



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 08:42 AM UTC

PDB ID : 7OVB / pdb_00007ovb
EMDB ID : EMD-13083
Title : L. pneumophila Type IV Coupling Complex (T4CC) with density for DotY
N-terminal and middle domains
Authors : Mace, K.; Meir, A.; Lukoyanova, N.; Waksman, G.
Deposited on : 2021-06-14
Resolution : 3.61 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:

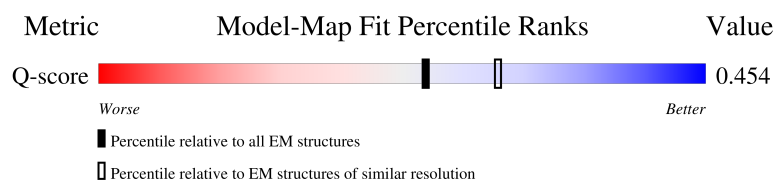
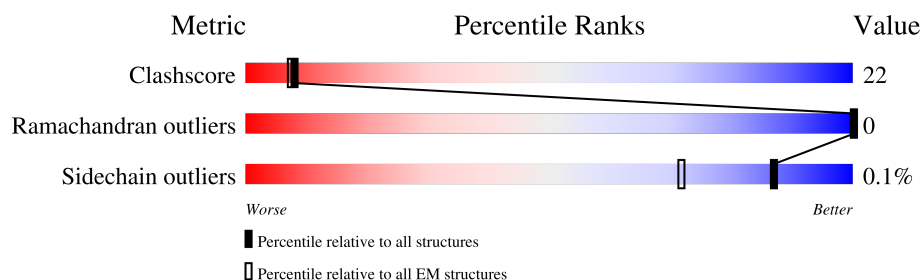
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.61 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11801 (3.11 - 4.10)

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	783	
2	B	380	
3	C	208	
4	D	294	

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Mol	Chain	Length	Quality of chain
5	E	230	28% 63% 18% • 18%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10854 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 IcmO (DotL).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	473	Total	C	N	O	S	0	0
			3665	2345	619	684	17		

- Molecule 2 is a protein called IcmP (DotM).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	259	Total	C	N	O	S	0	0
			2085	1326	367	377	15		

- Molecule 3 is a protein called IcmJ (DotN).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	202	Total	C	N	O	S	0	0
			1615	1024	277	304	10		

- Molecule 4 is a protein called DotZ.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	283	Total	C	N	O	S	0	0
			2284	1452	389	441	2		

- Molecule 5 is a protein called DotY.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	188	Total	C	N	O	S	0	0
			1204	742	218	240	4		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	C	1	Total	Zn	0
			1	1	

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

• Molecule 2: IcmP (DotM)

Chain B:  42% 26% 32%

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

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

TYR
R122
K123
E134
Q135
V138
M142
D148
Q152
D153
P158
M161
T164
P165
M166
E167
F168
K171
R176
K177
D178
D179
L182
D183
N184
P185
V186
P187
G188
E189
M191
T192
A193
G194
R202
V203
F204
Q207
L208
Y211
W212
F215
E216
R217

A222
Y223
A224
L225
S226
F229
M230
A231
R232
M233
N234
R235
D236
R237
A240
D248
F251
V252
D253
P256
D257
R262
M265
Y268
Q269
V274
Q275
V278
H281
A282
Y283
L288
A289
S290
L291
L292
R296
P302
S303
S304
F306
L307
W308
L309

D313
R314
R315
L316
W317
Y318
M319
L320
R326
Q326
E331
V332
P336
F336
A337
H338
W339
E342
M345
G346
R347
R348
S349
L350
V351
D355
E356
A357
T358
R359
A360
L361
V365
K366
E367
L370
T371
P372
R373
Q374
M375
E376
P380

• Molecule 3: IcmJ (DotN)

Chain C:  61% 37%

MET
ALA
ASP
ASN
GLN
E7
C8
E9
L10
L11
K11
L12
G17
S18
W19
R20
S23
A24
R25
K26
I27
D28
E29
R30
F31
K32
S33
Y34
E35
Q36
K37
C46
Q47
F48
F51
R54
L55
D58
D65
Y66
T67
N68
L71
S72
N73
C78
F80
Q83

E88
S89
Y90
G91
Y92
G93
L100
I101
Y102
L103
P104
Q108
L111
L114
C115
H116
V117
N124
Y128
Y136
R137
S138
F139
R142
S143
E147
E152
S155
I159
F160
G161
L163
M164
I165
D166
S167
G168
V169
H170
S171
E172
E173
I174
K177
L178
F179

