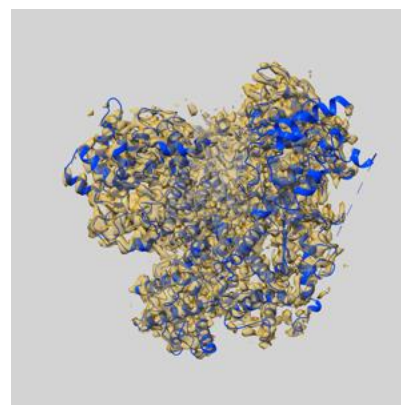
9.1 Map-model overlay [i](#)



X



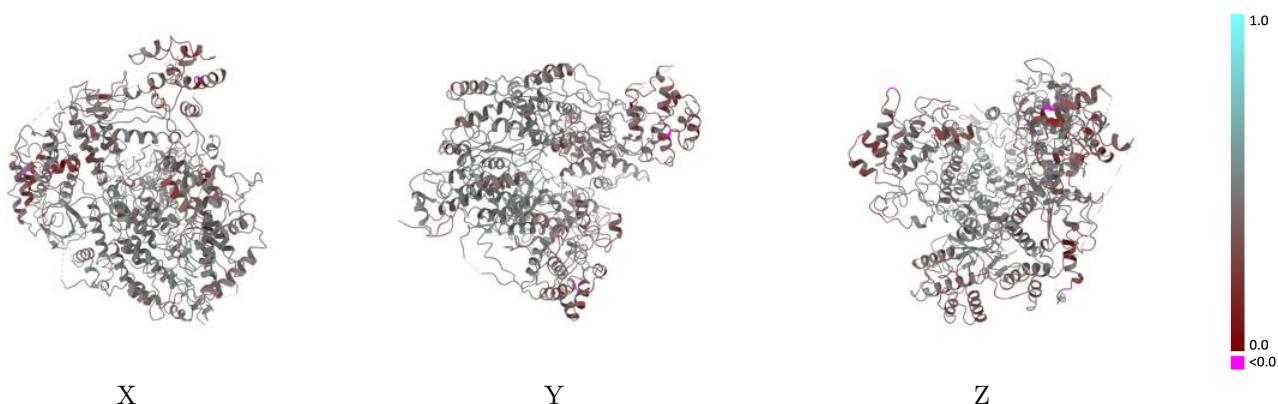
Y



Z

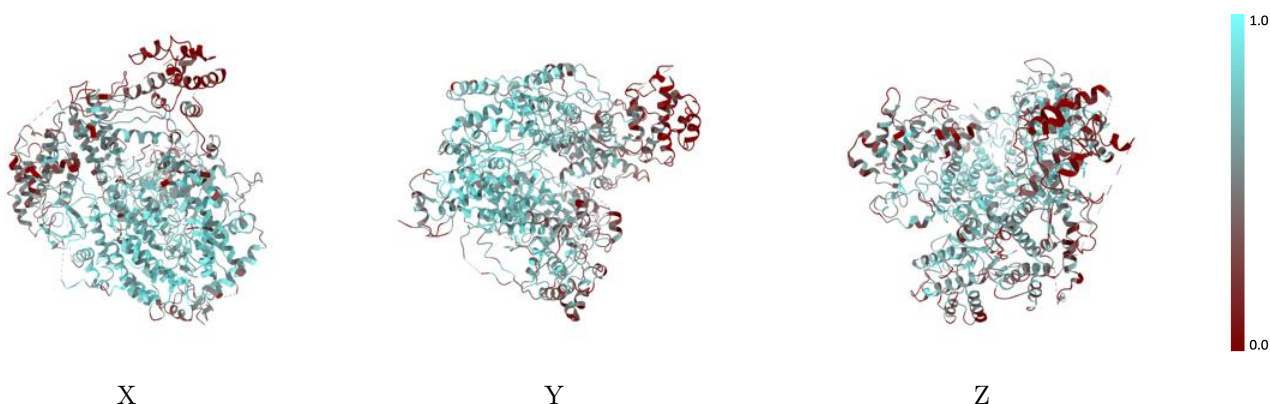
The images above show the 3D surface view of the map at the recommended contour level 0.067 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



