Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 03:06 pm GMT

PDB ID	:	5AJ2
EMDB ID	:	EMD-2901
Title	:	Cryo electron tomography of the Naip5-Nlrc4 inflammasome
Authors	:	Diebolder, C.A.; Halff, E.F.; Koster, A.J.; Huizinga, E.G.; Koning, R.I.
Deposited on	:	2015-02-20
Resolution	:	40.00 Å(reported)
Based on initial model	:	4KXF

This is a Full wwPDB EM Validation 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:

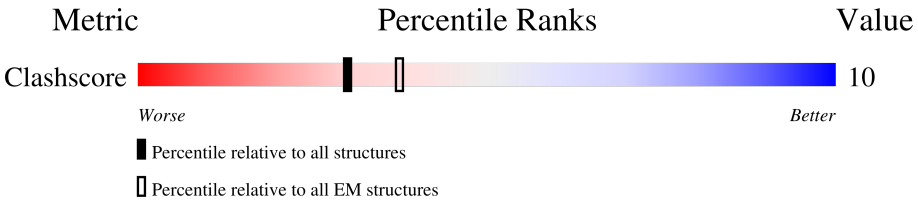
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 40.00 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	158937	4297

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	355	17% 74% · 26%
2	B	225	10% 97% ·
3	C	445	15% 92% · 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 904 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 NLR FAMILY CARD DOMAIN-CONTAINING PROTEIN 4.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
1	A	263	263	263	0	263

- Molecule 2 is a protein called NLR FAMILY CARD DOMAIN-CONTAINING PROTEIN 4.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
2	B	225	225	225	0	225

- Molecule 3 is a protein called NLR FAMILY CARD DOMAIN-CONTAINING PROTEIN 4.

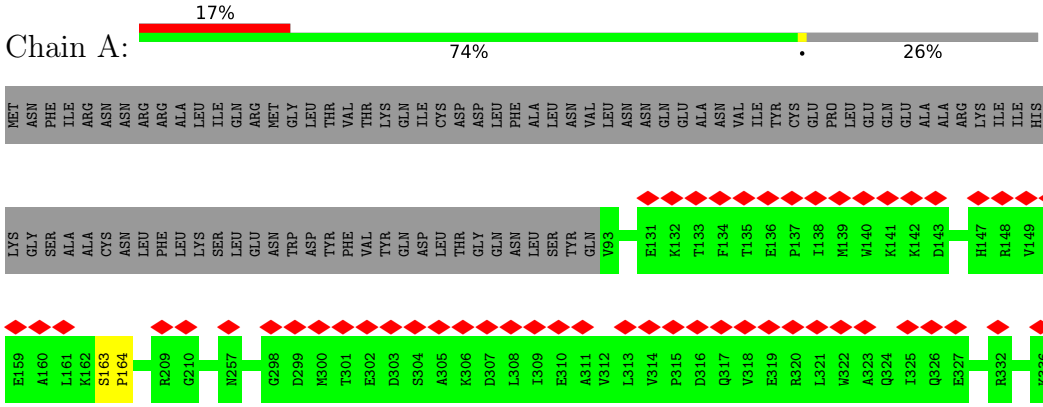
Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
3	C	416	416	416	0	416

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.

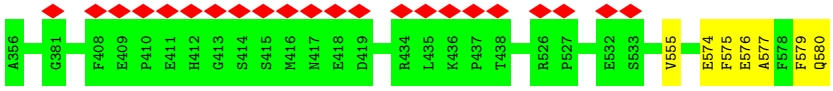
• Molecule 1: NLR FAMILY CARD DOMAIN-CONTAINING PROTEIN 4

Chain A:



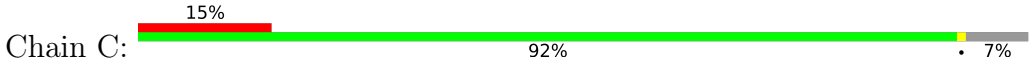
• Molecule 2: NLR FAMILY CARD DOMAIN-CONTAINING PROTEIN 4

