



## wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 07:06 PM UTC

PDB ID : 8UBF / pdb\_00008ubf  
EMDB ID : EMD-42085  
Title : Diversity-generating retroelement (DGR) ribonucleoprotein - Resting state 1c  
Authors : Biswas, T.; Handa, S.; Ghosh, P.  
Deposited on : 2023-09-22  
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](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:

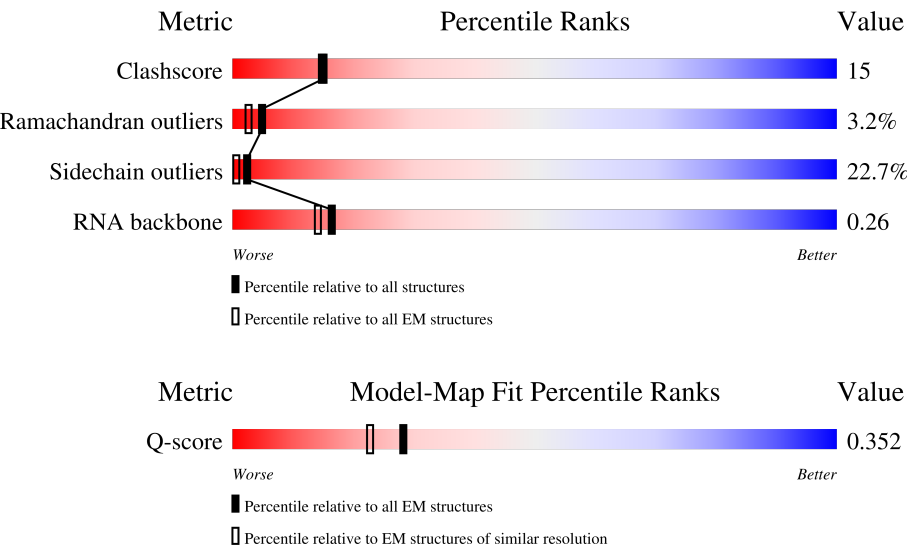
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance i

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.



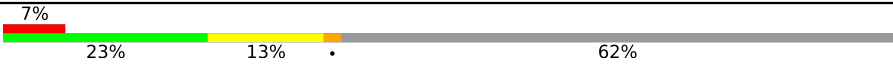
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| 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  $\geq 3$ , 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     | 328    |                  |
| 2   | B     | 290    |                  |
| 2   | C     | 290    |                  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 2   | D     | 290    |  |
| 2   | E     | 290    |  |
| 2   | F     | 290    |  |
| 3   | H     | 36     |  |
| 4   | I     | 140    |  |

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9291 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 Reverse transcriptase.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | A     | 317      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2593  | 1655 | 480 | 449 | 9 |         |       |

- Molecule 2 is a protein called Avd.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | B     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 976   | 631 | 172 | 166 | 7 |         |       |
| 2   | C     | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 888   | 578 | 157 | 148 | 5 |         |       |
| 2   | D     | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 888   | 577 | 161 | 145 | 5 |         |       |
| 2   | E     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 569 | 156 | 146 | 5 |         |       |
| 2   | F     | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 888   | 577 | 161 | 145 | 5 |         |       |

- Molecule 3 is a RNA chain called Diversity-generating retroelement (DGR) RNA TR.

| Mol | Chain | Residues | Atoms |    |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|----|---------|-------|
| 3   | H     | 10       | Total | C  | N  | O  | P  | 0       | 0     |
|     |       |          | 209   | 94 | 36 | 69 | 10 |         |       |

- Molecule 4 is a RNA chain called Diversity-generating retroelement (DGR) RNA Sp.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 4   | I     | 92       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1973  | 879 | 359 | 643 | 92 |         |       |



ALA  
SER  
VAL  
ILE  
THR  
GLU  
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HIS  
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PHE  
ALA  
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## ● Molecule 2: Avd

Chain C:  25% 11% 62%

MET  
GLU  
PRO  
ILE  
THR  
GLU  
GLN  
ALA  
THR  
LYS  
CYS  
Y11  
D12  
Q13  
M14  
I15  
I16  
V17  
E18  
E21  
A31  
R36  
K37  
H38  
G39  
V40  
E43  
M44  
F45  
I57  
K61  
S62  
N63  
Q64  
V65  
L68  
R79  
F80  
S81  
L82  
R83  
A86  
G87  
I88  
Q89  
K90  
P91  
H92  
A93  
H94  
T95

V99  
E100  
T101  
A102  
Q103  
V104  
L105  
I106  
V109  
G110  
R111  
R119  
V120  
N121  
ARG  
LYS  
GLY  
THR  
LYS  
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GLN  
VAL  
GLY  
GLU  
ALA  
LEU  
ILE  
ASN  
VAL  
GLY  
ASP  
GLY  
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## ● Molecule 2: Avd

Chain D:  7% 23% 13% 62%

MET  
GLU  
PRO  
ILE  
GLU  
GLU  
ALA  
THR  
LYS  
CYS  
TYR  
ASP  
Q13  
M14  
I15  
I16  
V17  
E18  
R19  
Y26  
L27  
A31  
R36  
K37  
E43  
M44  
F45  
L46  
K47  
Q52  
G60  
K61  
S62  
N63  
Q64  
V65  
S66  
K67  
L68  
Y69  
L75  
A76  
L82  
L85  
A86  
G87  
T88  
Q89  
K90  
P91

H92  
N94  
V99  
E100  
T101  
A102  
Q103  
V104  
L105  
I106  
V109  
L113  
G114  
S115  
W116  
I117  
A118  
R119  
V120  
N121  
R122  
K123  
GLY  
THR  
LYS  
VAL  
GLN  
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GLY  
GLY  
ALA  
LEU  
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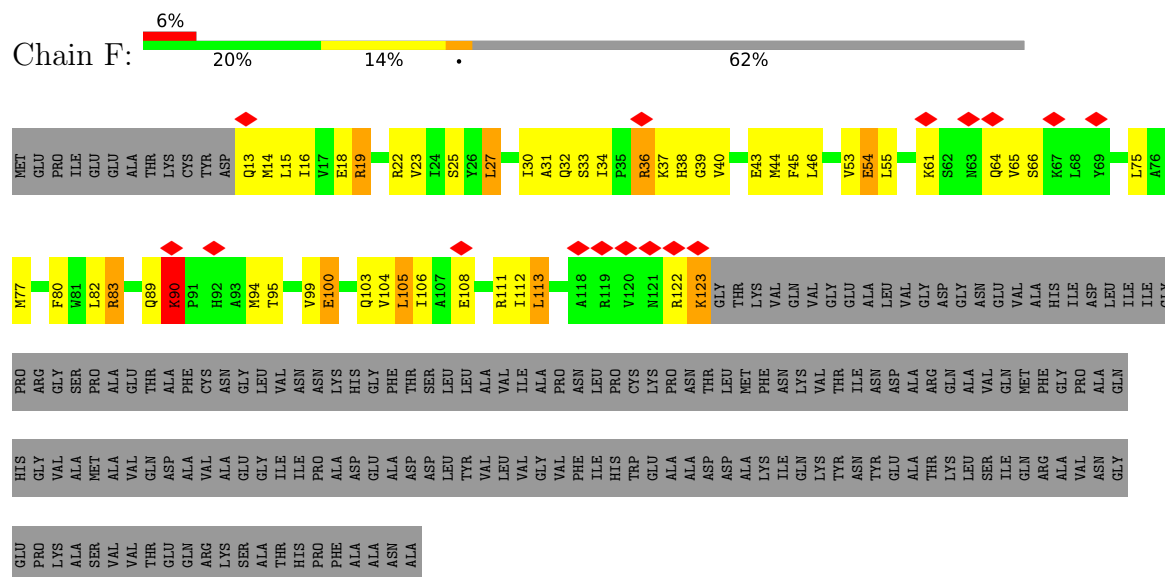
## ● Molecule 2: Avd

