



# wwPDB EM Validation Summary Report ⓘ

Oct 14, 2025 – 05:14 AM JST

PDB ID : 9JO9 / pdb\_00009jo9  
EMDB ID : EMD-61648  
Title : CRP-HCAb3 complex  
Authors : Li, Y.J.  
Deposited on : 2024-09-24  
Resolution : 3.65 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:

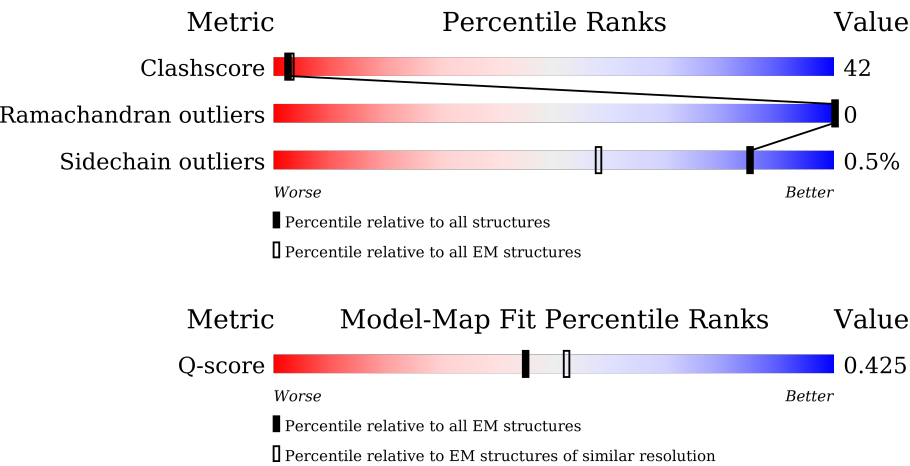
EMDB validation analysis : 0.0.1.dev129  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

# 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 3.65 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            | 210492                      | 15764                       | -  |
| Ramachandran outliers | 207382                      | 16835                       | -  |
| Sidechain outliers    | 206894                      | 16415                       | -  |
| Q-score               | -                           | 25397                       | 11564 ( 3.15 - 4.15 )                                    |

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     | 128    | <div><div></div><div>26%72%</div><div></div></div>   |
| 1   | C     | 128    | <div><div></div><div>26%67%5%</div><div></div></div> |
| 1   | E     | 128    | <div><div></div><div>26%71%</div><div></div></div>   |
| 1   | G     | 128    | <div><div></div><div>30%66%</div><div></div></div>   |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | I     | 128    |                  |
| 1   | K     | 128    |                  |
| 1   | M     | 128    |                  |
| 1   | O     | 128    |                  |
| 1   | P     | 128    |                  |
| 1   | R     | 128    |                  |
| 2   | B     | 206    |                  |
| 2   | D     | 206    |                  |
| 2   | F     | 206    |                  |
| 2   | H     | 206    |                  |
| 2   | J     | 206    |                  |
| 2   | L     | 206    |                  |
| 2   | N     | 206    |                  |
| 2   | Q     | 206    |                  |
| 2   | S     | 206    |                  |
| 2   | T     | 206    |                  |

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 42040 atoms, of which 15920 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 CRP specific recognition heavy chain antibody 3 (HCAb3).

| Mol | Chain | Residues | Atoms        |          |          |          |        | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|-------|
| 1   | O     | 125      | Total<br>980 | C<br>613 | N<br>171 | O<br>192 | S<br>4 | 0       | 0     |
| 1   | A     | 125      | Total<br>980 | C<br>613 | N<br>171 | O<br>192 | S<br>4 | 0       | 0     |
| 1   | C     | 125      | Total<br>980 | C<br>613 | N<br>171 | O<br>192 | S<br>4 | 0       | 0     |
| 1   | E     | 125      | Total<br>980 | C<br>613 | N<br>171 | O<br>192 | S<br>4 | 0       | 0     |
| 1   | G     | 125      | Total<br>980 | C<br>613 | N<br>171 | O<br>192 | S<br>4 | 0       | 0     |
| 1   | I     | 125      | Total<br>980 | C<br>613 | N<br>171 | O<br>192 | S<br>4 | 0       | 0     |
| 1   | K     | 125      | Total<br>980 | C<br>613 | N<br>171 | O<br>192 | S<br>4 | 0       | 0     |
| 1   | M     | 125      | Total<br>980 | C<br>613 | N<br>171 | O<br>192 | S<br>4 | 0       | 0     |
| 1   | P     | 125      | Total<br>980 | C<br>613 | N<br>171 | O<br>192 | S<br>4 | 0       | 0     |
| 1   | R     | 125      | Total<br>980 | C<br>613 | N<br>171 | O<br>192 | S<br>4 | 0       | 0     |

- Molecule 2 is a protein called C-reactive protein.

| Mol | Chain | Residues | Atoms         |           |           |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|-----------|-----------|----------|----------|--------|---------|-------|
| 2   | S     | 206      | Total<br>3224 | C<br>1058 | H<br>1592 | N<br>261 | O<br>309 | S<br>4 | 0       | 0     |
| 2   | B     | 206      | Total<br>3224 | C<br>1058 | H<br>1592 | N<br>261 | O<br>309 | S<br>4 | 0       | 0     |
| 2   | D     | 206      | Total<br>3224 | C<br>1058 | H<br>1592 | N<br>261 | O<br>309 | S<br>4 | 0       | 0     |
| 2   | F     | 206      | Total<br>3224 | C<br>1058 | H<br>1592 | N<br>261 | O<br>309 | S<br>4 | 0       | 0     |
| 2   | H     | 206      | Total<br>3224 | C<br>1058 | H<br>1592 | N<br>261 | O<br>309 | S<br>4 | 0       | 0     |

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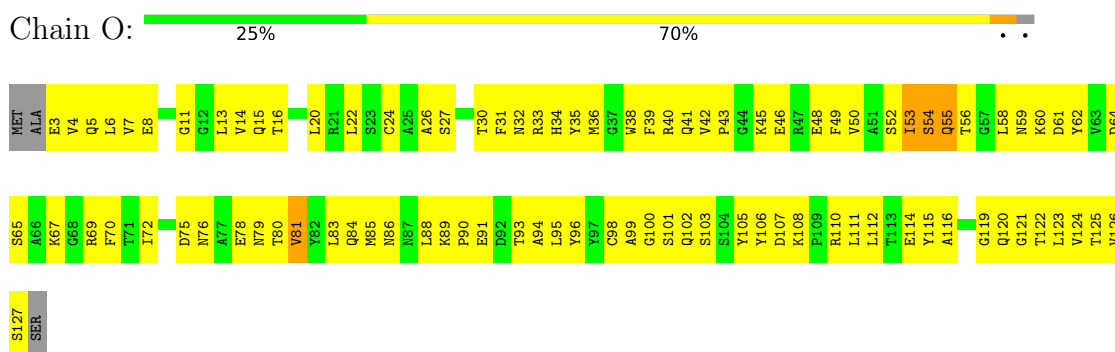
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| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 2   | J     | 206      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3224  | 1058 | 1592 | 261 | 309 | 4 |         |       |
| 2   | L     | 206      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3224  | 1058 | 1592 | 261 | 309 | 4 |         |       |
| 2   | N     | 206      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3224  | 1058 | 1592 | 261 | 309 | 4 |         |       |
| 2   | Q     | 206      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3224  | 1058 | 1592 | 261 | 309 | 4 |         |       |
| 2   | T     | 206      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3224  | 1058 | 1592 | 261 | 309 | 4 |         |       |

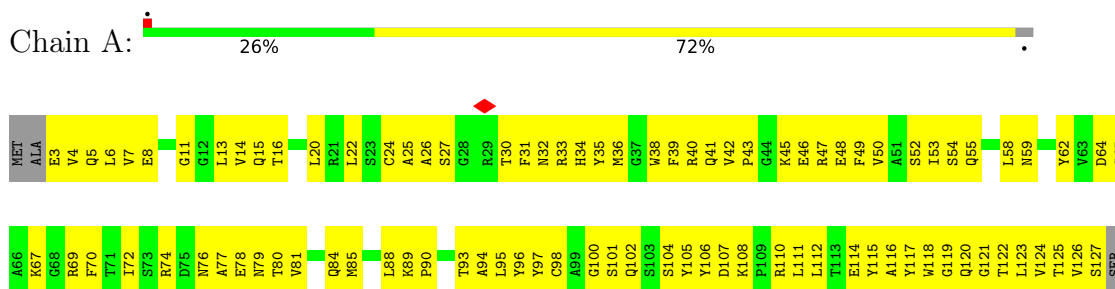
### 3 Residue-property plots

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.

