



## wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 05:07 AM UTC

PDB ID : 5AJ2 / pdb\_00005aj2  
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 wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

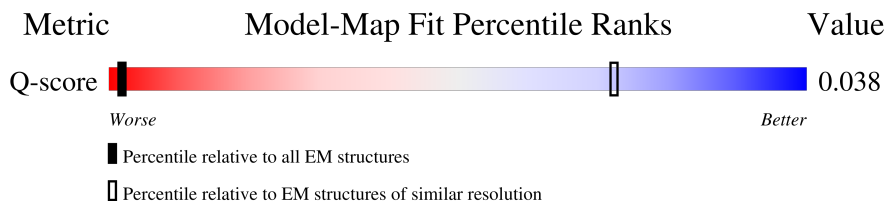
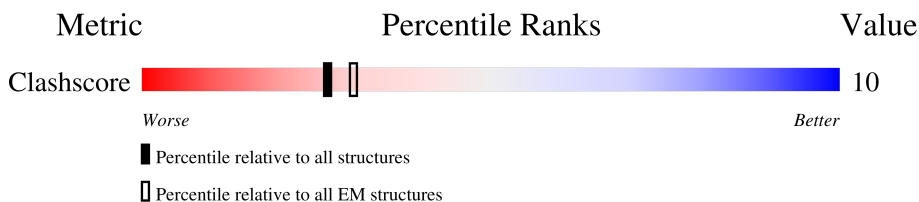
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

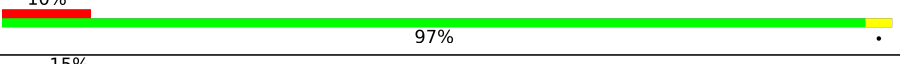
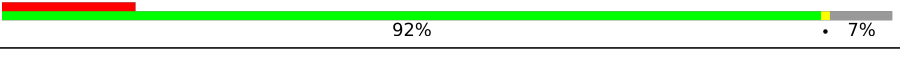
The reported resolution of this entry is 40.00 Å.

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<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore | 229148                      | 23984                       | -                                                        |
| Q-score    | -                           | 25397                       | 18 ( 40.00 - 40.00 )                                     |

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  $\geq 3$ , 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     | 355    |  |
| 2   | B     | 225    |  |
| 3   | C     | 445    |  |

## 2 Entry composition

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 |
|-----|-------|----------|-------|-----|---------|-------|
| 1   | A     | 263      | Total | C   | 0       | 263   |
|     |       |          | 263   | 263 |         |       |

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

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

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

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



## 4 Experimental information

| 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 ( $e^-/\text{\AA}^2$ ) | 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                                                                       | 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.

The worst 5 of 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              |

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 oligosaccharides 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.

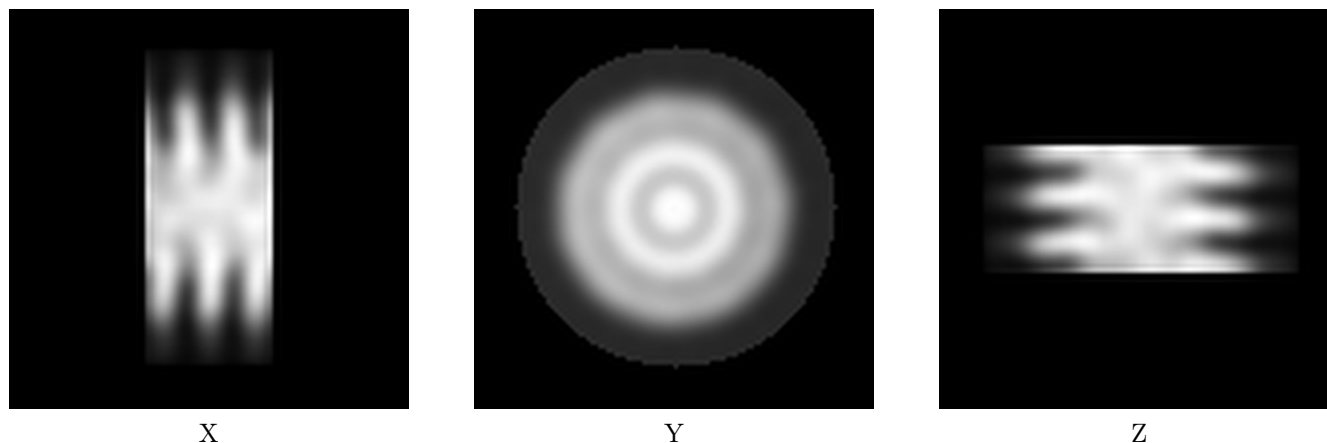
## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Tomogram visualisation [i](#)

