wwPDB EM Validation Summary Report (i)

Apr 29, 2024 – 11:44 am BST

PDB ID	:	2XKV
EMDB ID	:	EMD-1762
Title	:	Atomic Model of the SRP-FtsY Early Conformation
Authors	:	Estrozi, L.F.; Boehringer, D.; Shan, S.-o.; Ban, N.; Schaffitzel, C.
Deposited on	:	2010-07-13
Resolution	:	13.50 Å(reported)
Based on initial models	:	1DUL, 1OKK

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 (i) 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 (i)) were used in the production of this report:

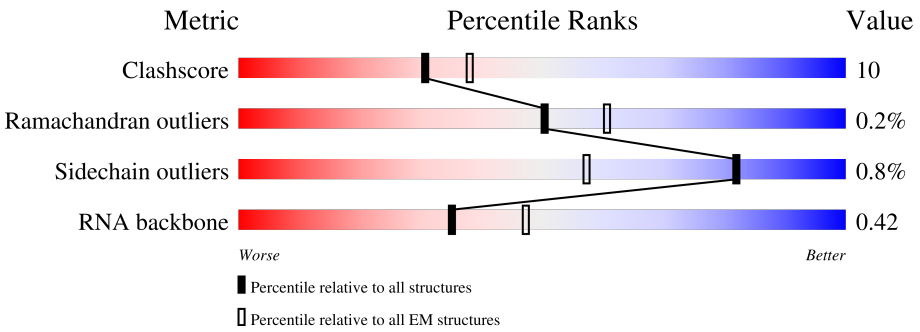
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 13.50 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
RNA backbone	4643	859

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 <=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	294	66%, 96%, • •
2	B	114	20%, 11%, 42%, 31%, 16%
3	C	69	23%, 61%, •, 36%
4	D	303	56%, 86%, •, 12%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6620 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 SIGNAL RECOGNITION PARTICLE PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	291	2231	1400	409	418	4	0	1

- Molecule 2 is a RNA chain called 4.5S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	96	2050	915	368	672	95	0	0

- Molecule 3 is a protein called SIGNAL RECOGNITION PARTICLE PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	44	334	205	67	58	4	0	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	58	SER	CYS	conflict	UNP P0AGD7

- Molecule 4 is a protein called CELL DIVISION PROTEIN FTSY.

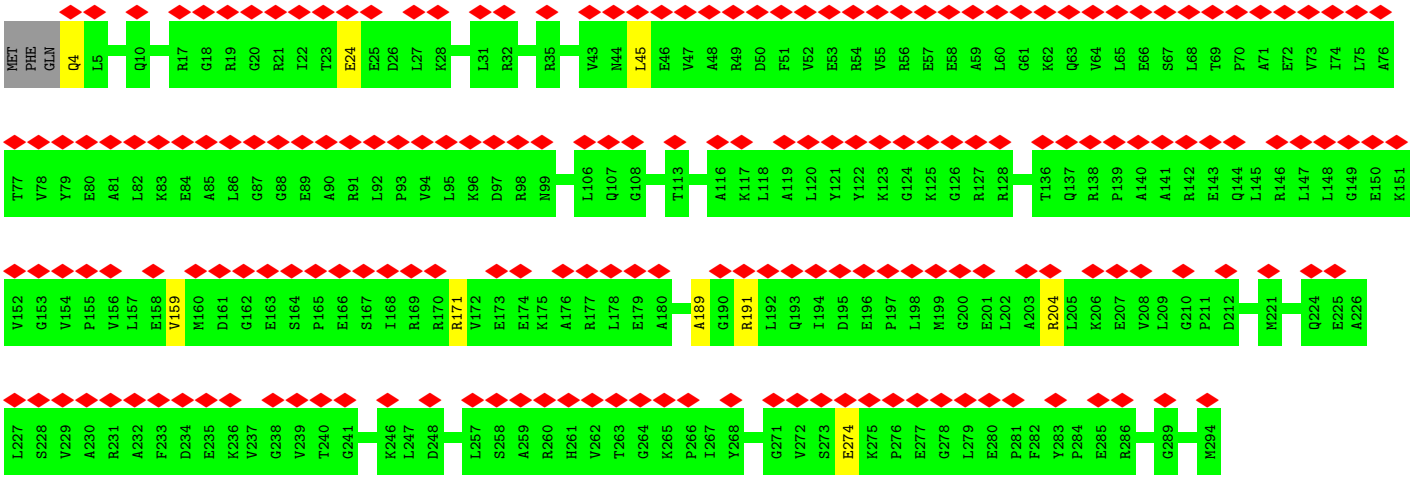
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	267	2005	1281	342	376	6	0	2

3 Residue-property plots (i)

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.