Chain E:  6% 24% 9% 62%

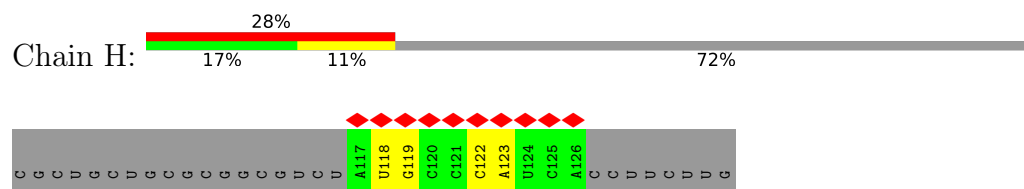
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D12  
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E21  
L27  
A31  
P35  
R36  
K37  
V40  
E43  
M44  
F45  
L50  
G51  
Q52  
V53  
G60  
K61  
S62  
N63  
Q64  
V65  
S66  
K67  
L68  
G74  
L75  
L82  
R83  
P84  
L85  
A86  
G87  
T88

Q89  
K90  
N94  
T95  
V99  
I106  
V109  
G110  
R111  
I112  
L113  
A118  
R119  
V120  
N121  
ARG  
LYS  
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THR  
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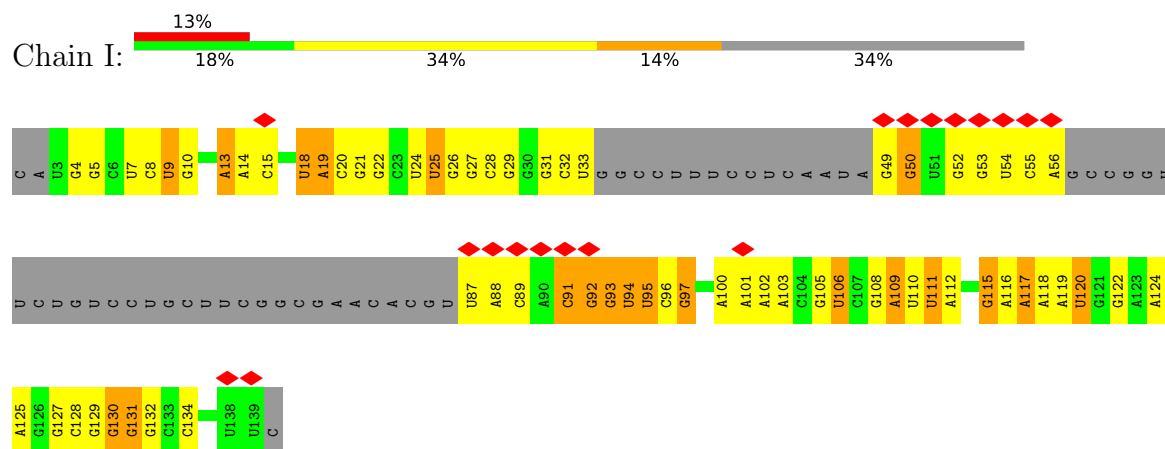
- Molecule 2: Avd



- Molecule 3: Diversity-generating retroelement (DGR) RNA TR



- Molecule 4: Diversity-generating retroelement (DGR) RNA Sp



## 4 Experimental information

| Property                             | Value               | Source    |
|--------------------------------------|---------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE     | Depositor |
| Imposed symmetry                     | POINT, Not provided |           |
| Number of particles used             | 66535               | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF   | Depositor |
| CTF correction method                | PHASE FLIPPING ONLY | Depositor |
| Microscope                           | FEI TITAN KRIOS     | Depositor |
| Voltage (kV)                         | 300                 | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 55                  | Depositor |
| Minimum defocus (nm)                 | 400                 | Depositor |
| Maximum defocus (nm)                 | 2000                | Depositor |
| Magnification                        | Not provided        |           |
| Image detector                       | GATAN K3 (6k x 4k)  | Depositor |
| Maximum map value                    | 0.936               | Depositor |
| Minimum map value                    | -0.579              | Depositor |
| Average map value                    | -0.000              | Depositor |
| Map value standard deviation         | 0.018               | Depositor |
| Recommended contour level            | 0.2                 | Depositor |
| Map size ( $\text{\AA}$ )            | 320.0, 320.0, 320.0 | wwPDB     |
| Map dimensions                       | 320, 320, 320       | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0    | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.0, 1.0, 1.0       | 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     | 0.34         | 0/2659        | 0.66        | 0/3590         |
| 2   | B     | 0.33         | 0/996         | 0.56        | 0/1345         |
| 2   | C     | 0.40         | 0/907         | 0.66        | 1/1226 (0.1%)  |
| 2   | D     | 0.57         | 3/906 (0.3%)  | 0.61        | 3/1222 (0.2%)  |
| 2   | E     | 0.33         | 0/894         | 0.53        | 0/1208         |
| 2   | F     | 0.29         | 0/906         | 0.58        | 0/1222         |
| 3   | H     | 0.29         | 0/232         | 0.42        | 0/358          |
| 4   | I     | 0.24         | 0/2205        | 0.44        | 0/3433         |
| All | All   | 0.35         | 3/9705 (0.0%) | 0.57        | 4/13604 (0.0%) |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 2   | D     | 90  | LYS  | N-CA  | -10.51 | 1.39        | 1.46     |
| 2   | D     | 90  | LYS  | CA-C  | 6.96   | 1.60        | 1.52     |
| 2   | D     | 90  | LYS  | C-O   | -6.86  | 1.18        | 1.24     |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | C     | 91  | PRO  | N-CA-CB | -7.29 | 95.59       | 103.25   |
| 2   | D     | 90  | LYS  | O-C-N   | 6.93  | 125.05      | 120.27   |
| 2   | D     | 90  | LYS  | CA-C-N  | -5.97 | 112.38      | 119.84   |
| 2   | D     | 90  | LYS  | C-N-CA  | -5.97 | 112.38      | 119.84   |

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     | 2593  | 0        | 2579     | 109     | 0            |
| 2   | B     | 976   | 0        | 1014     | 33      | 0            |
| 2   | C     | 888   | 0        | 923      | 31      | 0            |
| 2   | D     | 888   | 0        | 936      | 31      | 0            |
| 2   | E     | 876   | 0        | 914      | 31      | 0            |
| 2   | F     | 888   | 0        | 936      | 28      | 0            |
| 3   | H     | 209   | 0        | 109      | 4       | 0            |
| 4   | I     | 1973  | 0        | 996      | 31      | 0            |
| All | All   | 9291  | 0        | 8407     | 261     | 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 15.

The worst 5 of 261 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:E:86:ALA:HB2   | 2:E:99:VAL:HG21 | 1.45                     | 0.98              |
| 4:I:92:G:H3'     | 4:I:93:G:H4'    | 1.55                     | 0.88              |
| 2:E:35:PRO:HA    | 4:I:24:U:H5'    | 1.60                     | 0.83              |
| 1:A:213:TYR:HD1  | 1:A:311:ASP:OD2 | 1.64                     | 0.80              |
| 1:A:300:LEU:HD11 | 1:A:319:MET:HE1 | 1.64                     | 0.79              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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     | 313/328 (95%) | 253 (81%) | 45 (14%) | 15 (5%)  | <b>2</b> <b>15</b> |
| 2   | B     | 120/290 (41%) | 110 (92%) | 7 (6%)   | 3 (2%)   | <b>4</b> <b>25</b> |

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| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|---------|----------|-------------|----|
| 2   | C     | 109/290 (38%)  | 99 (91%)  | 5 (5%)  | 5 (5%)   | 2           | 15 |
| 2   | D     | 109/290 (38%)  | 100 (92%) | 7 (6%)  | 2 (2%)   | 6           | 31 |
| 2   | E     | 108/290 (37%)  | 98 (91%)  | 8 (7%)  | 2 (2%)   | 6           | 30 |
| 2   | F     | 109/290 (38%)  | 100 (92%) | 8 (7%)  | 1 (1%)   | 14          | 44 |
| All | All   | 868/1778 (49%) | 760 (88%) | 80 (9%) | 28 (3%)  | 5           | 21 |

