



wwPDB EM Validation Summary Report ⓘ

Feb 14, 2024 – 12:46 PM EST

PDB ID : 3LU0
EMDB ID : EMD-5169
Title : Molecular model of Escherichia coli core RNA polymerase
Authors : Darst, S.A.
Deposited on : 2010-02-16
Resolution : 11.20 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.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

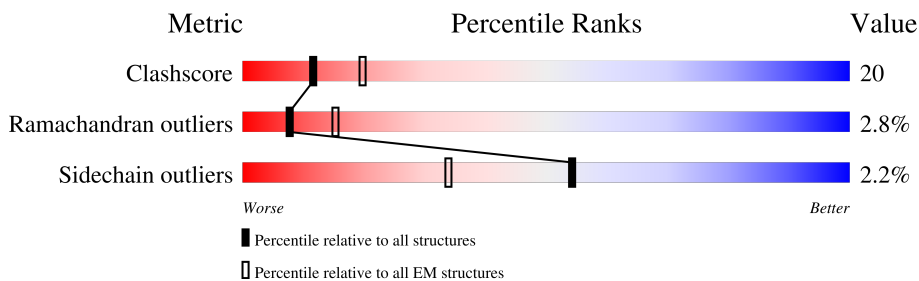
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 11.20 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	329	
1	B	329	
2	C	1342	
3	D	1407	
4	E	91	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 25410 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	235	Total	C	N	O	S	0	0
			1820	1132	323	358	7		
1	B	235	Total	C	N	O	S	0	0
			1820	1132	323	358	7		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	1335	Total	C	N	O	S	0	0
			10523	6602	1836	2042	43		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	516	VAL	ASP	conflict	UNP P0A8V2

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	1364	Total	C	N	O	S	0	0
			10547	6624	1879	1994	50		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

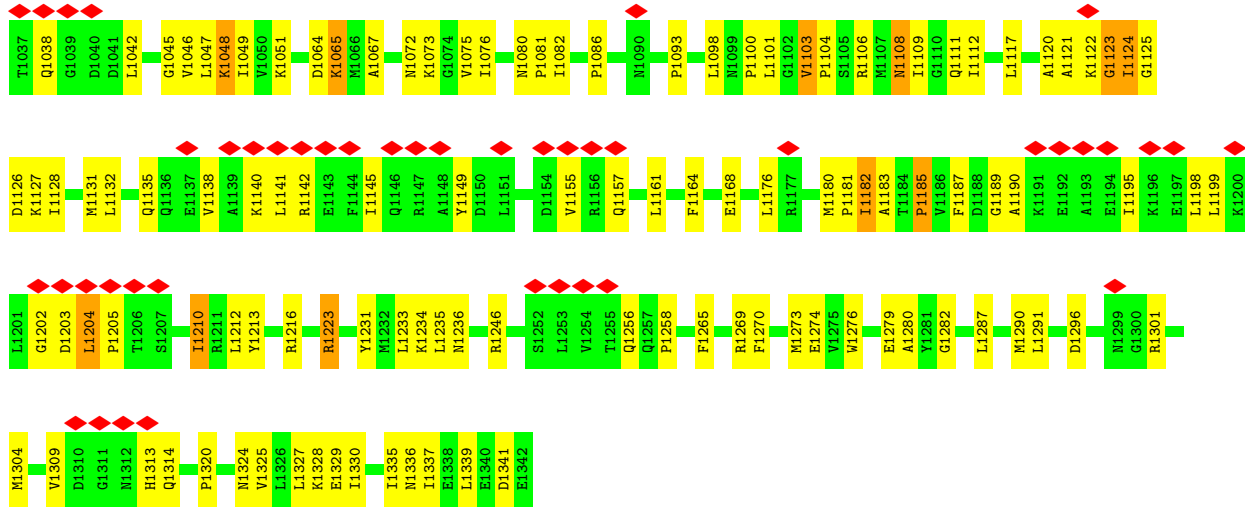
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	89	Total	C	N	O	S	0	0
			697	424	132	140	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