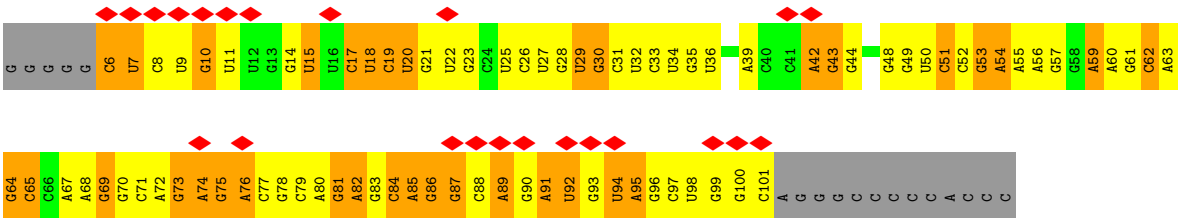
• Molecule 1: SIGNAL RECOGNITION PARTICLE PROTEIN

Chain A: 66% 96%



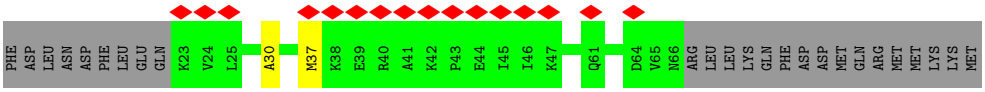
• Molecule 2: 4.5S RNA

Chain B: 20% 11% 42% 31% 16%



• Molecule 3: SIGNAL RECOGNITION PARTICLE PROTEIN

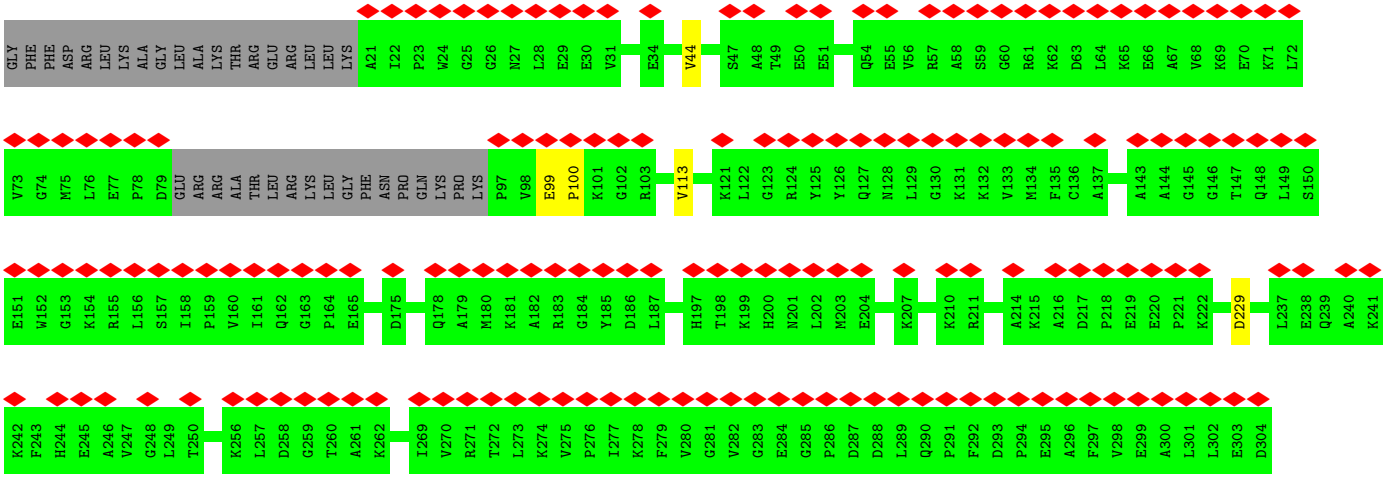
Chain C: 23% 61% 36%



• Molecule 4: CELL DIVISION PROTEIN FTSY

Chain D:

56%
86%
12%


GLY PHE PHE ASP ARG LEU LYS ALA GLY LEU ALA LYS THR ARG GLU ARG LEU LEU LYS A21 I22 P23 W24 G25 G26 N27 L28 E29 E30 V31 E34 V44 S47 A48 T49 E50 E51 Q54 E55 V56 R57 A58 S59 G60 R61 K62 D63 L64 K65 E66 A67 V68 K69 E70 K71 L72
V73 G74 M75 L76 E77 P78 D79 GLU ARG ARG ALA THR LEU ARG LYS LEU GLY PHE ASN PRO GLN LYS PRO LYS P97 V98 E99 P100 K101 G102 R103 V113 K121 L122 G123 R124 Y125 Y126 Q127 N128 L129 G130 K131 K132 V133 M134 F135 C136 A137 A143 A144 G145 G146 T147 Q148 L149 S150
E151 W152 G153 K154 R155 L156 S157 I158 P159 V160 I161 Q162 G163 P164 E165 D175 Q178 A179 M180 K181 A182 R183 G184 Y185 D186 L187 H197 T198 K199 H200 N201 L202 M203 E204 K207 K210 R211 A214 K215 A216 D217 P218 E219 E220 P221 K222 D229 L237 E238 Q239 A240 K241
K242 F243 H244 E245 A246 V247 G248 L249 T250 K256 L257 D258 G259 T260 A261 K262 I269 V270 R271 T272 L273 K274 V275 P276 I277 K278 F279 V280 G281 V282 G283 E284 G285 P286 D287 D288 L289 Q290 P291 F292 D293 P294 E295 A296 F297 V298 E299 A300 L301 L302 E303 D304

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	28822	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	0.101	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	354.33, 354.33, 354.33	wwPDB
Map dimensions	93, 93, 93	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	3.81, 3.81, 3.81	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	0.52	0/2255	0.62	0/3040
2	B	0.25	0/2292	0.70	0/3573
3	C	0.75	1/334 (0.3%)	0.57	0/441
4	D	0.58	0/2037	0.59	0/2755
All	All	0.49	1/6918 (0.0%)	0.64	0/9809

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	37	MET	CG-SD	5.10	1.94	1.81

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	2231	0	2332	3	0
2	B	2050	0	1036	114	0
3	C	334	0	369	2	0
4	D	2005	0	2074	2	0
All	All	6620	0	5811	119	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 10.

