



wwPDB EM Validation Summary Report ⓘ

May 29, 2024 – 02:17 PM JST

PDB ID : 8X01
EMDB ID : EMD-37964
Title : Structure of the Mumps Virus L Protein (state2) Bound by Phosphoprotein Tetramer
Authors : Li, T.H.; Shen, Q.T.
Deposited on : 2023-11-02
Resolution : 3.01 Å(reported)

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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.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

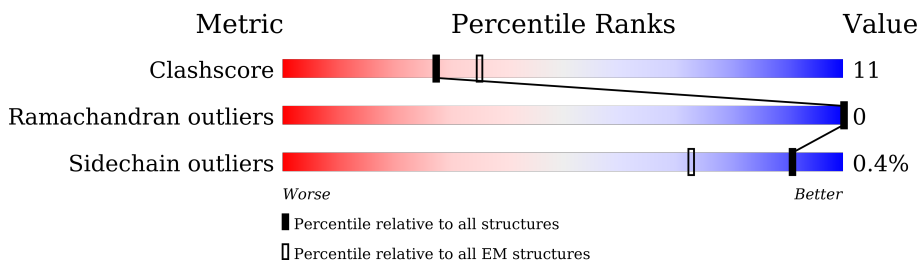
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.01 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 ≥ 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	2261	 47% 12% 40%
2	B	391	 13% 5% 82%
2	C	391	 13% 9% 78%
2	D	391	 7% 5% 87%
2	E	391	 8% 6% 86%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12742 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
			Total	C	N	O	S		
1	A	1350	10782	6893	1841	1987	61	0	0

- Molecule 2 is a protein called Phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	69	517	321	89	101	6	0	0
2	C	85	642	398	112	126	6	0	0
2	D	50	387	239	68	77	3	0	0
2	E	54	412	254	72	81	5	0	0

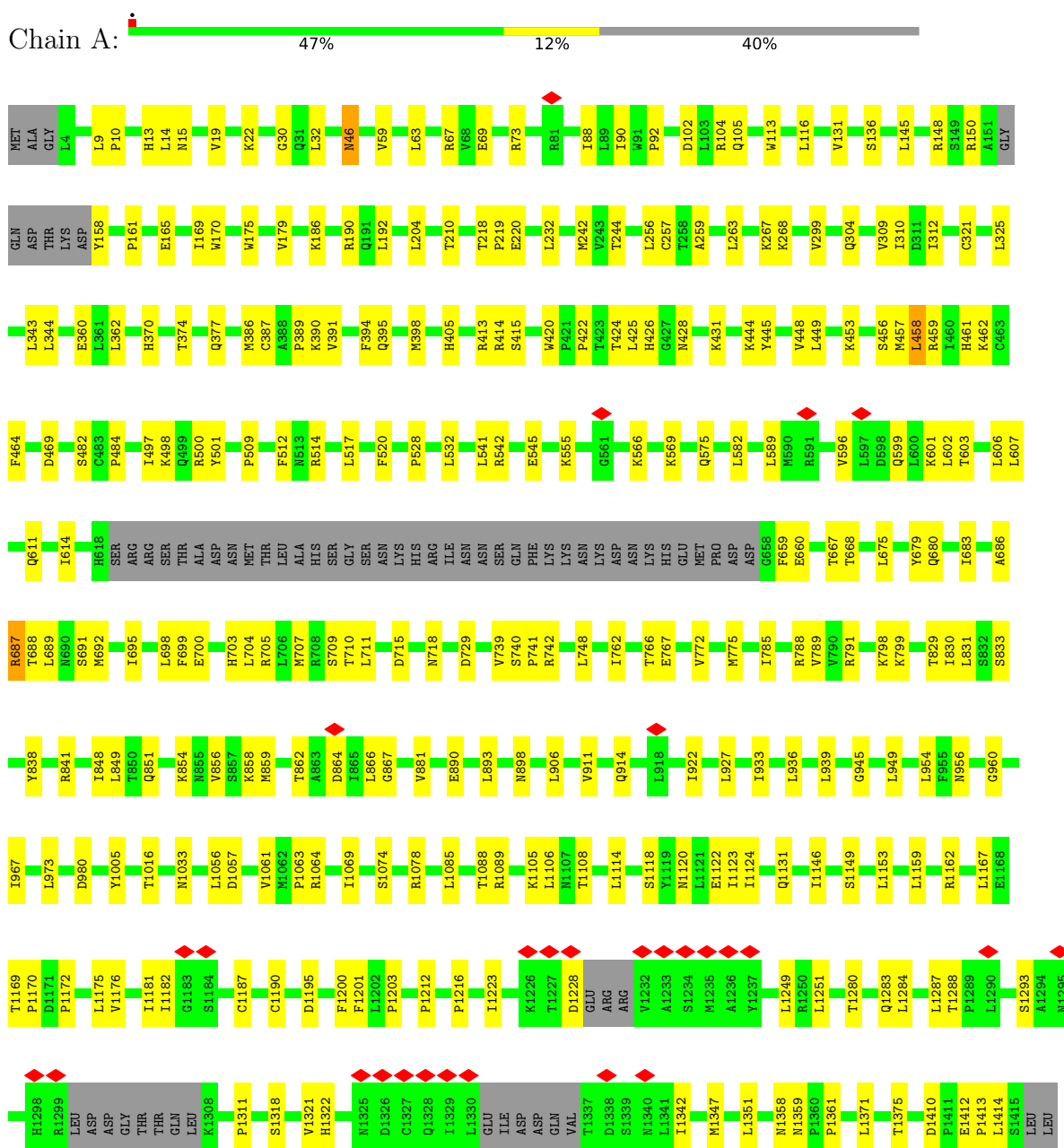
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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