5 of 28 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 7   | ASN  |
| 1   | A     | 109 | CYS  |
| 2   | C     | 88  | ILE  |
| 2   | C     | 91  | PRO  |
| 2   | C     | 92  | HIS  |

### 5.3.2 Protein sidechains ⓘ

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     | 267/278 (96%)  | 200 (75%) | 67 (25%)  | 0           | 4  |
| 2   | B     | 102/232 (44%)  | 79 (78%)  | 23 (22%)  | 1           | 6  |
| 2   | C     | 92/232 (40%)   | 79 (86%)  | 13 (14%)  | 3           | 17 |
| 2   | D     | 92/232 (40%)   | 76 (83%)  | 16 (17%)  | 2           | 11 |
| 2   | E     | 91/232 (39%)   | 72 (79%)  | 19 (21%)  | 1           | 7  |
| 2   | F     | 92/232 (40%)   | 63 (68%)  | 29 (32%)  | 0           | 2  |
| All | All   | 736/1438 (51%) | 569 (77%) | 167 (23%) | 2           | 6  |

5 of 167 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 103 | GLN  |
| 2   | F     | 19  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | E     | 13  | GLN  |
| 2   | E     | 67  | LYS  |
| 2   | F     | 54  | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | F     | 13  | GLN  |
| 2   | F     | 92  | HIS  |
| 2   | C     | 38  | HIS  |
| 2   | C     | 64  | GLN  |
| 2   | C     | 92  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed     | Backbone Outliers | Pucker Outliers |
|-----|-------|--------------|-------------------|-----------------|
| 3   | H     | 9/36 (25%)   | 0                 | 0               |
| 4   | I     | 90/140 (64%) | 46 (51%)          | 4 (4%)          |
| All | All   | 99/176 (56%) | 46 (46%)          | 4 (4%)          |

5 of 46 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | I     | 4   | G    |
| 4   | I     | 5   | G    |
| 4   | I     | 7   | U    |
| 4   | I     | 8   | C    |
| 4   | I     | 9   | U    |

All (4) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | I     | 20  | C    |
| 4   | I     | 87  | U    |
| 4   | I     | 94  | U    |
| 4   | I     | 100 | A    |

## 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.

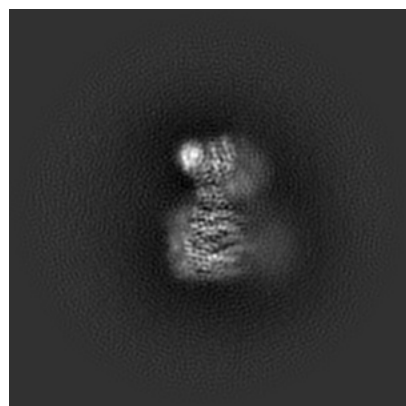
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42085. These allow visual inspection of the internal detail of the map and identification of artifacts.

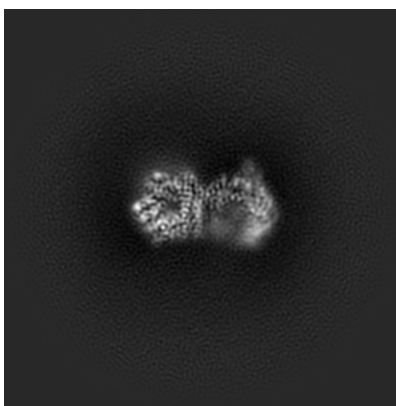
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

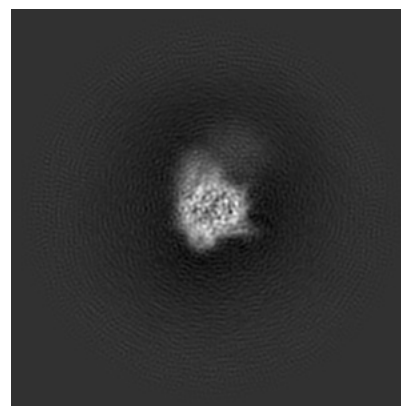
#### 6.1.1 Primary map



X

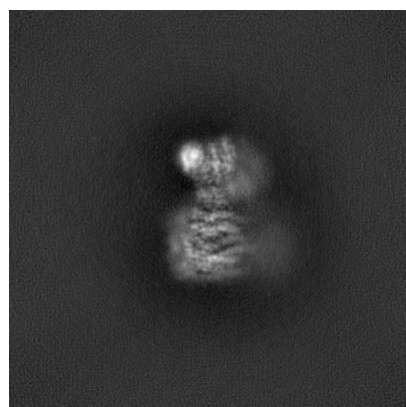


Y

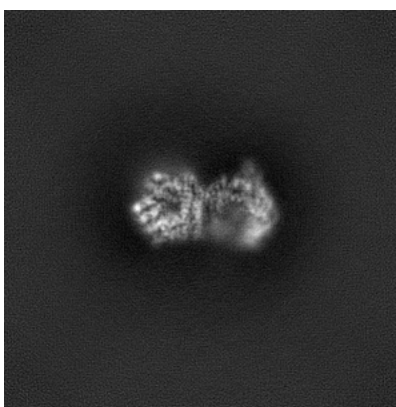


Z

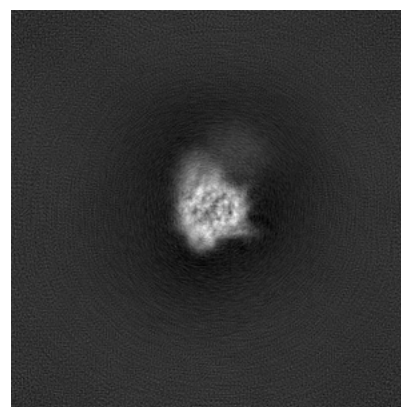
#### 6.1.2 Raw map



X



Y

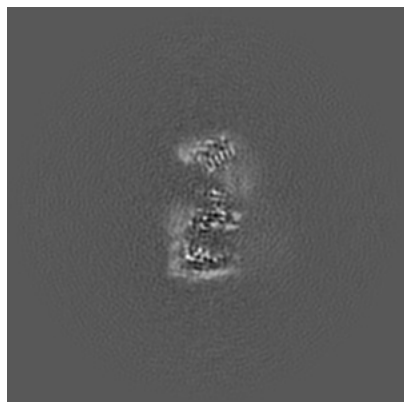


Z

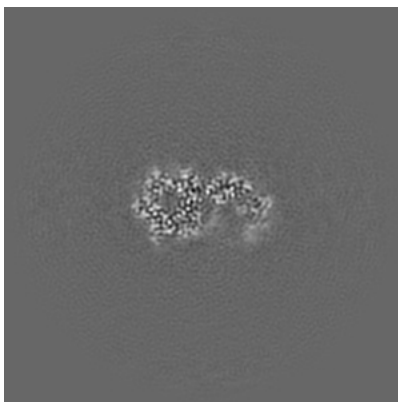
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