The worst 5 of 119 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)
2:B:93:G:H3'	2:B:94:U:H5"	1.26	1.12
2:B:88:C:H3'	2:B:89:A:H5"	1.23	1.11
2:B:74:A:H2'	2:B:75:G:H5"	1.46	0.96
2:B:88:C:H3'	2:B:89:A:C5'	2.01	0.89
2:B:93:G:H3'	2:B:94:U:C5'	2.03	0.89

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	289/294 (98%)	272 (94%)	17 (6%)	0	100	100
3	C	42/69 (61%)	40 (95%)	2 (5%)	0	100	100
4	D	263/303 (87%)	248 (94%)	14 (5%)	1 (0%)	34	72
All	All	594/666 (89%)	560 (94%)	33 (6%)	1 (0%)	50	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	44	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	229/233 (98%)	225 (98%)	4 (2%)	60	78
3	C	36/62 (58%)	36 (100%)	0	100	100
4	D	209/241 (87%)	209 (100%)	0	100	100
All	All	474/536 (88%)	470 (99%)	4 (1%)	82	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	24	GLU
1	A	204	ARG
1	A	274	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	96/114 (84%)	34 (35%)	6 (6%)

5 of 34 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	7	U
2	B	10	G
2	B	15	U
2	B	17	C
2	B	18	U

5 of 6 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	81	G
2	B	91	A
2	B	94	U
2	B	73	G
2	B	6	C

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.

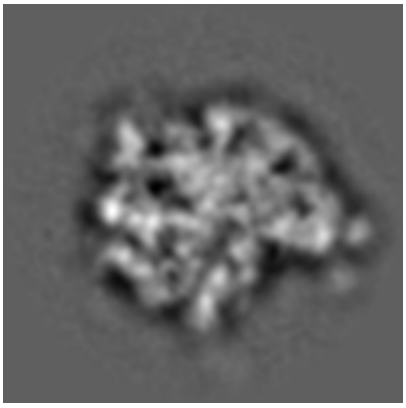
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-1762. These allow visual inspection of the internal detail of the map and identification of artifacts.

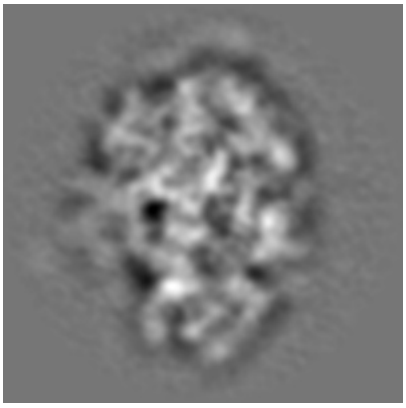
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

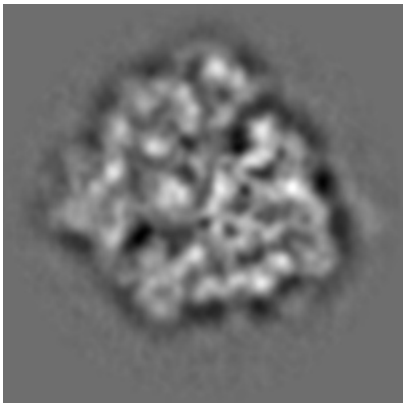
6.1.1 Primary map



X



Y

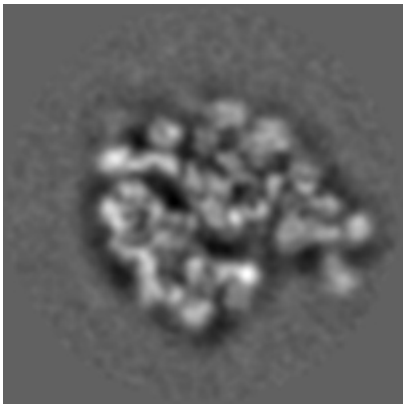


Z

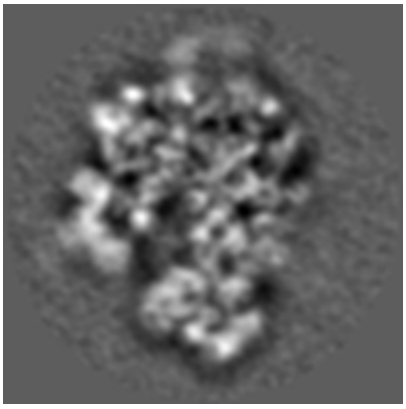
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