SER THR
THR GLU
GLU ASP
ASP ALA
ALA LEU
LEU ASN
ASN ASP
ASP ILE
ILE LYS
LYS ARG
ARG ASP
ASP ILE
ILE ILE
ILE ARG
ARG SER
SER ALA
ALA ILE

● Molecule 2: Phosphoprotein

Chain E:  8% 6%  86%

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

THR ALA
ALA SER
HIS HIS
SER SER
GLY GLY
GLY LYS
SER LYS
LEU LEU
ALA ALA
SER LYS
THR THR
GLY GLY
ARG ARG
SER SER
SER SER
GLY GLY
SER SER
THR THR
GLN GLN
THR THR
LEU LEU
ASP ASP
GLY GLY
THR THR
VAL VAL
TRP TRP
ASN ASN
PRO PRO
GLY GLY
SER SER
THR THR
SER SER
ALA ALA
ALA ALA
GLY GLY
THR THR
SER SER

SER TYR
TYR ARG
ARG SER
SER SER
VAL VAL
GLY GLY
SER LYS
LEU LEU
ALA ALA
SER LYS
THR THR
GLY GLY
LYS LYS
GLU GLU
ARG ARG
MET MET
ILE ILE
ILE ILE
ASN ASN
ARG ARG
PHE PHE
ILE ILE
VAL VAL
GLU GLU
LYS LYS
SER SER
PRO PRO
THR THR
THR THR
PHE PHE
LYS LYS
ARG ARG
GLY GLY
GLY GLY
PRO PRO
GLY GLY
ALA ALA
SER SER

LYS LYS
GLU GLU
ARG ARG
SER SER
GLY GLY
SER SER
LEU LEU
SER SER
ALA ALA
SER LYS
THR THR
LEU LEU
TYR TYR
ALA ALA
HIS HIS
SER SER
SER SER
PRO PRO
GLN GLN
VAL VAL
GLY GLY
SER SER
PRO PRO
ALA ALA
ASN ASN
VAL VAL
GLY GLY
VAL VAL
ILE ILE
THR THR
ALA ALA
PRO PRO
PHE PHE
SER SER
SER SER
ALA ALA
HIS HIS
SER SER
VAL VAL
M226
M227
M228
M229
M230
M231
M232
M233
M234
M235
M236
M237
M238
M239
M240
M241
M242
M243
M244
M245
M246
M247
M248
M249

T250 Q251
Q252 K253
K254 N254
E255 L256
S257 T258
T261 T262
T265 A271
THR VAL
LYS VAL
ILE ILE
MET MET
SER SER
ASN ASN
PRO PRO
GLY GLY
THR THR
VAL VAL
GLY GLY
VAL VAL
ILE ILE
THR THR
ALA ALA
PRO PRO
GLN GLN
SER SER
ILE ILE
LEU LEU
THR THR
LYS LYS
SER SER
PHE PHE
SER SER
ASP ASP
CYS CYS
VAL VAL
VAL VAL
ALA ALA
ASN ASN
PRO PRO
GLN GLN
SER SER
MET MET
LYS LYS
GLY GLY
PRO PRO
PHE PHE
SER SER
SER SER
ALA ALA
HIS HIS
SER SER
VAL VAL
M226
M227
M228
M229
M230
M231
M232
M233
M234
M235
M236
M237
M238
M239
M240
M241
M242
M243
M244
M245
M246
M247
M248
M249

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

GLU ASP
ASP ALA
ALA LEU
ASN ASN
ASP ILE
ILE LYS
LYS ARG
ARG ASP
SER SER
ALA ALA
ILE ILE

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	477568	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)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.626	Depositor
Minimum map value	-1.093	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.124	Depositor
Map size (\AA)	233.19998, 233.19998, 233.19998	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.53, 0.53, 0.53	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	0.28	0/11010	0.50	0/14946
2	B	0.37	0/520	0.58	0/701
2	C	0.45	0/648	0.62	0/874
2	D	0.35	0/387	0.59	0/519
2	E	0.47	0/412	0.63	0/551
All	All	0.31	0/12977	0.52	0/17591

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	10782	0	10909	213	0
2	B	517	0	545	38	0
2	C	642	0	665	39	0
2	D	387	0	408	25	0
2	E	412	0	434	20	0
3	A	2	0	0	0	0
All	All	12742	0	12961	278	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 11.

