



## wwPDB EM Validation Summary Report ⓘ

Jun 22, 2026 – 05:15 pm BST

PDB ID : 29RF / pdb\_000029rf  
EMDB ID : EMD-57322  
Title : Structure of Yeast RNA polymerase II elongation complex with NTP-state-III  
Authors : Yi, G.; Li, Q.; Zhang, P.; Wang, D.  
Deposited on : 2026-03-31  
Resolution : 3.02 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  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
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

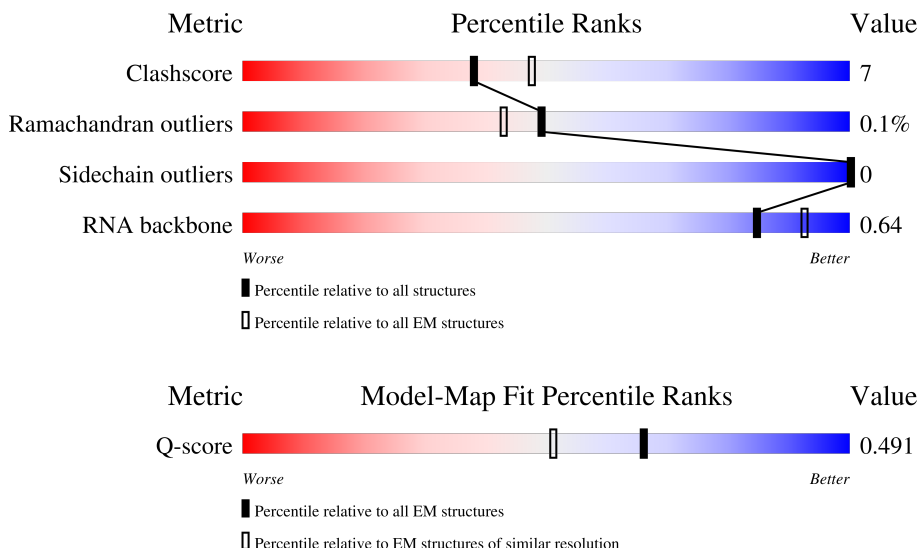
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.02 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                       | 13913 ( 2.52 - 3.52 )                                    |

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     | 1733   |                  |
| 2   | B     | 1224   |                  |
| 3   | C     | 318    |                  |

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| Mol | Chain | Length | Quality of chain       |
|-----|-------|--------|------------------------|
| 4   | D     | 221    | <p>76% 59% 16% 24%</p> |
| 5   | E     | 215    | <p>8% 85% 14%</p>      |
| 6   | F     | 155    | <p>43% 11% 46%</p>     |
| 7   | G     | 171    | <p>100% 82% 18%</p>    |
| 8   | H     | 146    | <p>5% 80% 12% 8%</p>   |
| 9   | I     | 122    | <p>13% 74% 18% 7%</p>  |
| 10  | J     | 70     | <p>71% 21% 7%</p>      |
| 11  | K     | 120    | <p>76% 18% 7%</p>      |
| 12  | L     | 70     | <p>6% 56% 9% 36%</p>   |
| 13  | N     | 74     | <p>7% 8% 14% 78%</p>   |
| 14  | R     | 19     | <p>26% 16% 11% 47%</p> |
| 15  | T     | 74     | <p>8% 19% 18% 64%</p>  |

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 32370 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | A     | 1396     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10993 | 6937 | 1916 | 2078 | 62 |         |       |

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 2   | B     | 1164     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 9268  | 5855 | 1627 | 1731 | 55 |         |       |

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | C     | 266      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2095  | 1317 | 348 | 417 | 13 |         |       |

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | D     | 167      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1327  | 821 | 230 | 273 | 3 |         |       |

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | E     | 213      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1744  | 1107 | 308 | 318 | 11 |         |       |

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | F     | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 670   | 428 | 114 | 125 | 3 |         |       |

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | G     | 171      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1340  | 861 | 222 | 249 | 8 |         |       |

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | H     | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1077  | 679 | 182 | 212 | 4 |         |       |

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 9   | I     | 114      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 926   | 570 | 167 | 178 | 11 |         |       |

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 10  | J     | 65       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 532   | 339 | 93 | 94 | 6 |         |       |

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | K     | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 904   | 580 | 154 | 168 | 2 |         |       |

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 12  | L     | 45       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 359   | 221 | 71 | 63 | 4 |         |       |

- Molecule 13 is a DNA chain called DNA (74-MER).

| Mol | Chain | Residues | Atoms |     |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|-------|
| 13  | N     | 16       | Total | C   | N  | O  | P  | 0       | 0     |
|     |       |          | 334   | 156 | 69 | 93 | 16 |         |       |

- Molecule 14 is a RNA chain called RNA (5'-R(\*AP\*UP\*CP\*GP\*AP\*GP\*AP\*GP\*GP\*AP

\*UP\*GP\*GP\*GP\*AP\*GP\*AP\*AP\*G)-3').

| Mol | Chain | Residues | Atoms |    |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|----|---------|-------|
| 14  | R     | 10       | Total | C  | N  | O  | P  | 0       | 0     |
|     |       |          | 223   | 99 | 47 | 67 | 10 |         |       |

- Molecule 15 is a DNA chain called DNA (74-MER).

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 15  | T     | 27       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 537   | 257 | 85 | 168 | 27 |         |       |

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 16  | A     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 16  | B     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 16  | C     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 16  | I     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 16  | J     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 16  | L     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 17  | R     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 18 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).

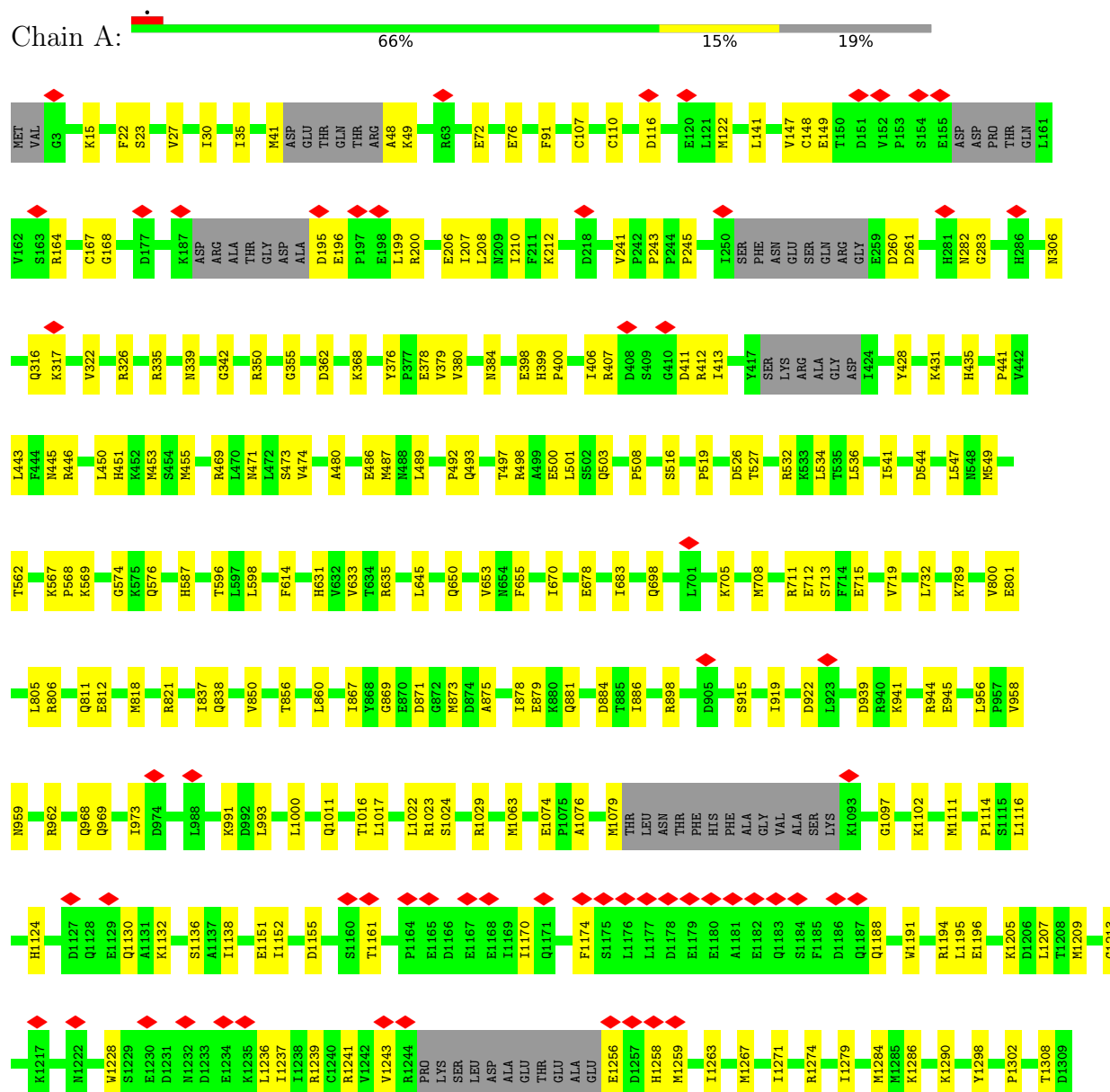


| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 18  | T     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |