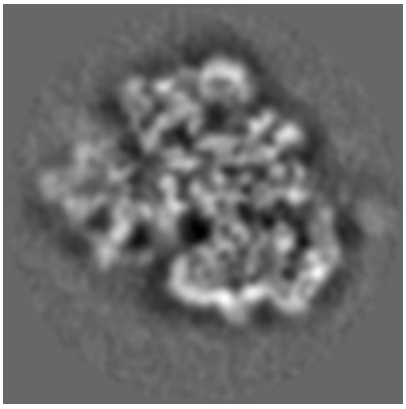
6.2.1 Primary map



X Index: 46



Y Index: 46

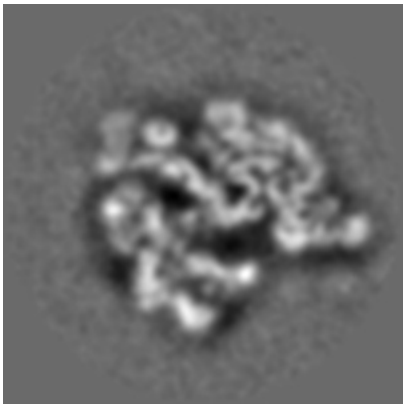


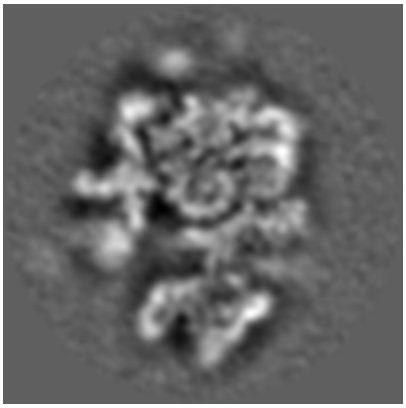
Z Index: 46

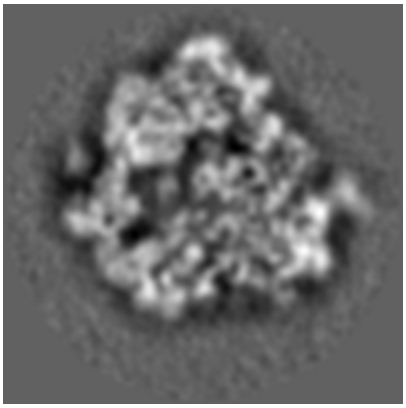
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 44

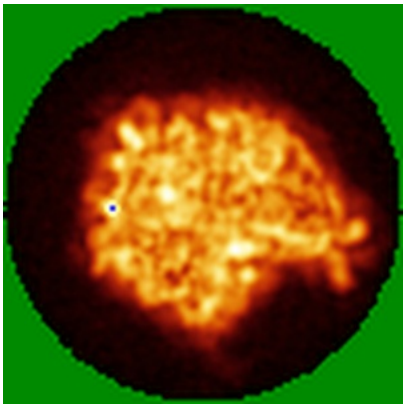

Y Index: 50

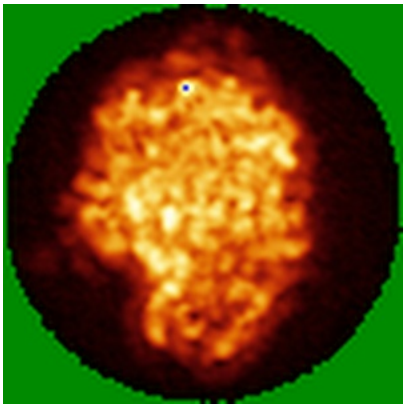

Z Index: 41

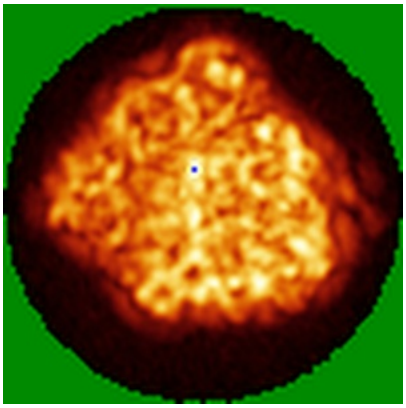
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map


X

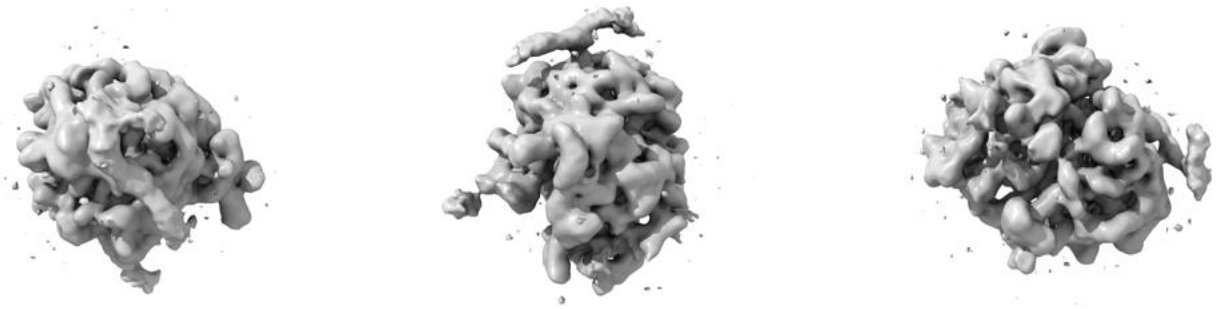

Y


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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