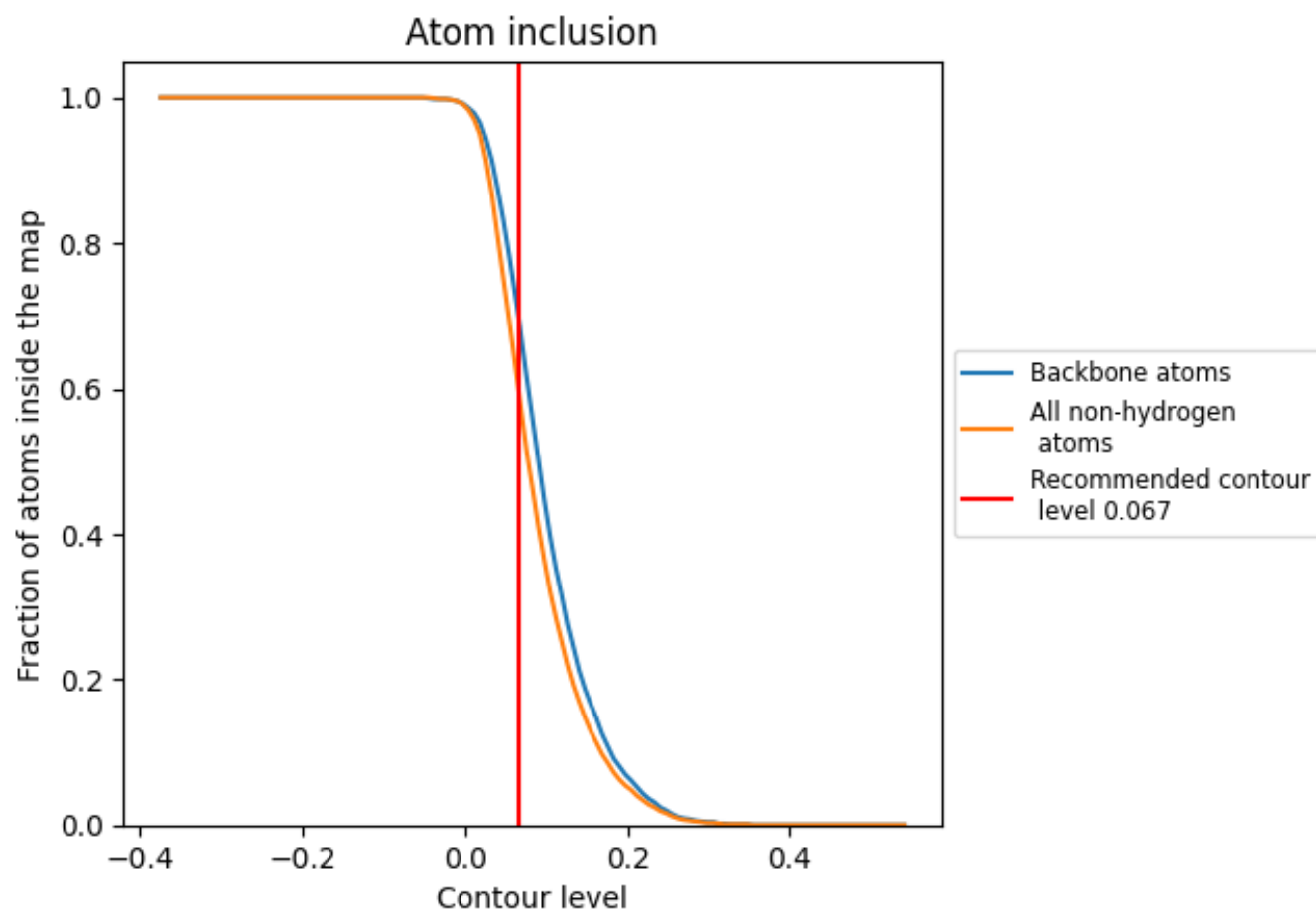
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.067).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 59% 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 (0.067) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5880	<div></div> 0.4400
A	<div></div> 0.5900	<div></div> 0.4400
B	<div></div> 0.5280	<div></div> 0.4580