### 3 Residue-property plots

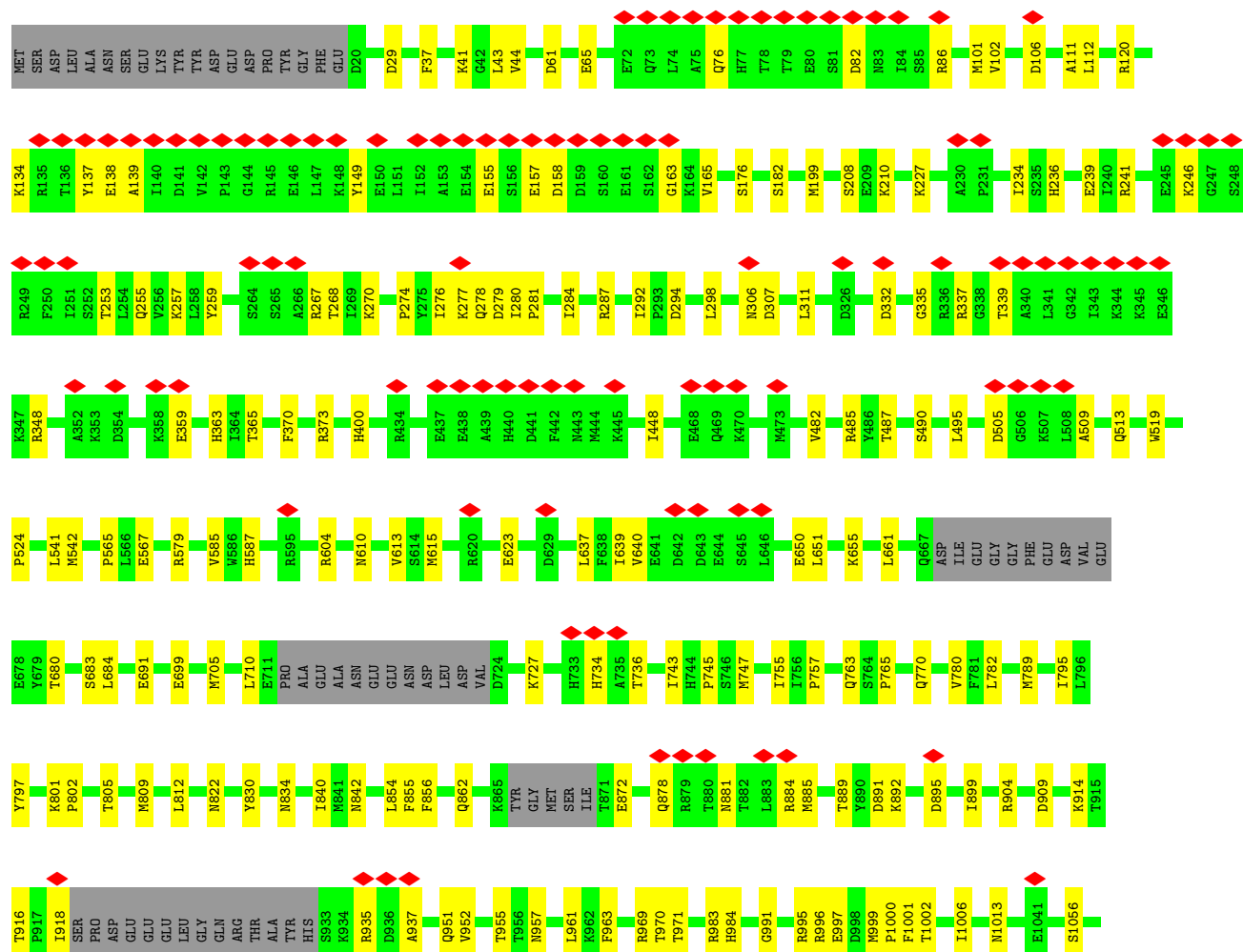
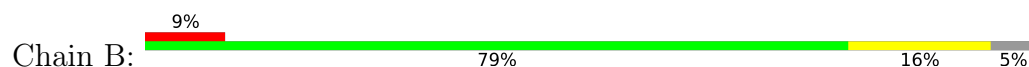
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: DNA-directed RNA polymerase II subunit RPB1

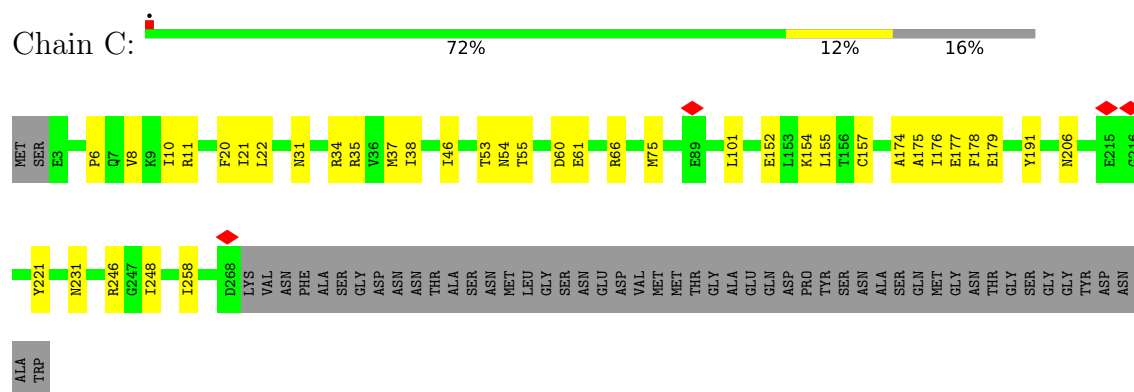




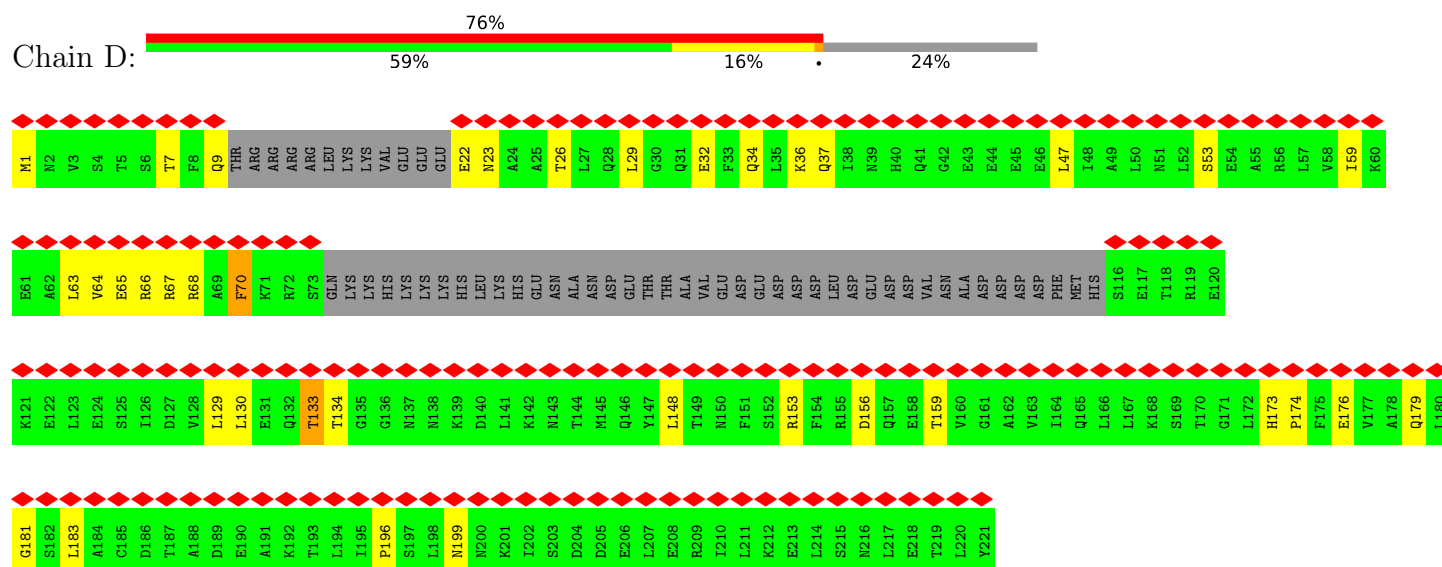
- Molecule 2: DNA-directed RNA polymerase II subunit RPB2



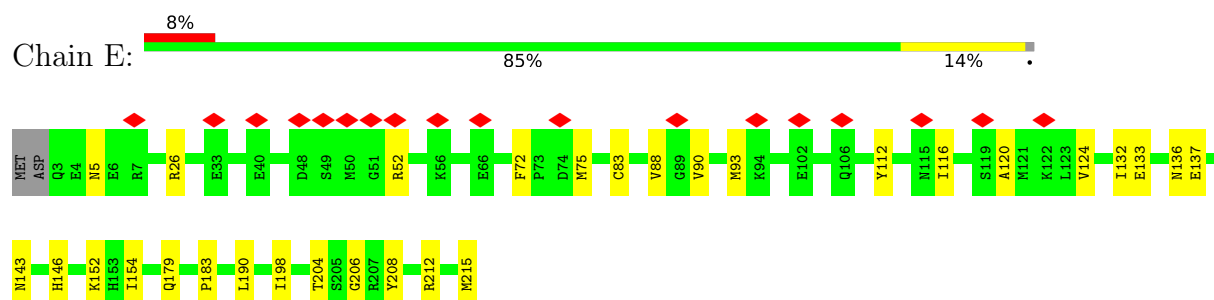
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3



- Molecule 4: DNA-directed RNA polymerase II subunit RPB4



- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1




- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



MET SER GLN ASP TYR GLU ARG ALA PHE ASN ASP GLY GLU ASN GLU ASN PHE GLU ASP PHE ASP VAL GLU HIS PHE SER ASP GLU GLU THR TVR GLU LYS LYS PRO GLN PHE LYS LYS ASP GLY THR THR ASP ASP ALA ASN GLY LYS THR THR ILE VAL THR GLY ASN GLY ASP PRO GLU ASP PHE GLN

HIS GLU GLN ILE ARG ARG LYS THR LEU LYS K72 T81 T82 E89 R90 I93 V107 F108 V109 D110 L111 D116 R119 I120 V133 I134 R135 R136 W146 S147 D154 LEU