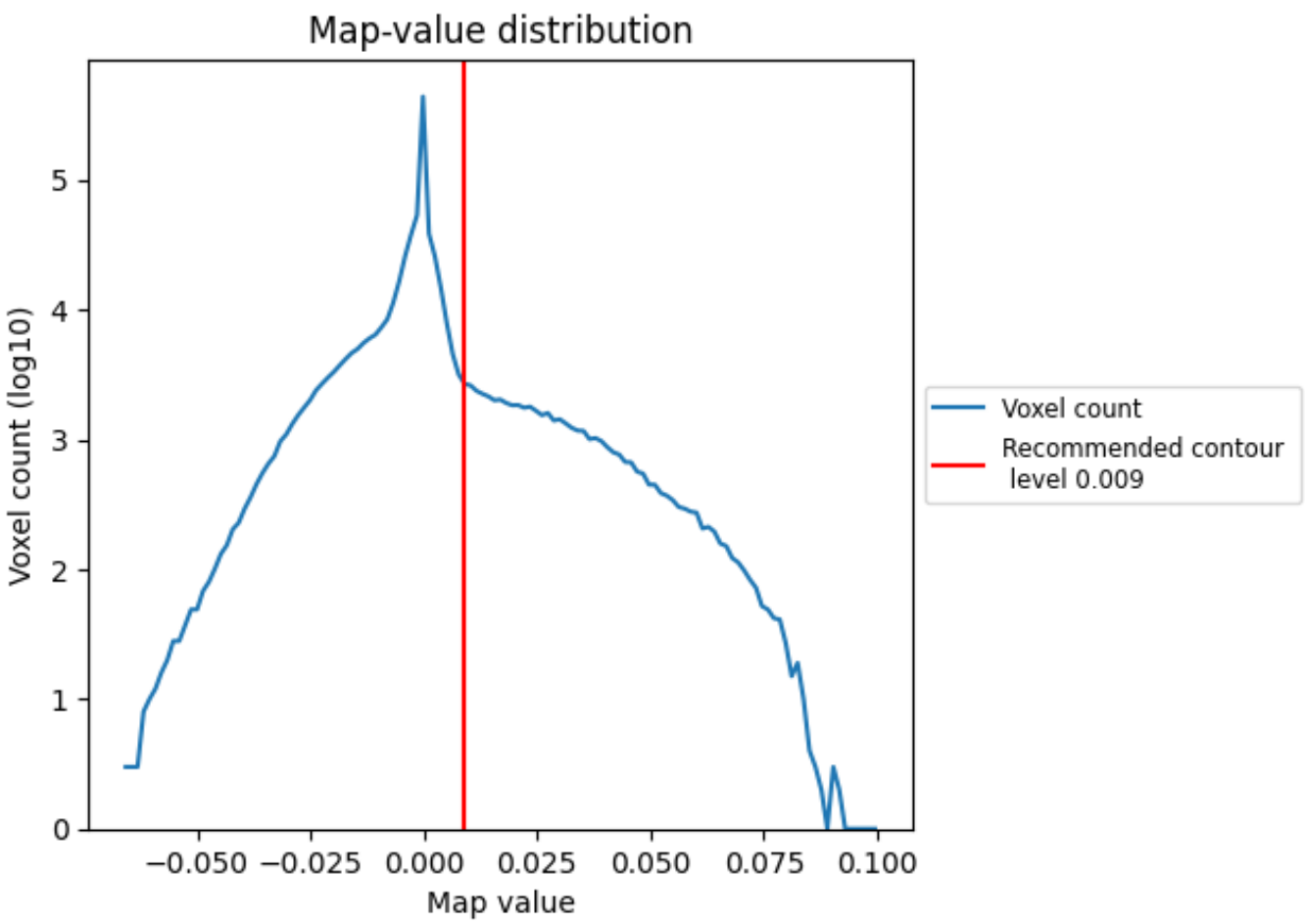
6.6 Mask visualisation (i)