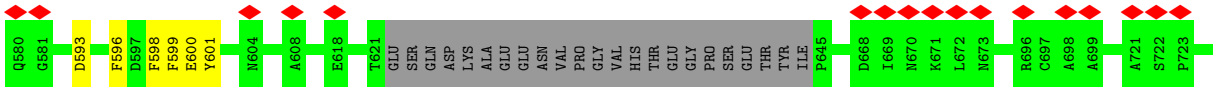
Chain B:

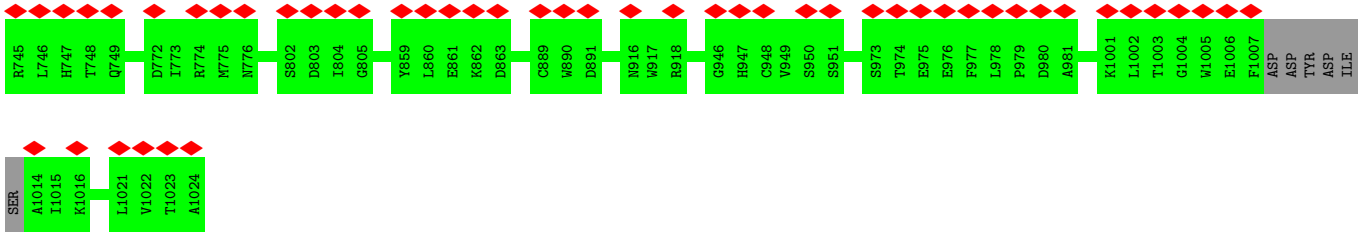


• Molecule 3: NLR FAMILY CARD DOMAIN-CONTAINING PROTEIN 4

Chain C:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of tilted images used	50	Depositor
Resolution determination method	Not provided	
CTF correction method	TOMOCTF	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	100	Depositor
Minimum defocus (nm)	6500	Depositor
Maximum defocus (nm)	7500	Depositor
Magnification	18000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum voxel value	255.000	Depositor
Minimum voxel value	0.000	Depositor
Average voxel value	16.017	Depositor
Voxel value standard deviation	46.347	Depositor
Recommended contour level	175.0	Depositor
Tomogram size (Å)	546.3, 546.3, 546.3	wwPDB
Tomogram dimensions	100, 100, 100	wwPDB
Tomogram angles (°)	90.0, 90.0, 90.0	wwPDB
Grid spacing (Å)	5.463, 5.463, 5.463	Depositor

5 Model quality

5.1 Standard geometry

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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

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	263	0	0	1	0
2	B	225	0	0	8	0
3	C	416	0	0	8	0
All	All	904	0	0	9	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.

All (9) 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:579:PHE:CA	3:C:596:PHE:CA	1.76	1.63
2:B:575:PHE:CA	3:C:600:GLU:CA	1.92	1.46
2:B:576:GLU:CA	3:C:600:GLU:CA	1.98	1.41
2:B:576:GLU:CA	3:C:599:PHE:CA	2.22	1.18
2:B:580:GLN:CA	3:C:598:PHE:CA	2.35	1.04
2:B:574:GLU:CA	3:C:601:TYR:CA	2.68	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:577:ALA:CA	3:C:601:TYR:CA	2.72	0.68
2:B:555:VAL:CA	3:C:593:ASP:CA	2.82	0.57
1:A:163:SER:CA	1:A:164:PRO:CA	2.90	0.49

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

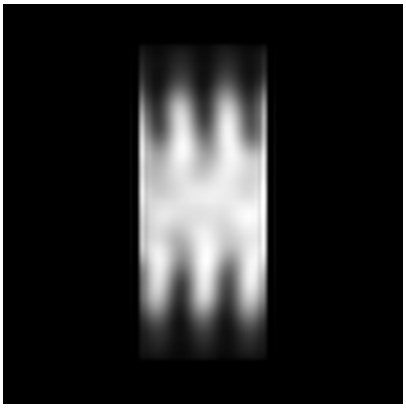
5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

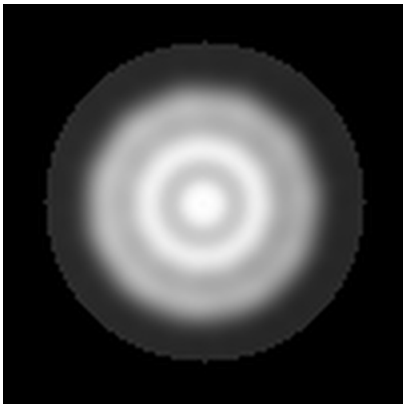
6 Tomogram visualisation

This section contains visualisations of the EMDB entry EMD-2901. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections