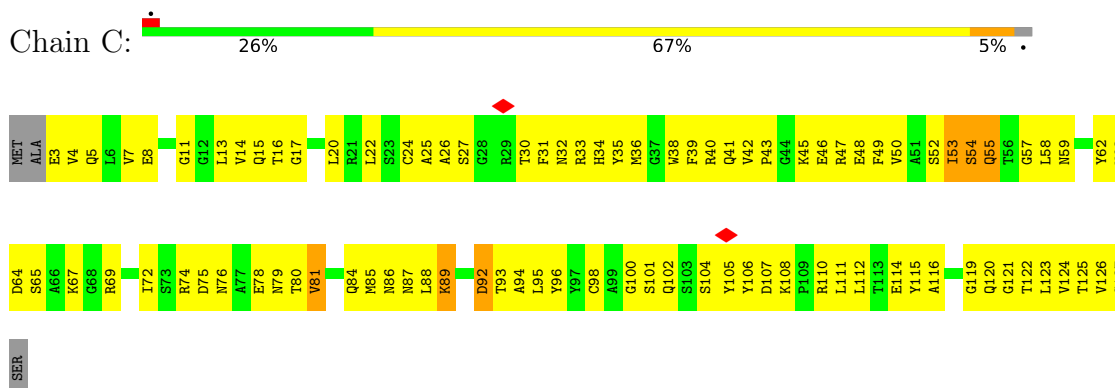
- Molecule 1: CRP specific recognition heavy chain antibody 3 (HCAb3)



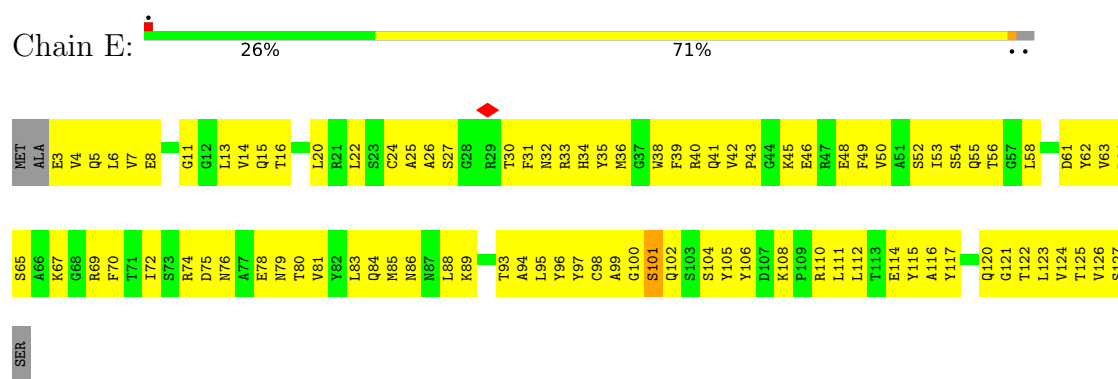
- Molecule 1: CRP specific recognition heavy chain antibody 3 (HCAb3)



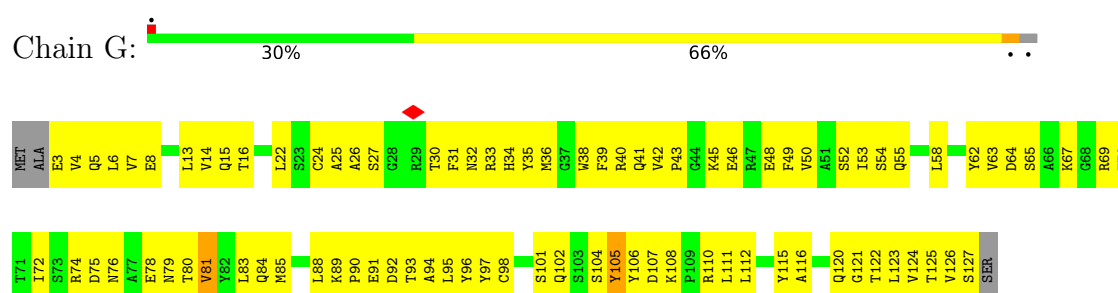
- Molecule 1: CRP specific recognition heavy chain antibody 3 (HCAb3)



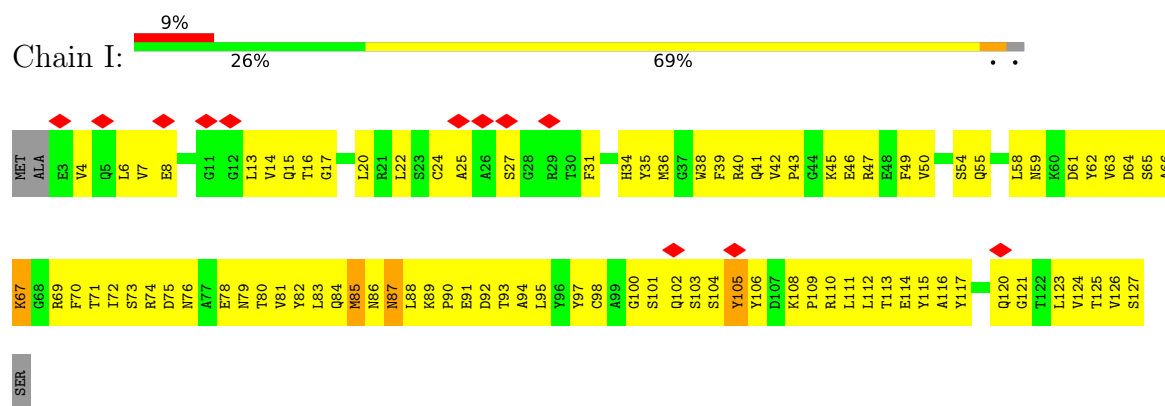
- Molecule 1: CRP specific recognition heavy chain antibody 3 (HCAb3)



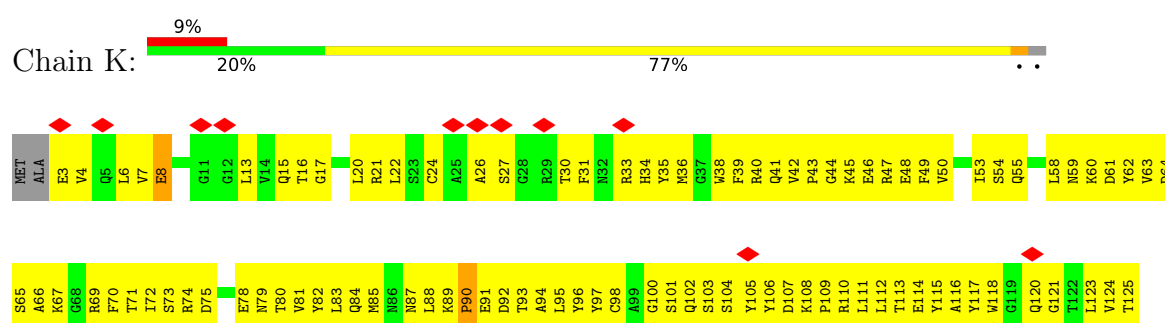
- Molecule 1: CRP specific recognition heavy chain antibody 3 (HCAb3)



- Molecule 1: CRP specific recognition heavy chain antibody 3 (HCAb3)



- Molecule 1: CRP specific recognition heavy chain antibody 3 (HCAb3)



V126  
S127  
SER

- Molecule 1: CRP specific recognition heavy chain antibody 3 (HCAb3)

Chain M: 

MET ALA E3 V4 Q5 L6 V7 G11 G12 L13 V14 Q15 T16 G17 L20 L21 R21 L22 S23 C24 A25 A26 A27 G28 R29 T30 R33 H34 Y35 M36 G37 W38 F39 R40 Q41 V42 P43 G44 K45 E46 R47 E48 F49 V50 A51 S52 I53 S54 Q55 T56 G57 L58 M59 K60 D61 V62 Y63 V64 D64

S65 A66 K67 G68 R69 F70 T71 I72 S73 R74 D75 E78 N79 T80 V81 Q84 M85 R86 L88 M89 P90 E91 D92 T93 A94 Y95 Y96 Y97 C98 A99 G100 S101 Q102 S103 W104 Y105 Y106 D107 K108 P109 R110 L111 L112 T113 E114 Y115 A116 Y117 W118 G119 Q120 L123 V124 T125 V126 S127

SER

- Molecule 1: CRP specific recognition heavy chain antibody 3 (HCAb3)

Chain P: 

MET ALA E3 V4 Q5 L6 V7 E8 G11 G12 L13 V14 Q15 T16 G17 L20 L21 R21 L22 S23 C24 A25 A26 A27 S27 G28 R29 T30 F31 N32 R33 H34 Y35 M36 G37 W38 F39 R40 Q41 V42 P43 G44 K45 E46 R47 E48 F49 V50 I53 S54 Q55 N59 K60 D61 V62 Y63 V64 D64 S65

A66 K67 G68 R69 F70 T71 I72 S73 R74 D75 N76 A77 E78 N79 T80 V81 Q84 M85 R86 L88 M89 P90 E91 D92 T93 A94 Y95 Y96 Y97 C98 A99 G100 S101 Q102 S103 W104 Y105 Y106 D107 K108 P109 R110 L111 L112 T113 E114 Y115 Q120 G121 T122 L123 V124 T125 V126 S127 SER

- Molecule 1: CRP specific recognition heavy chain antibody 3 (HCAb3)

Chain R: 

MET ALA E3 V4 Q5 L6 V7 E8 G11 G12 L13 V14 Q15 T16 G17 L20 L21 R21 L22 S23 C24 A25 A26 A27 S27 G28 R29 T30 F31 H34 Y35 M36 G37 W38 F39 R40 Q41 V42 P43 G44 K45 E46 R47 E48 F49 V50 I53 S54 Q55 L58 M59 K60 D61 V62 Y63 V64 D64 S65

A66 R69 F70 T71 I72 D75 N76 A77 E78 N79 T80 V81 Y82 L83 Q84 M85 R86 L88 M89 P90 E91 D92 T93 A94 Y95 Y96 Y97 C98 A99 G100 S101 Q102 S103 W104 Y105 Y106 D107 K108 P109 R110 L111 L112 T113 E114 Y115 A116 Y117 Q120 G121 T122 L123 V124 T125 V126 S127 SER

- Molecule 2: C-reactive protein

Chain S: 