The worst 5 of 278 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:729:ASP:O	2:C:286:VAL:HG12	1.51	1.09
1:A:394:PHE:HE2	2:B:269:MET:HG3	1.22	1.04
1:A:459:ARG:HB2	2:C:303:PRO:HG3	1.49	0.95
1:A:459:ARG:HB2	2:C:303:PRO:CG	2.01	0.91
1:A:687:ARG:HH21	2:B:284:VAL:HG22	1.38	0.86

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	1338/2261 (59%)	1315 (98%)	23 (2%)	0	100	100
2	B	67/391 (17%)	66 (98%)	1 (2%)	0	100	100
2	C	83/391 (21%)	79 (95%)	4 (5%)	0	100	100
2	D	48/391 (12%)	48 (100%)	0	0	100	100
2	E	52/391 (13%)	51 (98%)	1 (2%)	0	100	100
All	All	1588/3825 (42%)	1559 (98%)	29 (2%)	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	1214/2037 (60%)	1208 (100%)	6 (0%)	88	96
2	B	59/324 (18%)	59 (100%)	0	100	100
2	C	74/324 (23%)	74 (100%)	0	100	100
2	D	44/324 (14%)	44 (100%)	0	100	100
2	E	46/324 (14%)	46 (100%)	0	100	100
All	All	1437/3333 (43%)	1431 (100%)	6 (0%)	91	97

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	458	LEU
1	A	687	ARG
1	A	980	ASP
1	A	170	TRP
1	A	46	ASN

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	697	HIS
1	A	887	ASN
2	E	254	ASN

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](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

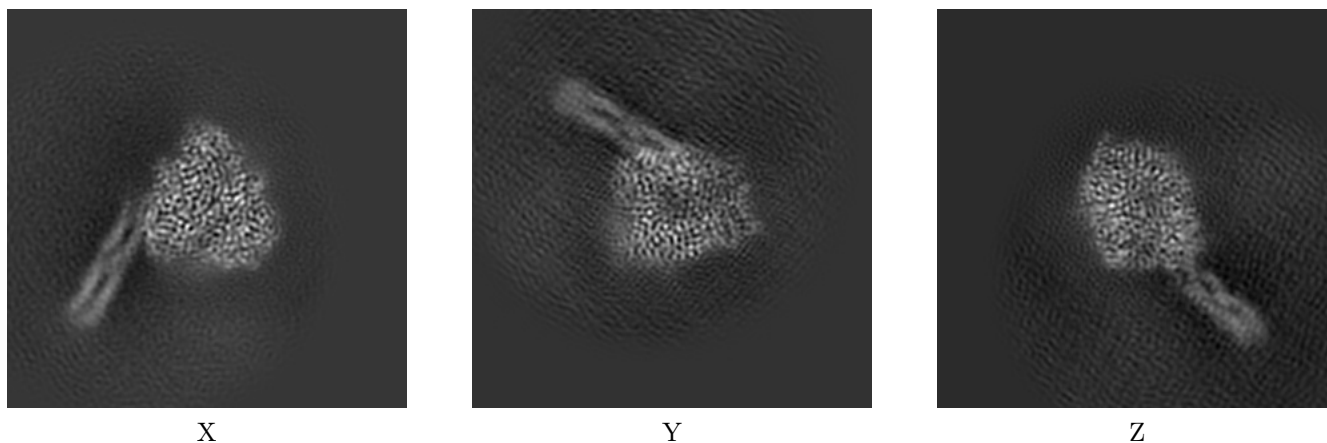
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37964. 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](#)