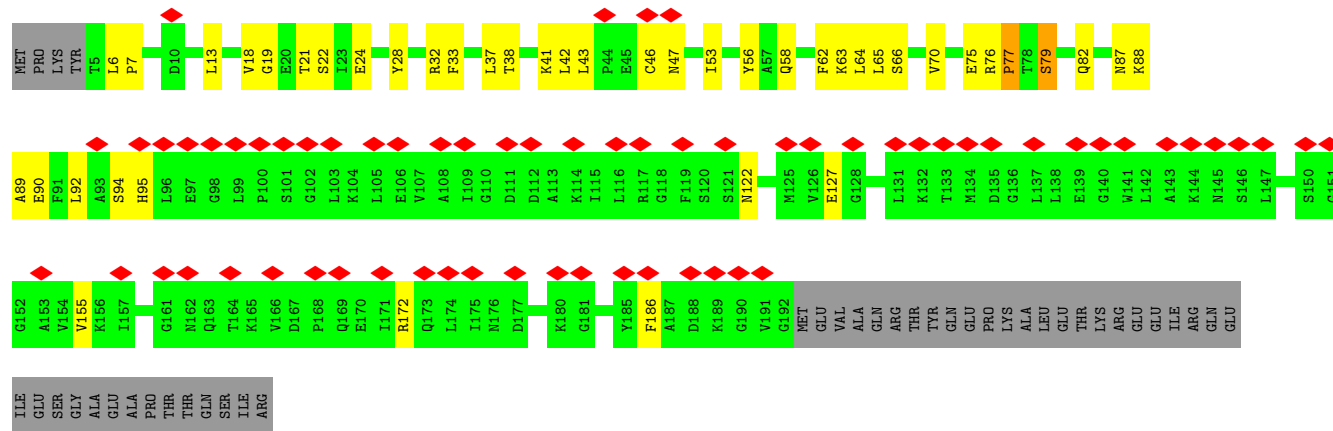
K180
N181
L185
P186
S187
F191
R192
K193
Q194
I195
E196
K197
W198
L203
D208

• Molecule 4: DotZ

Chain D:  6% 54% 42%

MET
ASP
GLU
ILE
LYS
ASP
ASP
GLU
GLU
LEU
S11
D12
W13
T19
T20
T21
A22
E23
R24
I31
S32
L33
F34
Q35
D36
E37
L38
L39
E40
A41
M43
I44
P45
Y49
R50
H51
Q54
L57
V60
L61
N62
V65
L66
S70
D71
A76
Q77
K78
L79
L80

I81
D82
Y83
L84
L85
K91
D94
S95
Q96
G97
R101
E102
S103
L104
E107
Q109
R110
L111
V112
Q113
L114
L121
Q125
L128
I129
A130
S131
S132
S135
K138
W143
E148
L151
M155
Y158
K159
M160
H162
S163
K164
I165
K166
K167
M168



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	183397	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 ($e^-/\text{\AA}^2$)	54	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	38.624	Depositor
Minimum map value	-21.045	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	8	Depositor
Map size (Å)	315.0, 315.0, 315.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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	0.51	0/3727	0.65	0/5031
2	B	0.63	0/2132	0.69	0/2883
3	C	0.66	0/1646	0.69	0/2213
4	D	0.58	0/2318	0.68	0/3131
5	E	0.44	0/1218	0.69	1/1659 (0.1%)
All	All	0.57	0/11041	0.68	1/14917 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	77	PRO	N-CA-C	-6.97	100.29	111.03

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	3665	0	3720	211	0
2	B	2085	0	2098	90	0
3	C	1615	0	1578	75	0
4	D	2284	0	2327	105	0
5	E	1204	0	965	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	1	0	0	0	0
All	All	10854	0	10688	475	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 22.

The worst 5 of 475 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:289:PHE:HB3	1:A:297:VAL:HB	1.44	1.00
4:D:101:ARG:NH1	4:D:102:GLU:OE1	2.06	0.88
1:A:219:MET:HB2	1:A:252:MET:HE1	1.55	0.87
1:A:371:VAL:O	1:A:374:ARG:NH2	2.10	0.85
1:A:273:ASN:HB3	1:A:279:ARG:HH12	1.42	0.83

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	465/783 (59%)	426 (92%)	39 (8%)	0	100	100
2	B	257/380 (68%)	225 (88%)	32 (12%)	0	100	100
3	C	200/208 (96%)	177 (88%)	23 (12%)	0	100	100
4	D	281/294 (96%)	247 (88%)	34 (12%)	0	100	100
5	E	186/230 (81%)	153 (82%)	33 (18%)	0	100	100
All	All	1389/1895 (73%)	1228 (88%)	161 (12%)	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	397/676 (59%)	397 (100%)	0	100	100
2	B	222/332 (67%)	222 (100%)	0	100	100
3	C	173/179 (97%)	173 (100%)	0	100	100
4	D	256/269 (95%)	256 (100%)	0	100	100
5	E	81/192 (42%)	80 (99%)	1 (1%)	63	70
All	All	1129/1648 (68%)	1128 (100%)	1 (0%)	87	87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	79	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	12	GLN
4	D	54	GLN
5	E	87	ASN
4	D	67	GLN
3	C	116	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](#)

Of 1 ligands modelled in this entry, 1 is 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.