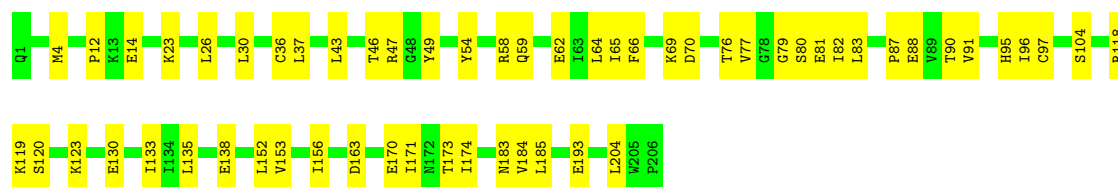
Q1 K12 P13 K14 E14 S18 L22 L26 L30 V35 C36 C38 L37 H38 L43 R47 G48 Y49 S50 I51 F52 Y54 K57 R58 E62 I63 I65 I66 F66 W67 T76 T77 S80 E81 I82 L83 P87 E88 V89 A92 C97 E108 V111 D112

R118 K119 S120 L121 K122 Y125 T126 V127 G128 A129 S132 I133 C134 L135 H136 D140 S141 F142 N145 L152 V153 S154 V155 V156 M157 M158 M159 M160 M161 D162 D163 P168 D169 I170 I171 I172 I173 I174 I175 L176 N183 V184 L185 N186 Y187 R188 A189 L190 Q195 V198 W205 P206

- Molecule 2: C-reactive protein

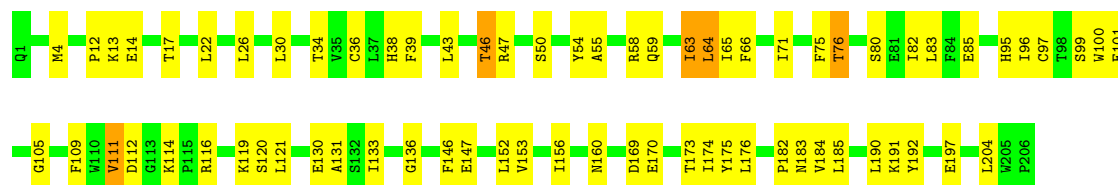


Chain B:  72% 28%



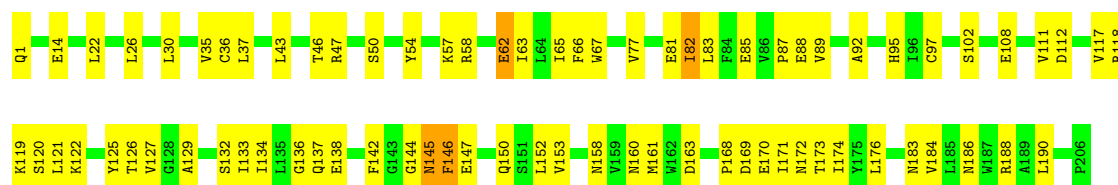
• Molecule 2: C-reactive protein

Chain D:  66% 32% •



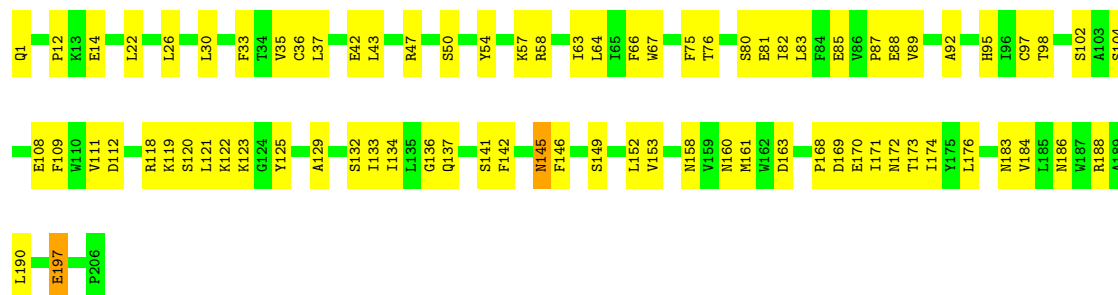
• Molecule 2: C-reactive protein

Chain F:  63% 35% •



• Molecule 2: C-reactive protein

Chain H:  62% 37% •



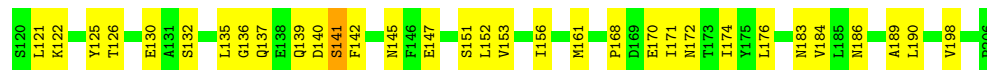
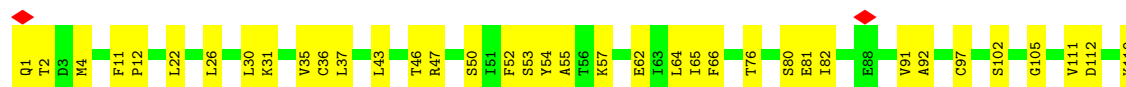
• Molecule 2: C-reactive protein

Chain J:  66% 33% •

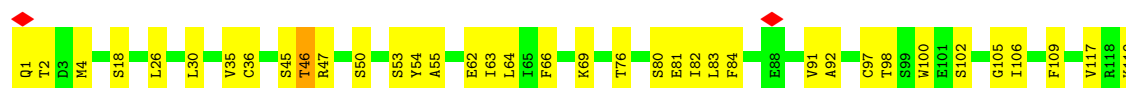




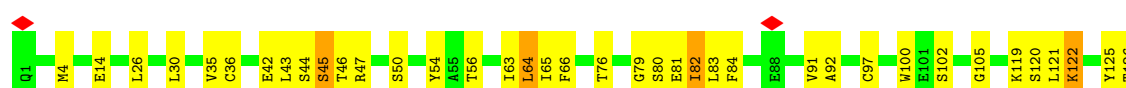
• Molecule 2: C-reactive protein



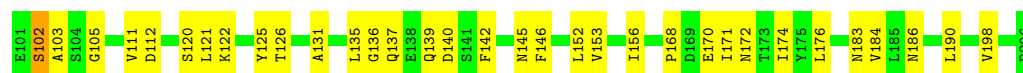
• Molecule 2: C-reactive protein



• Molecule 2: C-reactive protein



• Molecule 2: C-reactive protein



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C5                               | Depositor |
| Number of particles used             | 249262                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 30                                      | Depositor |
| Minimum defocus (nm)                 | 1500                                    | Depositor |
| Maximum defocus (nm)                 | 2500                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.610                                   | Depositor |
| Minimum map value                    | -0.226                                  | Depositor |
| Average map value                    | 0.003                                   | Depositor |
| Map value standard deviation         | 0.036                                   | Depositor |
| Recommended contour level            | 0.0959                                  | Depositor |
| Map size (Å)                         | 218.88, 218.88, 218.88                  | wwPDB     |
| Map dimensions                       | 256, 256, 256                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.855, 0.855, 0.855                     | 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).

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$     | RMSZ        | # $ Z  > 5$     |
| 1   | A     | 0.30         | 0/1000          | 0.50        | 0/1352          |
| 1   | C     | 0.33         | 1/1000 (0.1%)   | 0.60        | 2/1352 (0.1%)   |
| 1   | E     | 0.32         | 1/1000 (0.1%)   | 0.43        | 0/1352          |
| 1   | G     | 0.34         | 0/1000          | 0.56        | 1/1352 (0.1%)   |
| 1   | I     | 0.39         | 1/1000 (0.1%)   | 0.59        | 3/1352 (0.2%)   |
| 1   | K     | 0.44         | 3/1000 (0.3%)   | 0.48        | 0/1352          |
| 1   | M     | 0.44         | 1/1000 (0.1%)   | 0.65        | 3/1352 (0.2%)   |
| 1   | O     | 0.32         | 0/1000          | 0.52        | 3/1352 (0.2%)   |
| 1   | P     | 0.50         | 5/1000 (0.5%)   | 0.63        | 1/1352 (0.1%)   |
| 1   | R     | 0.48         | 2/1000 (0.2%)   | 0.55        | 1/1352 (0.1%)   |
| 2   | B     | 0.34         | 1/1678 (0.1%)   | 0.67        | 1/2279 (0.0%)   |
| 2   | D     | 0.51         | 7/1678 (0.4%)   | 0.76        | 7/2279 (0.3%)   |
| 2   | F     | 0.46         | 4/1678 (0.2%)   | 0.79        | 7/2279 (0.3%)   |
| 2   | H     | 0.28         | 0/1678          | 0.76        | 4/2279 (0.2%)   |
| 2   | J     | 0.48         | 3/1678 (0.2%)   | 0.77        | 6/2279 (0.3%)   |
| 2   | L     | 0.41         | 1/1678 (0.1%)   | 0.74        | 6/2279 (0.3%)   |
| 2   | N     | 0.44         | 1/1678 (0.1%)   | 0.77        | 5/2279 (0.2%)   |
| 2   | Q     | 0.51         | 6/1678 (0.4%)   | 0.81        | 3/2279 (0.1%)   |
| 2   | S     | 0.33         | 1/1678 (0.1%)   | 0.76        | 2/2279 (0.1%)   |
| 2   | T     | 0.42         | 2/1678 (0.1%)   | 0.76        | 4/2279 (0.2%)   |
| All | All   | 0.41         | 40/26780 (0.1%) | 0.69        | 59/36310 (0.2%) |

The worst 5 of 40 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | N     | 46  | THR  | C-N   | 8.34  | 1.45        | 1.33     |
| 1   | M     | 12  | GLY  | C-N   | 8.20  | 1.44        | 1.33     |
| 2   | L     | 53  | SER  | C-N   | -8.10 | 1.22        | 1.33     |
| 2   | D     | 63  | ILE  | C-N   | 8.03  | 1.44        | 1.33     |
| 2   | B     | 65  | ILE  | C-N   | -7.94 | 1.23        | 1.33     |