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

7 Map analysis (i)

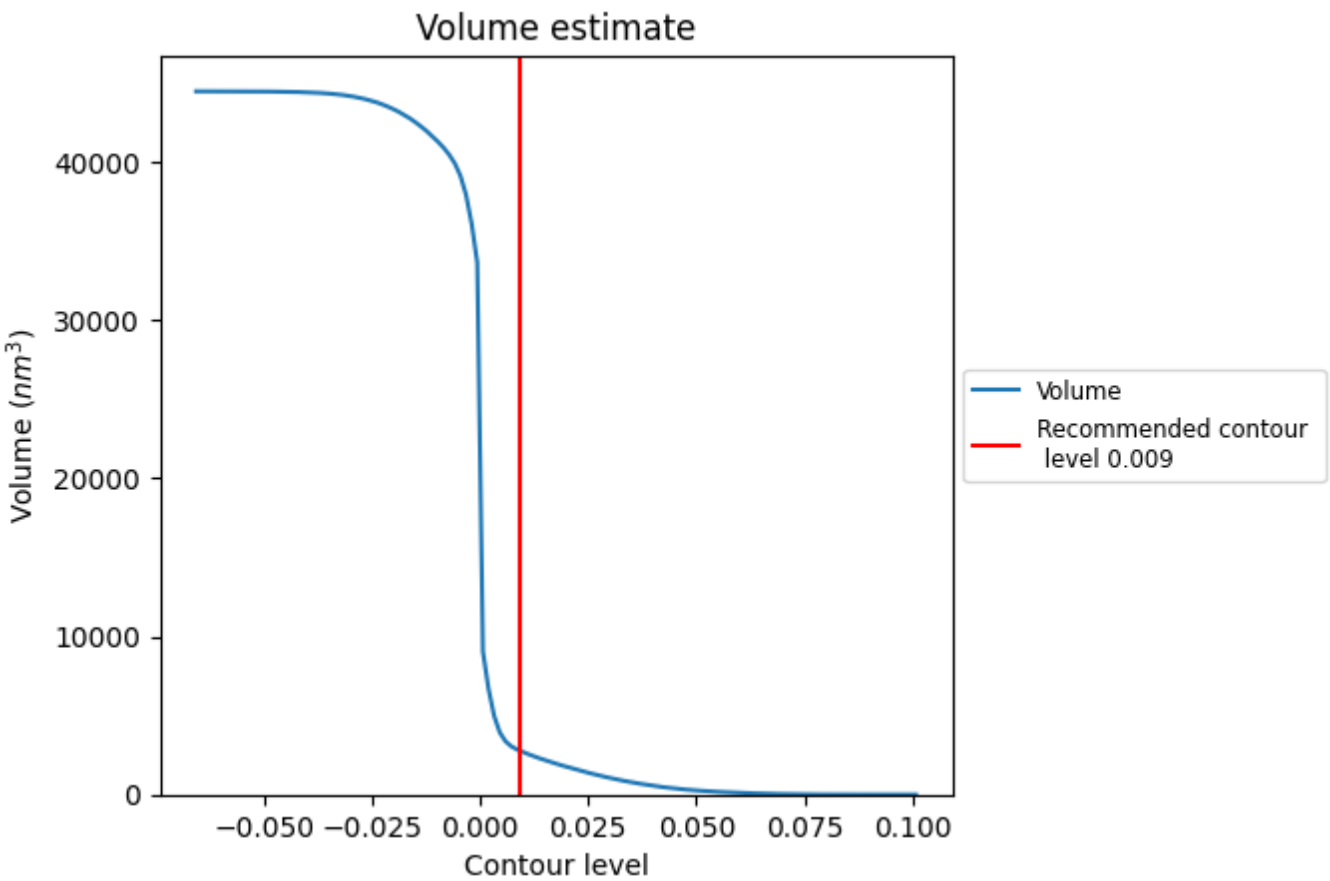
This section contains the results of statistical analysis of the map.

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.

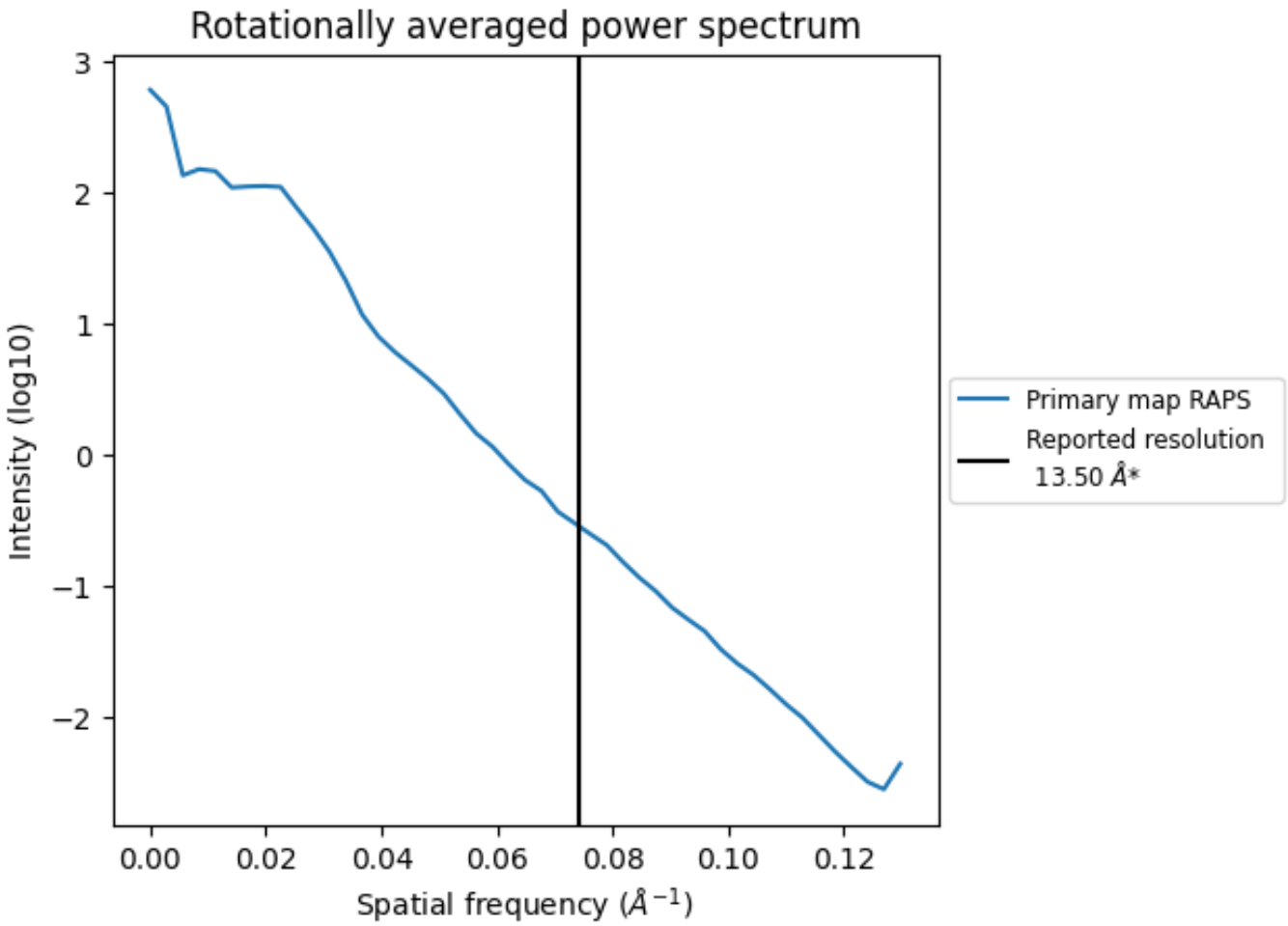
7.2 Volume estimate (i)