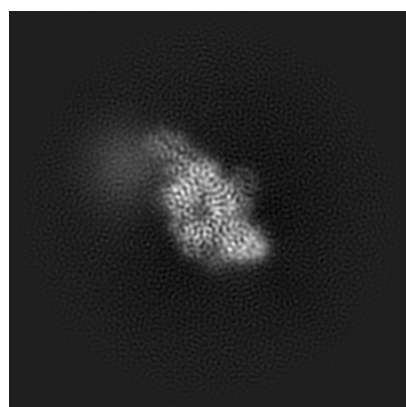
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13083. These allow visual inspection of the internal detail of the map and identification of artifacts.

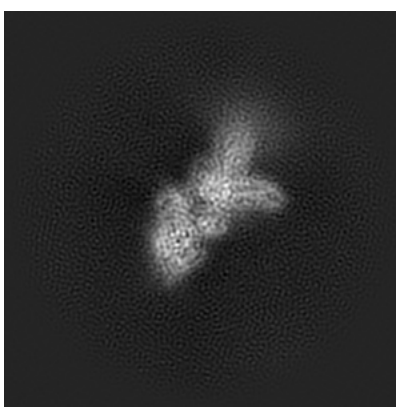
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

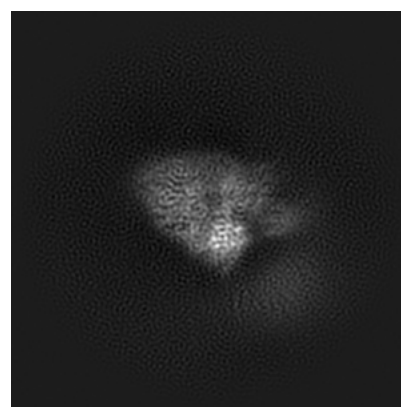
6.1.1 Primary map



X



Y

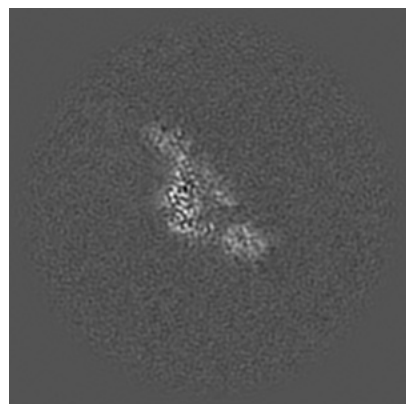


Z

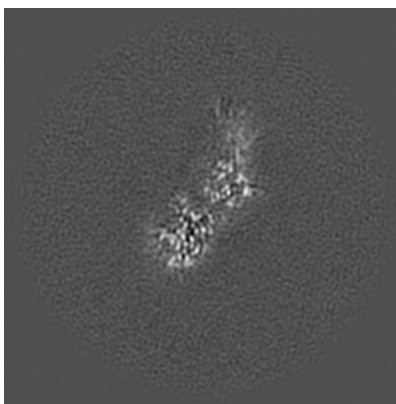
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

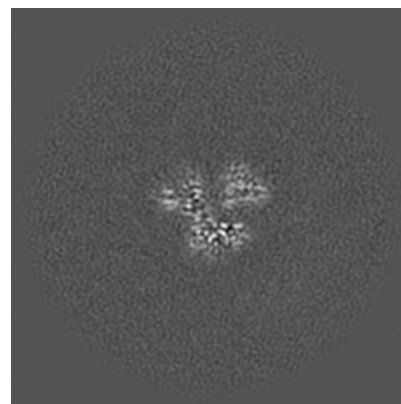
6.2.1 Primary map



X Index: 150



Y Index: 150

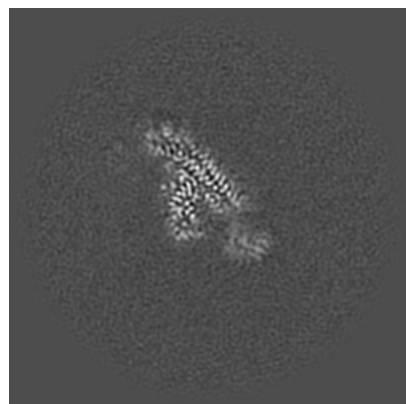


Z Index: 150

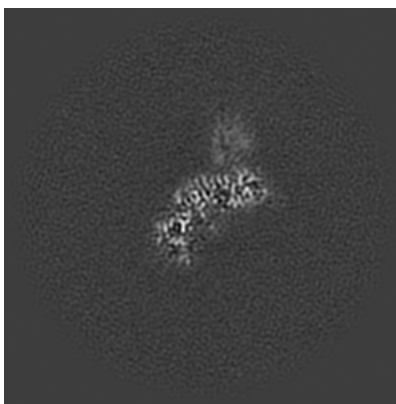
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