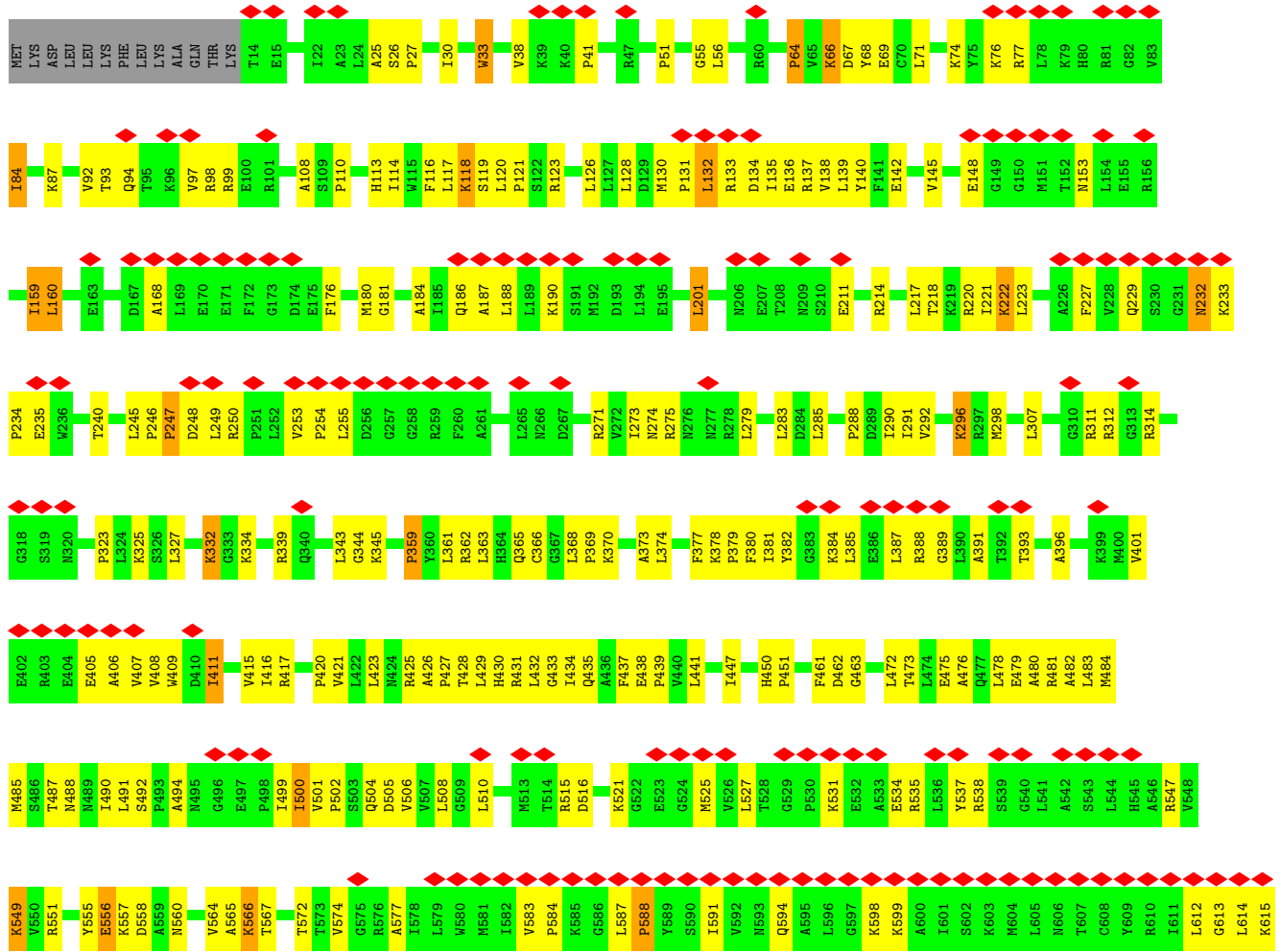
Mol	Chain	Residues	Atoms		AltConf
5	D	1	Total	Mg	0
			1	1	

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
6	D	2	2	2	0



• Molecule 3: DNA-directed RNA polymerase subunit beta'



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	42000	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	10	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	69.984	Depositor
Minimum map value	-1.475	Depositor
Average map value	0.803	Depositor
Map value standard deviation	3.186	Depositor
Recommended contour level	11.0	Depositor
Map size (\AA)	252, 252, 252	wwPDB
Map dimensions	90, 90, 90	wwPDB
Map angles ($^\circ$)	90, 90, 90	wwPDB
Pixel spacing (\AA)	2.8, 2.8, 2.8	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: MG, 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	0.19	0/1842	0.37	0/2495
1	B	0.19	0/1842	0.36	0/2495
2	C	0.21	1/10690 (0.0%)	0.34	0/14422
3	D	0.26	0/10710	0.63	3/14470 (0.0%)
4	E	1.09	2/699 (0.3%)	1.79	4/942 (0.4%)
All	All	0.29	3/25783 (0.0%)	0.56	7/34824 (0.0%)

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
3	D	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	49	ILE	C-N	5.62	1.47	1.34
2	C	951	MET	CG-SD	5.51	1.95	1.81
4	E	49	ILE	CA-C	5.30	1.66	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1360	GLY	CA-C-N	-50.05	7.09	117.20
4	E	81	GLN	CG-CD-OE1	-38.65	44.30	121.60
3	D	1360	GLY	C-N-CA	-31.89	41.97	121.70
4	E	81	GLN	CG-CD-NE2	-9.65	93.55	116.70
4	E	49	ILE	C-N-CA	8.22	142.25	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	1360	GLY	Peptide

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	1820	0	1850	78	0
1	B	1820	0	1850	59	0
2	C	10523	0	10551	327	0
3	D	10547	0	10751	495	0
4	E	697	0	706	209	0
5	D	1	0	0	0	0
6	D	2	0	0	0	0
All	All	25410	0	25708	1011	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 20.