The volume at the recommended contour level is 2796 nm^3; this corresponds to an approximate mass of 2526 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 0.074 Å^{-1}

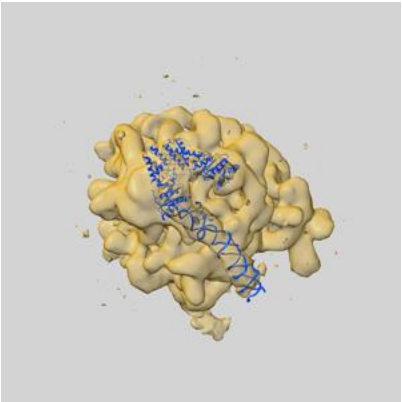
8 Fourier-Shell correlation (i)

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

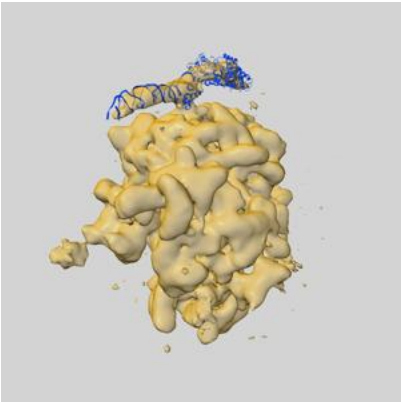
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-1762 and PDB model 2XKV. Per-residue inclusion information can be found in section 3 on page 4.

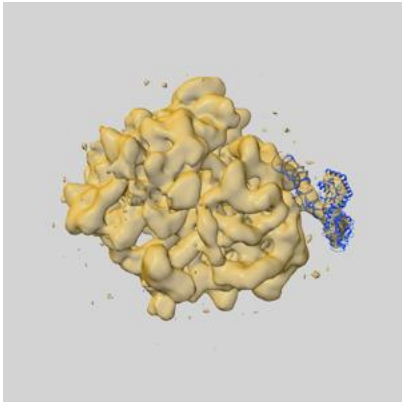
9.1 Map-model overlay (i)