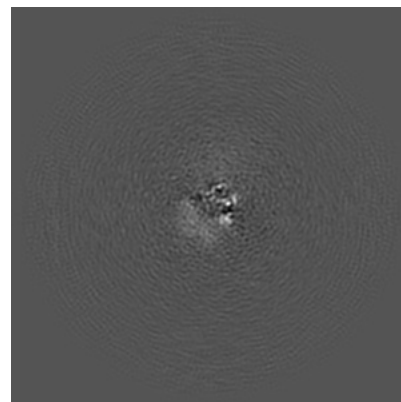
### 6.2.1 Primary map



X Index: 160

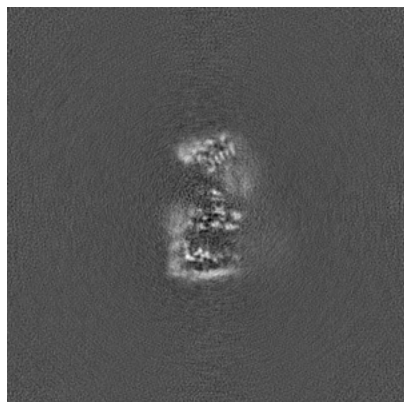


Y Index: 160

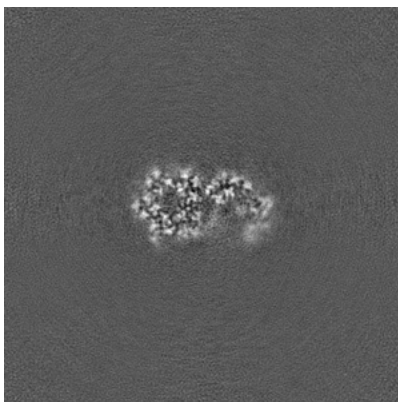


Z Index: 160

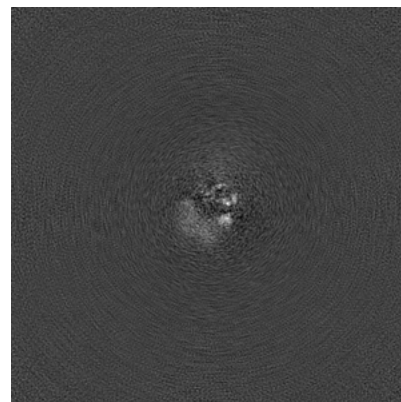
### 6.2.2 Raw map



X Index: 160



Y Index: 160



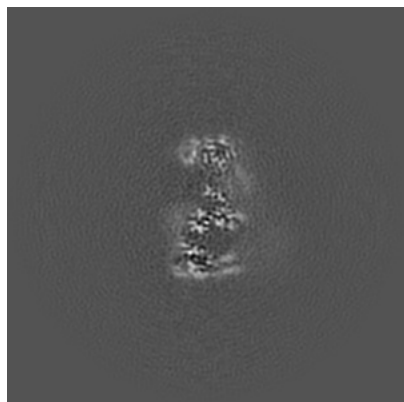
Z Index: 160

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

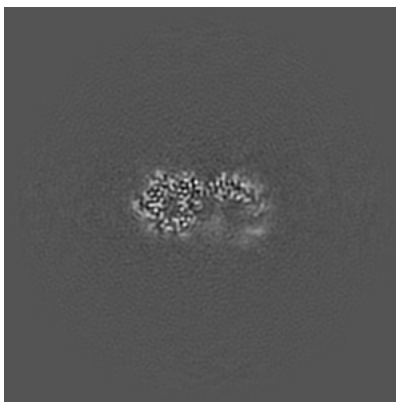


## 6.3 Largest variance slices [i](#)

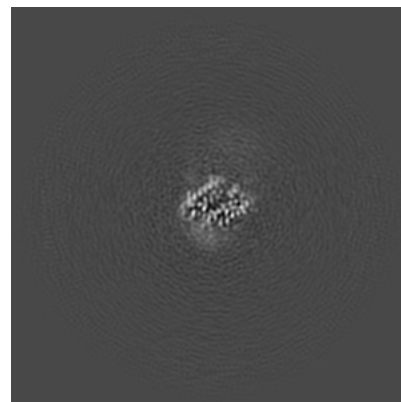
### 6.3.1 Primary map



X Index: 163

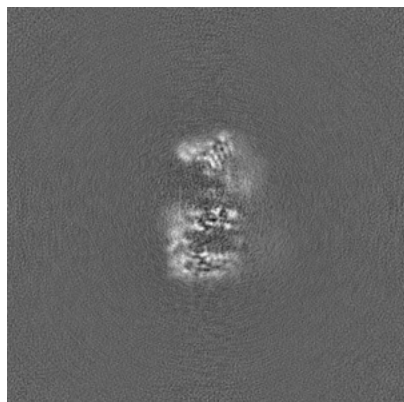


Y Index: 155

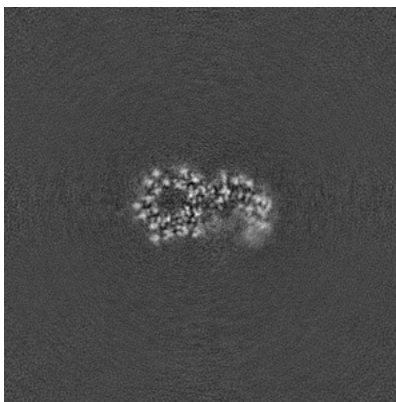


Z Index: 144

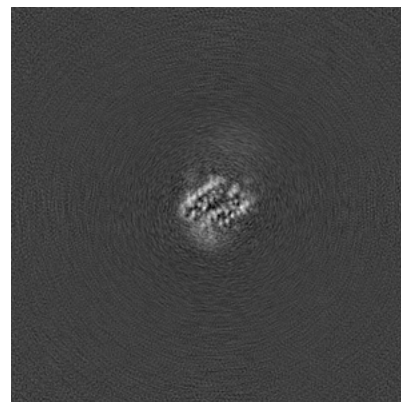
### 6.3.2 Raw map



X Index: 158



Y Index: 163



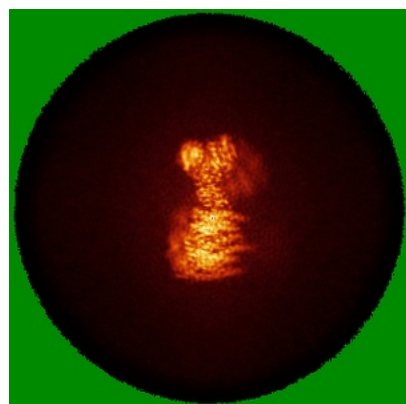
Z Index: 144