The worst 5 of 59 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | I     | 105 | TYR  | N-CA-C | 7.75 | 121.54      | 109.07   |
| 2   | J     | 53  | SER  | CA-C-N | 7.67 | 133.58      | 123.00   |
| 2   | J     | 53  | SER  | C-N-CA | 7.67 | 133.58      | 123.00   |
| 2   | H     | 145 | ASN  | N-CA-C | 7.33 | 121.74      | 111.92   |
| 1   | P     | 106 | TYR  | N-CA-C | 7.20 | 117.37      | 107.73   |

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     | 980   | 0        | 941      | 160     | 0            |
| 1   | C     | 980   | 0        | 939      | 185     | 0            |
| 1   | E     | 980   | 0        | 939      | 153     | 0            |
| 1   | G     | 980   | 0        | 939      | 160     | 0            |
| 1   | I     | 980   | 0        | 941      | 128     | 0            |
| 1   | K     | 980   | 0        | 941      | 184     | 0            |
| 1   | M     | 980   | 0        | 941      | 164     | 0            |
| 1   | O     | 980   | 0        | 941      | 192     | 0            |
| 1   | P     | 980   | 0        | 941      | 131     | 0            |
| 1   | R     | 980   | 0        | 941      | 145     | 0            |
| 2   | B     | 1632  | 1592     | 1595     | 62      | 0            |
| 2   | D     | 1632  | 1592     | 1595     | 65      | 0            |
| 2   | F     | 1632  | 1592     | 1595     | 75      | 0            |
| 2   | H     | 1632  | 1592     | 1595     | 70      | 0            |
| 2   | J     | 1632  | 1592     | 1595     | 66      | 0            |
| 2   | L     | 1632  | 1592     | 1595     | 64      | 0            |
| 2   | N     | 1632  | 1592     | 1595     | 60      | 0            |
| 2   | Q     | 1632  | 1592     | 1595     | 50      | 0            |
| 2   | S     | 1632  | 1592     | 1595     | 81      | 0            |
| 2   | T     | 1632  | 1592     | 1595     | 60      | 0            |
| All | All   | 26120 | 15920    | 25354    | 2134    | 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 42.

The worst 5 of 2134 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) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:O:105:TYR:O   | 1:O:106:TYR:CD2 | 1.84                     | 1.31              |
| 1:A:35:TYR:CE2  | 1:A:102:GLN:HB2 | 1.65                     | 1.29              |
| 1:O:95:LEU:CD1  | 1:P:13:LEU:HD21 | 1.61                     | 1.27              |
| 1:C:95:LEU:CD1  | 1:K:13:LEU:HD21 | 1.63                     | 1.26              |
| 1:C:13:LEU:HD21 | 1:K:95:LEU:CD1  | 1.68                     | 1.22              |

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     | 123/128 (96%) | 114 (93%) | 9 (7%)   | 0        | 100         | 100 |
| 1   | C     | 123/128 (96%) | 115 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 1   | E     | 123/128 (96%) | 115 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 1   | G     | 123/128 (96%) | 116 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 1   | I     | 123/128 (96%) | 112 (91%) | 11 (9%)  | 0        | 100         | 100 |
| 1   | K     | 123/128 (96%) | 117 (95%) | 6 (5%)   | 0        | 100         | 100 |
| 1   | M     | 123/128 (96%) | 118 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 1   | O     | 123/128 (96%) | 114 (93%) | 9 (7%)   | 0        | 100         | 100 |
| 1   | P     | 123/128 (96%) | 118 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 1   | R     | 123/128 (96%) | 111 (90%) | 12 (10%) | 0        | 100         | 100 |
| 2   | B     | 204/206 (99%) | 189 (93%) | 15 (7%)  | 0        | 100         | 100 |
| 2   | D     | 204/206 (99%) | 194 (95%) | 10 (5%)  | 0        | 100         | 100 |
| 2   | F     | 204/206 (99%) | 195 (96%) | 9 (4%)   | 0        | 100         | 100 |
| 2   | H     | 204/206 (99%) | 196 (96%) | 8 (4%)   | 0        | 100         | 100 |
| 2   | J     | 204/206 (99%) | 194 (95%) | 10 (5%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 2   | L     | 204/206 (99%)   | 196 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 2   | N     | 204/206 (99%)   | 193 (95%)  | 11 (5%)  | 0        | 100         | 100 |
| 2   | Q     | 204/206 (99%)   | 193 (95%)  | 11 (5%)  | 0        | 100         | 100 |
| 2   | S     | 204/206 (99%)   | 196 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 2   | T     | 204/206 (99%)   | 197 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| All | All   | 3270/3340 (98%) | 3093 (95%) | 177 (5%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 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     | 104/106 (98%)  | 104 (100%) | 0        | 100         | 100 |
| 1   | C     | 104/106 (98%)  | 101 (97%)  | 3 (3%)   | 37          | 58  |
| 1   | E     | 104/106 (98%)  | 104 (100%) | 0        | 100         | 100 |
| 1   | G     | 104/106 (98%)  | 103 (99%)  | 1 (1%)   | 73          | 82  |
| 1   | I     | 104/106 (98%)  | 102 (98%)  | 2 (2%)   | 52          | 69  |
| 1   | K     | 104/106 (98%)  | 104 (100%) | 0        | 100         | 100 |
| 1   | M     | 104/106 (98%)  | 102 (98%)  | 2 (2%)   | 52          | 69  |
| 1   | O     | 104/106 (98%)  | 103 (99%)  | 1 (1%)   | 73          | 82  |
| 1   | P     | 104/106 (98%)  | 104 (100%) | 0        | 100         | 100 |
| 1   | R     | 104/106 (98%)  | 103 (99%)  | 1 (1%)   | 73          | 82  |
| 2   | B     | 180/180 (100%) | 179 (99%)  | 1 (1%)   | 84          | 90  |
| 2   | D     | 180/180 (100%) | 179 (99%)  | 1 (1%)   | 84          | 90  |
| 2   | F     | 180/180 (100%) | 180 (100%) | 0        | 100         | 100 |
| 2   | H     | 180/180 (100%) | 179 (99%)  | 1 (1%)   | 84          | 90  |
| 2   | J     | 180/180 (100%) | 180 (100%) | 0        | 100         | 100 |
| 2   | L     | 180/180 (100%) | 180 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 2   | N     | 180/180 (100%)  | 180 (100%)  | 0        | 100         | 100 |
| 2   | Q     | 180/180 (100%)  | 180 (100%)  | 0        | 100         | 100 |
| 2   | S     | 180/180 (100%)  | 179 (99%)   | 1 (1%)   | 84          | 90  |
| 2   | T     | 180/180 (100%)  | 180 (100%)  | 0        | 100         | 100 |
| All | All   | 2840/2860 (99%) | 2826 (100%) | 14 (0%)  | 85          | 92  |

5 of 14 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 81  | VAL  |
| 2   | H     | 197 | GLU  |
| 1   | R     | 7   | VAL  |
| 1   | M     | 67  | LYS  |
| 1   | M     | 72  | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 15  | GLN  |
| 2   | Q     | 203 | GLN  |
| 1   | M     | 87  | ASN  |
| 2   | N     | 203 | GLN  |
| 1   | R     | 87  | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

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.

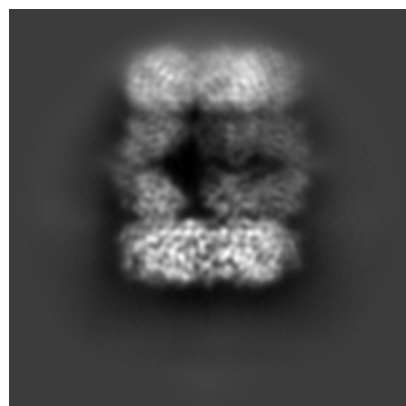
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61648. These allow visual inspection of the internal detail of the map and identification of artifacts.

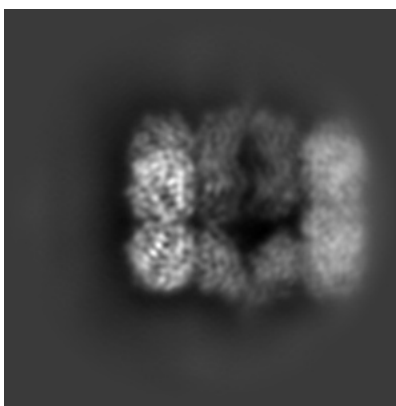
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