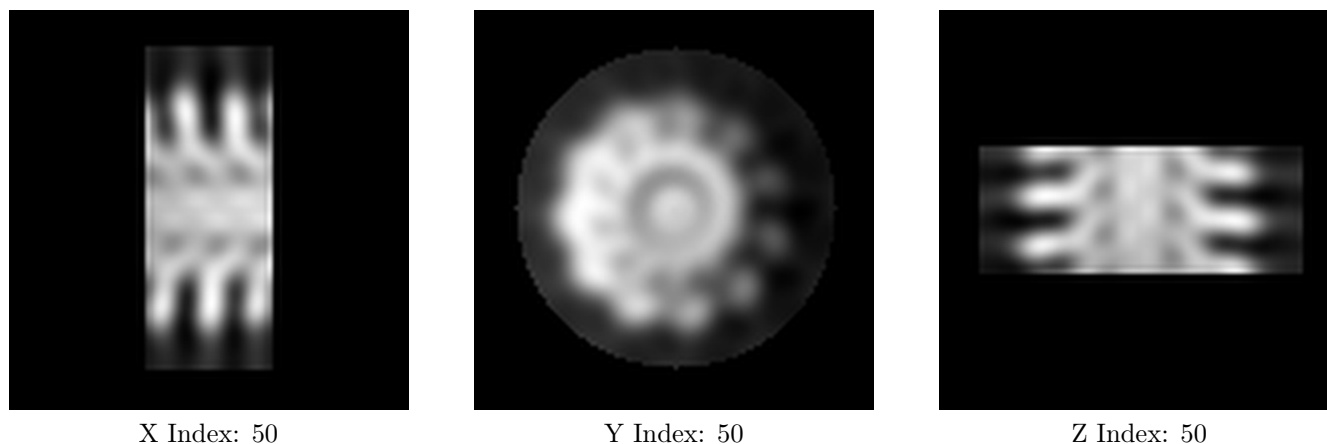
This section contains visualisations of the EMDB entry EMD-2901. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

### 6.1 Orthogonal projections [i](#)



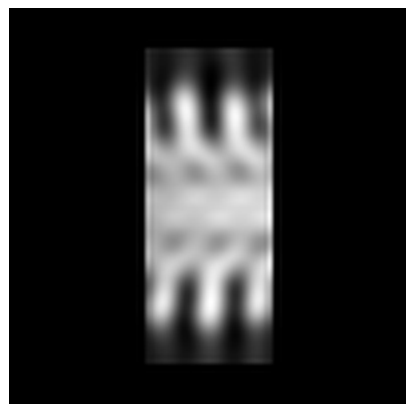
The images above show the tomogram projected in three orthogonal directions.

### 6.2 Central slices [i](#)

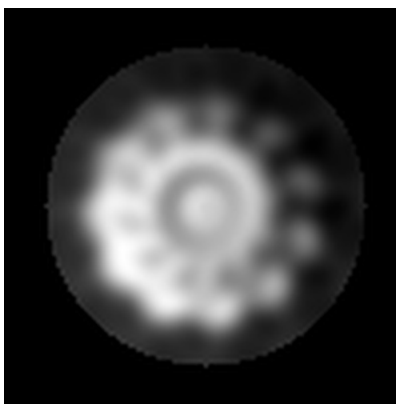


The images above show central slices of the tomogram in three orthogonal directions.