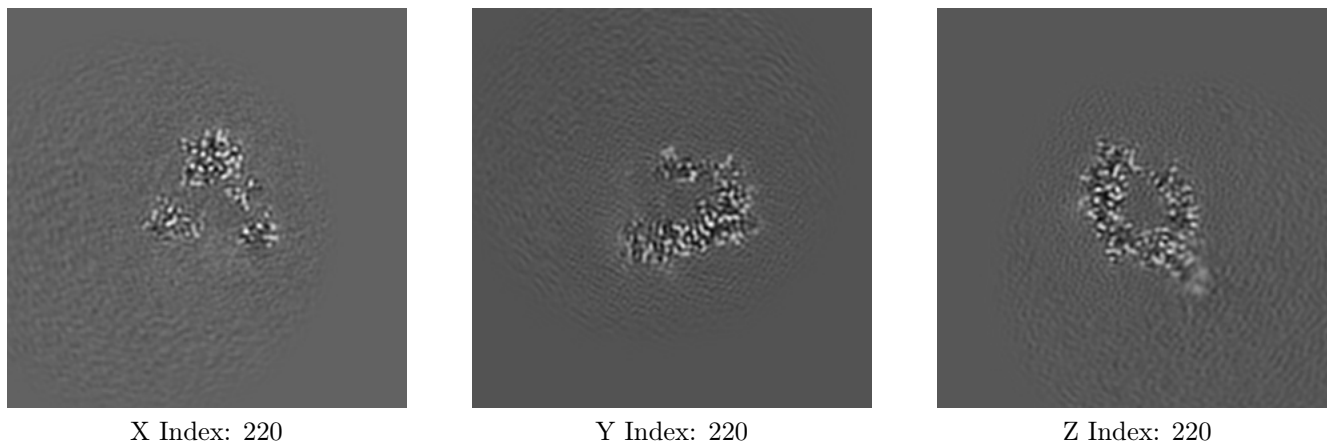
6.1.1 Primary map



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

6.2 Central slices [i](#)

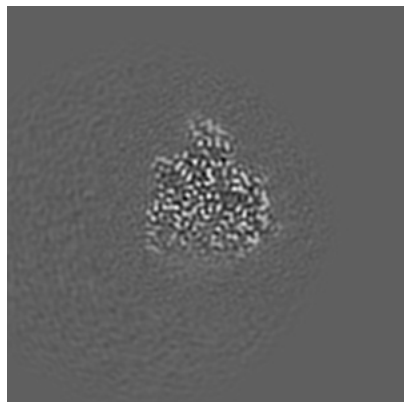
6.2.1 Primary map



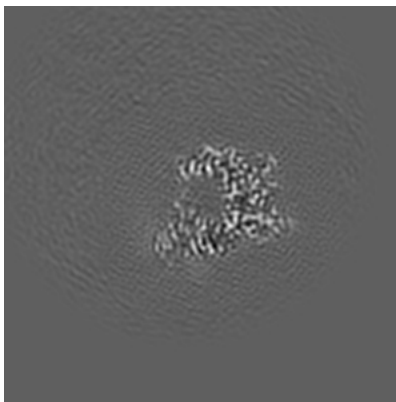
The images above show central slices of the map in three orthogonal directions.

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

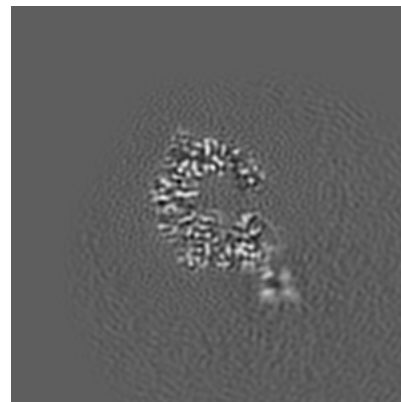
6.3.1 Primary map



X Index: 193



Y Index: 208

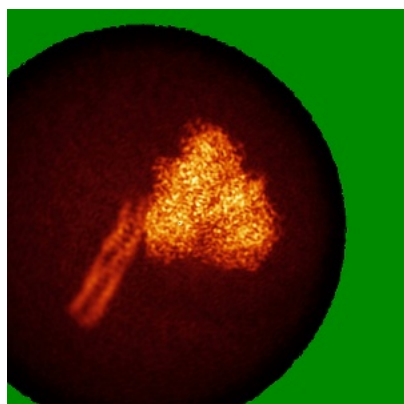


Z Index: 195

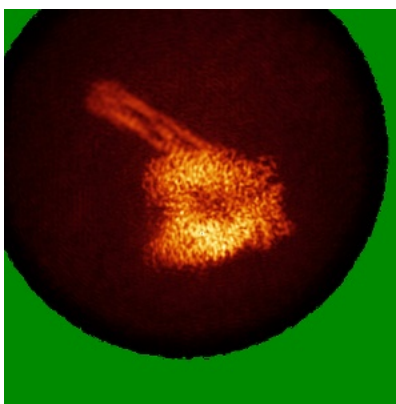
The images above show the largest variance slices of the map in three orthogonal directions.