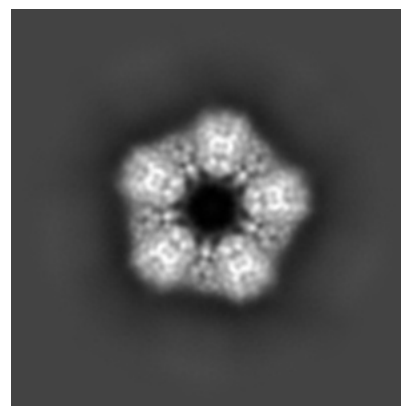
#### 6.1.1 Primary map



X

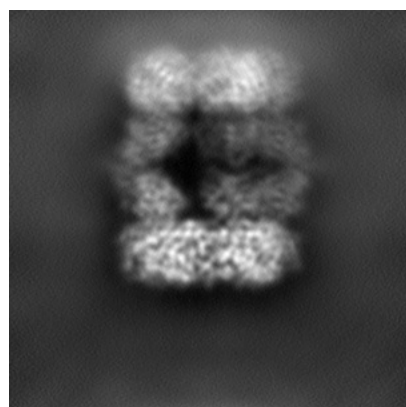


Y

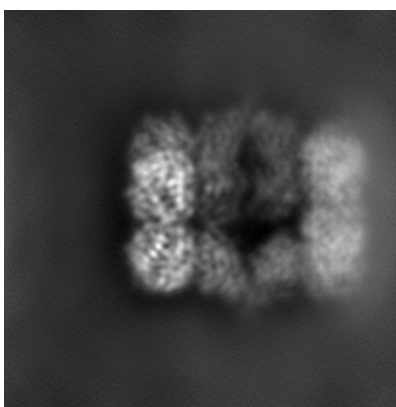


Z

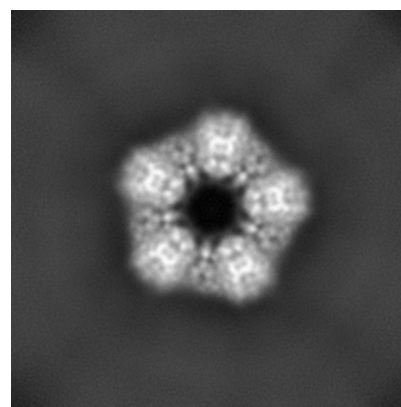
#### 6.1.2 Raw map



X



Y

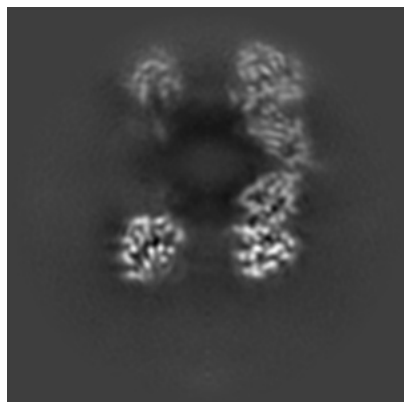


Z

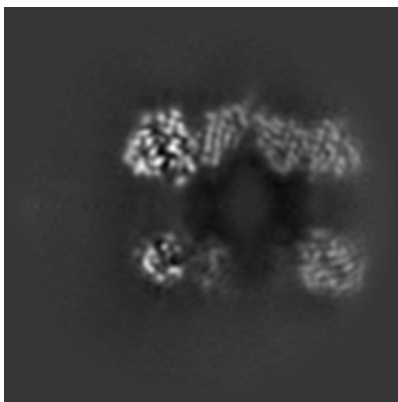
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

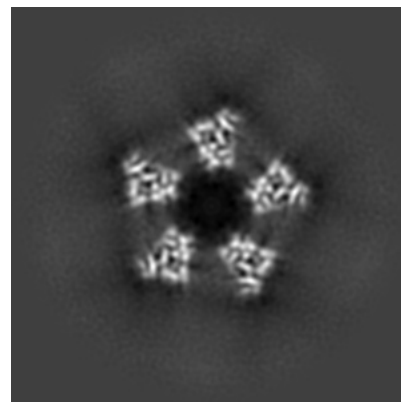
### 6.2.1 Primary map



X Index: 128

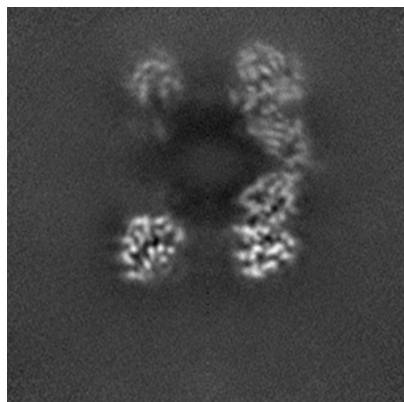


Y Index: 128

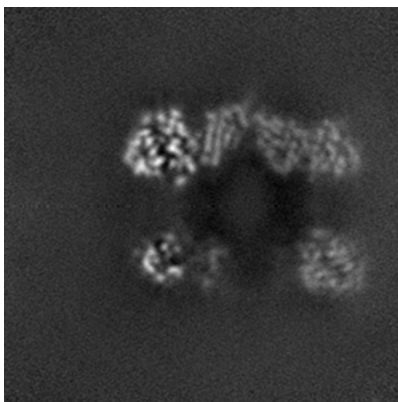


Z Index: 128

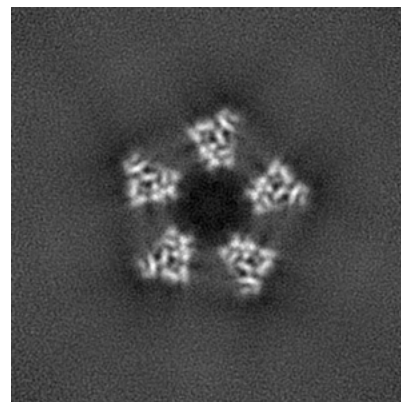
### 6.2.2 Raw map



X Index: 128



Y Index: 128

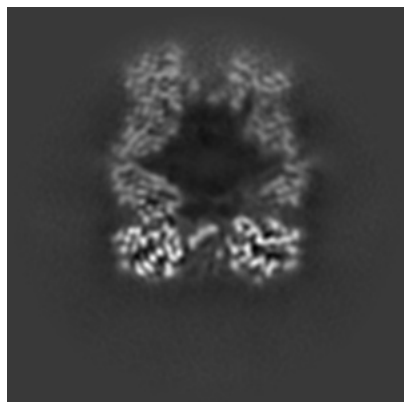


Z Index: 128

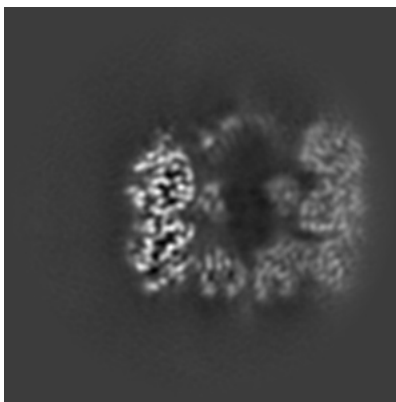
The images above show central slices of the map in three orthogonal directions.

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

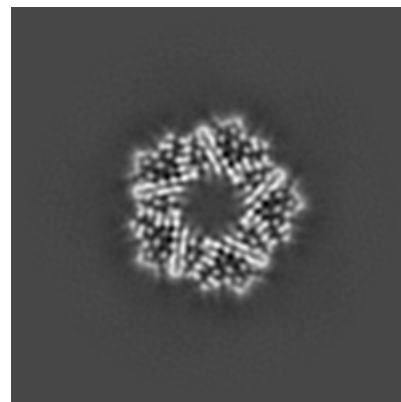
### 6.3.1 Primary map



X Index: 145

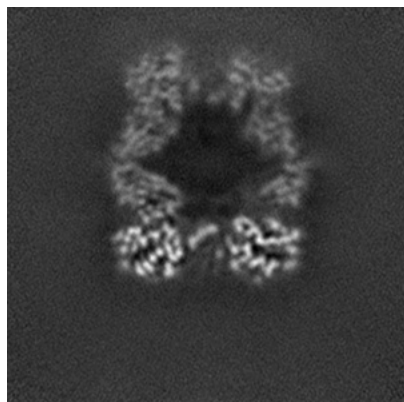


Y Index: 154

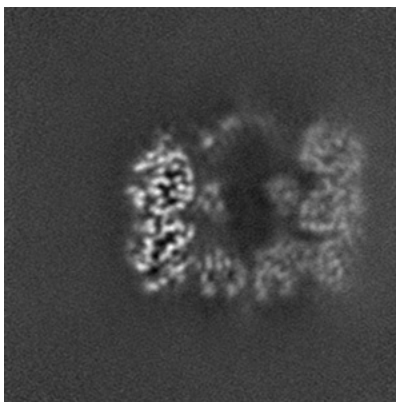


Z Index: 100

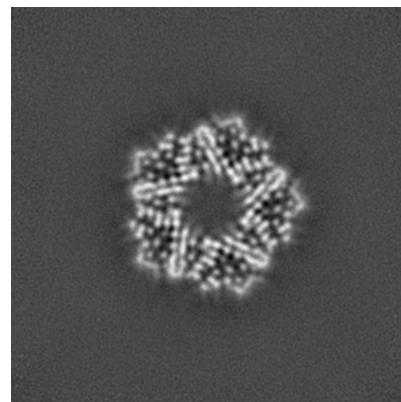
### 6.3.2 Raw map



X Index: 145



Y Index: 154

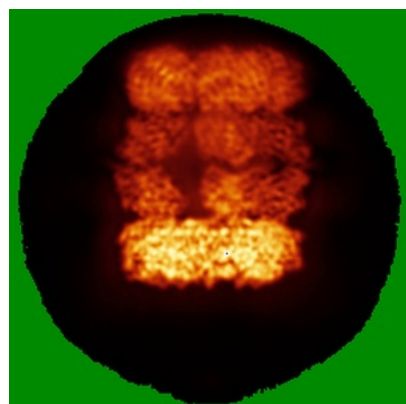


Z Index: 100

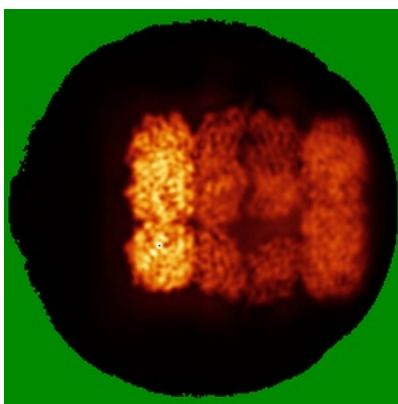
The images above show the largest variance slices of the map in three orthogonal directions.