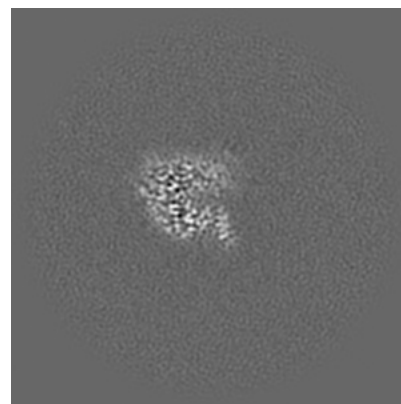
6.3.1 Primary map



X Index: 161



Y Index: 137

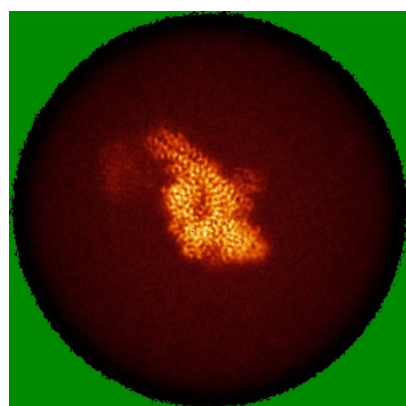


Z Index: 130

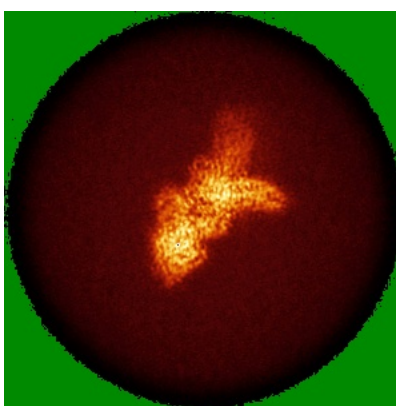
The images above show the largest variance slices of the map in three orthogonal directions.

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

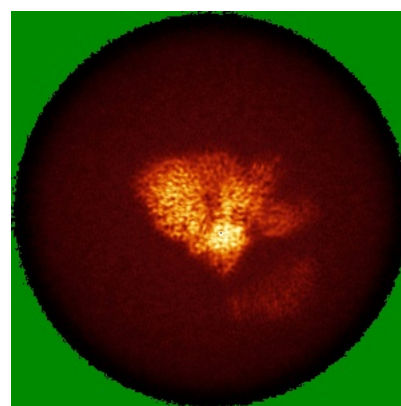
6.4.1 Primary map



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

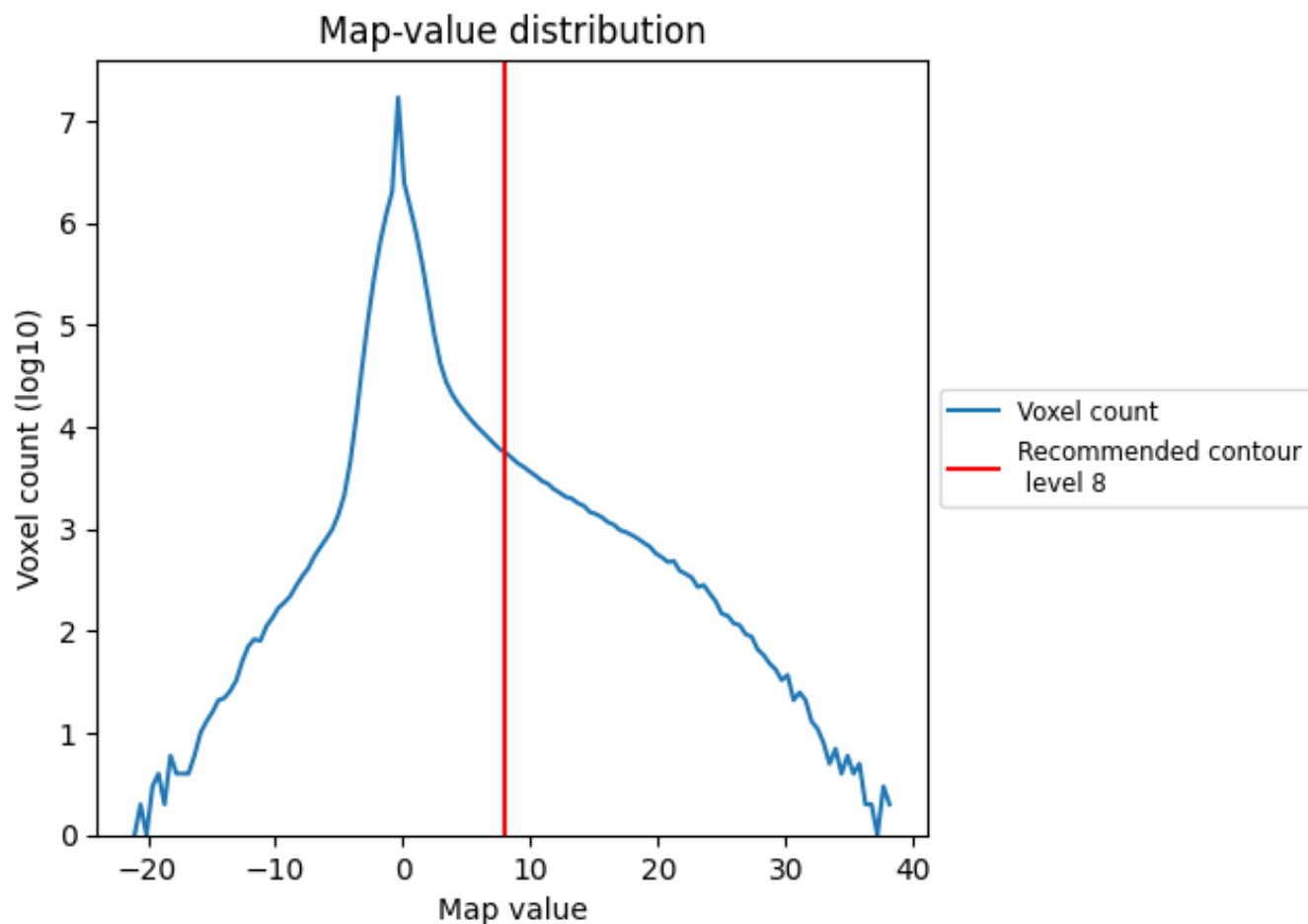
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