The worst 5 of 1011 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)
3:D:615:LYS:CD	4:E:5:THR:CA	1.80	1.59
3:D:615:LYS:CE	4:E:5:THR:HA	1.37	1.53
3:D:615:LYS:CD	4:E:5:THR:HA	1.34	1.46
3:D:615:LYS:HD3	4:E:5:THR:C	1.31	1.46
3:D:615:LYS:HD3	4:E:5:THR:CA	1.34	1.45

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	233/329 (71%)	196 (84%)	31 (13%)	6 (3%)	5	31
1	B	233/329 (71%)	197 (84%)	28 (12%)	8 (3%)	3	26
2	C	1333/1342 (99%)	1109 (83%)	190 (14%)	34 (3%)	5	31
3	D	1362/1407 (97%)	1124 (82%)	198 (14%)	40 (3%)	4	29
4	E	87/91 (96%)	74 (85%)	10 (12%)	3 (3%)	3	26
All	All	3248/3498 (93%)	2700 (83%)	457 (14%)	91 (3%)	8	30

5 of 91 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	ILE
1	A	166	ARG
1	B	124	VAL
2	C	489	PRO
2	C	582	ASN

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	202/286 (71%)	195 (96%)	7 (4%)	36	59
1	B	202/286 (71%)	199 (98%)	3 (2%)	65	80
2	C	1150/1157 (99%)	1139 (99%)	11 (1%)	76	86
3	D	1129/1168 (97%)	1091 (97%)	38 (3%)	37	60

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	E	73/75 (97%)	71 (97%)	2 (3%)	44 65
All	All	2756/2972 (93%)	2695 (98%)	61 (2%)	54 71

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	222	LYS
3	D	1266	ILE
3	D	549	LYS
3	D	1263	LYS
4	E	31	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	680	ASN
3	D	1238	GLN
3	D	762	ASN
3	D	921	GLN
3	D	1383	GLN

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 3 ligands modelled in this entry, 3 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.

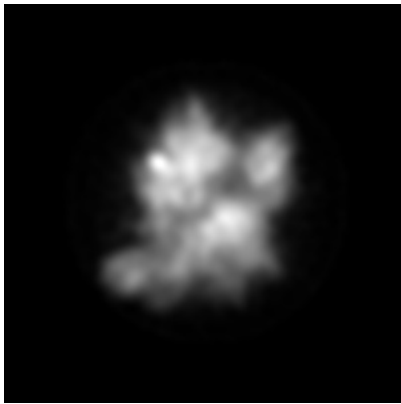
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5169. These allow visual inspection of the internal detail of the map and identification of artifacts.

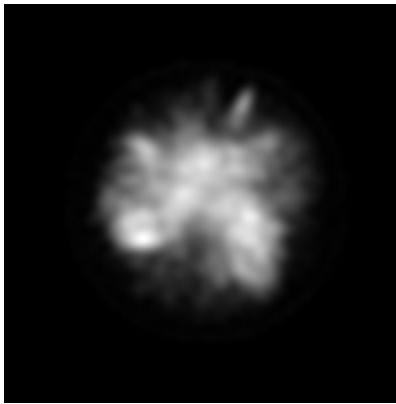
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

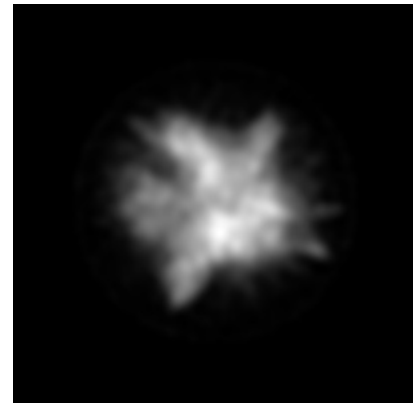
6.1.1 Primary map



X



Y

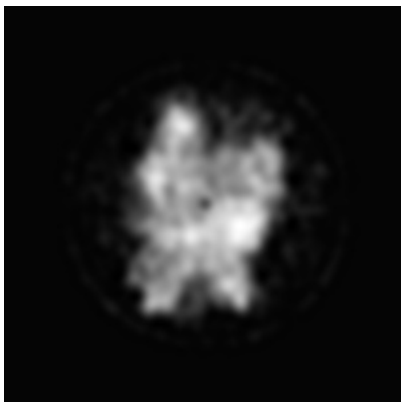


Z

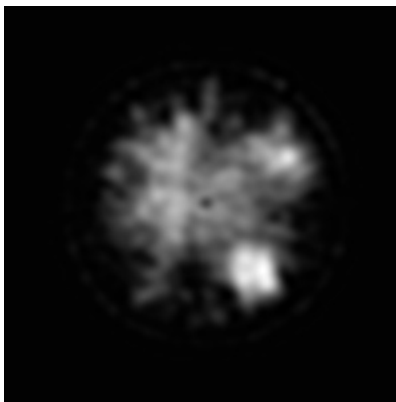
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