X

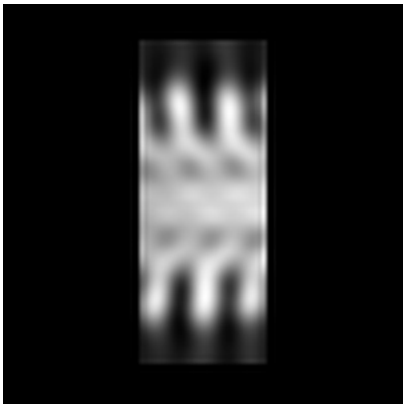


Y

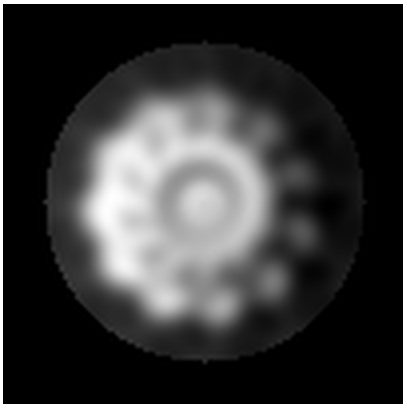
Z

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

6.2 Central slices



X Index: 50

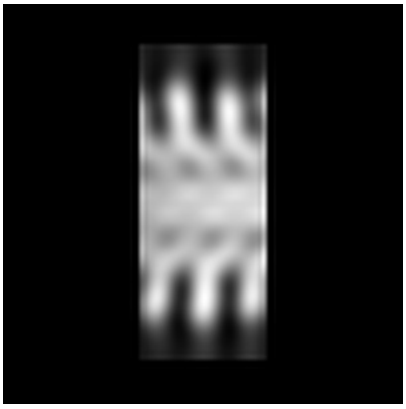


Y Index: 50

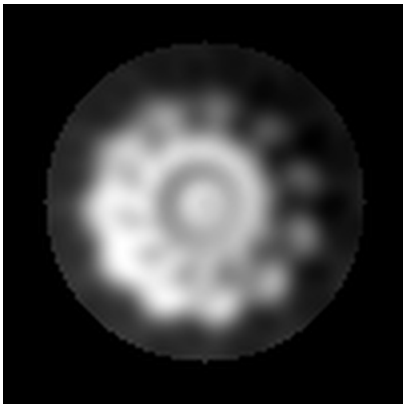
Z Index: 50

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

6.3 Largest variance slices (i)



X Index: 49



Y Index: 51

Z Index: 48

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