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

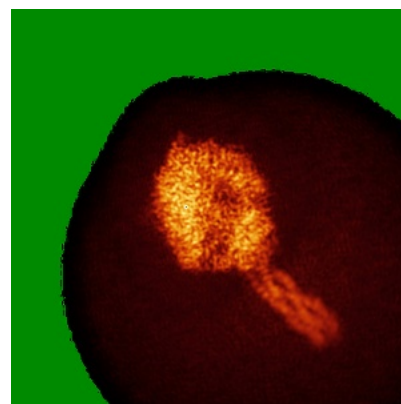
6.4.1 Primary map



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

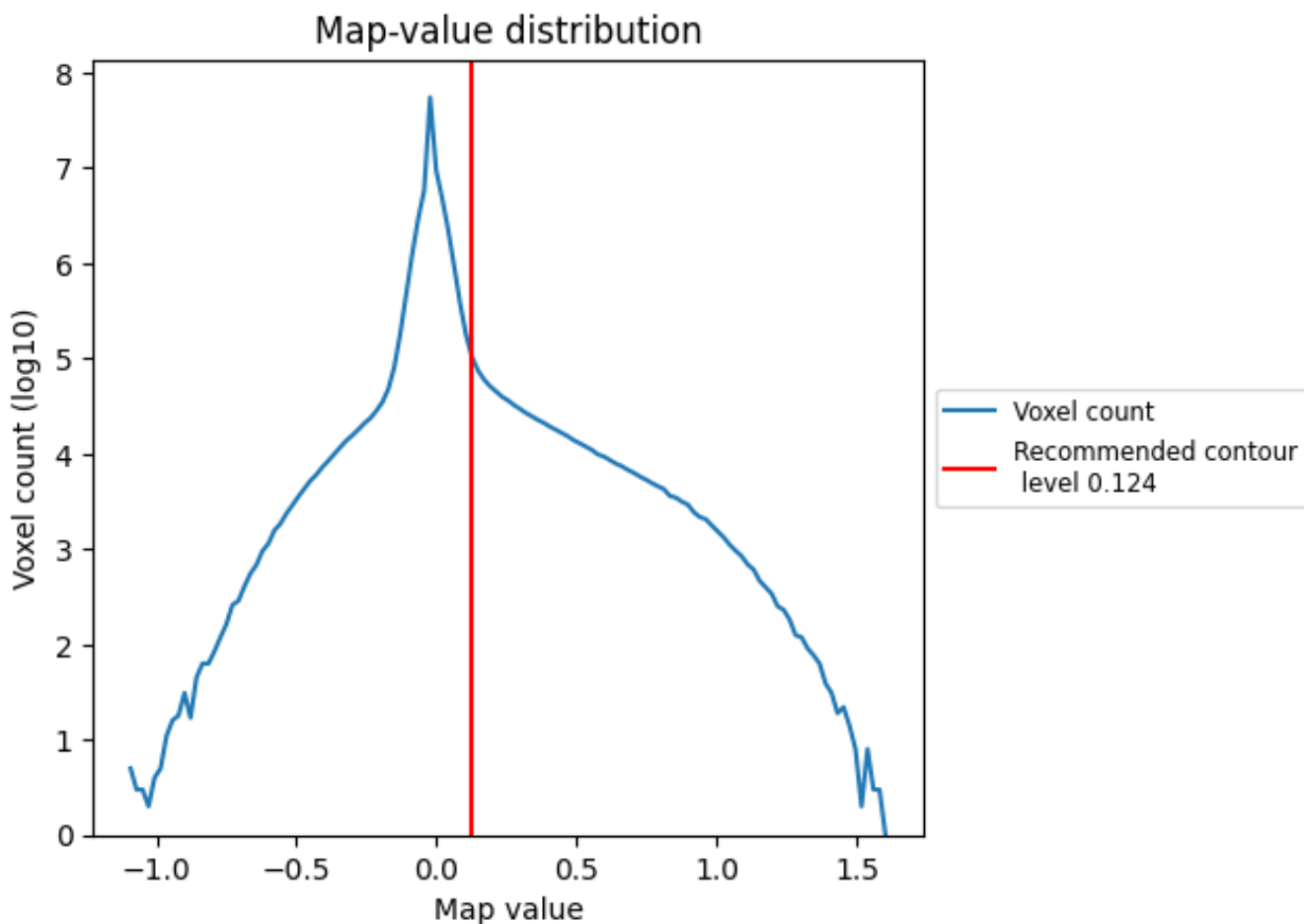
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

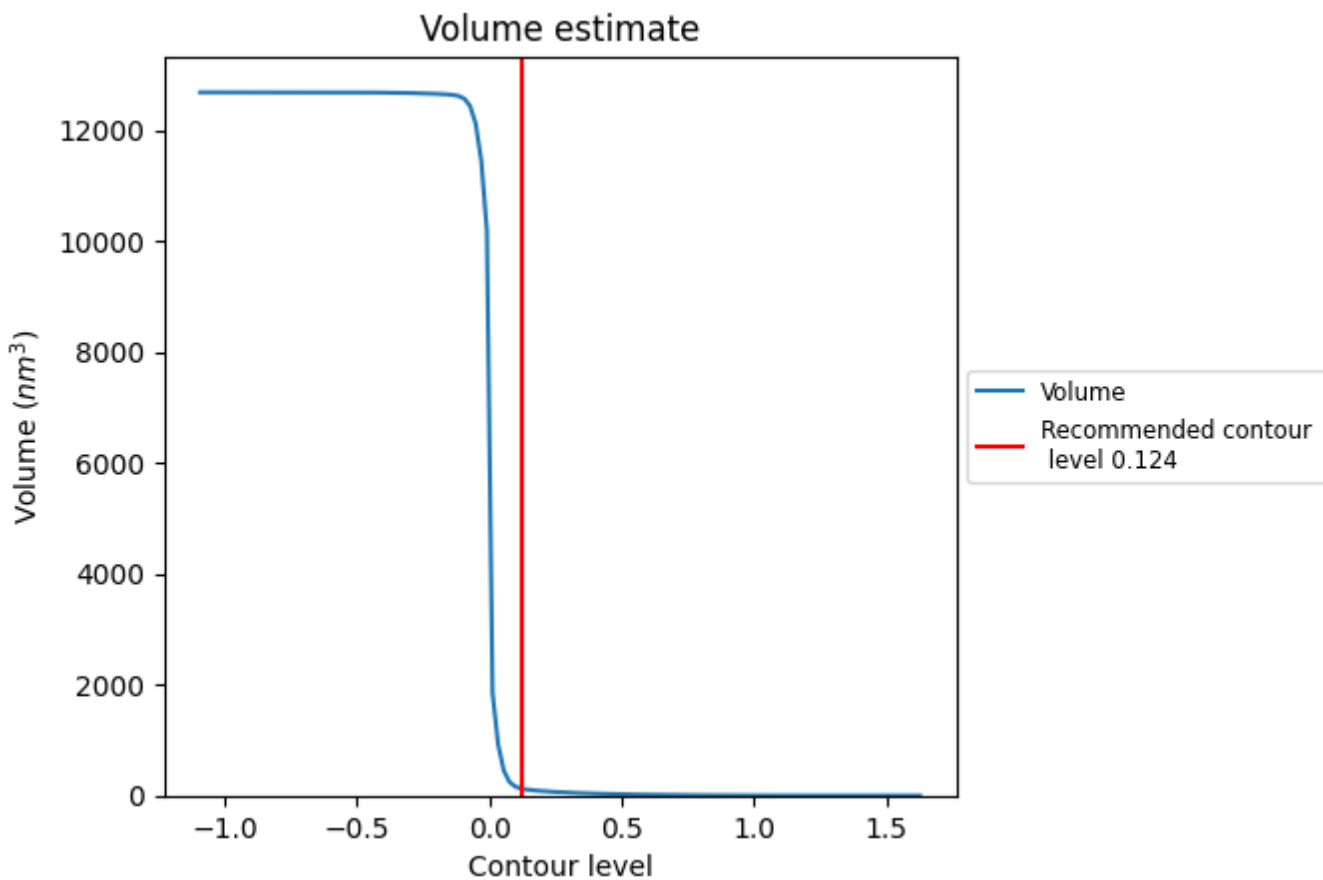
This section contains the results of statistical analysis of the map.