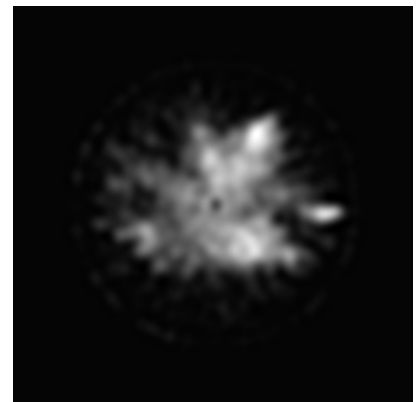
6.2.1 Primary map



X Index: 45



Y Index: 45

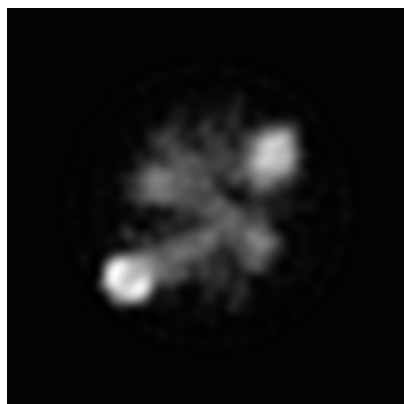


Z Index: 45

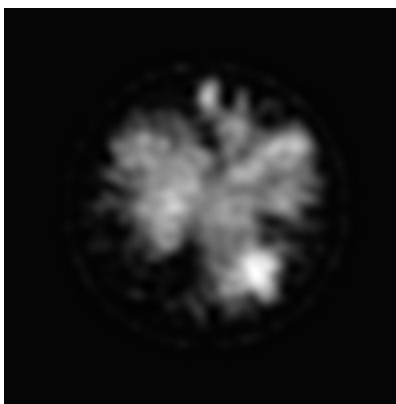
The images above show central slices of the map in three orthogonal directions.

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

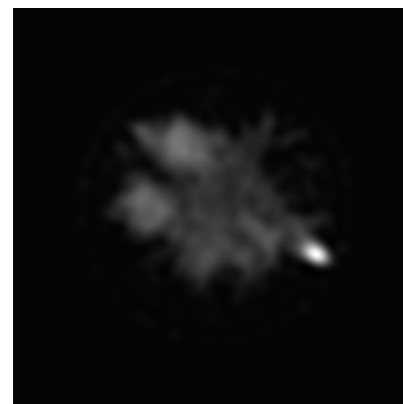
6.3.1 Primary map



X Index: 38



Y Index: 42

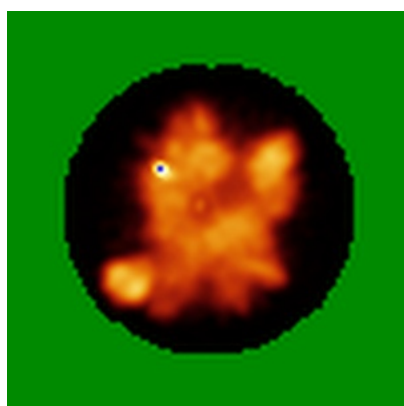


Z Index: 54

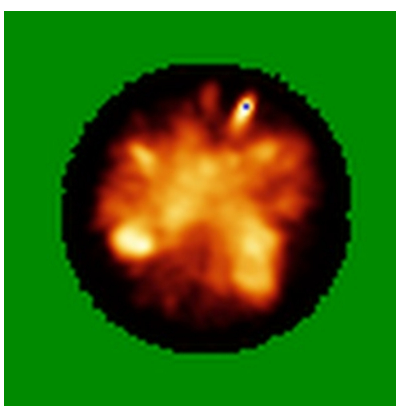
The images above show the largest variance slices of the map in three orthogonal directions.

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

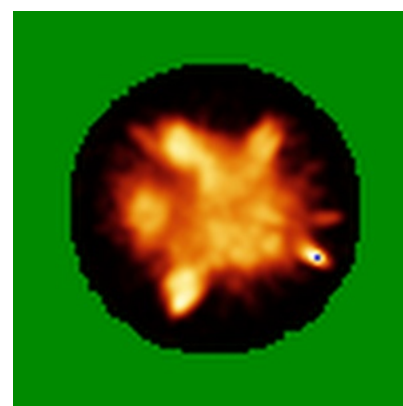
6.4.1 Primary map



X



Y

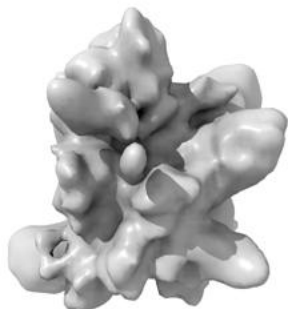


Z

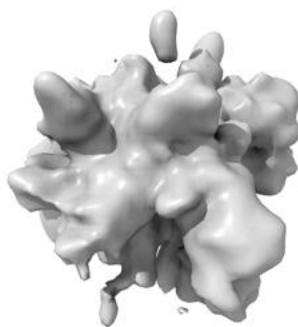
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

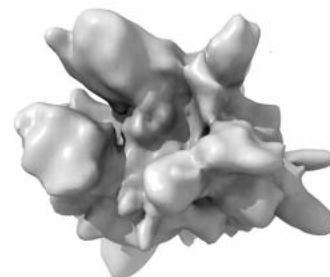
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 11.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