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

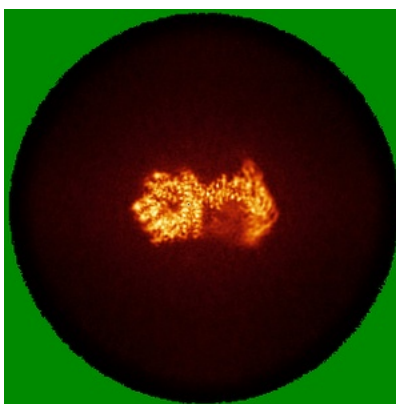


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

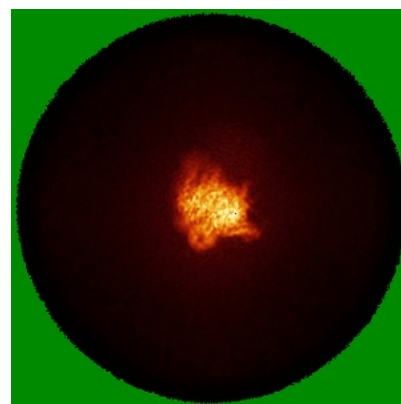
### 6.4.1 Primary map



X

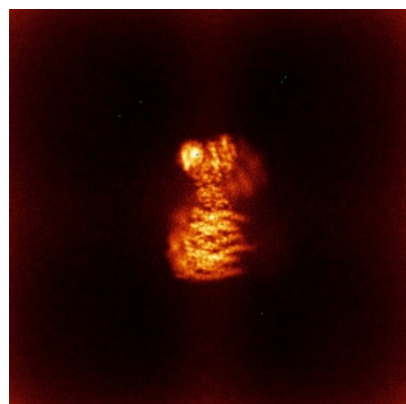


Y

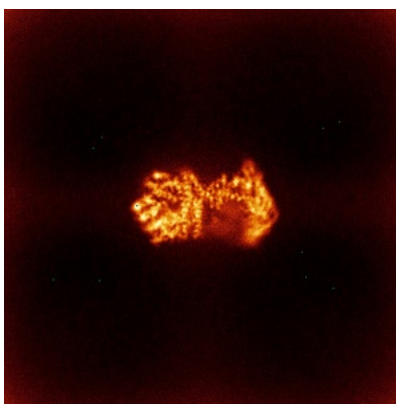


Z

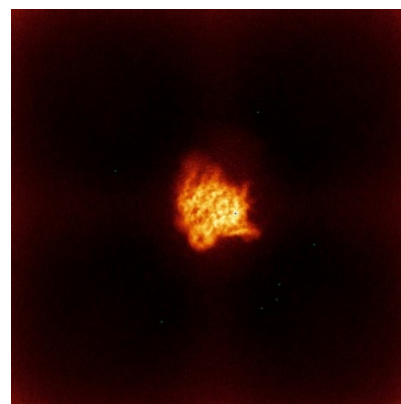
### 6.4.2 Raw map



X



Y

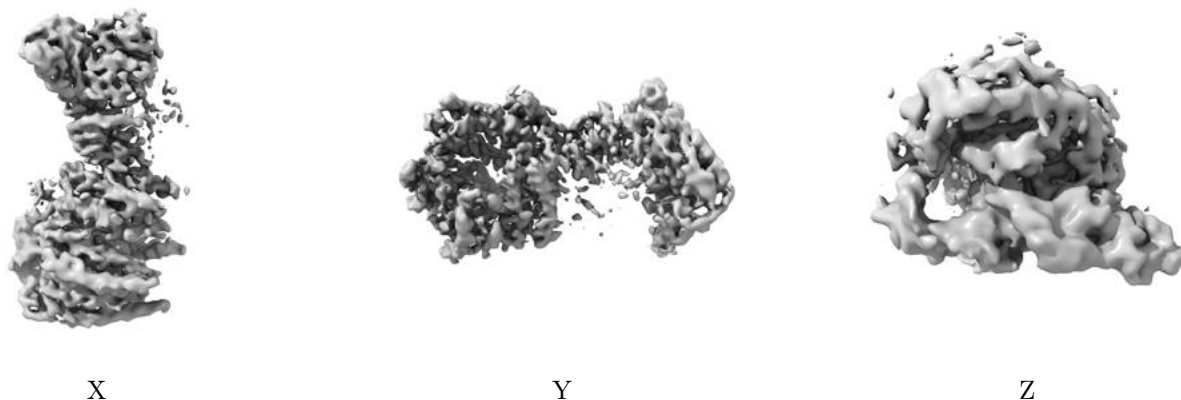


Z

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.

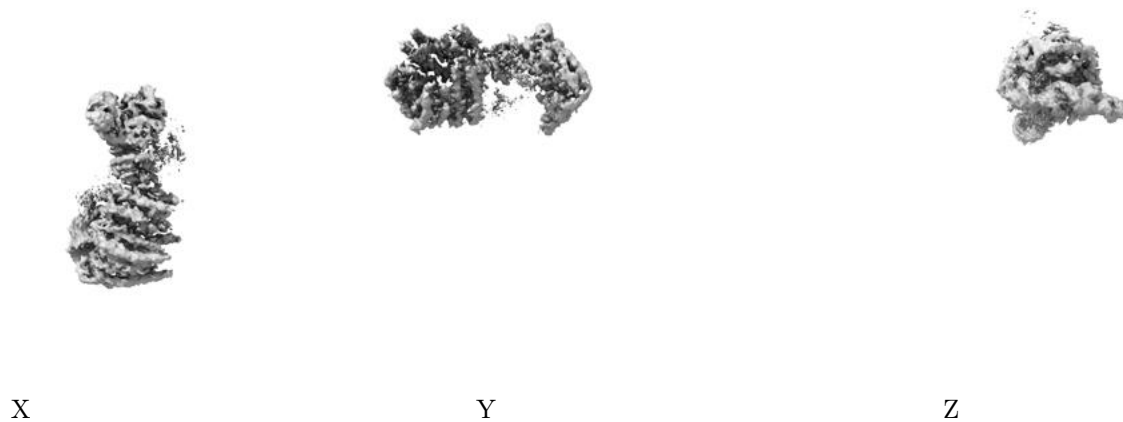
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

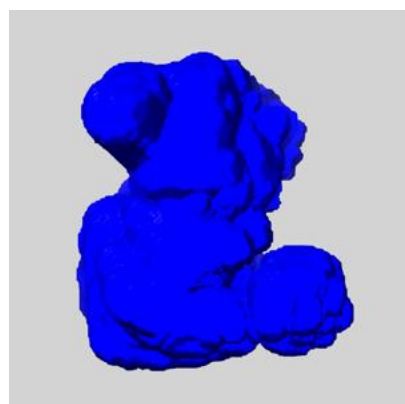
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

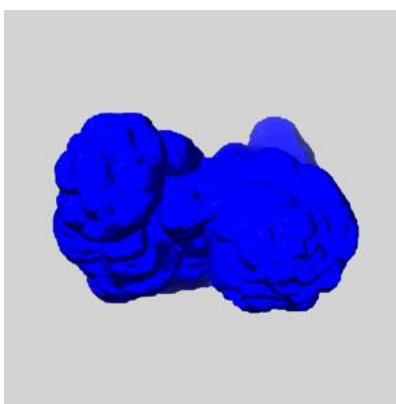
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

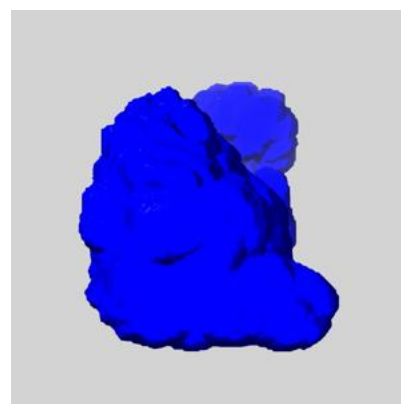
### 6.6.1 emd\_42085\_msk\_1.map [i](#)