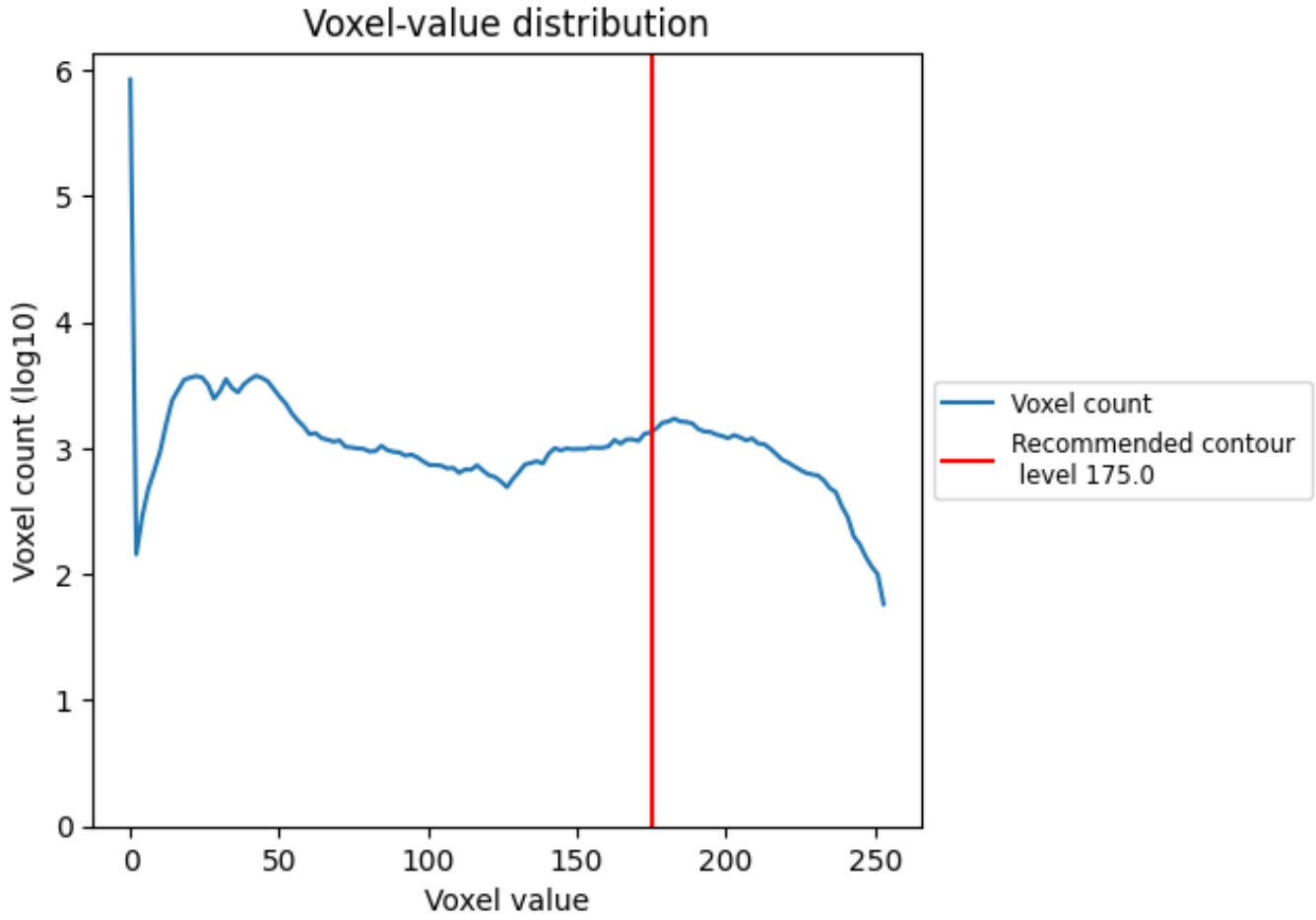
6.4 Mask visualisation (i)

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

7 Tomogram analysis

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

7.1 Voxel-value distribution



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

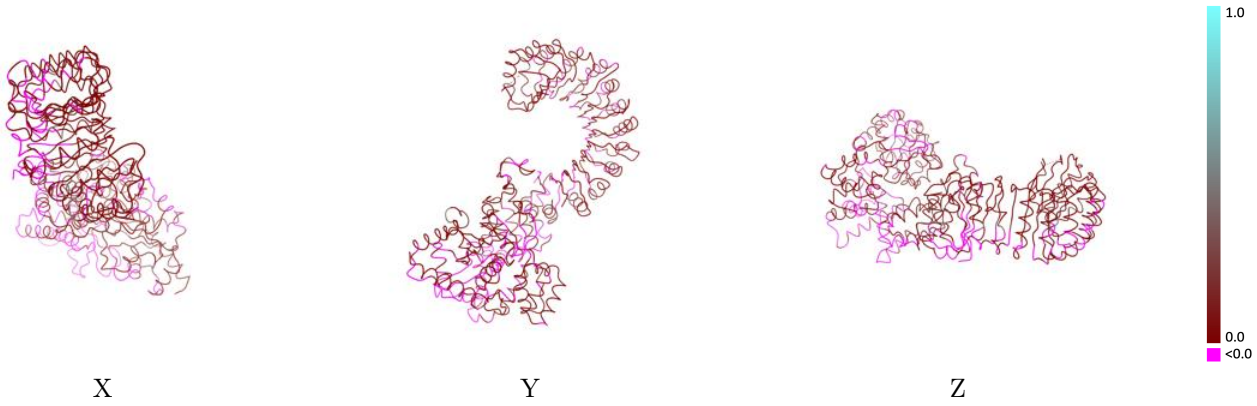
8 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2901 and PDB model 5AJ2. Per-residue inclusion information can be found in section 3 on page 4.