• Molecule 7: DNA-directed RNA polymerase II subunit RPB7


Chain G:  100%  
82% 18%

M1 F2 F3 I4 K5 D6 L7 S8 L9 M10 M11 T12 L13 H14 P15 S16 F17 F18 G19 P20 M22 K23 Q24 Y25 L26 K27 T28 K29 L30 L31 E32 E33 V34 E35 G36 S37 C38 T39 G40 K41 F42 G43 Y44 I45 L46 C47 V48 L49 D50 Y51 D52 N53 I54 D55 T56 Q57 R58 G59 R60

L61 L62 P63 T64 D65 G66 S67 A68 E69 F70 M71 V72 K73 L74 Y75 A76 V77 V78 F79 K80 P81 F82 K83 G84 E85 V86 V87 D88 G89 T90 V91 V92 S93 S94 S95 Q96 H97 G98 F99 E100 I101 Q102 V103 G104 P105 M106 K107 V108 F109 V110 T111 K112 H113 L114 M115 P116 Q117 D118 L119 T120

F121 M122 A123 G124 S125 M126 P127 P128 S129 Y130 Q131 S132 S133 E134 D135 V136 I137 T138 I139 K140 S141 L142 I143 R144 V145 K146 I147 E148 G149 C150 I151 S152 Q153 S155 S156 I157 H158 A159 I160 G161 I162 I163 K164 E165 D166 Y167 L168 G169 I171

• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:  5%  
80% 12% 8%

MET S2 D8 I9 F10 P17 C24 A28 Q35 L38 P48 T59 L65 GLU ASP THR PRO ALA ASN ASP SER SER ALA THR R77 A84 G85 D86 H87 K103 S108 K109 D110 Y115 L122 M123 R130 K136 R146

• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:  13%  
74% 18% 7%

M1 T2 T3 F4 R5 F6 C7 C10 M11 M12 M13 L14 N22 N23 R24 L25 C29 R30 T31 C32 S33 E36 E37 S40 P41 L42 V43 Y44 R45 H46 E47 T50 T55 V58 V59 Q60 T67 E74 C75 S80 R81 R82 R83 D84 R87 V98

L99 I109 D113 Q114 LYS ASN LYS ARG THR GLN PHE SER

• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:  71%  
21% 7%

M1 I2 V3 F8 S9 C10 G11 E27 R43 Y44 C45 C46 R47 R48 M49 T52 L56 P65 LEU GLU LYS ARG ASP

• Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain K:  76%  
18% 7%



## 4 Experimental information

| Property                             | Value                         | Source    |
|--------------------------------------|-------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE               | Depositor |
| Imposed symmetry                     | POINT, Not provided           |           |
| Number of particles used             | 39522                         | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF             | Depositor |
| CTF correction method                | NONE                          | Depositor |
| Microscope                           | TFS KRIOS                     | Depositor |
| Voltage (kV)                         | 300                           | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                            | Depositor |
| Minimum defocus (nm)                 | 500                           | Depositor |
| Maximum defocus (nm)                 | 2500                          | Depositor |
| Magnification                        | Not provided                  |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value                    | 1.632                         | Depositor |
| Minimum map value                    | -0.917                        | Depositor |
| Average map value                    | 0.000                         | Depositor |
| Map value standard deviation         | 0.055                         | Depositor |
| Recommended contour level            | 0.25                          | Depositor |
| Map size ( $\text{\AA}$ )            | 346.496, 346.496, 346.496     | wwPDB     |
| Map dimensions                       | 320, 320, 320                 | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0              | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.0828, 1.0828, 1.0828        | Depositor |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, GTP

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     | 0.14         | 0/11187        | 0.33        | 2/15122 (0.0%) |
| 2   | B     | 0.13         | 0/9448         | 0.29        | 0/12738        |
| 3   | C     | 0.13         | 0/2133         | 0.30        | 0/2891         |
| 4   | D     | 2.18         | 8/1336 (0.6%)  | 0.66        | 7/1794 (0.4%)  |
| 5   | E     | 0.11         | 0/1780         | 0.30        | 0/2395         |
| 6   | F     | 0.12         | 0/682          | 0.29        | 0/922          |
| 7   | G     | 0.09         | 0/1368         | 0.27        | 0/1844         |
| 8   | H     | 0.11         | 0/1095         | 0.26        | 0/1482         |
| 9   | I     | 0.15         | 0/944          | 0.39        | 0/1272         |
| 10  | J     | 0.13         | 0/541          | 0.32        | 0/727          |
| 11  | K     | 0.13         | 0/922          | 0.30        | 0/1244         |
| 12  | L     | 0.10         | 0/361          | 0.27        | 0/478          |
| 13  | N     | 0.16         | 0/376          | 0.34        | 0/579          |
| 14  | R     | 0.12         | 0/251          | 0.32        | 0/391          |
| 15  | T     | 0.20         | 0/596          | 0.41        | 0/914          |
| All | All   | 0.46         | 8/33020 (0.0%) | 0.33        | 9/44793 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 9   | I     | 0                   | 1                   |

The worst 5 of 8 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | D     | 133 | THR  | CA-CB   | 35.27 | 2.09        | 1.53     |
| 4   | D     | 70  | PHE  | CD2-CE2 | 32.51 | 2.36        | 1.38     |
| 4   | D     | 70  | PHE  | CE1-CZ  | 32.00 | 2.34        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | D     | 70  | PHE  | CD1-CE1 | 31.50 | 2.33        | 1.38     |
| 4   | D     | 70  | PHE  | CE2-CZ  | 31.48 | 2.33        | 1.38     |

The worst 5 of 9 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | D     | 133 | THR  | CA-CB-CG2  | 14.48 | 135.12      | 110.50   |
| 4   | D     | 133 | THR  | CA-CB-OG1  | 12.35 | 128.12      | 109.60   |
| 4   | D     | 133 | THR  | OG1-CB-CG2 | -8.59 | 92.13       | 109.30   |
| 4   | D     | 133 | THR  | N-CA-C     | -8.47 | 102.12      | 111.36   |
| 4   | D     | 133 | THR  | CB-CA-C    | 7.83  | 124.17      | 110.85   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 9   | I     | 40  | SER  | Peptide |

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 10993 | 0        | 11071    | 175     | 0            |
| 2   | B     | 9268  | 0        | 9287     | 136     | 0            |
| 3   | C     | 2095  | 0        | 2051     | 30      | 0            |
| 4   | D     | 1327  | 0        | 1331     | 68      | 0            |
| 5   | E     | 1744  | 0        | 1772     | 18      | 0            |
| 6   | F     | 670   | 0        | 690      | 13      | 0            |
| 7   | G     | 1340  | 0        | 1357     | 22      | 0            |
| 8   | H     | 1077  | 0        | 1050     | 10      | 0            |
| 9   | I     | 926   | 0        | 879      | 16      | 0            |
| 10  | J     | 532   | 0        | 542      | 13      | 0            |
| 11  | K     | 904   | 0        | 911      | 15      | 0            |
| 12  | L     | 359   | 0        | 381      | 4       | 0            |
| 13  | N     | 334   | 0        | 178      | 9       | 0            |
| 14  | R     | 223   | 0        | 109      | 3       | 0            |
| 15  | T     | 537   | 0        | 306      | 9       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 16  | A     | 2     | 0        | 0        | 0       | 0            |
| 16  | B     | 1     | 0        | 0        | 0       | 0            |
| 16  | C     | 1     | 0        | 0        | 0       | 0            |
| 16  | I     | 2     | 0        | 0        | 0       | 0            |
| 16  | J     | 1     | 0        | 0        | 0       | 0            |
| 16  | L     | 1     | 0        | 0        | 0       | 0            |
| 17  | R     | 1     | 0        | 0        | 0       | 0            |
| 18  | T     | 32    | 0        | 12       | 1       | 0            |
| All | All   | 32370 | 0        | 31927    | 475     | 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 7.

The worst 5 of 475 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) |
|----------------|-----------------|--------------------------|-------------------|
| 4:D:70:PHE:CD2 | 4:D:70:PHE:CG   | 1.84                     | 1.64              |
| 4:D:70:PHE:CG  | 4:D:70:PHE:CD1  | 1.84                     | 1.60              |
| 4:D:133:THR:CB | 4:D:133:THR:CG2 | 1.83                     | 1.54              |
| 4:D:70:PHE:CE1 | 4:D:133:THR:HB  | 1.42                     | 1.50              |
| 4:D:70:PHE:CD1 | 4:D:133:THR:HA  | 1.53                     | 1.43              |

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     | 1380/1733 (80%) | 1331 (96%) | 47 (3%) | 2 (0%)   | 48          | 79  |
| 2   | B     | 1154/1224 (94%) | 1116 (97%) | 38 (3%) | 0        | 100         | 100 |
| 3   | C     | 264/318 (83%)   | 263 (100%) | 1 (0%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 4   | D     | 161/221 (73%)   | 159 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 5   | E     | 211/215 (98%)   | 203 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 6   | F     | 81/155 (52%)    | 80 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 7   | G     | 169/171 (99%)   | 163 (96%)  | 6 (4%)   | 0        | 100         | 100 |
| 8   | H     | 130/146 (89%)   | 128 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 9   | I     | 112/122 (92%)   | 97 (87%)   | 13 (12%) | 2 (2%)   | 6           | 29  |
| 10  | J     | 63/70 (90%)     | 63 (100%)  | 0        | 0        | 100         | 100 |
| 11  | K     | 110/120 (92%)   | 108 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 12  | L     | 43/70 (61%)     | 41 (95%)   | 1 (2%)   | 1 (2%)   | 5           | 23  |
| All | All   | 3878/4565 (85%) | 3752 (97%) | 121 (3%) | 5 (0%)   | 49          | 79  |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | I     | 40  | SER  |
| 9   | I     | 41  | PRO  |
| 1   | A     | 958 | VAL  |
| 1   | A     | 922 | ASP  |
| 12  | L     | 45  | ALA  |