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

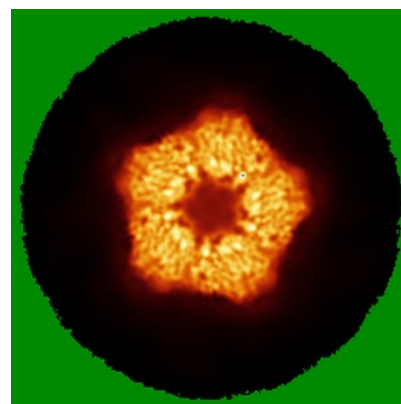
### 6.4.1 Primary map



X

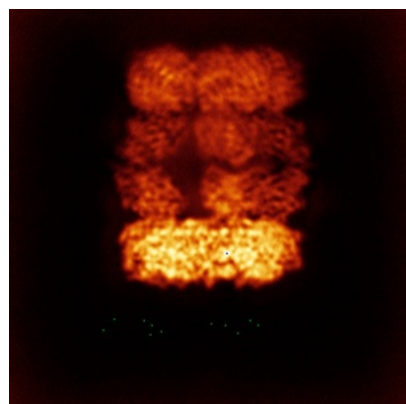


Y

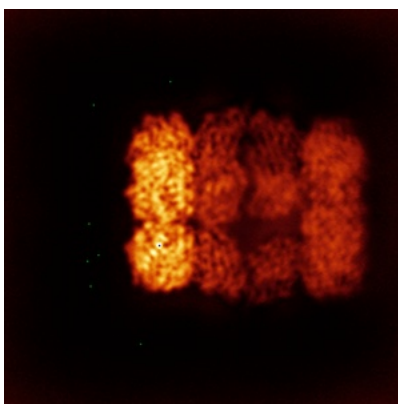


Z

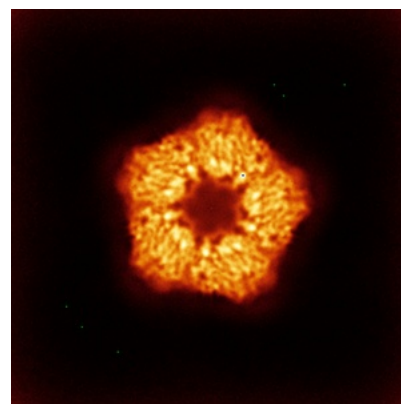
### 6.4.2 Raw map



X



Y

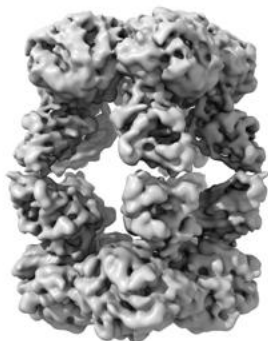


Z

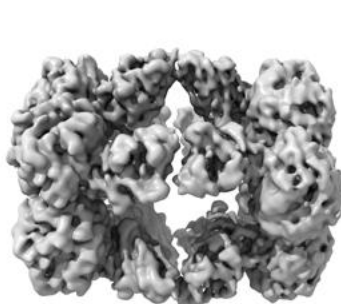
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

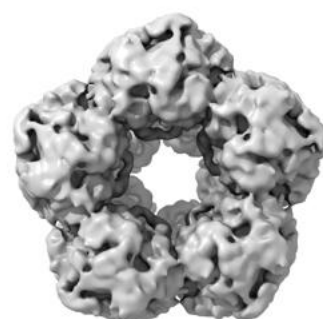
### 6.5.1 Primary map



X



Y



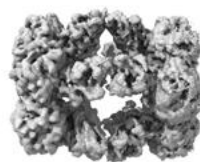
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0959. 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



X



Y



Z

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.

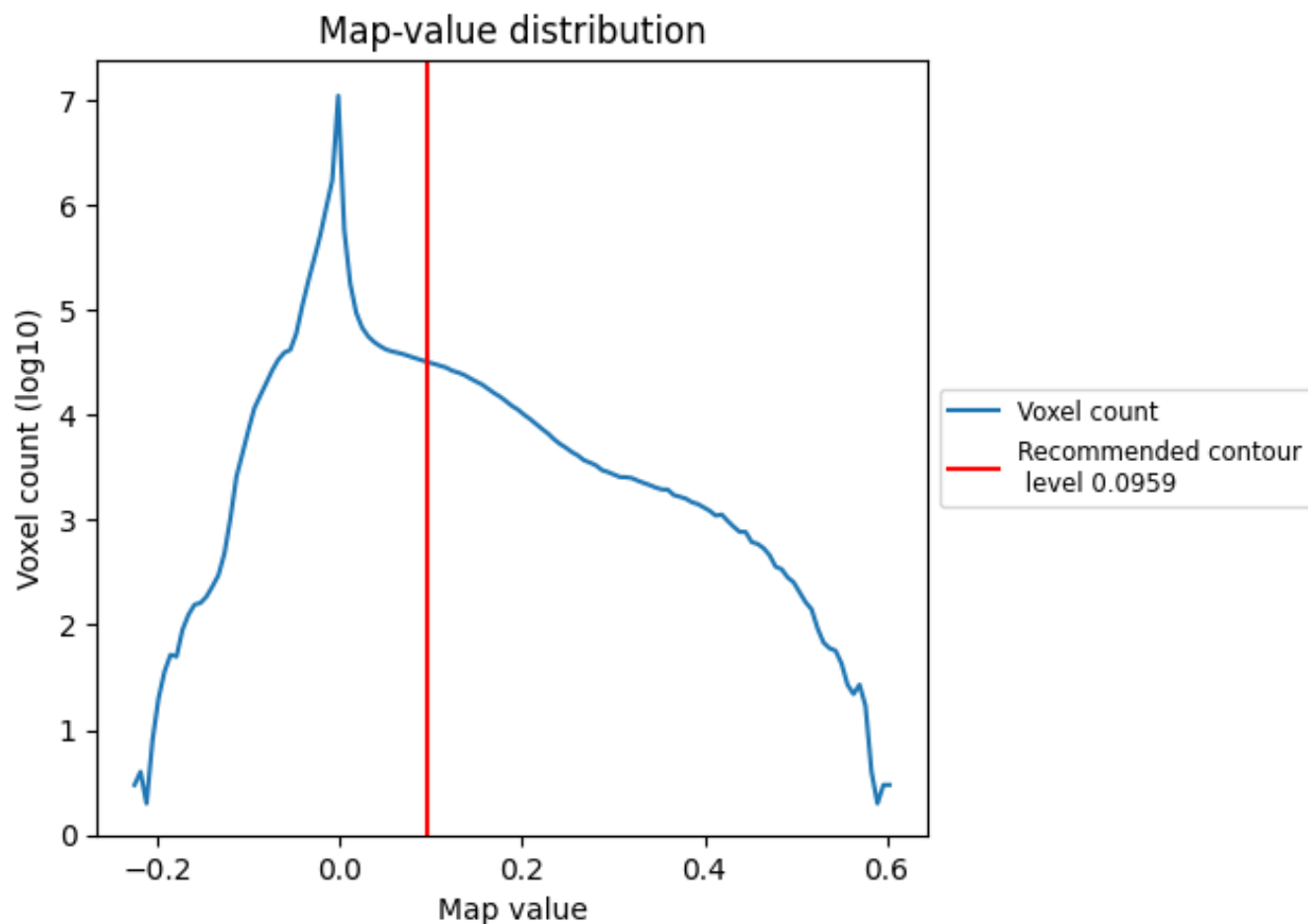
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

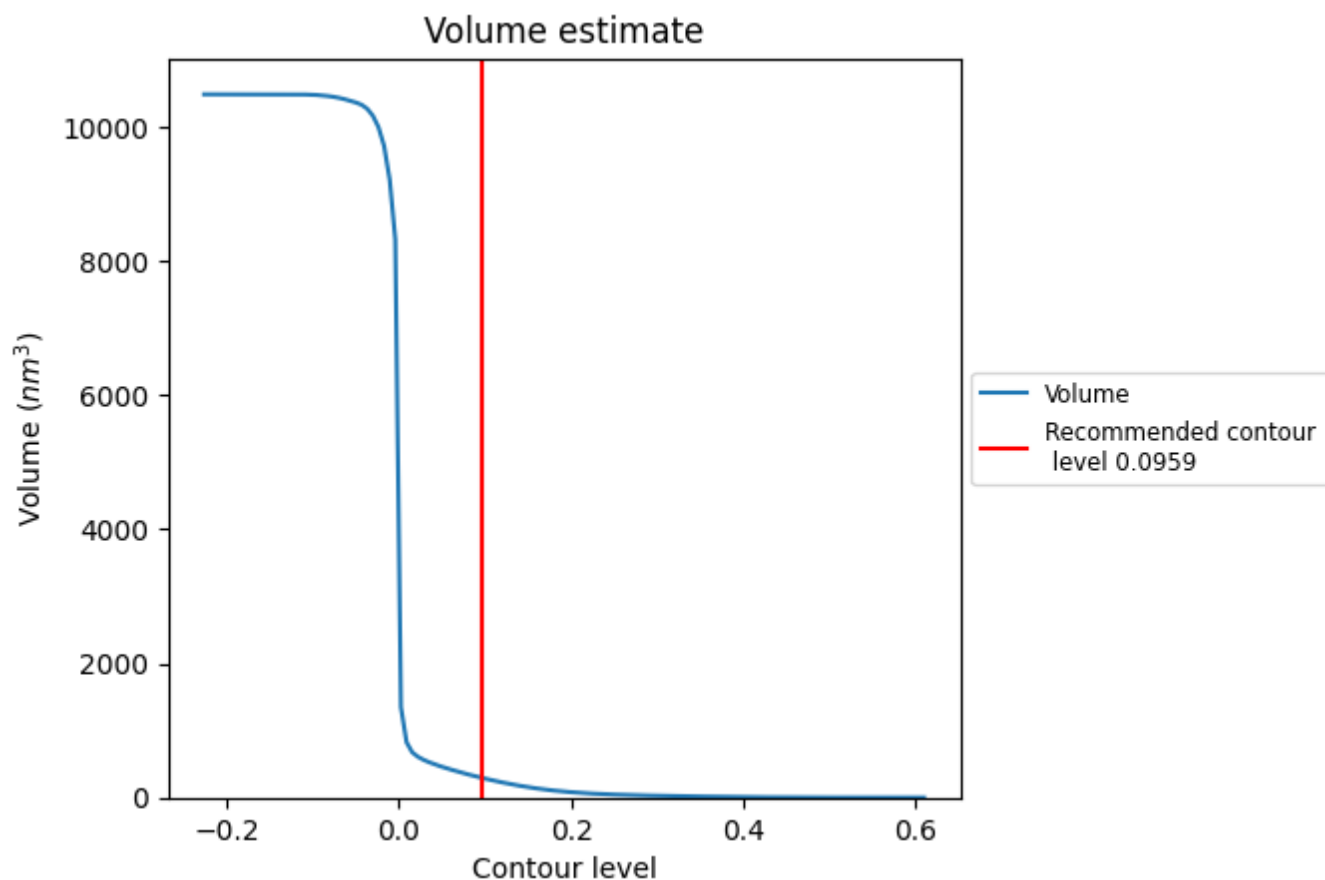
This section contains the results of statistical analysis of the map.