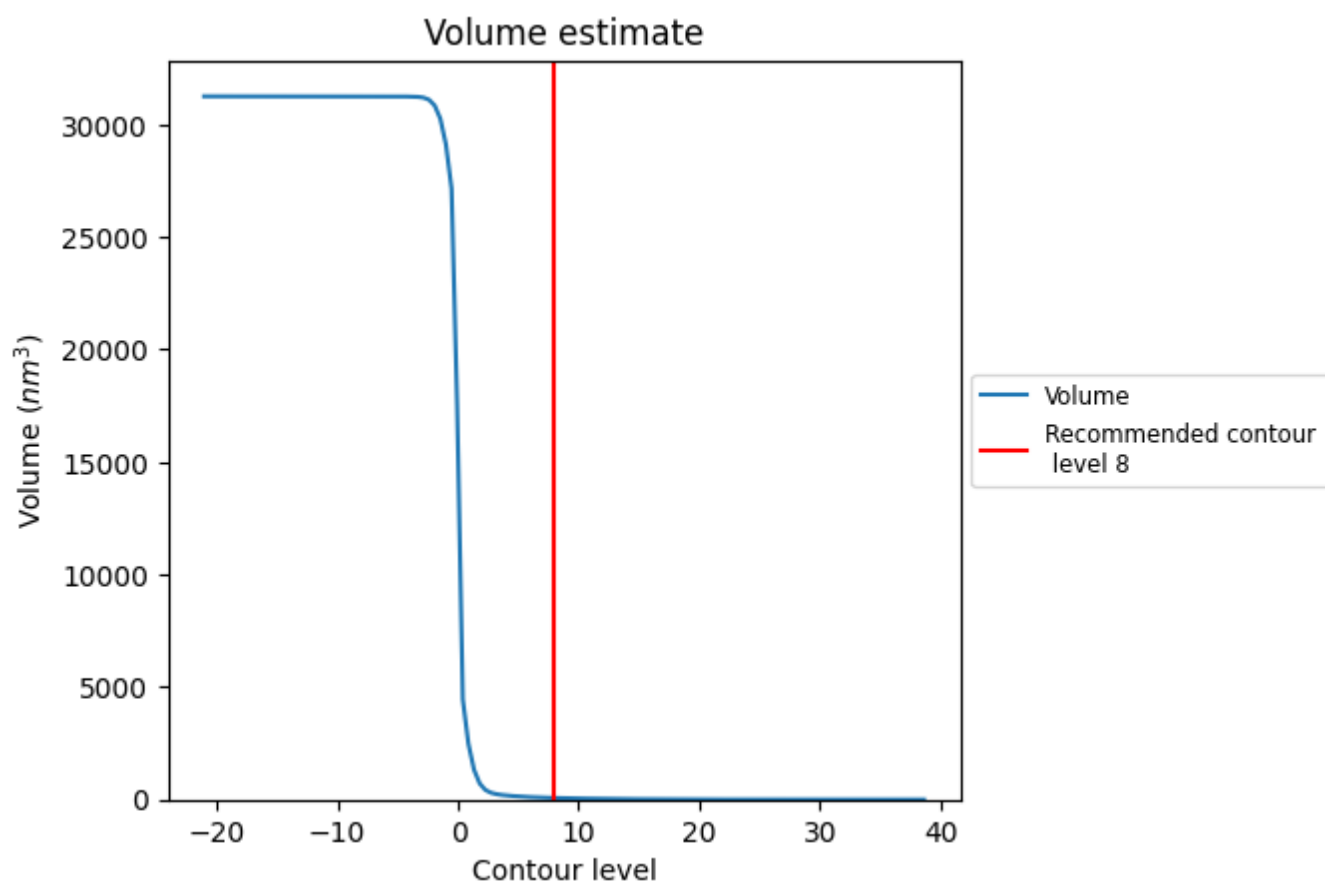
This section contains the results of statistical analysis of the map.