X



Y

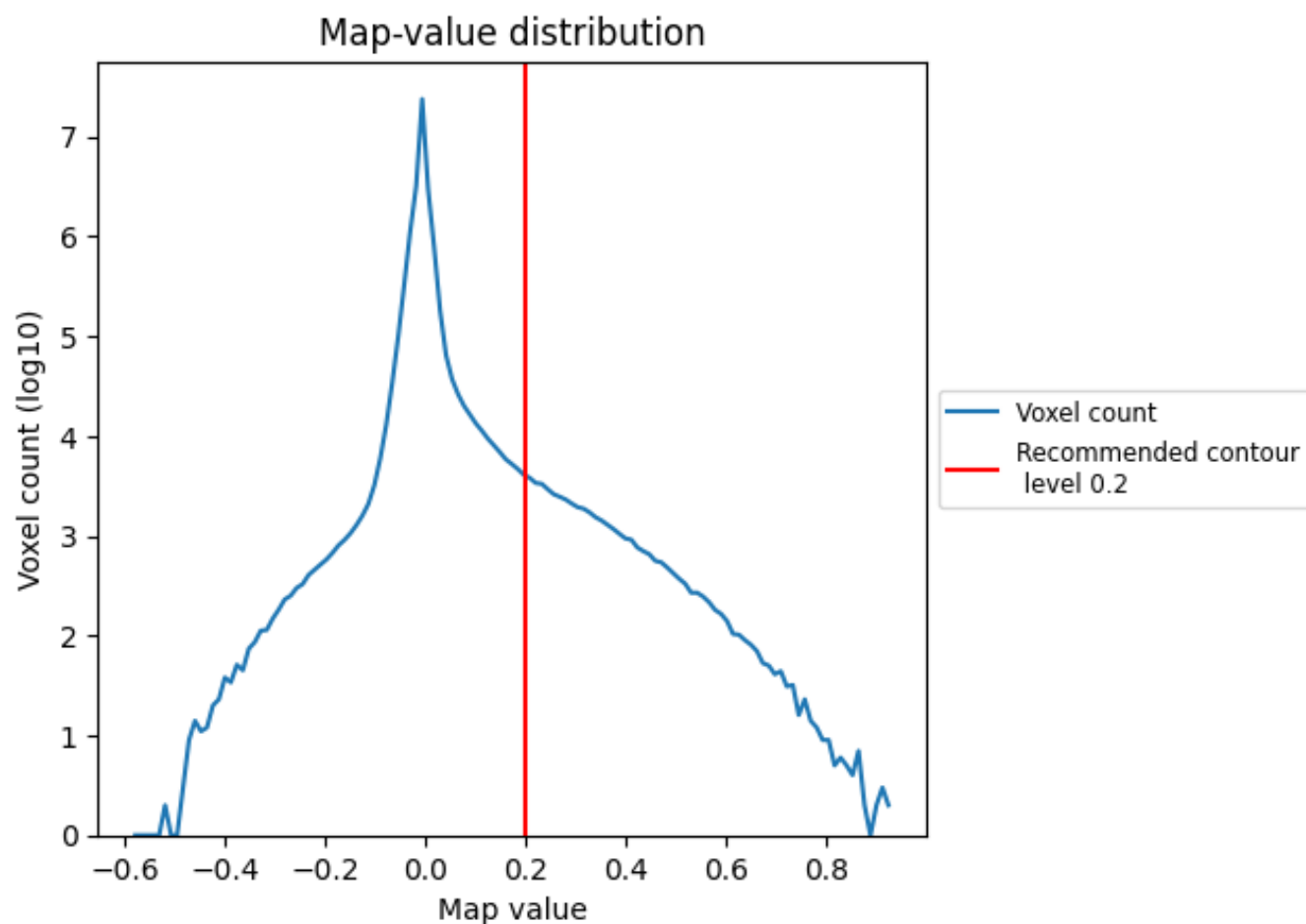


Z

## 7 Map analysis [i](#)

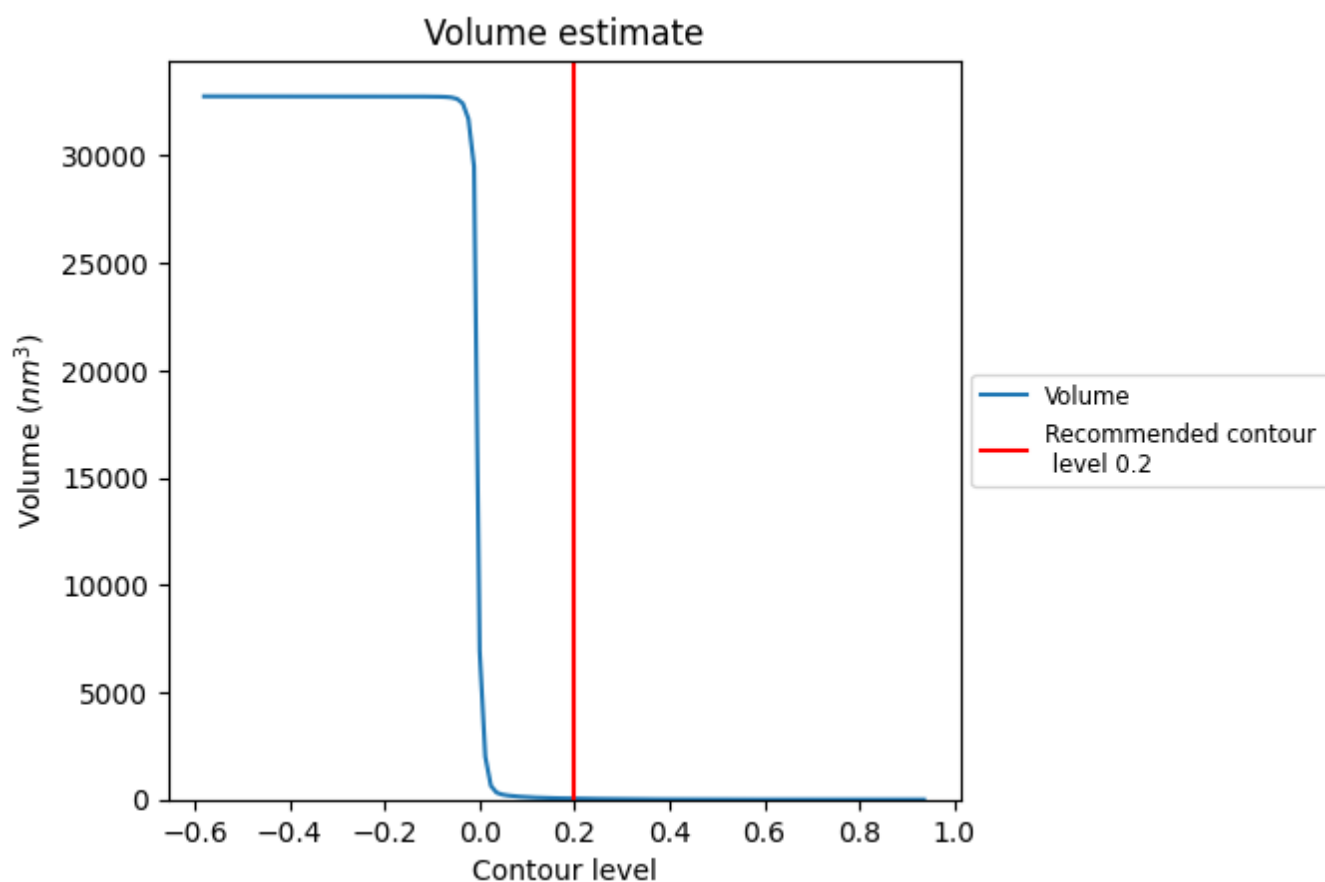
This section contains the results of statistical analysis of the map.

### 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.

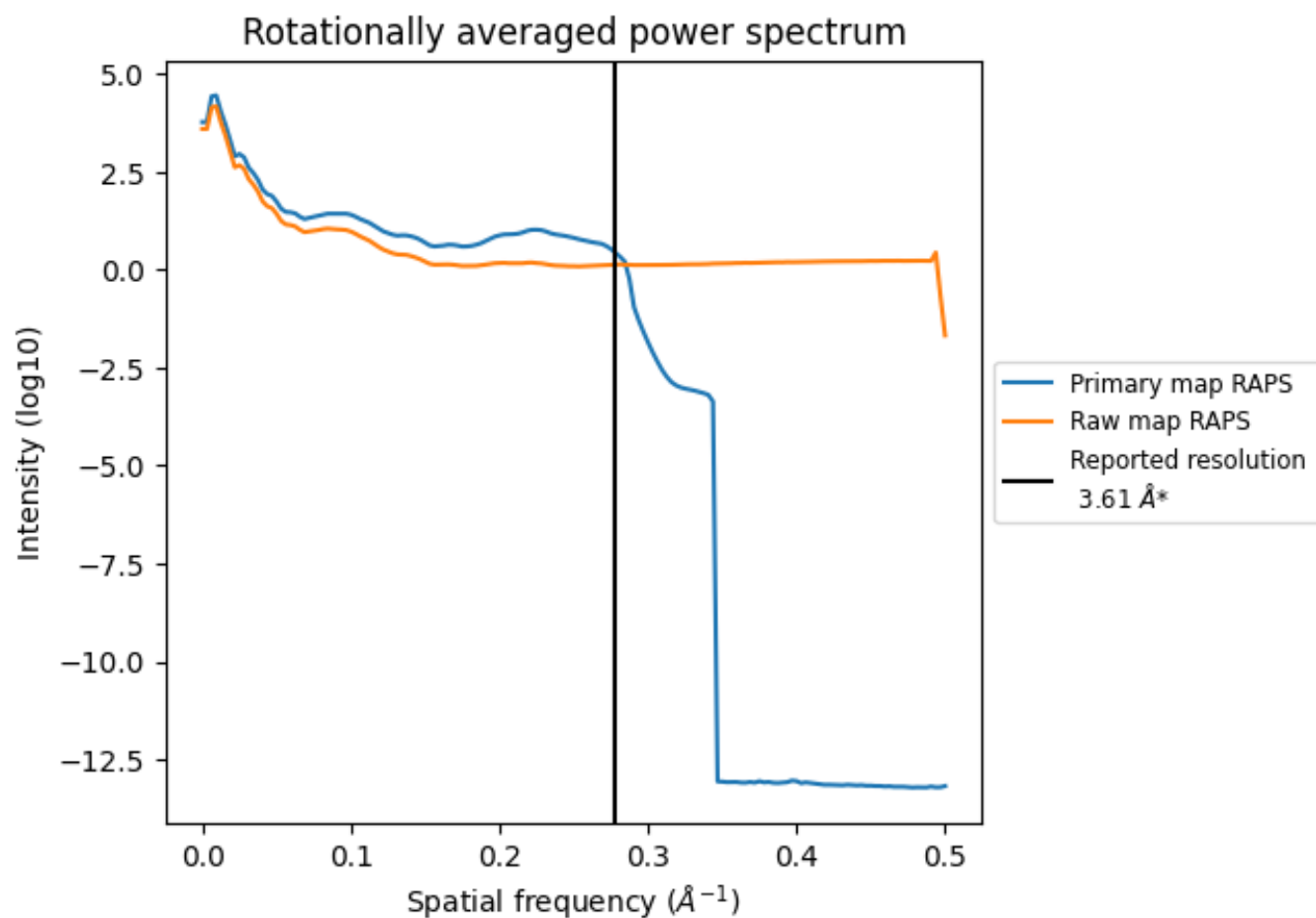
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 47 nm<sup>3</sup>; this corresponds to an approximate mass of 42 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 ⓘ