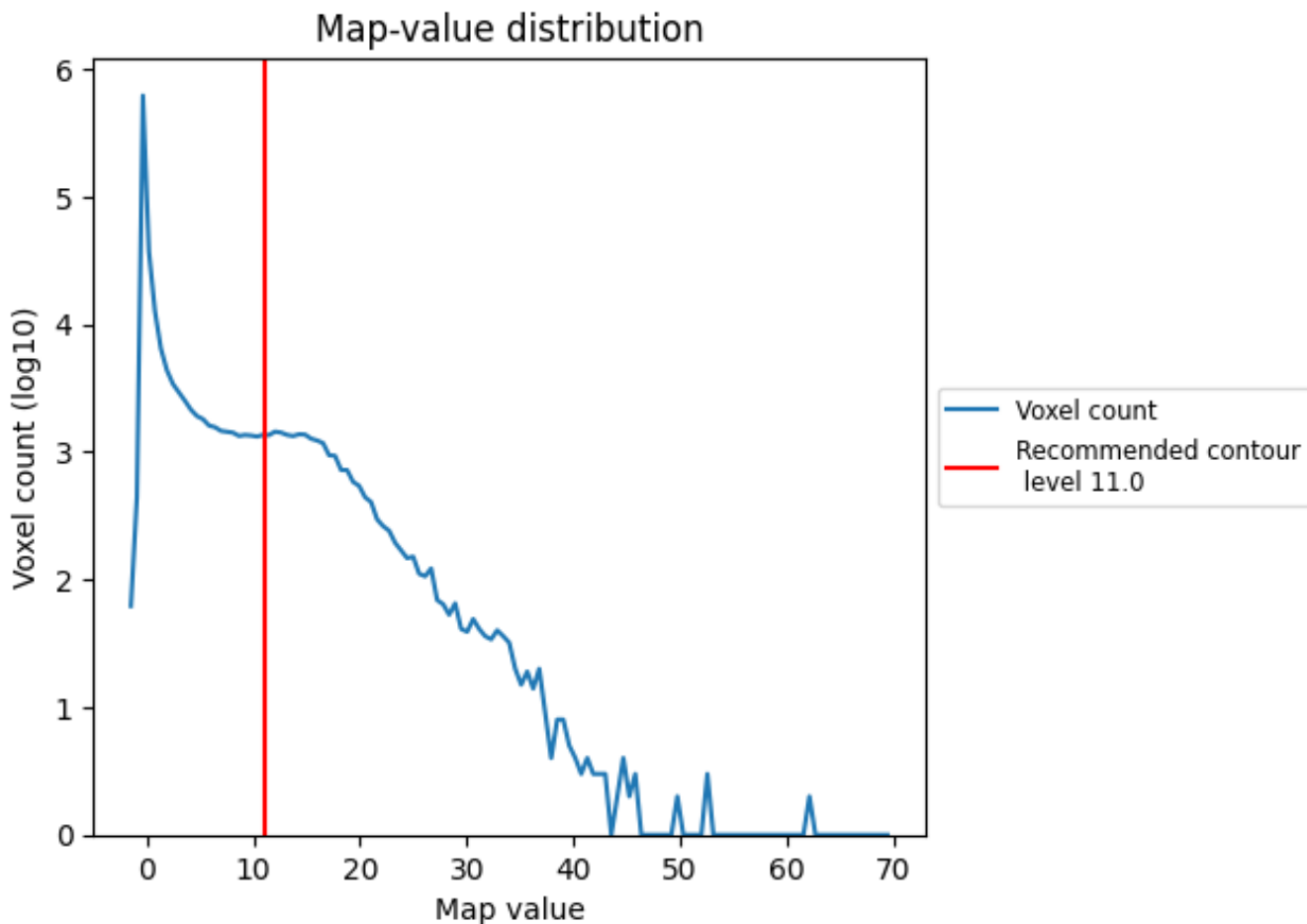
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

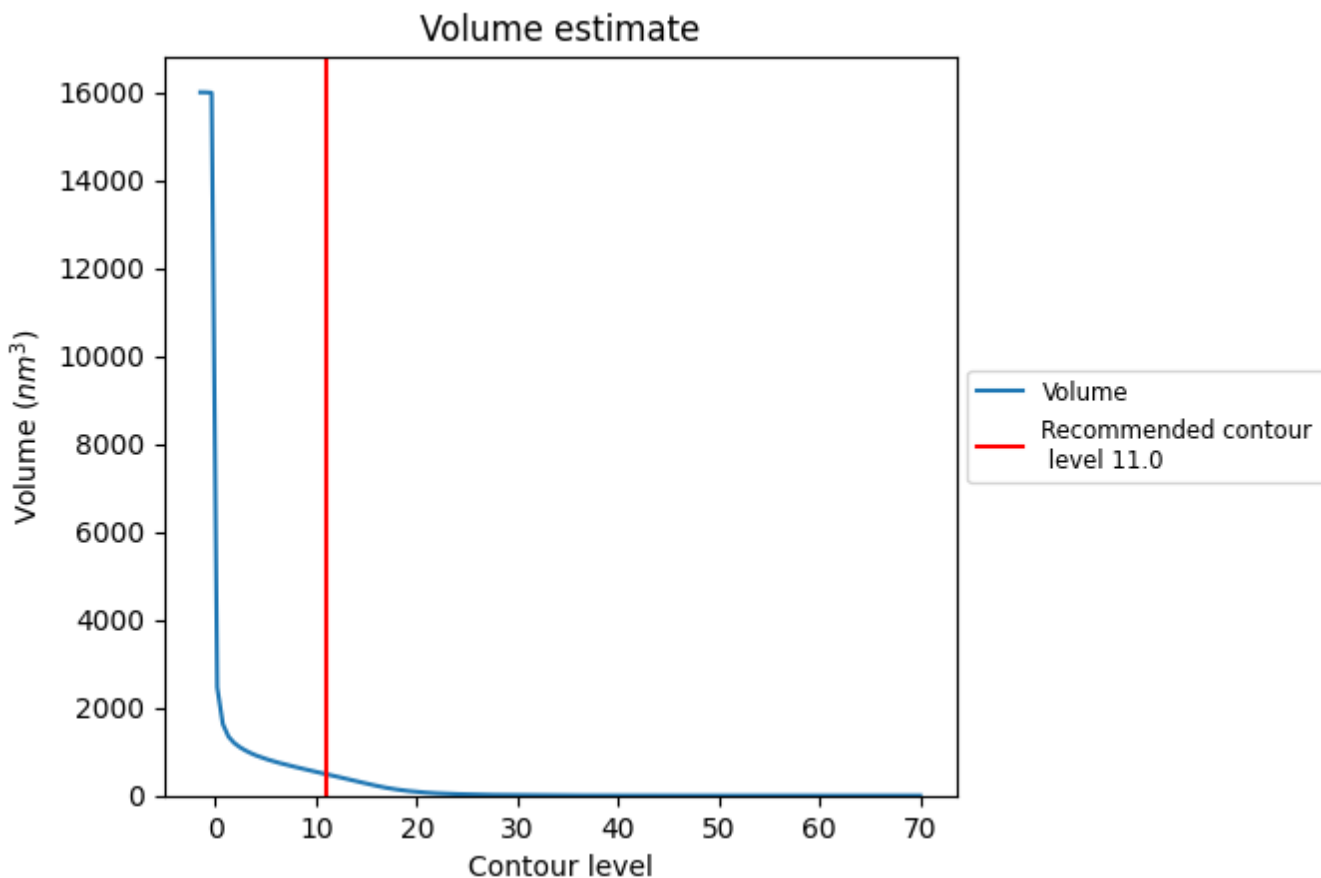
This section contains the results of statistical analysis of the map.