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



X Index: 49



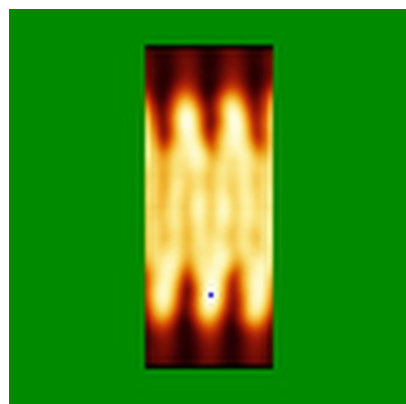
Y Index: 51



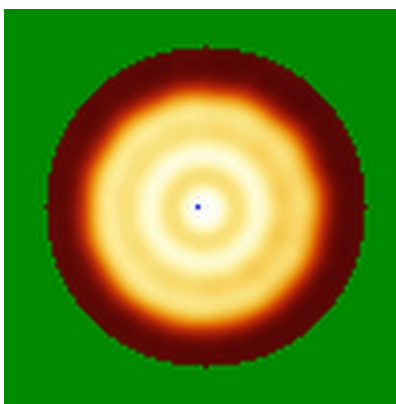
Z Index: 48

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

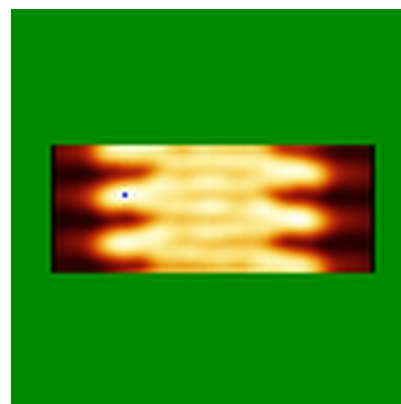
### 6.4 Orthogonal standard-deviation projections (False-color) [i](#)



X



Y



Z

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

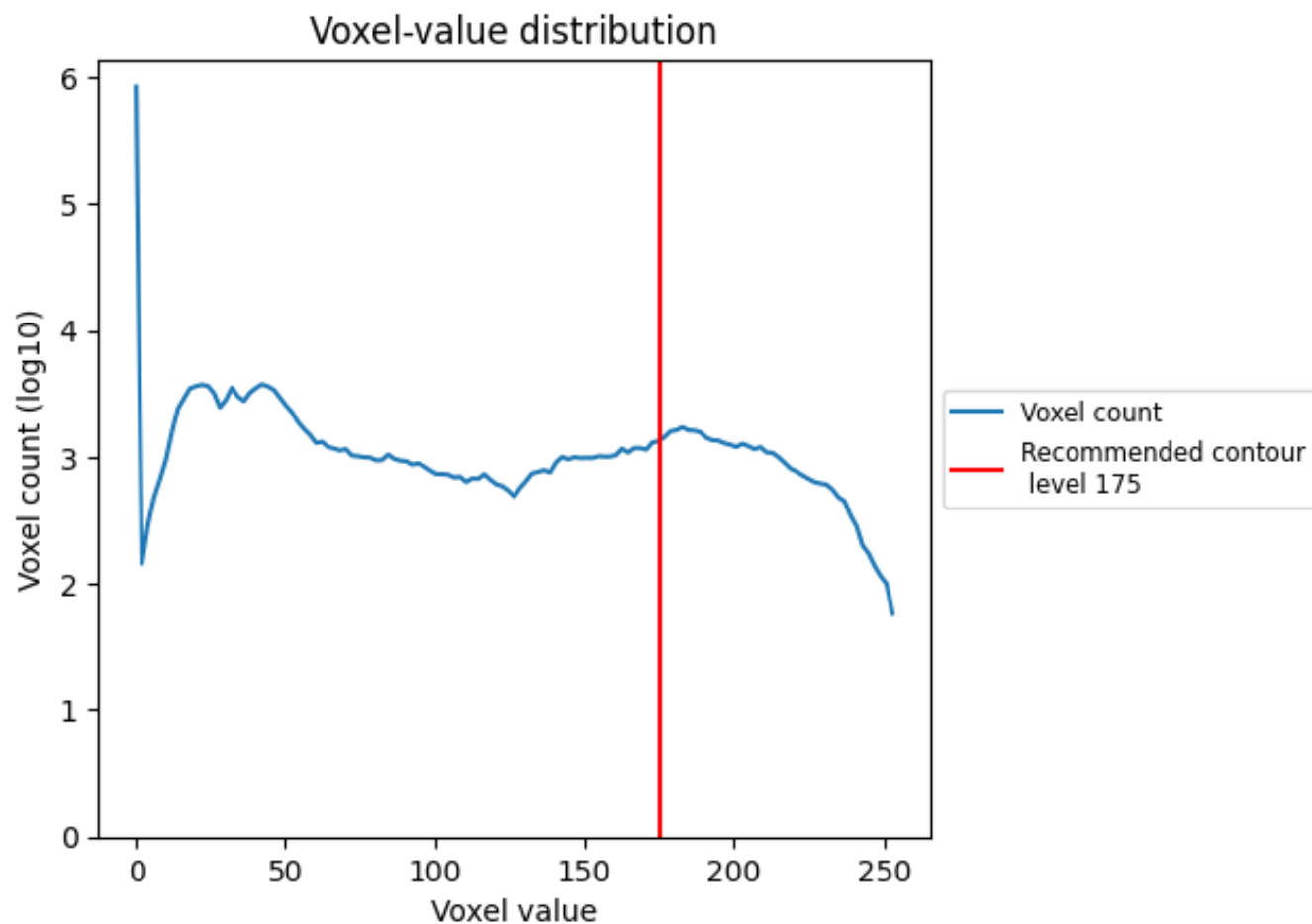
### 6.5 Mask visualisation [i](#)