X



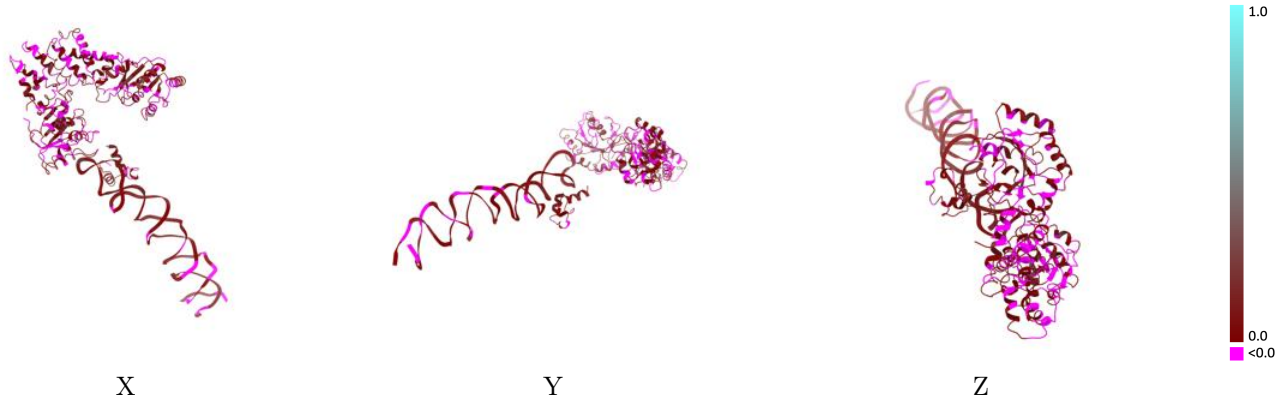
Y



Z

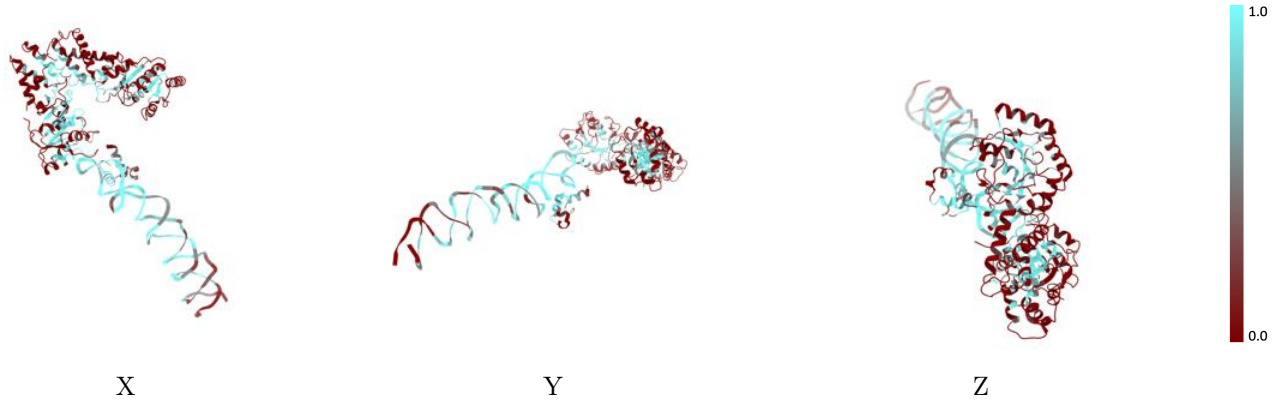
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



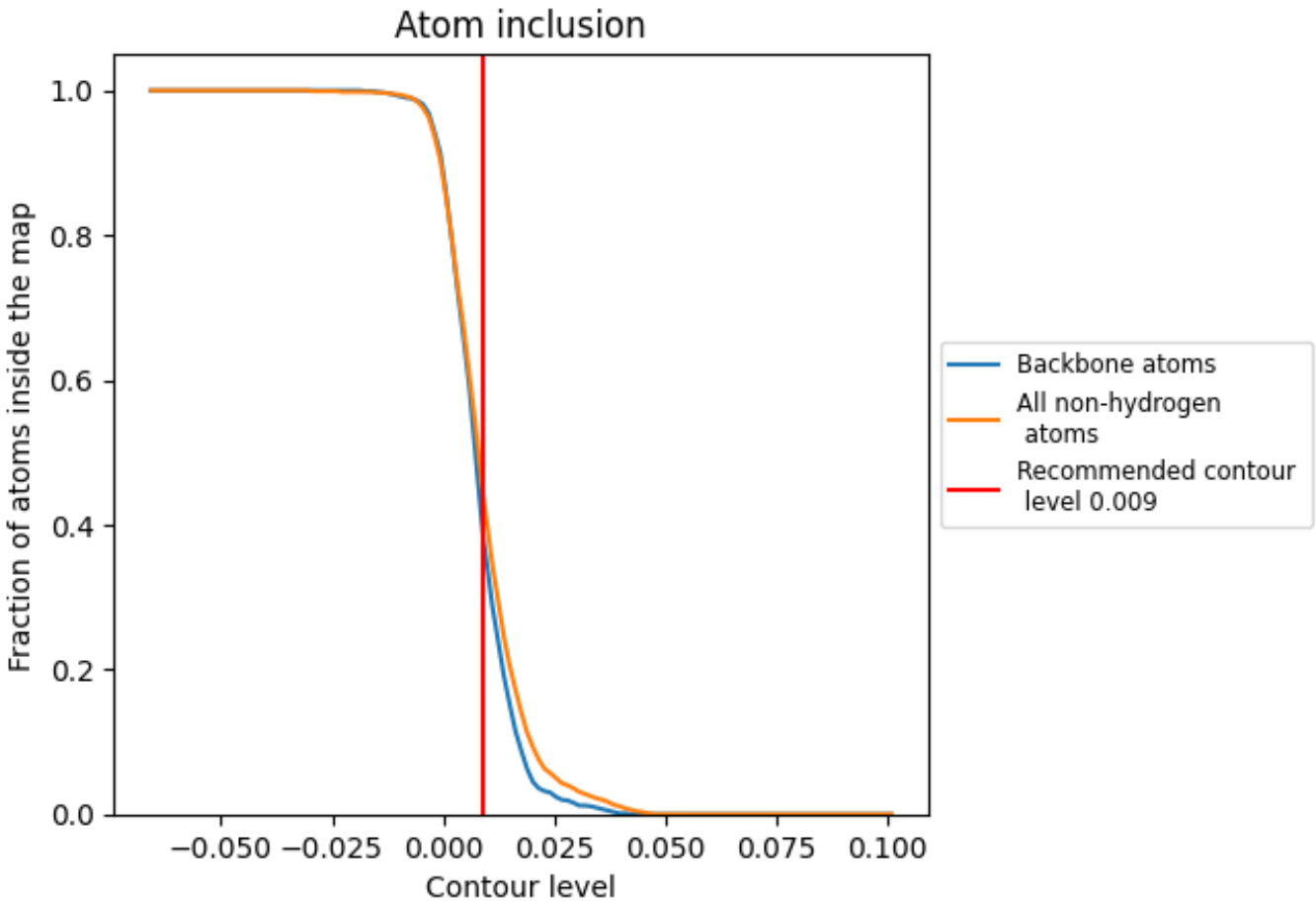
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.009).

9.4 Atom inclusion (i)



At the recommended contour level, 38% of all backbone atoms, 44% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4390	0.0440
A	0.2960	0.0370
B	0.6660	0.0640
C	0.5520	0.0500
D	0.3440	0.0300