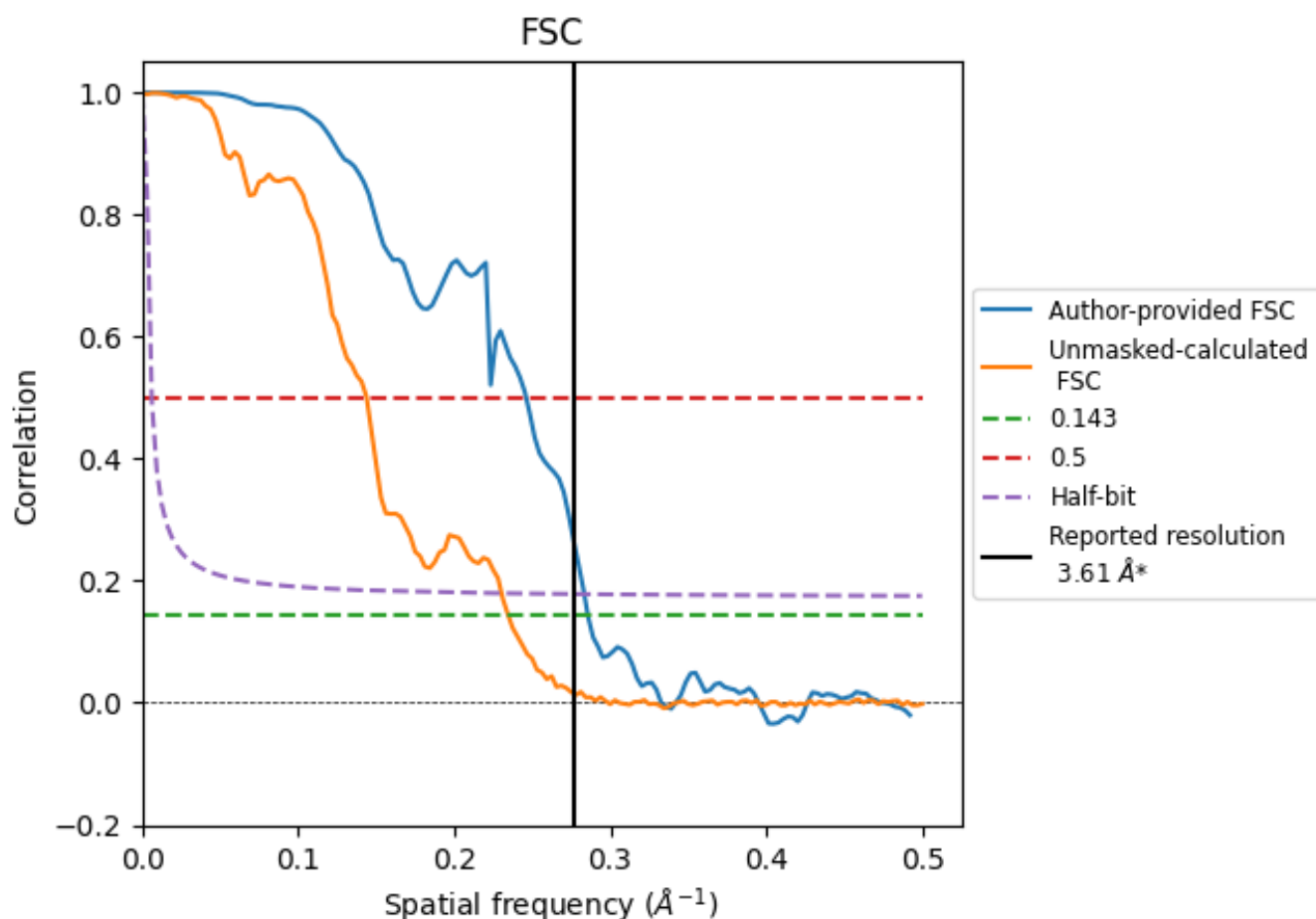


\*Reported resolution corresponds to spatial frequency of 0.277 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.277 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.61                               | -    | -        |
| Author-provided FSC curve | 3.50                               | 4.06 | 3.53     |
| Unmasked-calculated*      | 4.26                               | 6.95 | 4.34     |

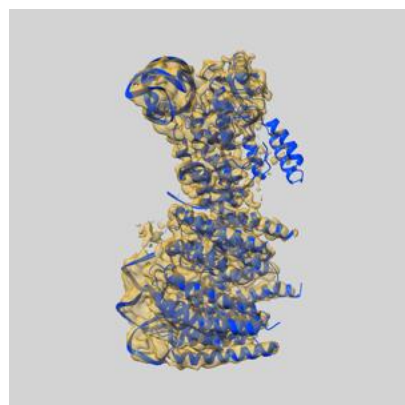
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.26 differs from the reported value 3.61 by more than 10 %



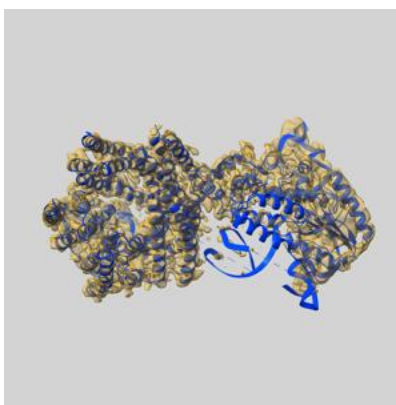
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42085 and PDB model 8UBF. Per-residue inclusion information can be found in section [3](#) on page [5](#).