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.

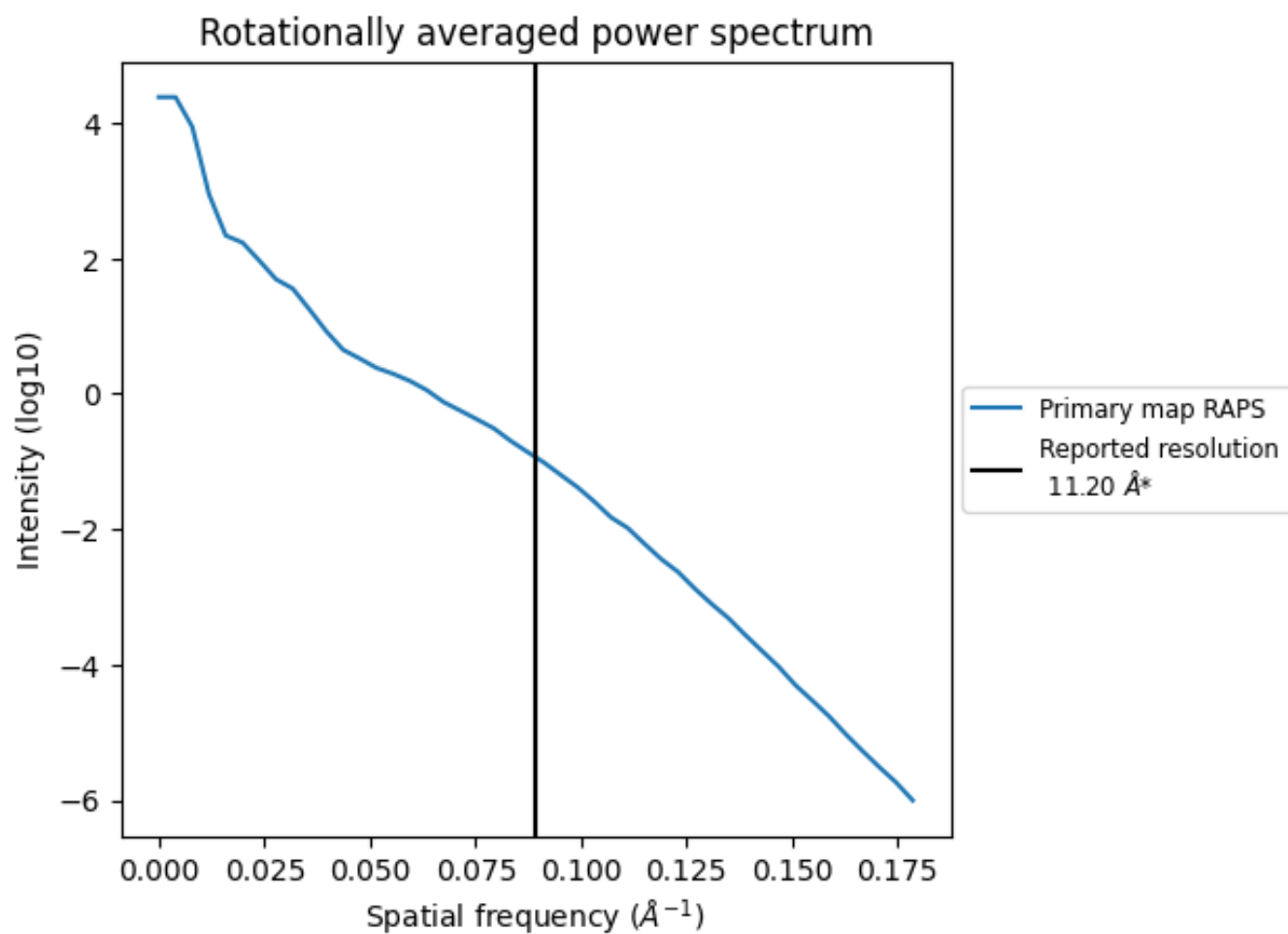
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 488 nm³; this corresponds to an approximate mass of 441 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 0.089 Å⁻¹