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.

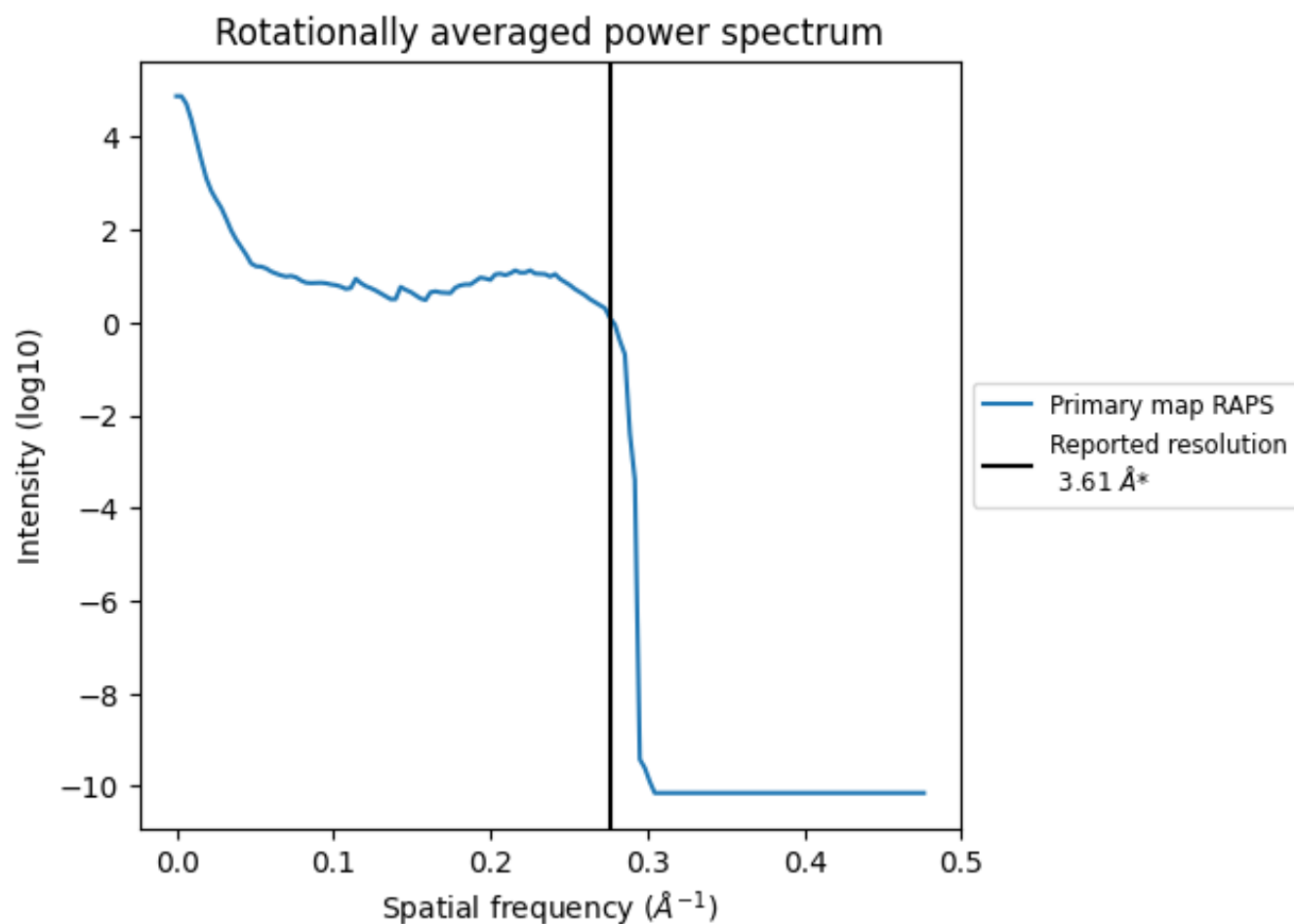
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 71 nm^3 ; this corresponds to an approximate mass of 64 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 0.277 Å⁻¹