### 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     | 1222/1520 (80%) | 1222 (100%) | 0        | 100         | 100 |
| 2   | B     | 1010/1061 (95%) | 1010 (100%) | 0        | 100         | 100 |
| 3   | C     | 234/274 (85%)   | 234 (100%)  | 0        | 100         | 100 |
| 4   | D     | 149/200 (74%)   | 149 (100%)  | 0        | 100         | 100 |
| 5   | E     | 195/197 (99%)   | 195 (100%)  | 0        | 100         | 100 |
| 6   | F     | 73/137 (53%)    | 73 (100%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 7   | G     | 152/152 (100%)  | 152 (100%)  | 0        | 100         | 100 |
| 8   | H     | 118/128 (92%)   | 118 (100%)  | 0        | 100         | 100 |
| 9   | I     | 108/116 (93%)   | 108 (100%)  | 0        | 100         | 100 |
| 10  | J     | 60/65 (92%)     | 60 (100%)   | 0        | 100         | 100 |
| 11  | K     | 97/102 (95%)    | 97 (100%)   | 0        | 100         | 100 |
| 12  | L     | 40/57 (70%)     | 40 (100%)   | 0        | 100         | 100 |
| All | All   | 3458/4009 (86%) | 3458 (100%) | 0        | 100         | 100 |

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | E     | 115  | ASN  |
| 5   | E     | 146  | HIS  |
| 9   | I     | 90   | GLN  |
| 1   | A     | 1130 | GLN  |
| 1   | A     | 1078 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed    | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 14  | R     | 10/19 (52%) | 2 (20%)           | 1 (10%)         |

All (2) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | R     | 10  | A    |
| 14  | R     | 16  | G    |

All (1) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | R     | 9   | G    |

## 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](#)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 18  | GTP  | T     | 101 | -    | 30,34,34     | 3.62 | 19 (63%)    | 46,54,54    | 1.76 | 12 (26%)    |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 18  | GTP  | T     | 101 | -    | -       | 2/22/38/38 | 0/3/3/3 |

The worst 5 of 19 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 18  | T     | 101 | GTP  | C2'-C3' | -10.53 | 1.24        | 1.53     |
| 18  | T     | 101 | GTP  | C4-N3   | 6.30   | 1.49        | 1.34     |
| 18  | T     | 101 | GTP  | C2-N3   | 5.80   | 1.47        | 1.33     |
| 18  | T     | 101 | GTP  | O4'-C1' | -5.57  | 1.28        | 1.42     |
| 18  | T     | 101 | GTP  | C2-N2   | 5.15   | 1.46        | 1.34     |

The worst 5 of 12 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 18  | T     | 101 | GTP  | C5-C4-N3 | -5.09 | 120.21      | 128.46   |
| 18  | T     | 101 | GTP  | C2-N3-C4 | 4.34  | 120.03      | 112.30   |
| 18  | T     | 101 | GTP  | N9-C4-N3 | 2.98  | 131.93      | 125.94   |
| 18  | T     | 101 | GTP  | C2-N1-C6 | -2.93 | 119.75      | 125.10   |
| 18  | T     | 101 | GTP  | C4-C5-N7 | -2.80 | 106.29      | 110.72   |

There are no chirality outliers.

All (2) torsion outliers are listed below:

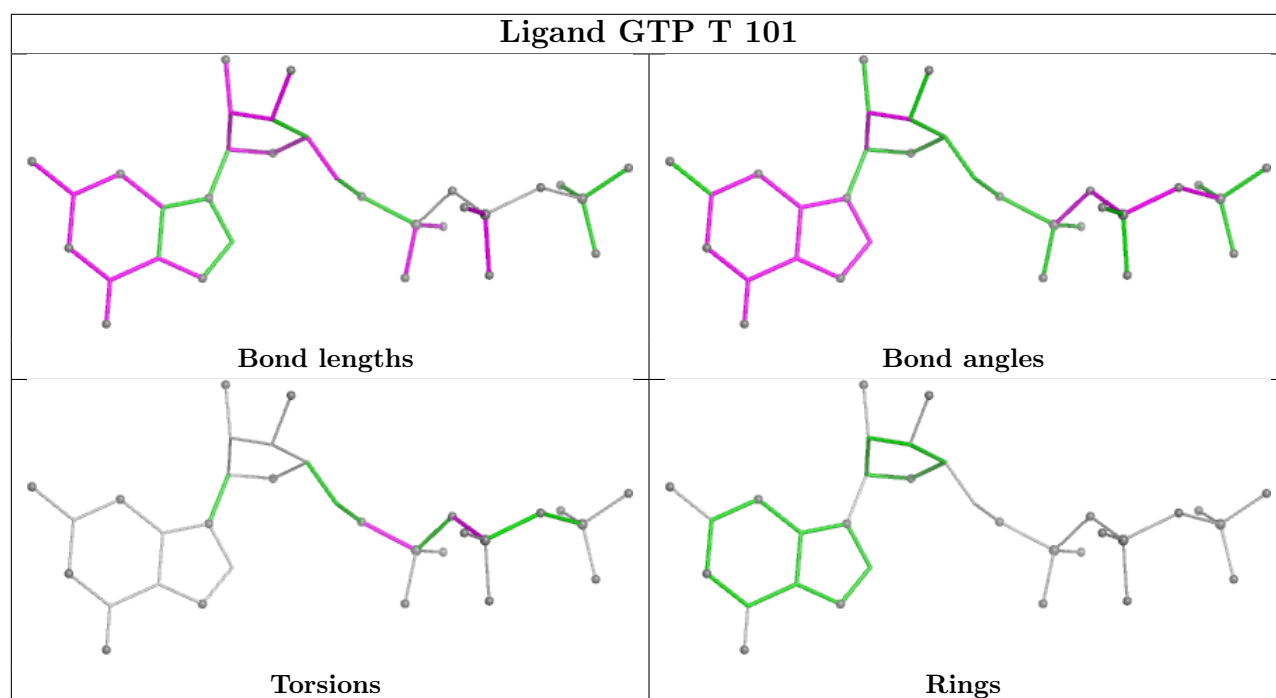
| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 18  | T     | 101 | GTP  | PA-O3A-PB-O2B  |
| 18  | T     | 101 | GTP  | C5'-O5'-PA-O1A |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 18  | T     | 101 | GTP  | 1       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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.

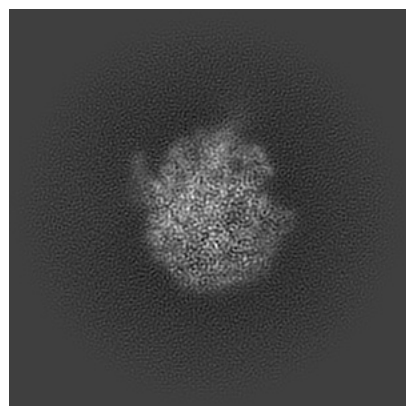
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-57322. These allow visual inspection of the internal detail of the map and identification of artifacts.

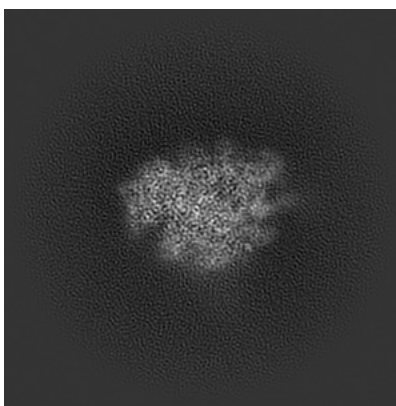
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