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

## 7 Tomogram analysis [i](#)

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

### 7.1 Voxel-value distribution [i](#)



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

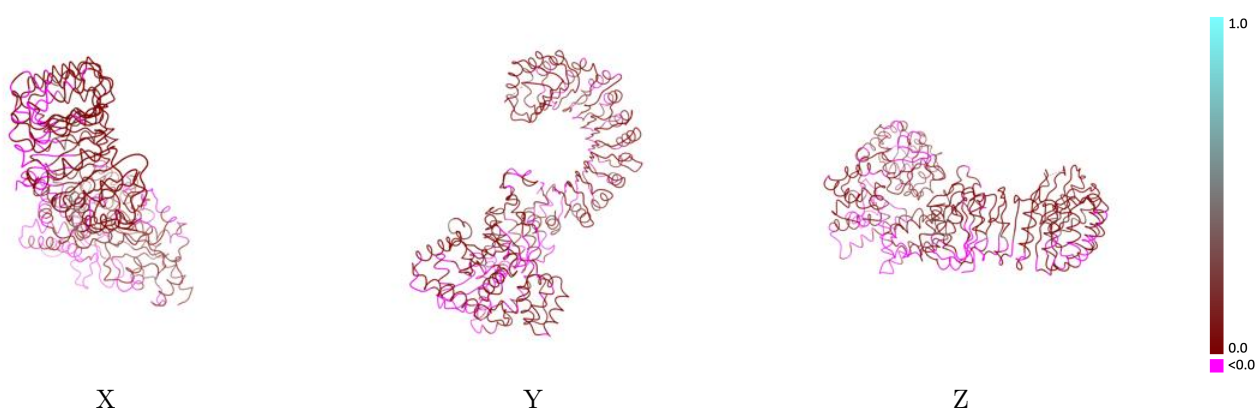
## 8 Map-model fit [i](#)

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 [i](#)

This section was not generated.