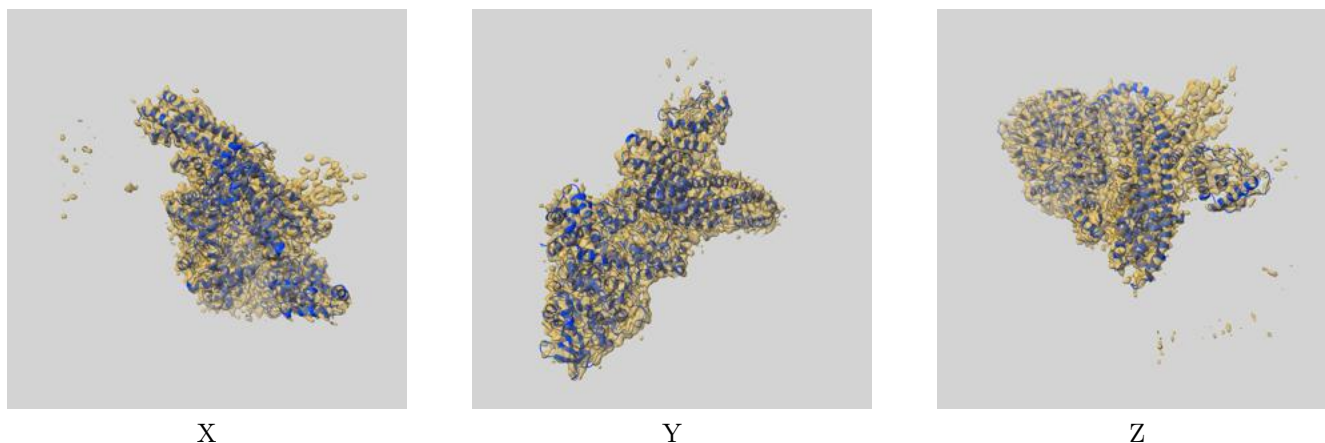
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

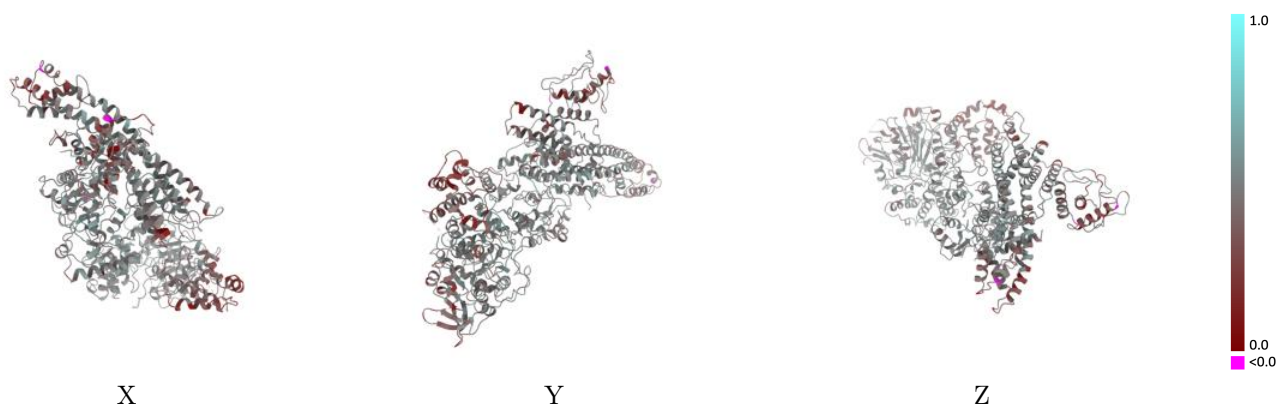
This section contains information regarding the fit between EMDB map EMD-13083 and PDB model 7OVB. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



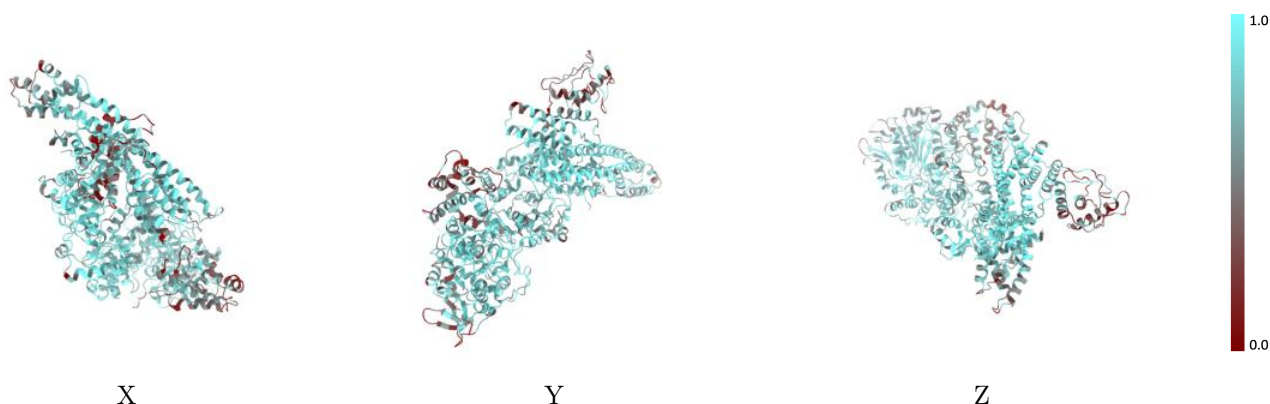
The images above show the 3D surface view of the map at the recommended contour level 8.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