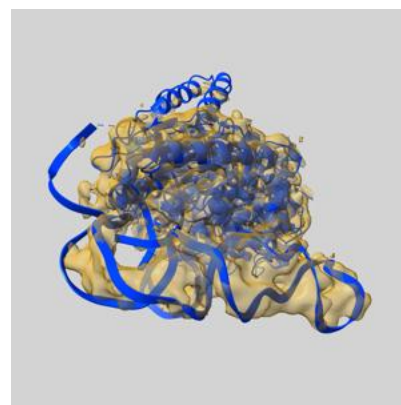
### 9.1 Map-model overlay [i](#)



X



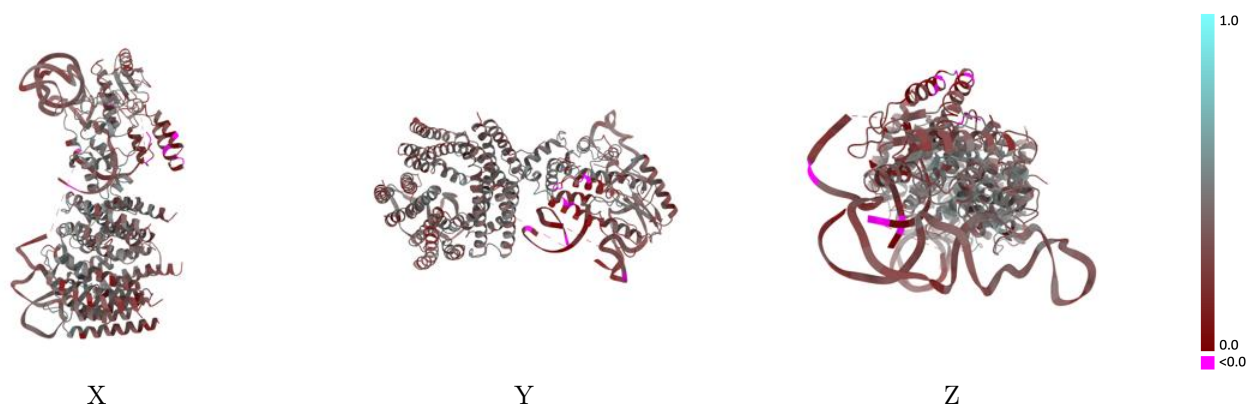
Y



Z

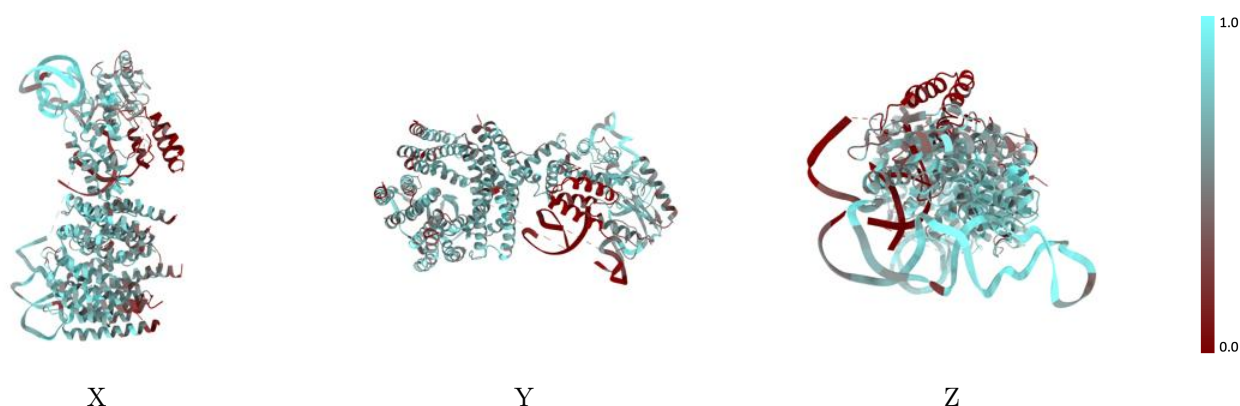
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



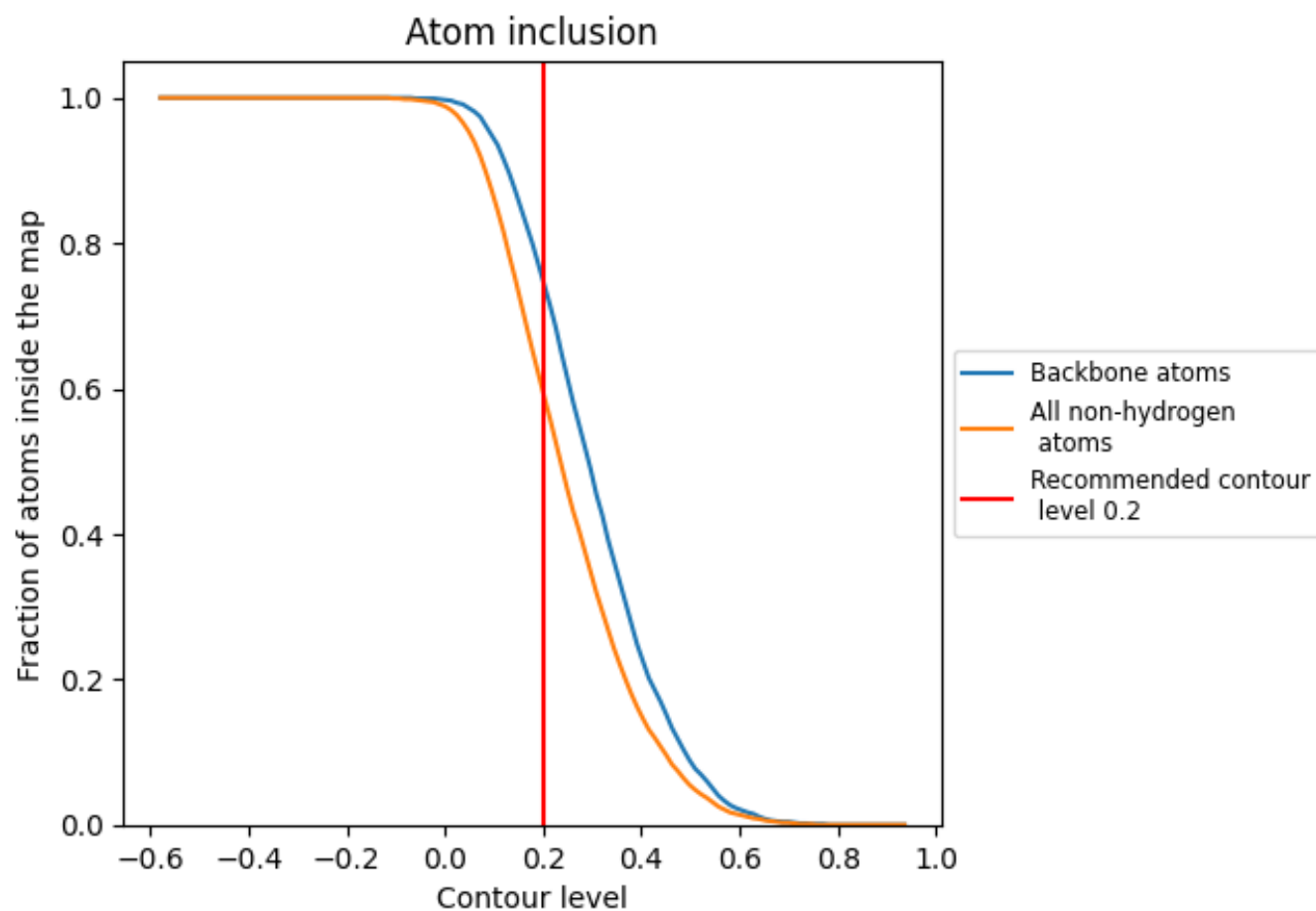
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 59% 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 (0.2) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.5940 | <div></div> 0.3520 |
| A     | <div></div> 0.5160 | <div></div> 0.3520 |
| B     | <div></div> 0.6690 | <div></div> 0.4130 |
| C     | <div></div> 0.6840 | <div></div> 0.4100 |
| D     | <div></div> 0.6340 | <div></div> 0.3810 |
| E     | <div></div> 0.6510 | <div></div> 0.3670 |
| F     | <div></div> 0.6340 | <div></div> 0.3640 |
| H     | <div></div> 0.0140 | <div></div> 0.1390 |
| I     | <div></div> 0.6200 | <div></div> 0.2950 |

1.0

0.0

<0.0