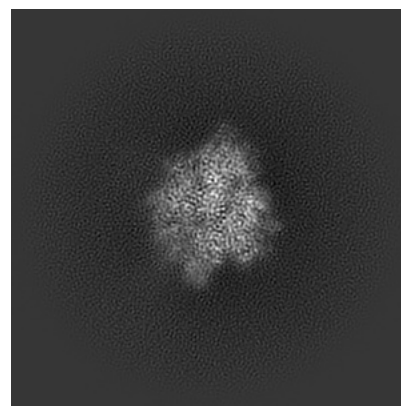
#### 6.1.1 Primary map



X

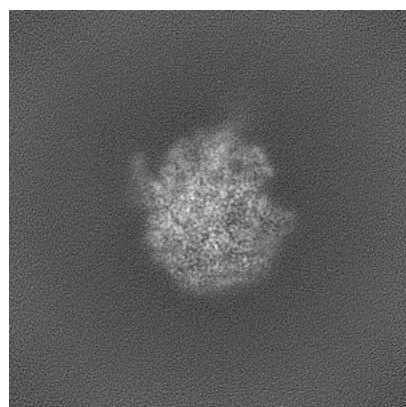


Y

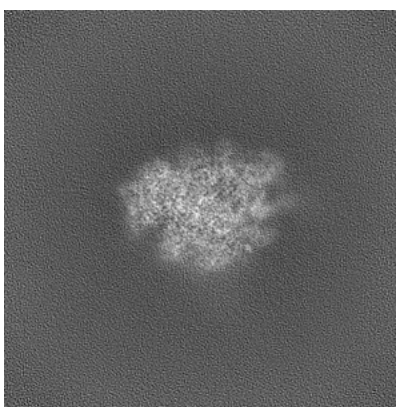


Z

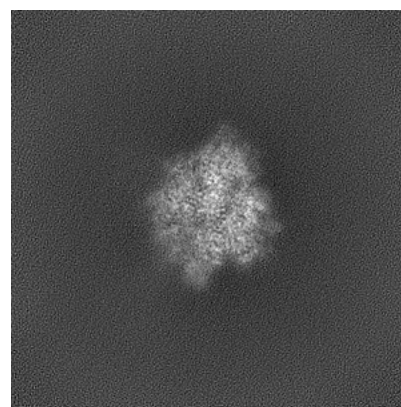
#### 6.1.2 Raw map



X



Y



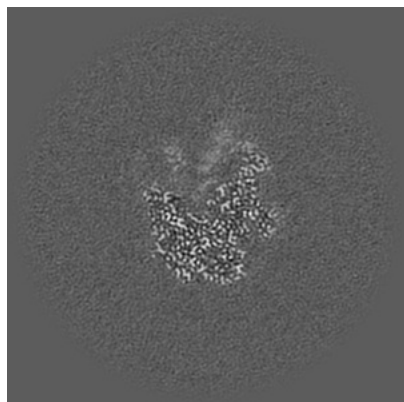
Z

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

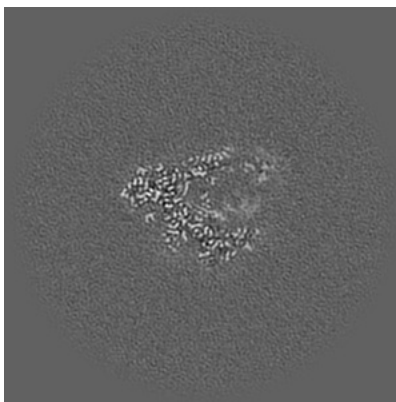


## 6.2 Central slices [i](#)

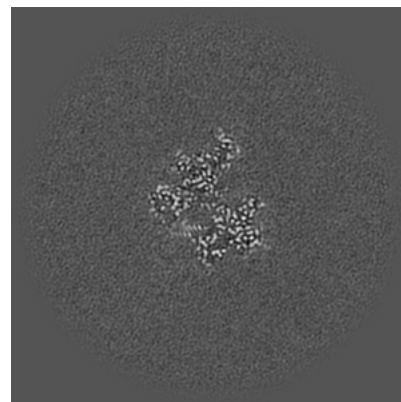
### 6.2.1 Primary map



X Index: 160

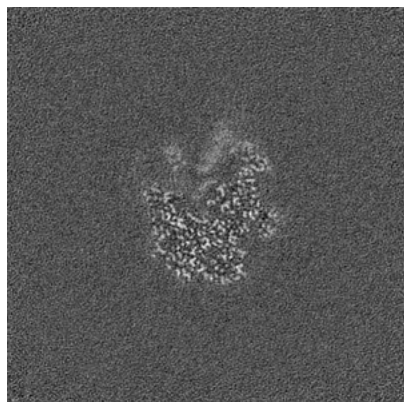


Y Index: 160

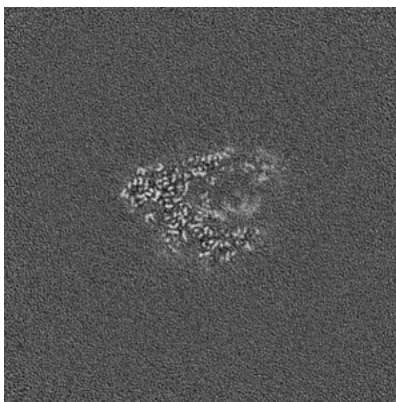


Z Index: 160

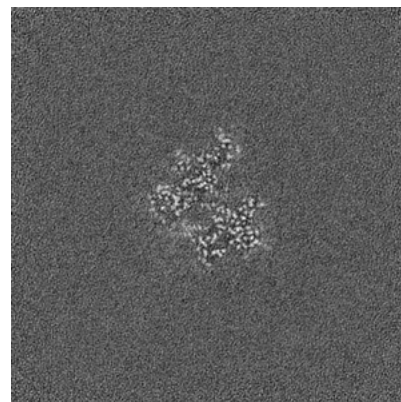
### 6.2.2 Raw map



X Index: 160



Y Index: 160

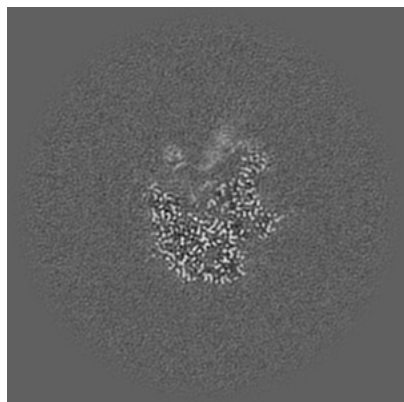


Z Index: 160

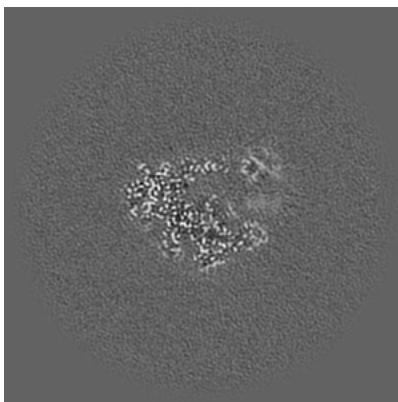
The images above show central slices of the map in three orthogonal directions.