### 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](#)

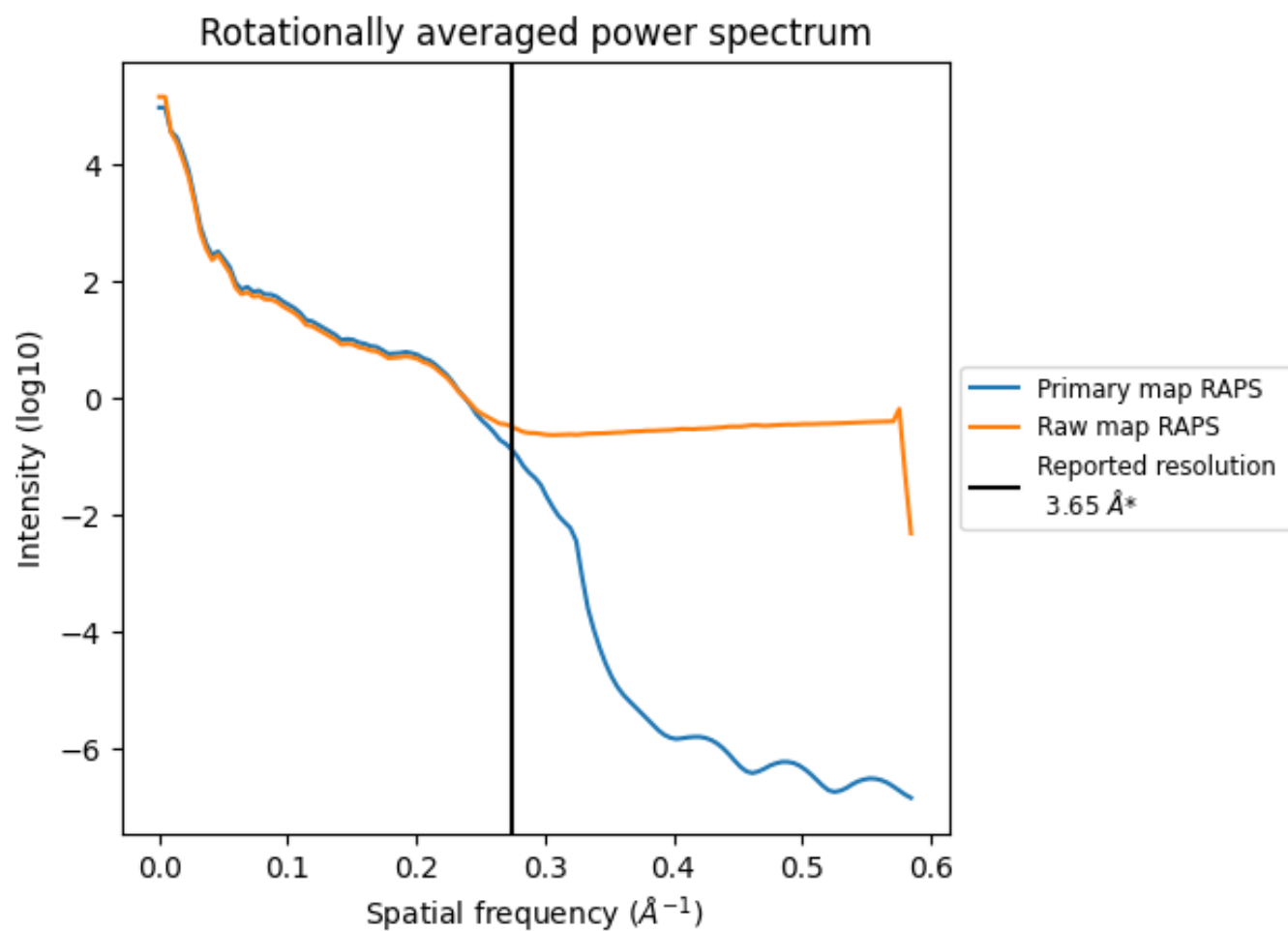


The volume at the recommended contour level is 296 nm<sup>3</sup>; this corresponds to an approximate mass of 267 kDa.

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 ⓘ

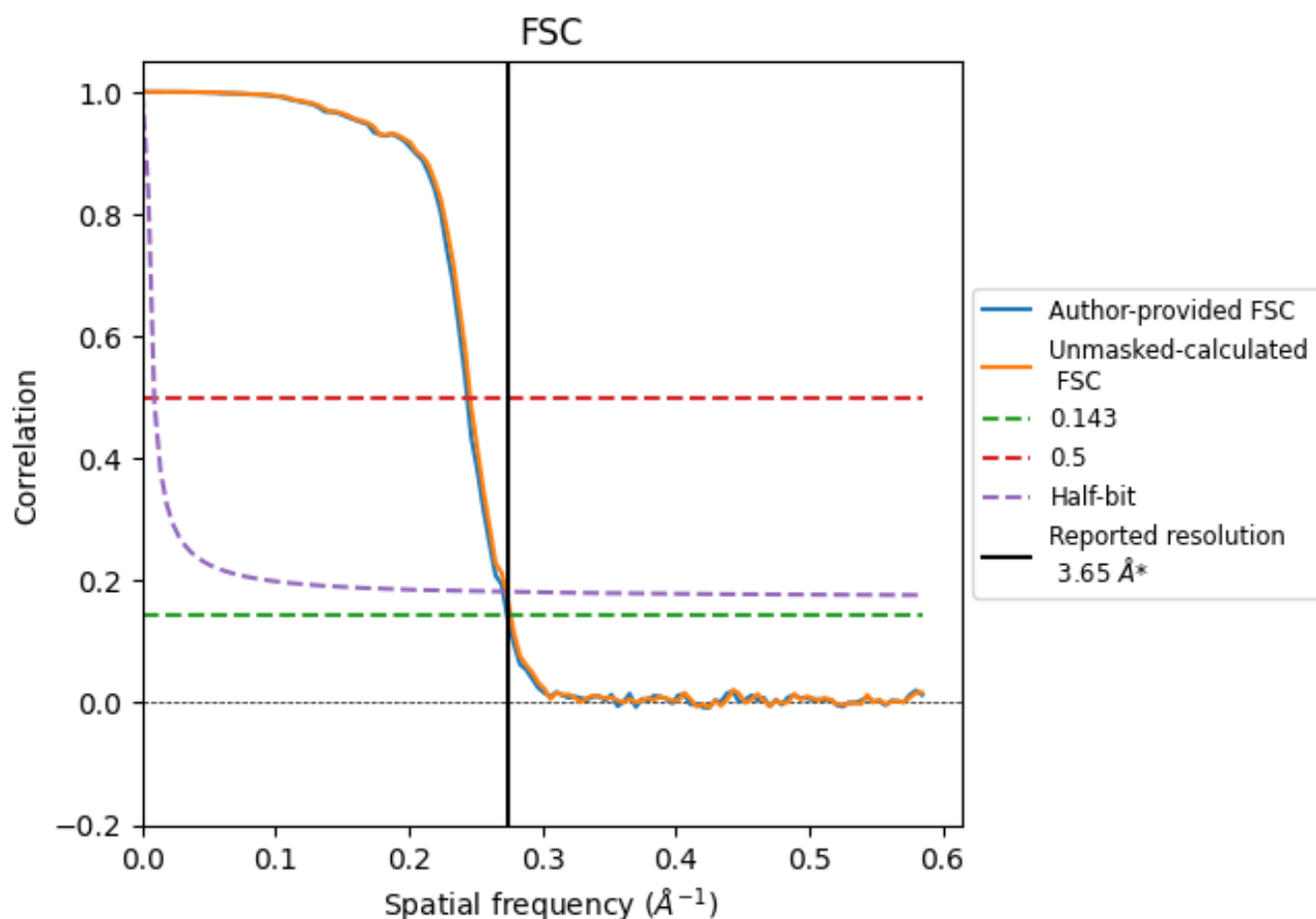


\*Reported resolution corresponds to spatial frequency of 0.274 Å<sup>-1</sup>

## 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  $0.274 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

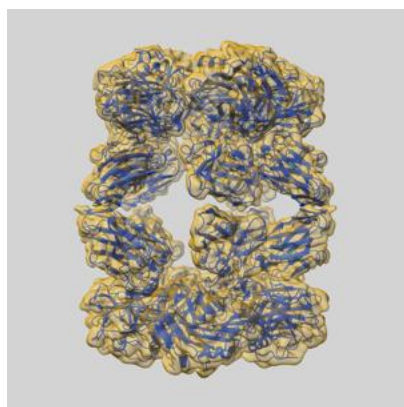
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.65                               | -    | -        |
| Author-provided FSC curve | 3.65                               | 4.10 | 3.70     |
| Unmasked-calculated*      | 3.62                               | 4.07 | 3.67     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

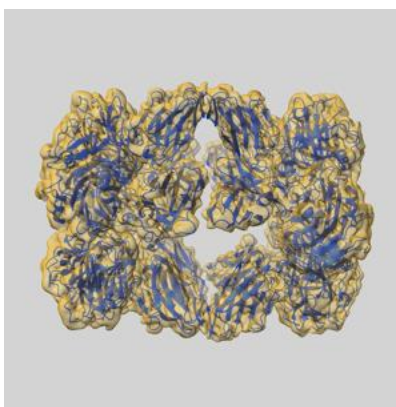
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61648 and PDB model 9JO9. Per-residue inclusion information can be found in section [3](#) on page [6](#).