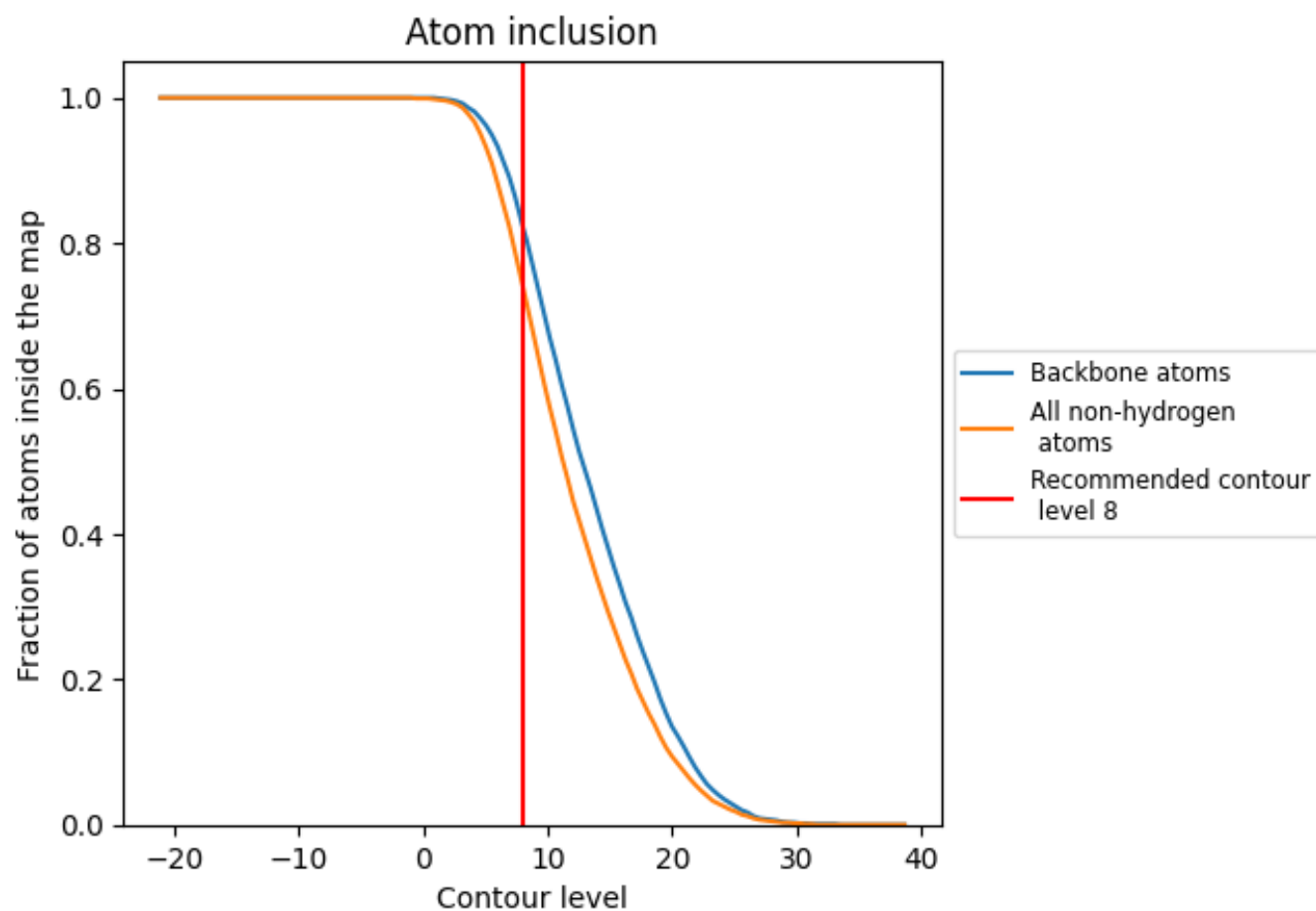
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 74% 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 (8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7410	0.4540
A	0.6820	0.4290
B	0.7960	0.4870
C	0.8560	0.5030
D	0.7780	0.4510
E	0.6010	0.4170