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

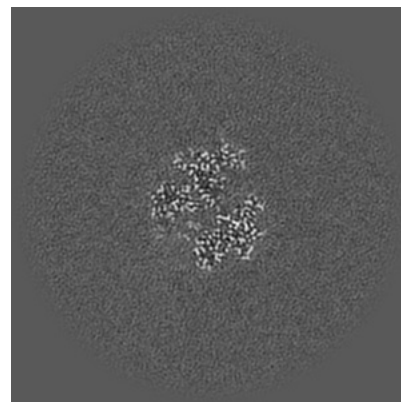
### 6.3.1 Primary map



X Index: 161

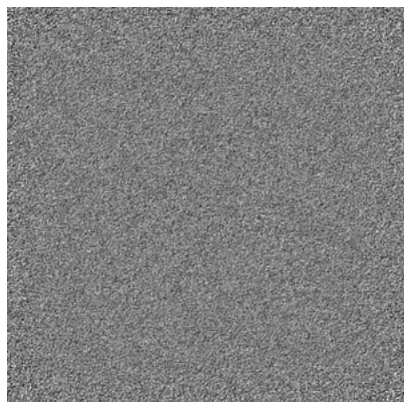


Y Index: 166

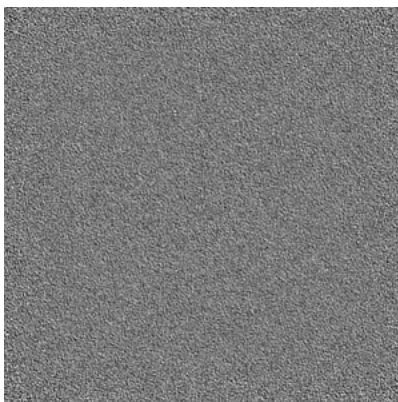


Z Index: 164

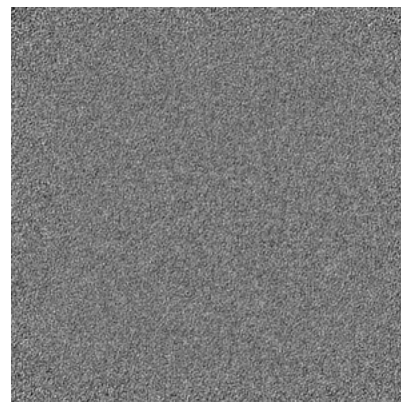
### 6.3.2 Raw map



X Index: 0



Y Index: 0



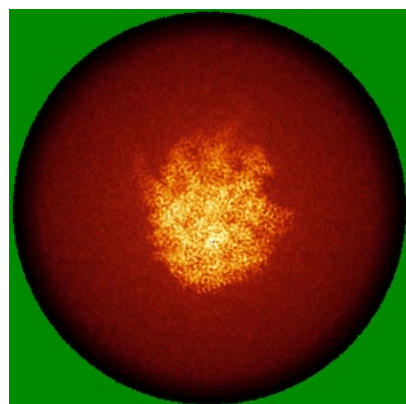
Z Index: 0

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

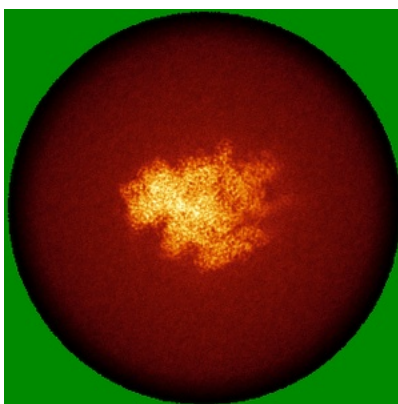


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

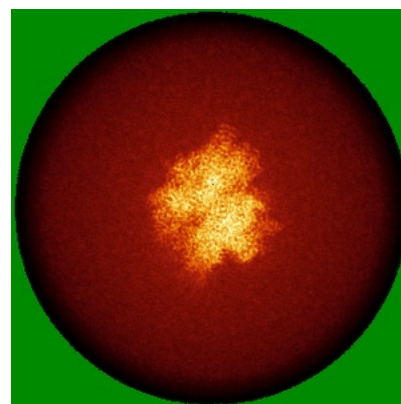
### 6.4.1 Primary map



X

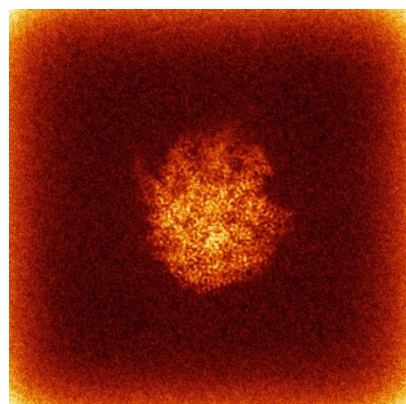


Y

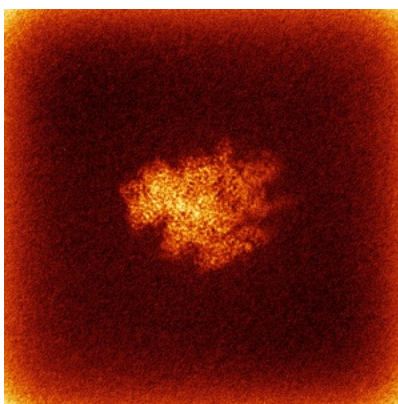


Z

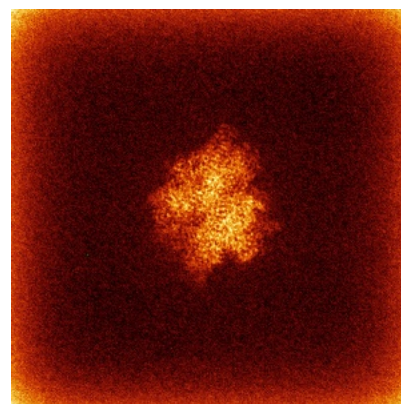
### 6.4.2 Raw map



X



Y

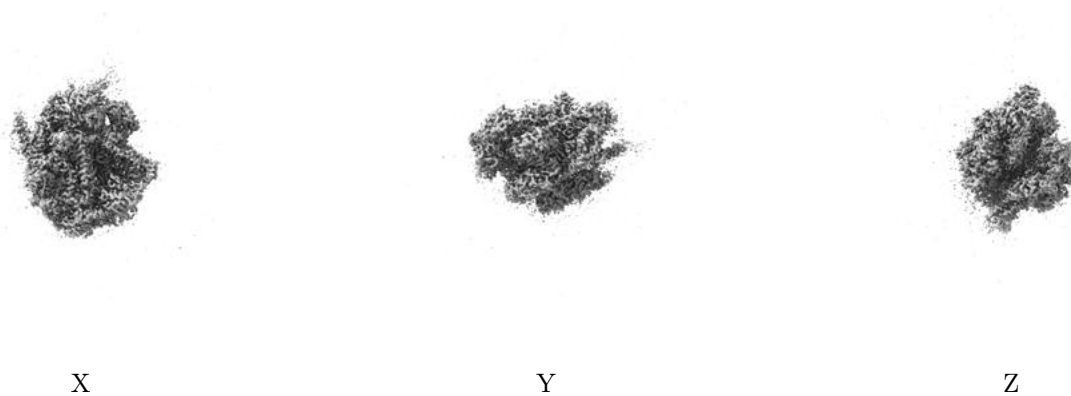


Z

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.

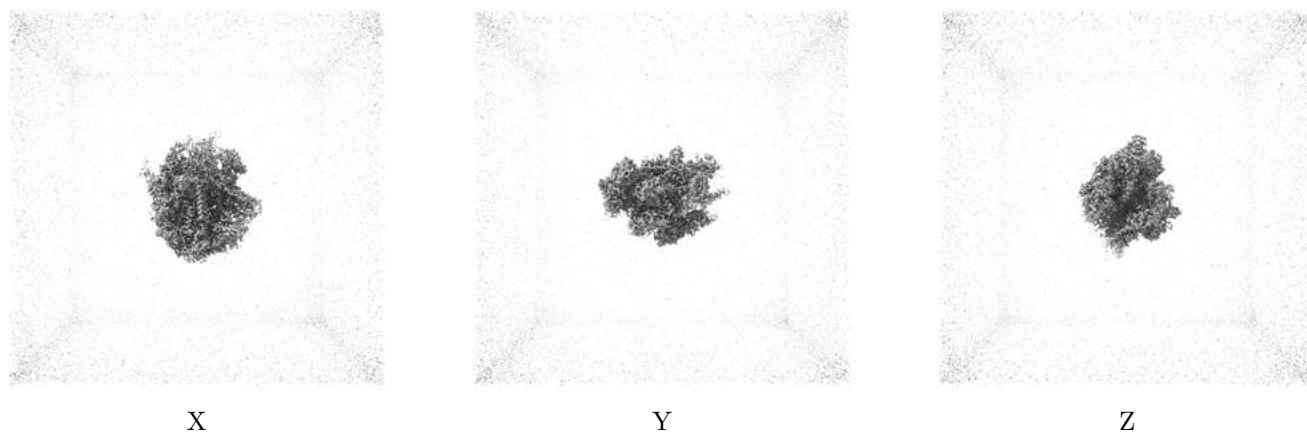
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

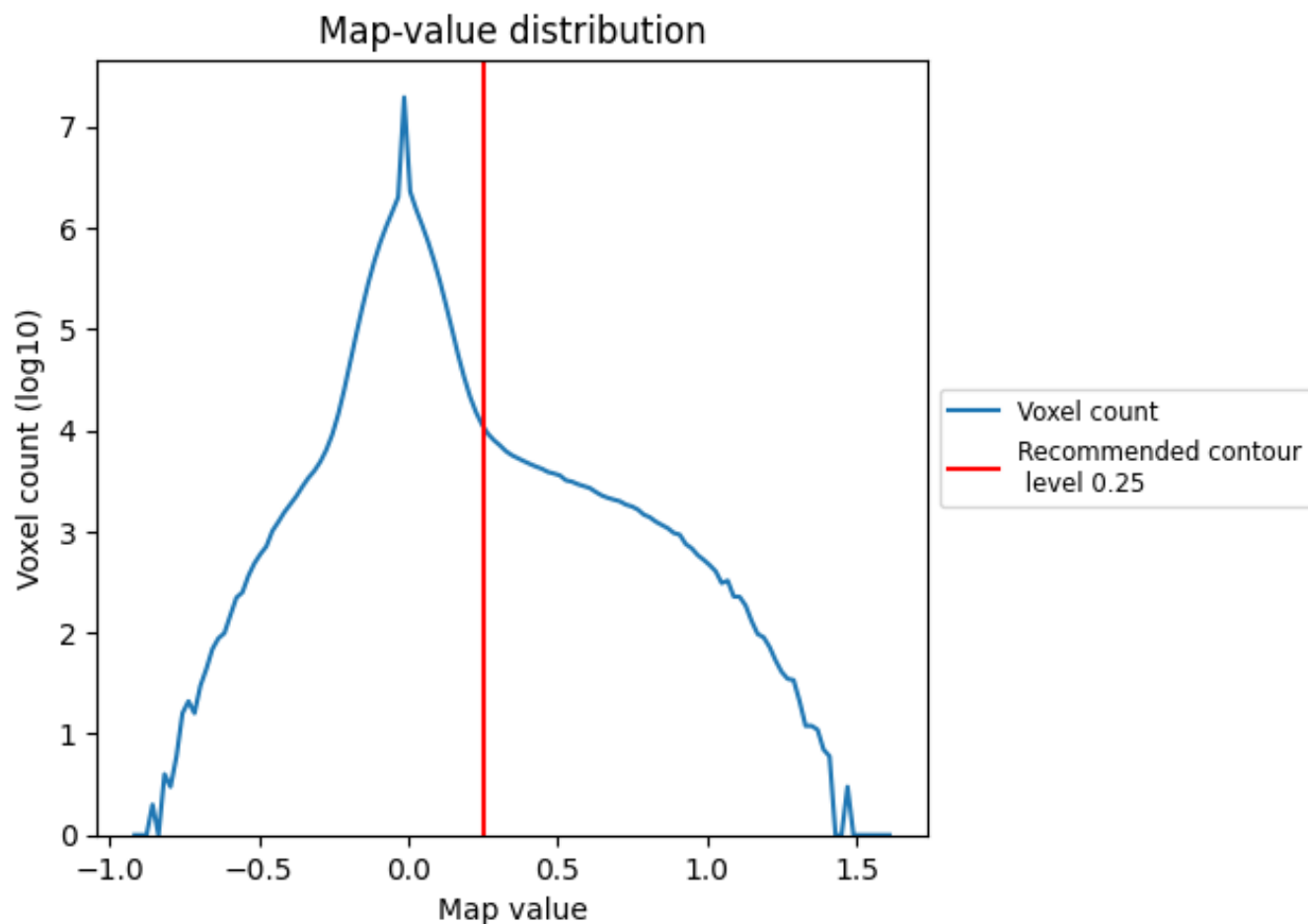
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

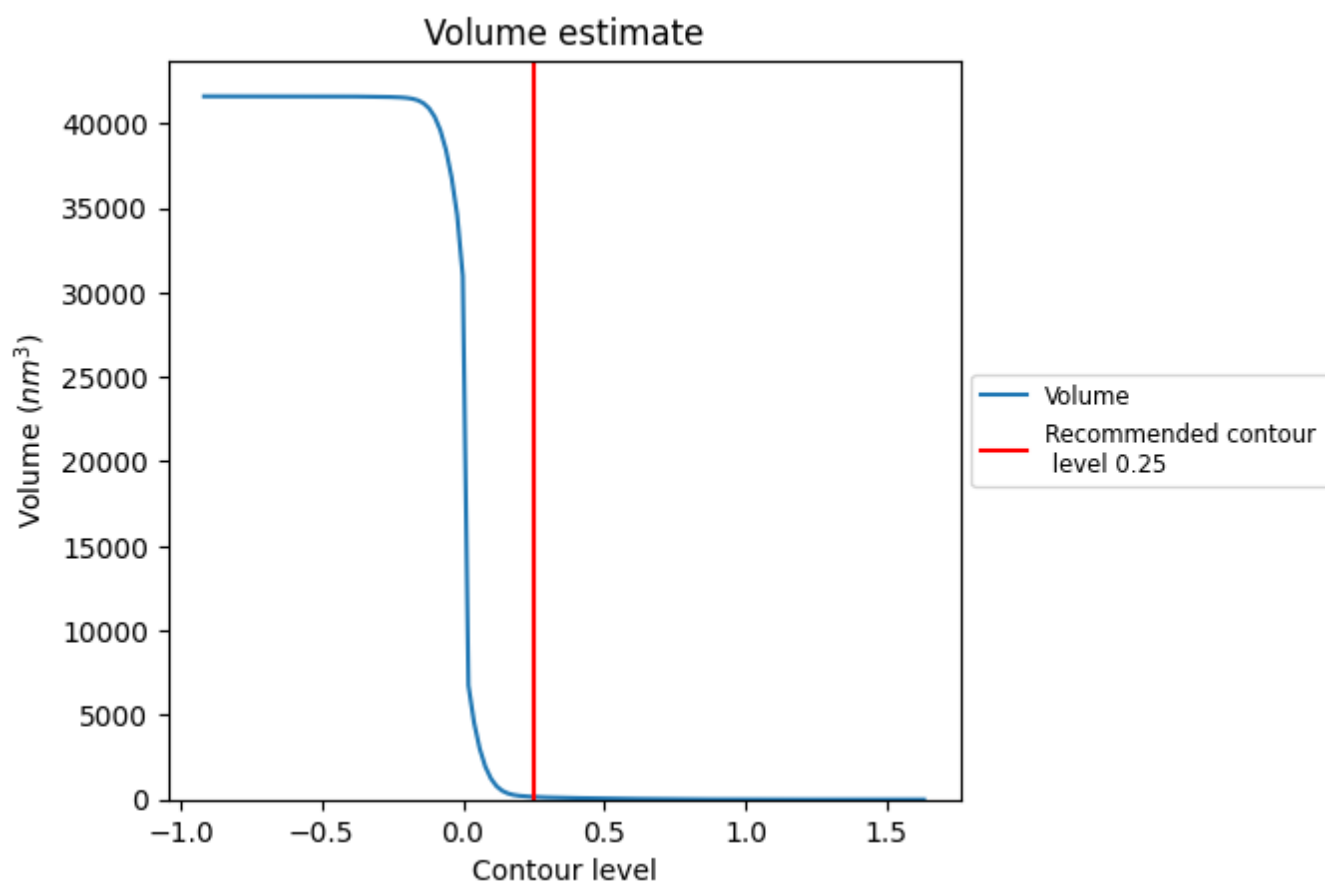
This section contains the results of statistical analysis of the map.