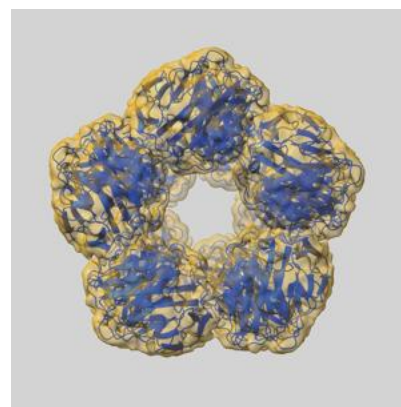
### 9.1 Map-model overlay [i](#)



X



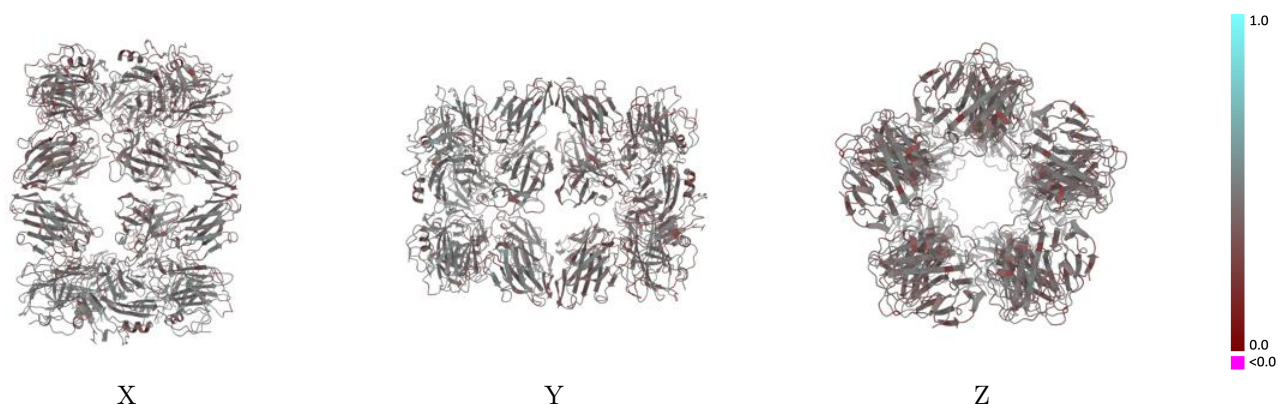
Y



Z

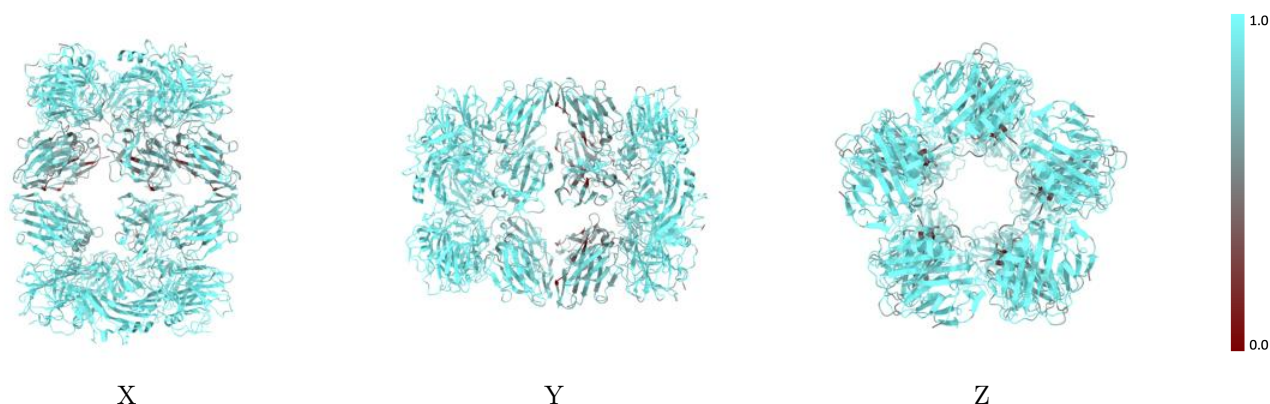
The images above show the 3D surface view of the map at the recommended contour level 0.0959 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



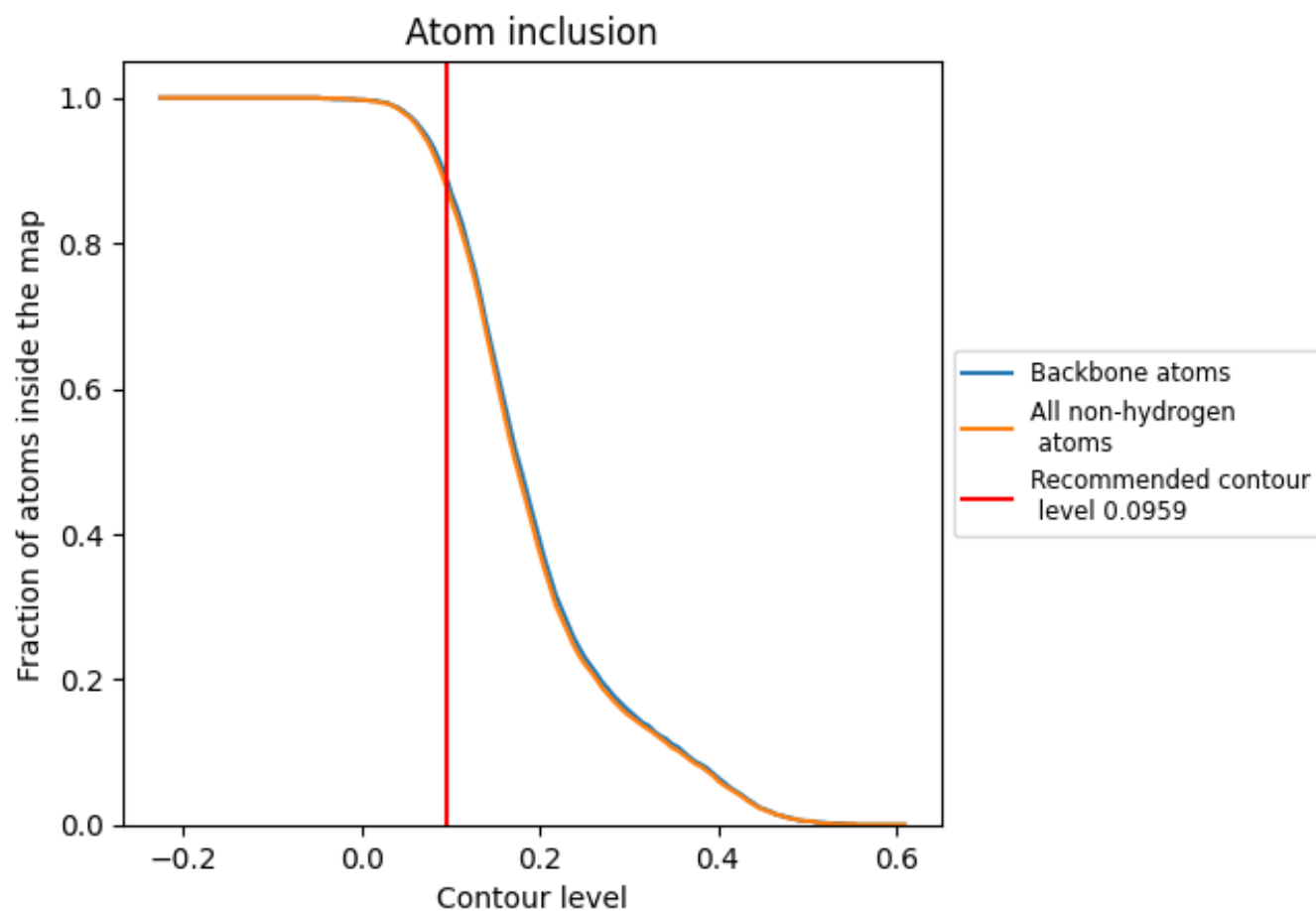
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0959).











































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% 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 (0.0959) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.8760   |  0.4250   |
| A     |  0.8730   |  0.4230   |
| B     |  0.9580   |  0.4560   |
| C     |  0.8660   |  0.4170   |
| D     |  0.9580   |  0.4560   |
| E     |  0.8710   |  0.4270   |
| F     |  0.9560   |  0.4480   |
| G     |  0.8680   |  0.4200   |
| H     |  0.9580   |  0.4500   |
| I     |  0.7190   |  0.4050   |
| J     |  0.9090   |  0.4130   |
| K     |  0.7100   |  0.4050   |
| L     |  0.9110   |  0.4130   |
| M     |  0.7230   |  0.4010   |
| N     |  0.9090  |  0.4130  |
| O     |  0.8700 |  0.4270 |
| P     |  0.7190 |  0.4040 |
| Q     |  0.9140 |  0.4130 |
| R     |  0.7180 |  0.4000 |
| S     |  0.9580 |  0.4500 |
| T     |  0.9110 |  0.4110 |