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.

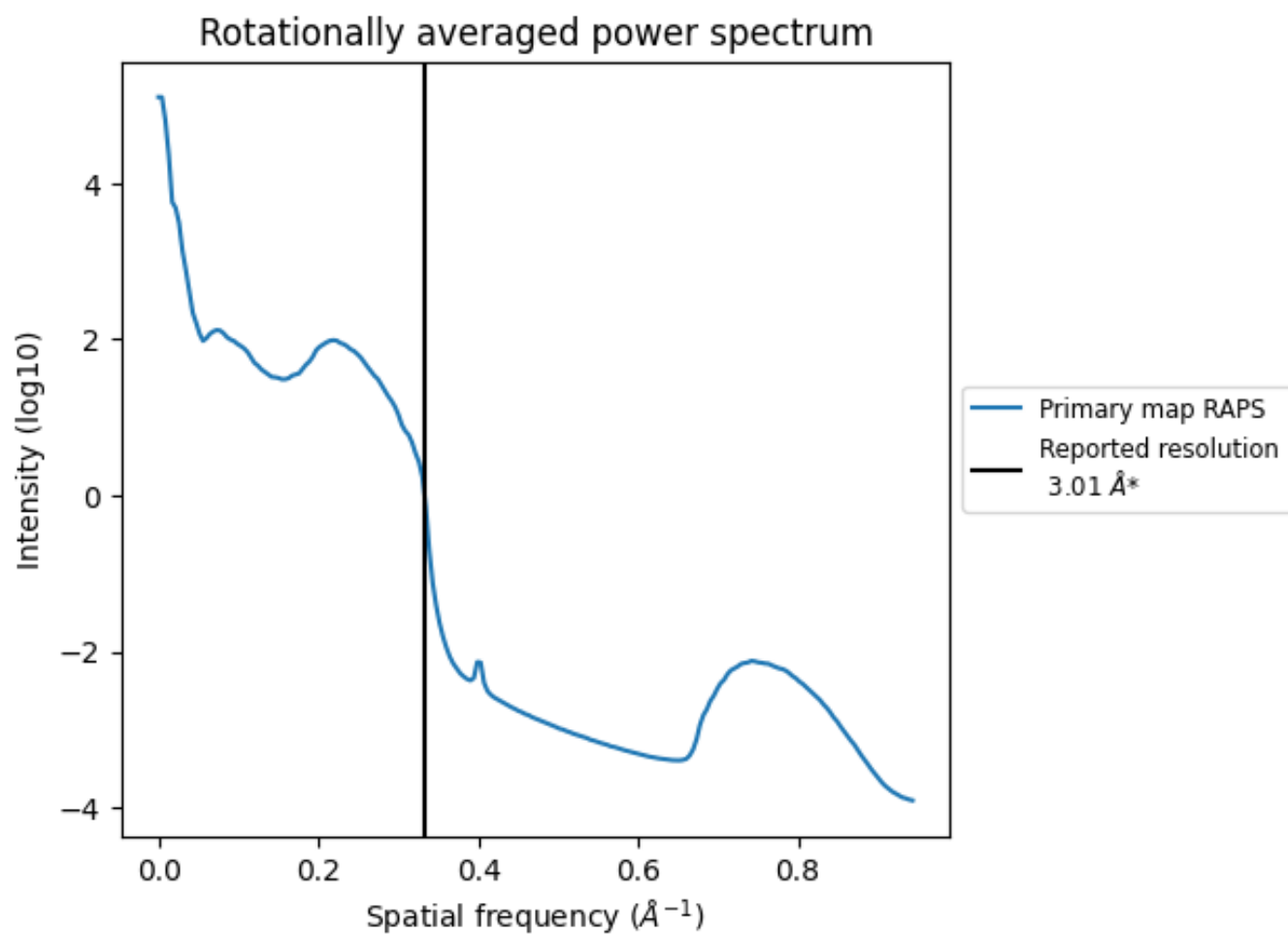
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 123 nm³; this corresponds to an approximate mass of 111 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.332\AA^{-1}