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

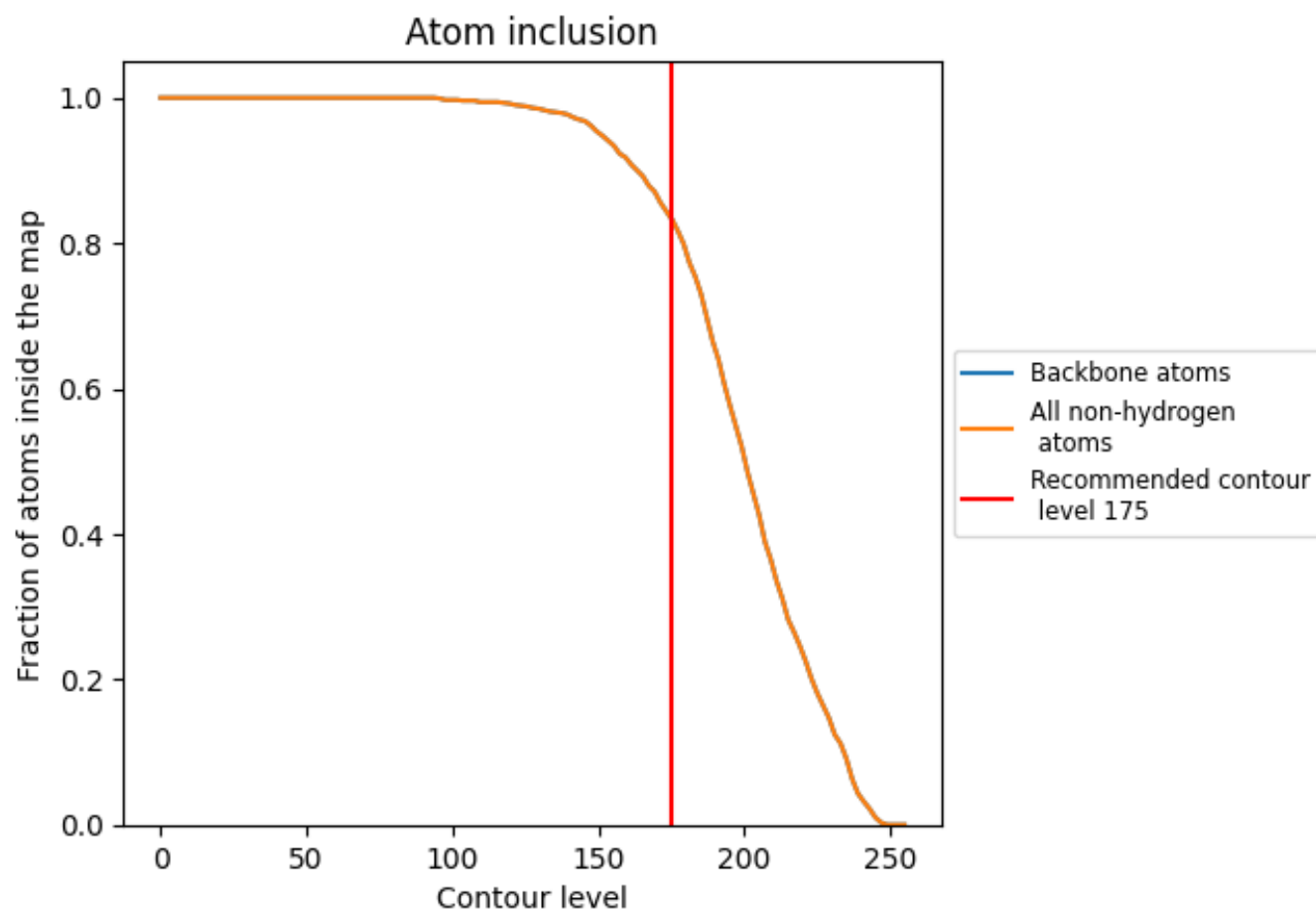


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

### 8.3 Atom inclusion mapped to coordinate model [i](#)

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) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.8340 | <div></div> 0.0380 |
| A     | <div></div> 0.7680 | <div></div> 0.0410 |
| B     | <div></div> 0.9020 | <div></div> 0.0190 |
| C     | <div></div> 0.8390 | <div></div> 0.0470 |