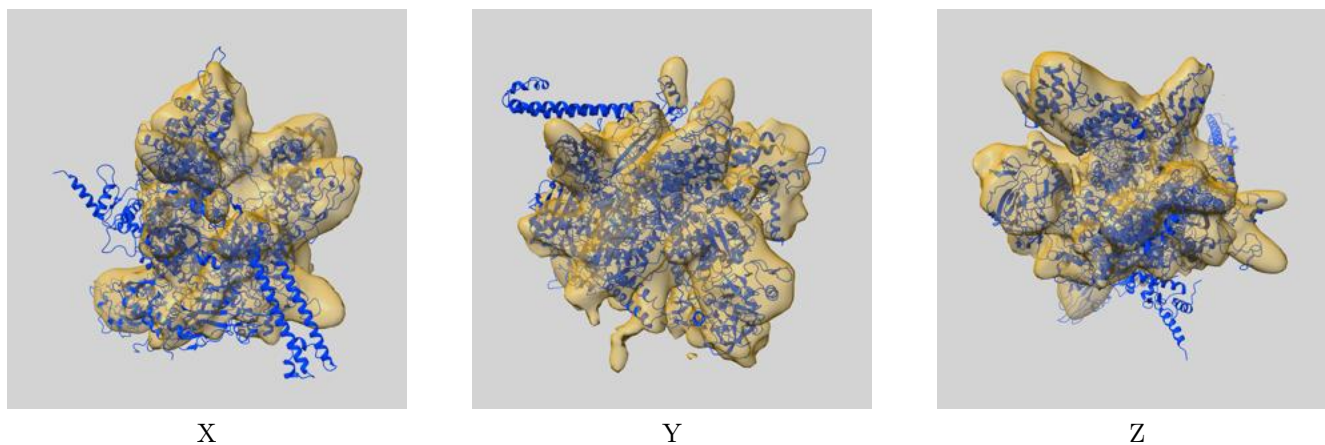
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

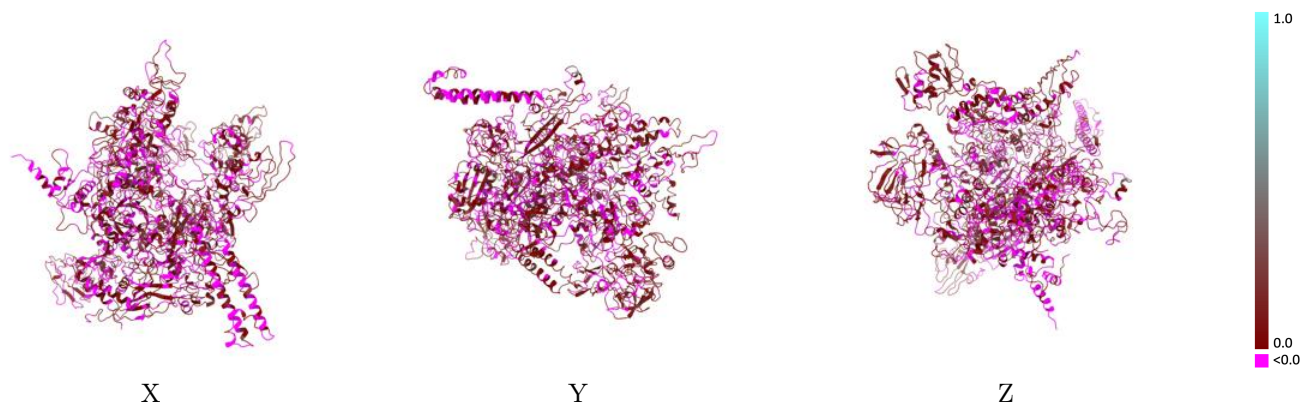
This section contains information regarding the fit between EMDB map EMD-5169 and PDB model 3LU0. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