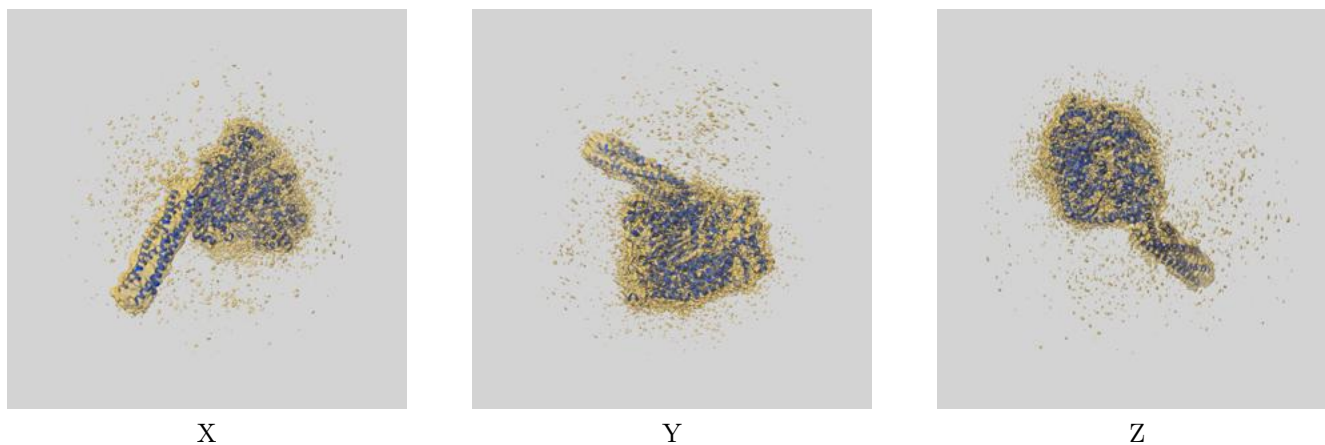
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

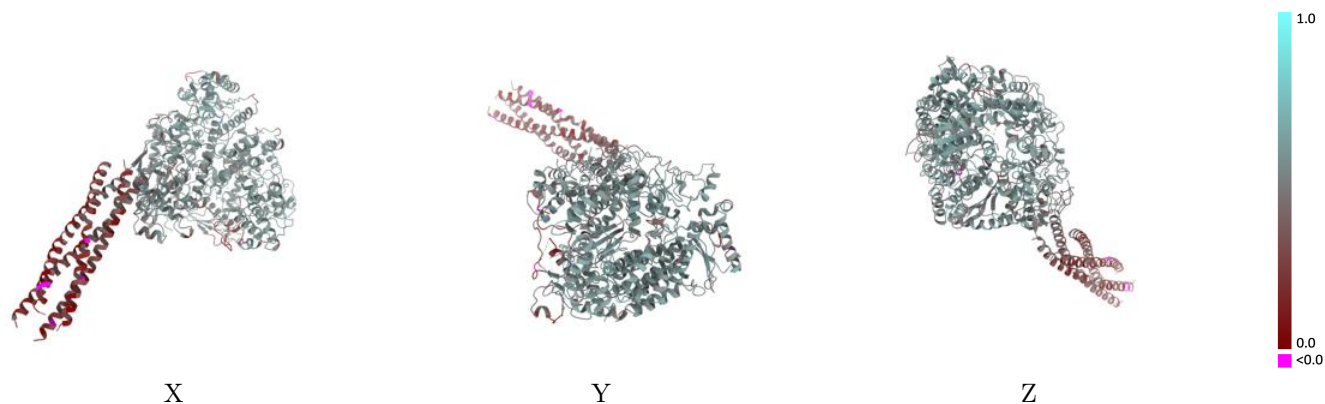
This section contains information regarding the fit between EMDB map EMD-37964 and PDB model 8X01. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