### 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.

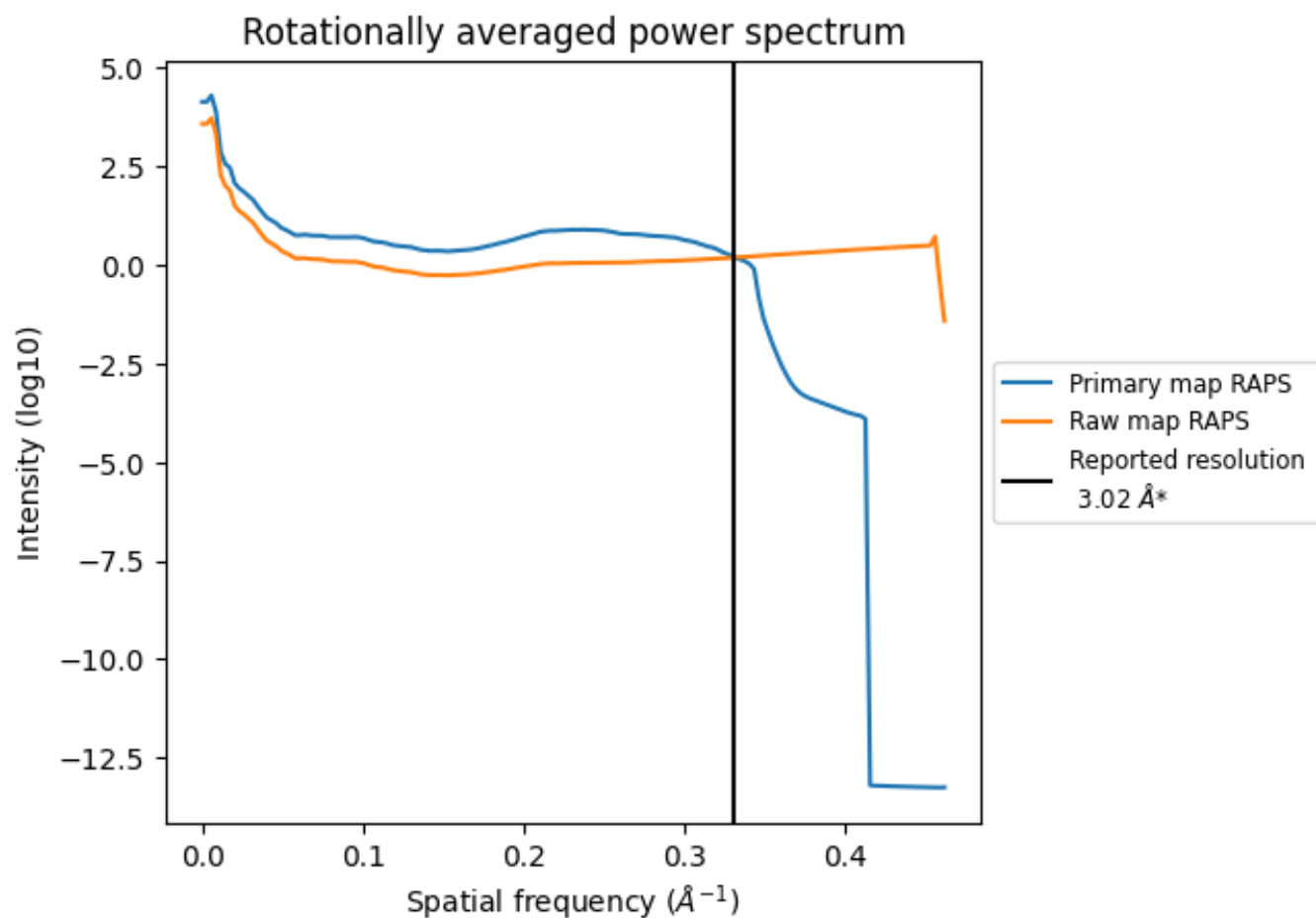
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 159  $\text{nm}^3$ ; this corresponds to an approximate mass of 144 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 ⓘ

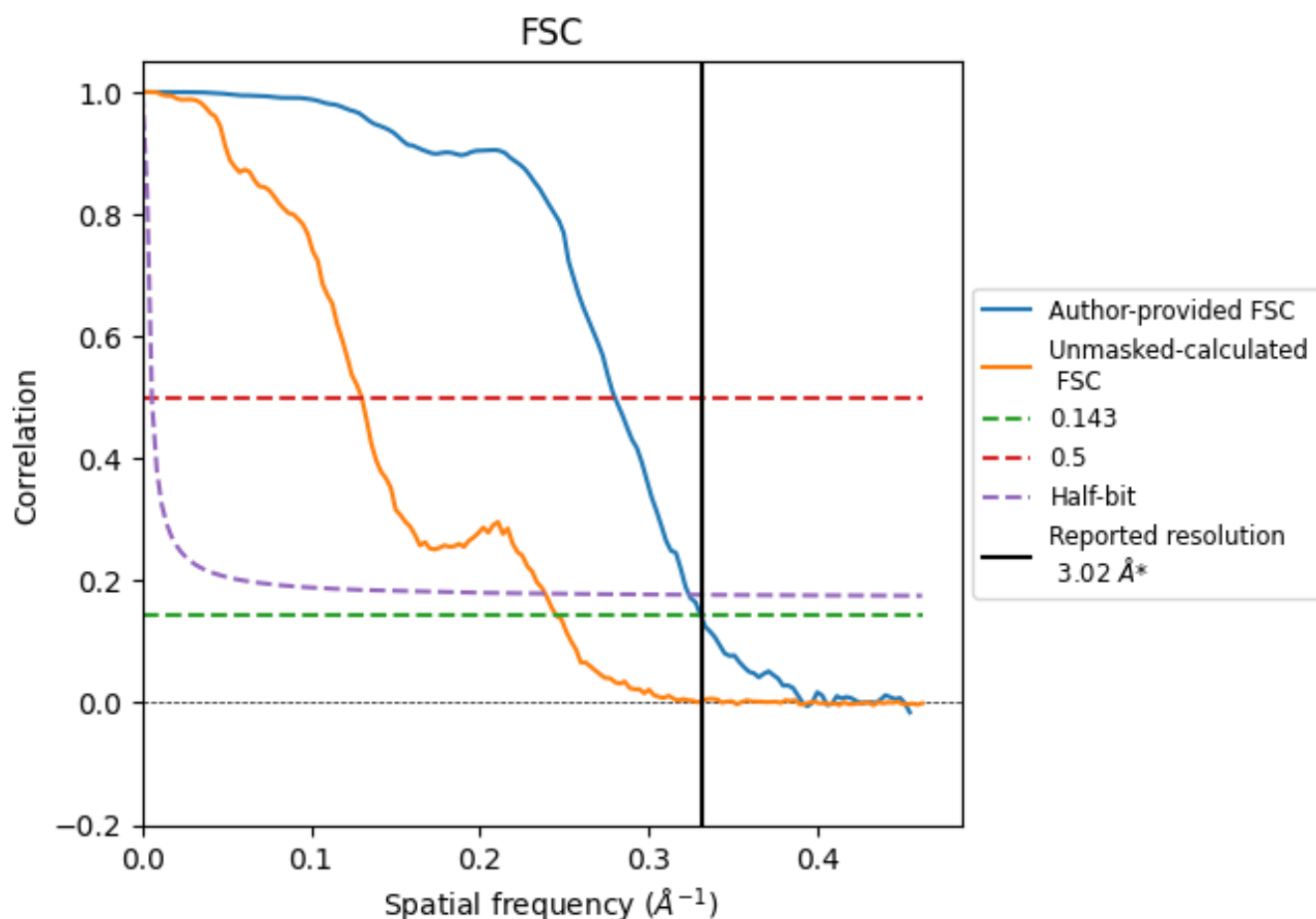


\*Reported resolution corresponds to spatial frequency of 0.331 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