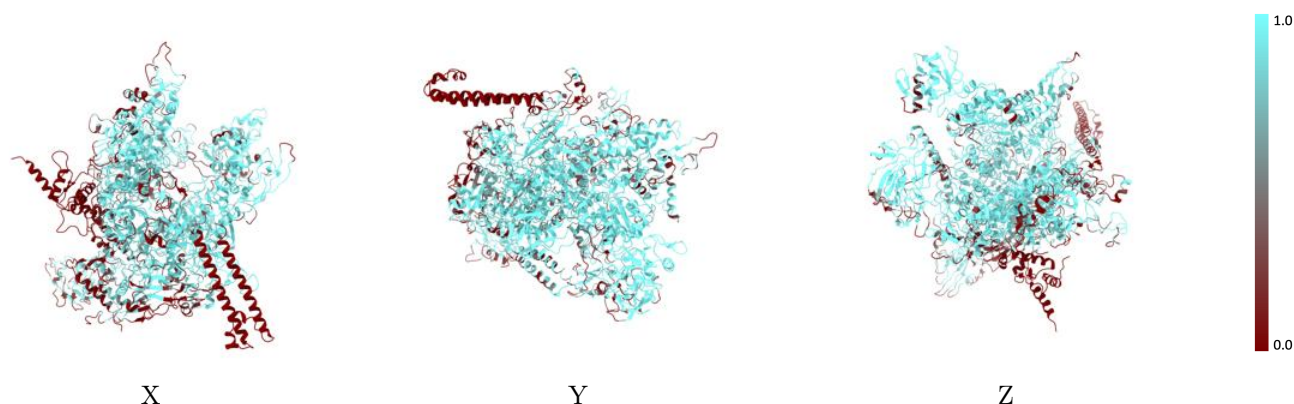
The images above show the 3D surface view of the map at the recommended contour level 11.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



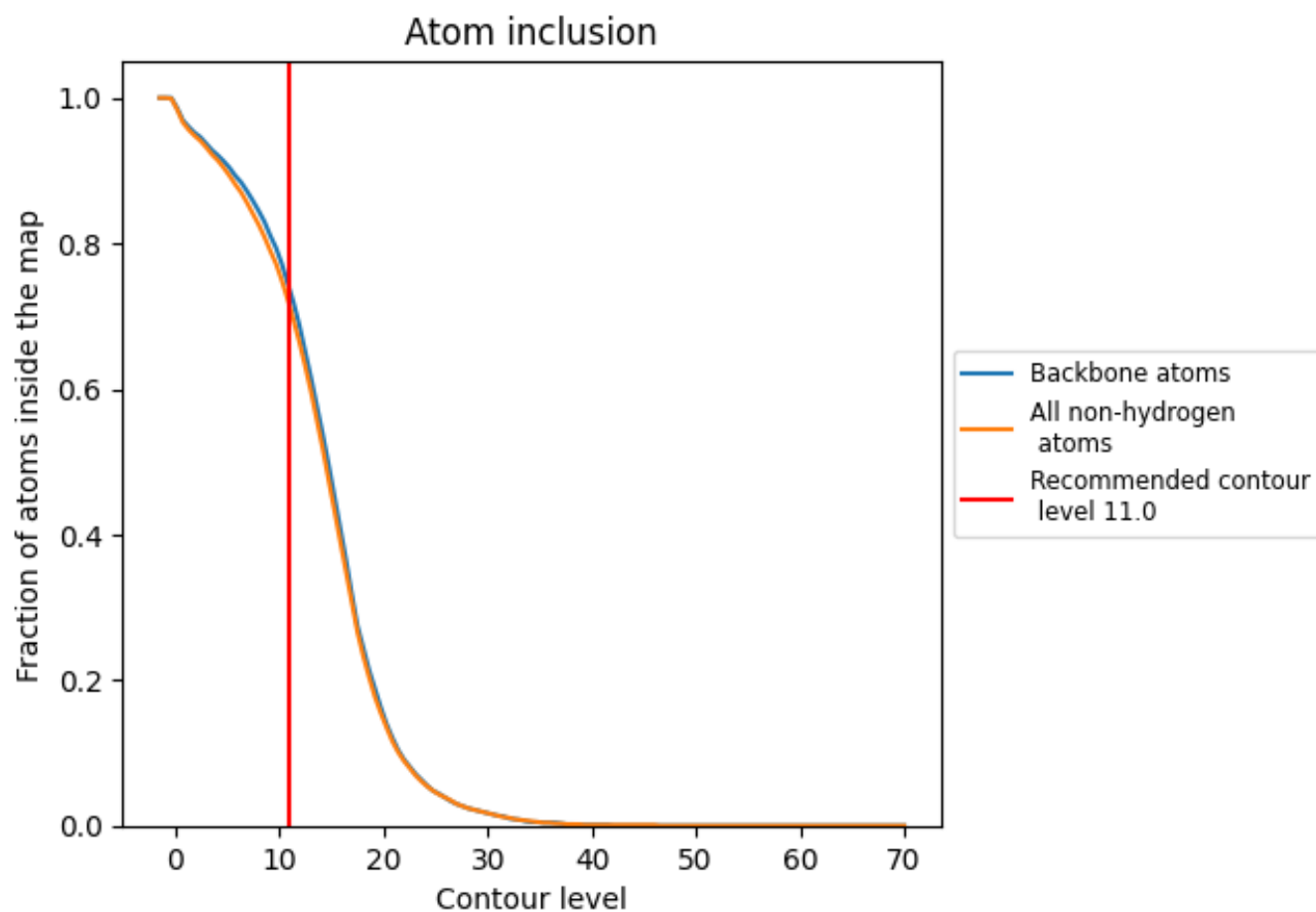
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (11.0).













9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 71% 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 (11.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7140	 0.0350
A	 0.5290	 0.0420
B	 0.5290	 0.0160
C	 0.7860	 0.0390
D	 0.7530	 0.0370
E	 0.0030	 -0.0260