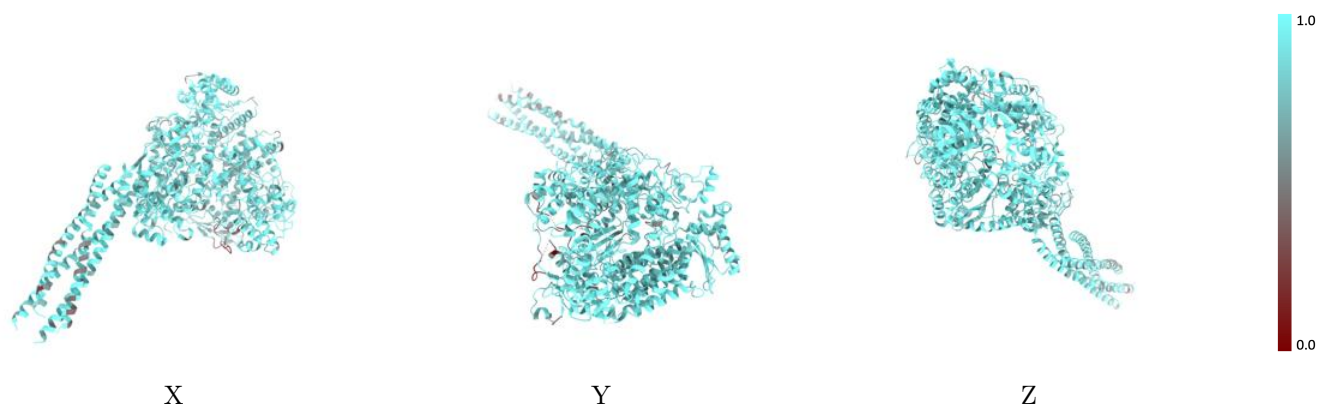
The images above show the 3D surface view of the map at the recommended contour level 0.124 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



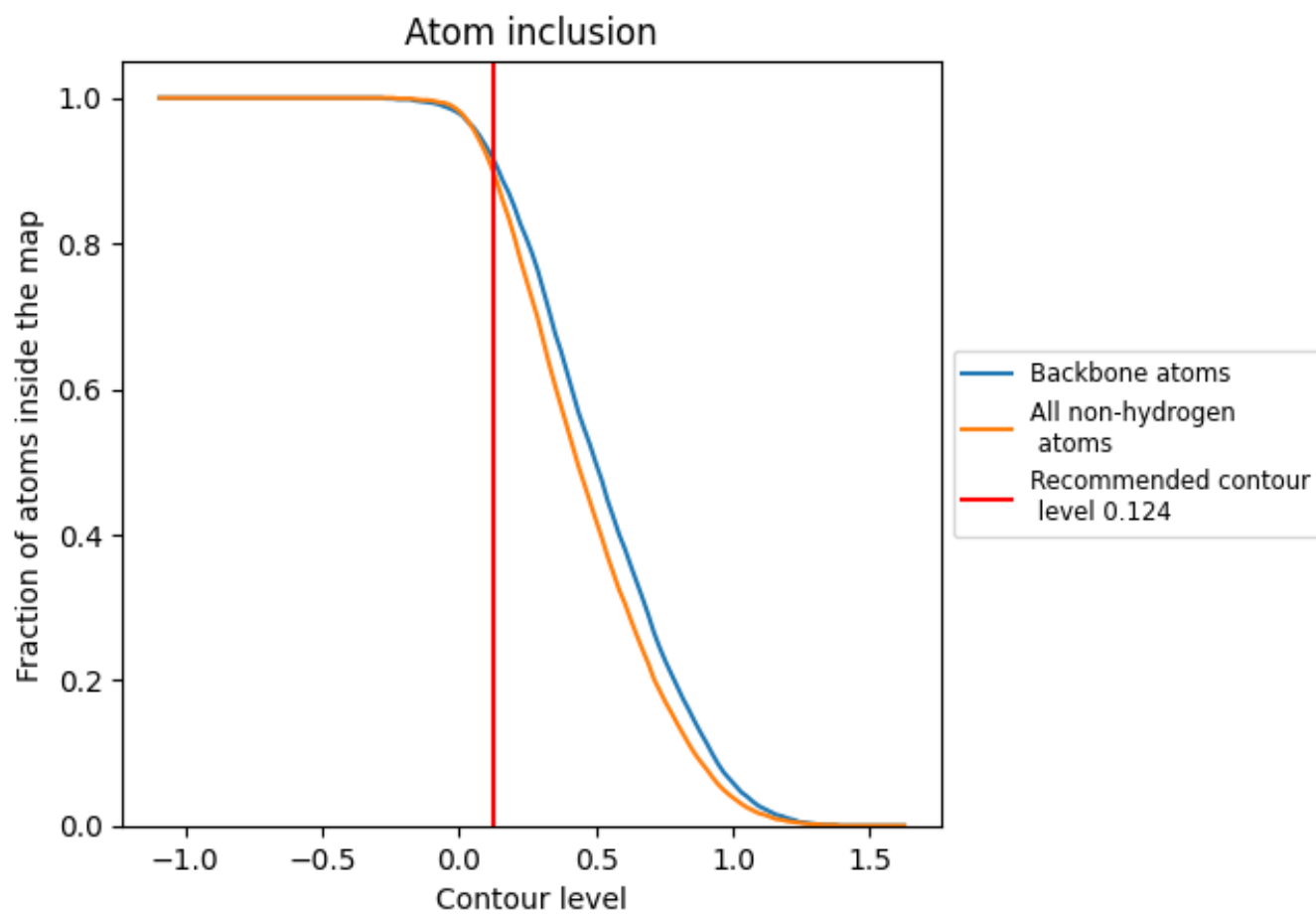
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.124).













9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 90% 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 (0.124) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9000	 0.4950
A	 0.9090	 0.5340
B	 0.8950	 0.3300
C	 0.8310	 0.3240
D	 0.7880	 0.2080
E	 0.8850	 0.2350