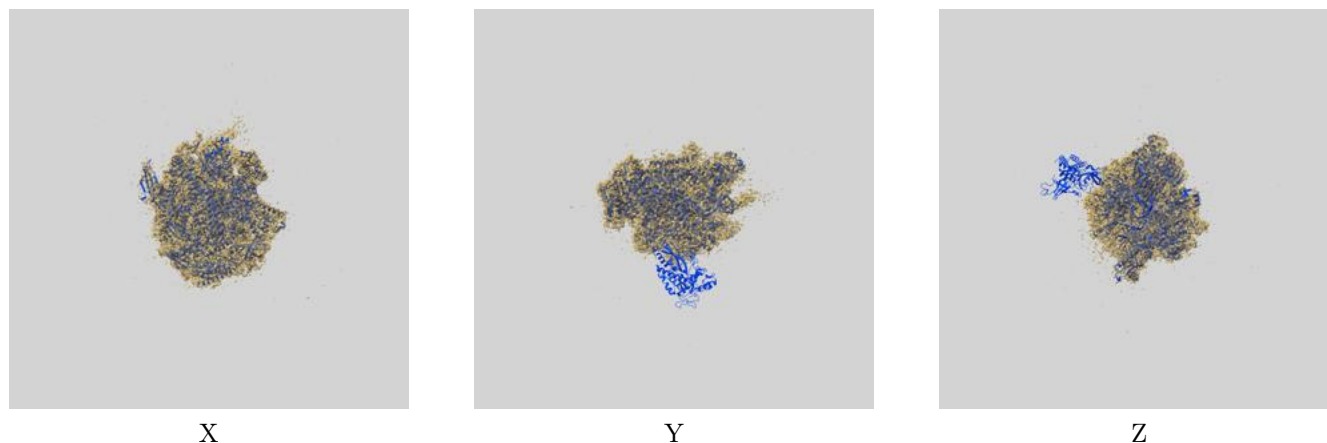
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.02                               | -    | -        |
| Author-provided FSC curve | 3.02                               | 3.57 | 3.09     |
| Unmasked-calculated*      | 4.08                               | 7.70 | 4.19     |

\*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 4.08 differs from the reported value 3.02 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-57322 and PDB model 29RF. Per-residue inclusion information can be found in section [3](#) on page [8](#).

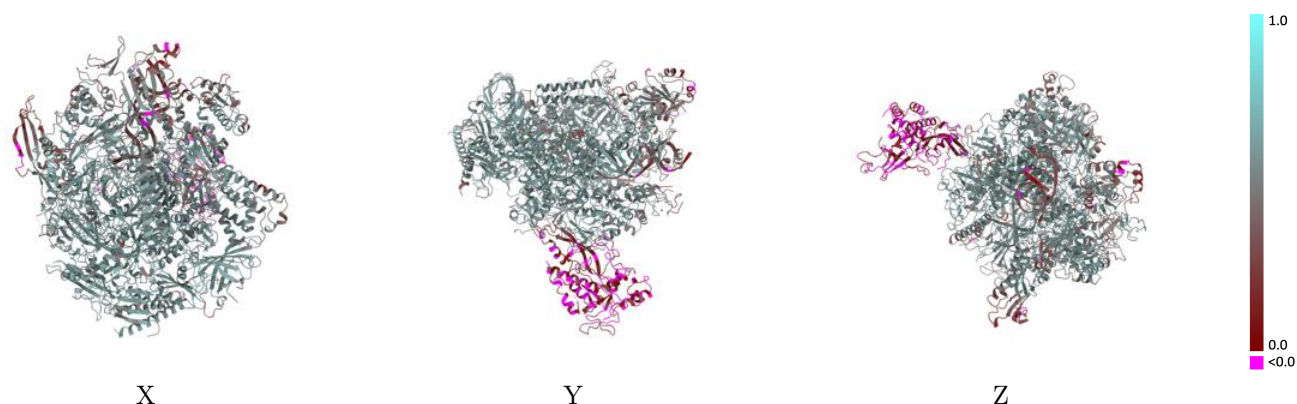
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.25 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.

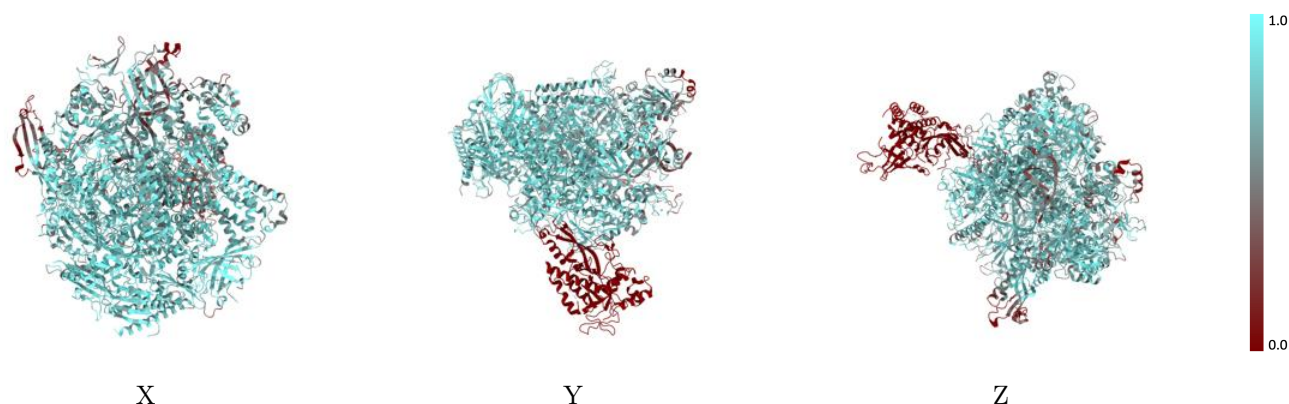


## 9.2 Q-score mapped to coordinate model [i](#)



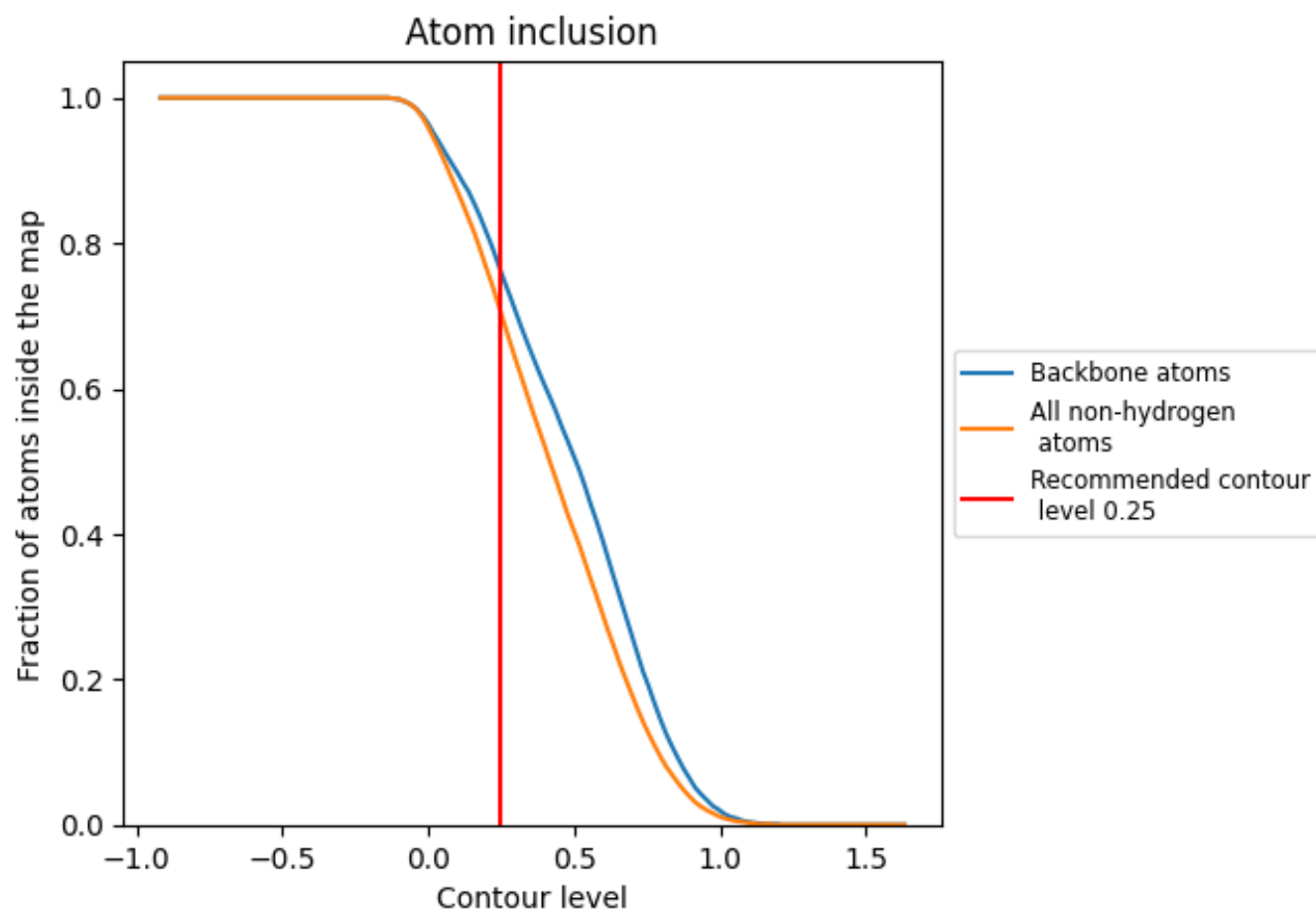
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 70% 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 (0.25) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.7030   |  0.4910   |
| A     |  0.7750   |  0.5350   |
| B     |  0.7640   |  0.5310   |
| C     |  0.8340   |  0.5620   |
| D     |  0.0010   |  0.0320   |
| E     |  0.7350   |  0.5150   |
| F     |  0.8160   |  0.5640   |
| G     |  0.0010   |  0.0930   |
| H     |  0.7790   |  0.5470   |
| I     |  0.6700   |  0.4690   |
| J     |  0.8670   |  0.5750   |
| K     |  0.8250   |  0.5760   |
| L     |  0.6570   |  0.4900   |
| N     |  0.4460   |  0.2790   |
| R     |  0.8390  |  0.5410  |
| T     |  0.5910 |  0.3860 |