8.1 Map-model overlay

This section was not generated.

8.2 Q-score mapped to coordinate model

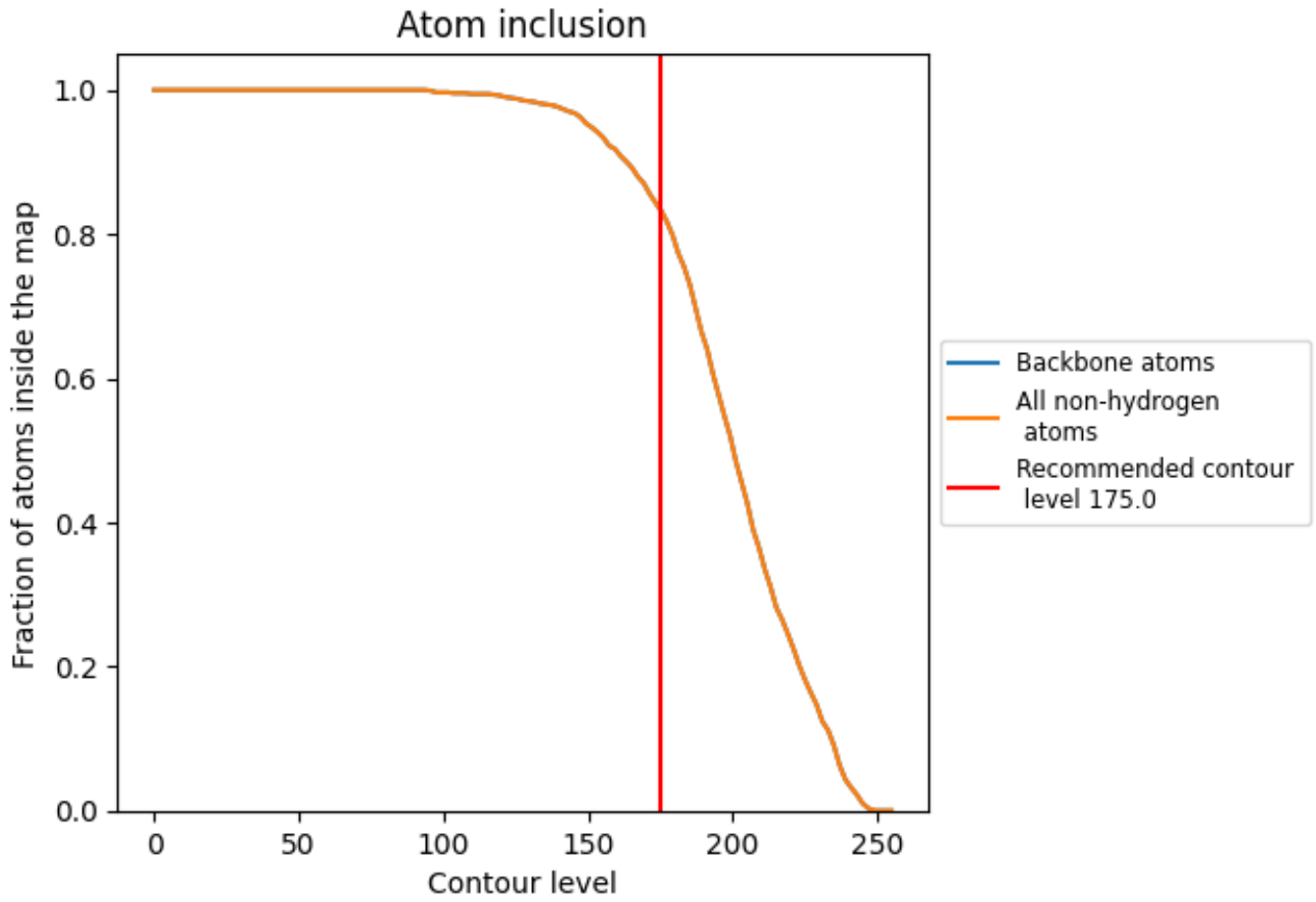


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

8.3 Atom inclusion mapped to coordinate model

This section was not generated.

8.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (175.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8341	0.0390
A	0.7681	0.0410
B	0.9022	0.0220
C	0.8389	0.0480