



## wwPDB EM Validation Summary Report ⓘ

Jun 10, 2024 – 12:29 PM JST

PDB ID : 8W8E  
EMDB ID : EMD-37352  
Title : human co-transcriptional RNA capping enzyme RNGTT  
Authors : Li, Y.; Wang, Q.; Xu, Y.; Li, Z.  
Deposited on : 2023-09-02  
Resolution : 3.90 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.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

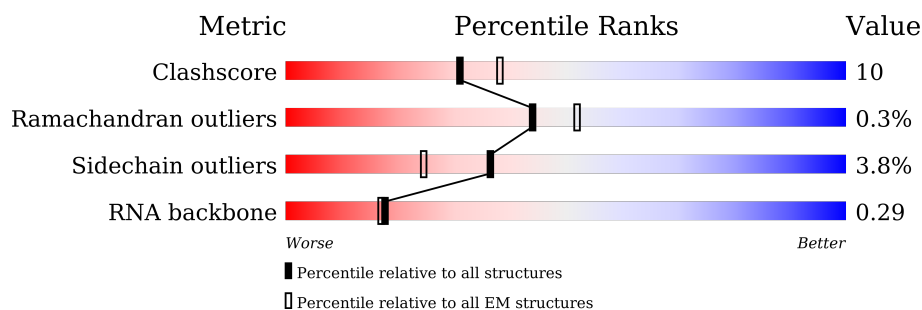
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 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.




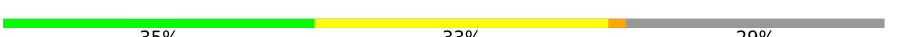

| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 158937                      | 4297                        |
| Ramachandran outliers | 154571                      | 4023                        |
| Sidechain outliers    | 154315                      | 3826                        |
| RNA backbone          | 4643                        | 859                         |

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     | 1970   |                  |
| 2   | B     | 1174   |                  |
| 3   | C     | 271    |                  |
| 4   | D     | 142    |                  |
| 5   | E     | 210    |                  |
| 6   | F     | 127    |                  |
| 7   | G     | 172    |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 8   | H     | 150    |    |
| 9   | I     | 125    |    |
| 10  | J     | 67     |    |
| 11  | K     | 117    |    |
| 12  | L     | 58     |    |
| 13  | N     | 48     |    |
| 14  | P     | 16     |    |
| 15  | T     | 48     |    |
| 16  | U     | 528    |    |
| 17  | V     | 580    |    |
| 18  | W     | 584    |    |
| 19  | X     | 380    |    |
| 20  | Y     | 121    |  |
| 21  | Z     | 1087   |  |
| 22  | a     | 597    |  |

## 2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 50912 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 subunit.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | A     | 1426     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 11299 | 7111 | 2020 | 2099 | 69 |         |       |

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

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 2   | B     | 1133     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 9046  | 5723 | 1594 | 1665 | 64 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | C     | 258      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2072  | 1301 | 353 | 412 | 6 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | D     | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 997   | 629 | 169 | 195 | 4 |         |       |

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | E     | 209      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1721  | 1089 | 300 | 324 | 8 |         |       |

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit F.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | F     | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 658   | 418 | 113 | 122 | 5 |         |       |

- 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     |
|     |       |          | 1305  | 852 | 205 | 240 | 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     | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1186  | 750 | 194 | 237 | 5 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 9   | I     | 117      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 950   | 587 | 169 | 183 | 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     | 67       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 533   | 345 | 90 | 92 | 6 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | K     | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 920   | 593 | 152 | 173 | 2 |         |       |

- Molecule 12 is a protein called RPB12.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 12  | L     | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 389   | 241 | 75 | 67 | 6 |         |       |

- Molecule 13 is a DNA chain called DNA (36-MER).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 13  | N     | 34       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 714   | 333 | 147 | 200 | 34 |         |       |

- Molecule 14 is a RNA chain called RNA (5'-D(\*(GTP))-R(P\*AP\*GP\*AP\*GP\*AP\*GP\*G

P\*GP\*AP\*AP\*CP\*CP\*CP\*AP\*CP\*U)-3').

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 14  | P     | 16       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 347   | 155 | 69 | 107 | 16 |         |       |

- Molecule 15 is a DNA chain called DNA (45-MER).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 15  | T     | 45       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 910   | 432 | 156 | 277 | 45 |         |       |

- Molecule 16 is a protein called Negative elongation factor A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | U     | 183      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1410  | 895 | 239 | 269 | 7 |         |       |

- Molecule 17 is a protein called Negative elongation factor B.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 17  | V     | 550      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4411  | 2825 | 752 | 810 | 24 |         |       |

- Molecule 18 is a protein called Negative elongation factor C/D.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 18  | W     | 532      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3823  | 2419 | 664 | 720 | 20 |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| W     | 7       | SER      | -      | expression tag | UNP Q8IXH7 |
| W     | 8       | ASN      | -      | expression tag | UNP Q8IXH7 |
| W     | 9       | ALA      | -      | expression tag | UNP Q8IXH7 |

- Molecule 19 is a protein called Negative elongation factor E.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 19  | X     | 37       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 293   | 191 | 50 | 51 | 1 |         |       |

- Molecule 20 is a protein called Transcription elongation factor SPT4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | Y     | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 911   | 570 | 159 | 173 | 9 |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| Y     | -3      | GLY      | -      | expression tag | UNP P63272 |
| Y     | -2      | PRO      | -      | expression tag | UNP P63272 |
| Y     | -1      | GLY      | -      | expression tag | UNP P63272 |
| Y     | 0       | SER      | -      | expression tag | UNP P63272 |

- Molecule 21 is a protein called Transcription elongation factor SPT5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 21  | Z     | 360      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2880  | 1835 | 495 | 537 | 13 |         |       |

- Molecule 22 is a protein called mRNA-capping enzyme.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 22  | a     | 506      | Total | C    | N   | O   | S  | 5       | 0     |
|     |       |          | 4096  | 2614 | 710 | 740 | 32 |         |       |

- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 23  | A     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

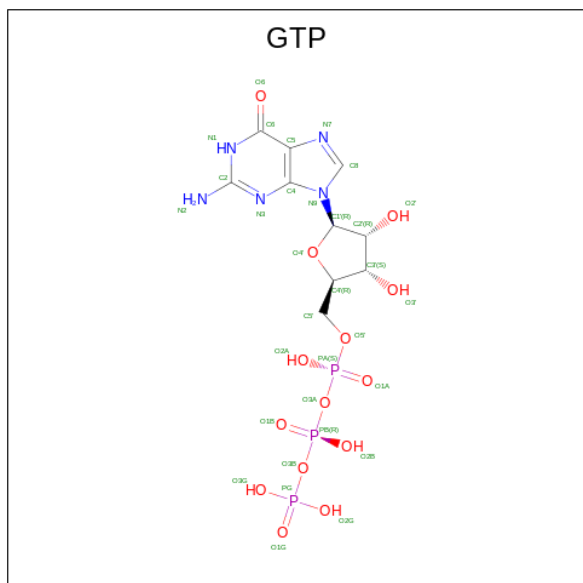
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 24  | A     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 24  | B     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 24  | C     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

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| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 24  | I     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 24  | L     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 24  | Y     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 25 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ) (labeled as "Ligand of Interest" by depositor).



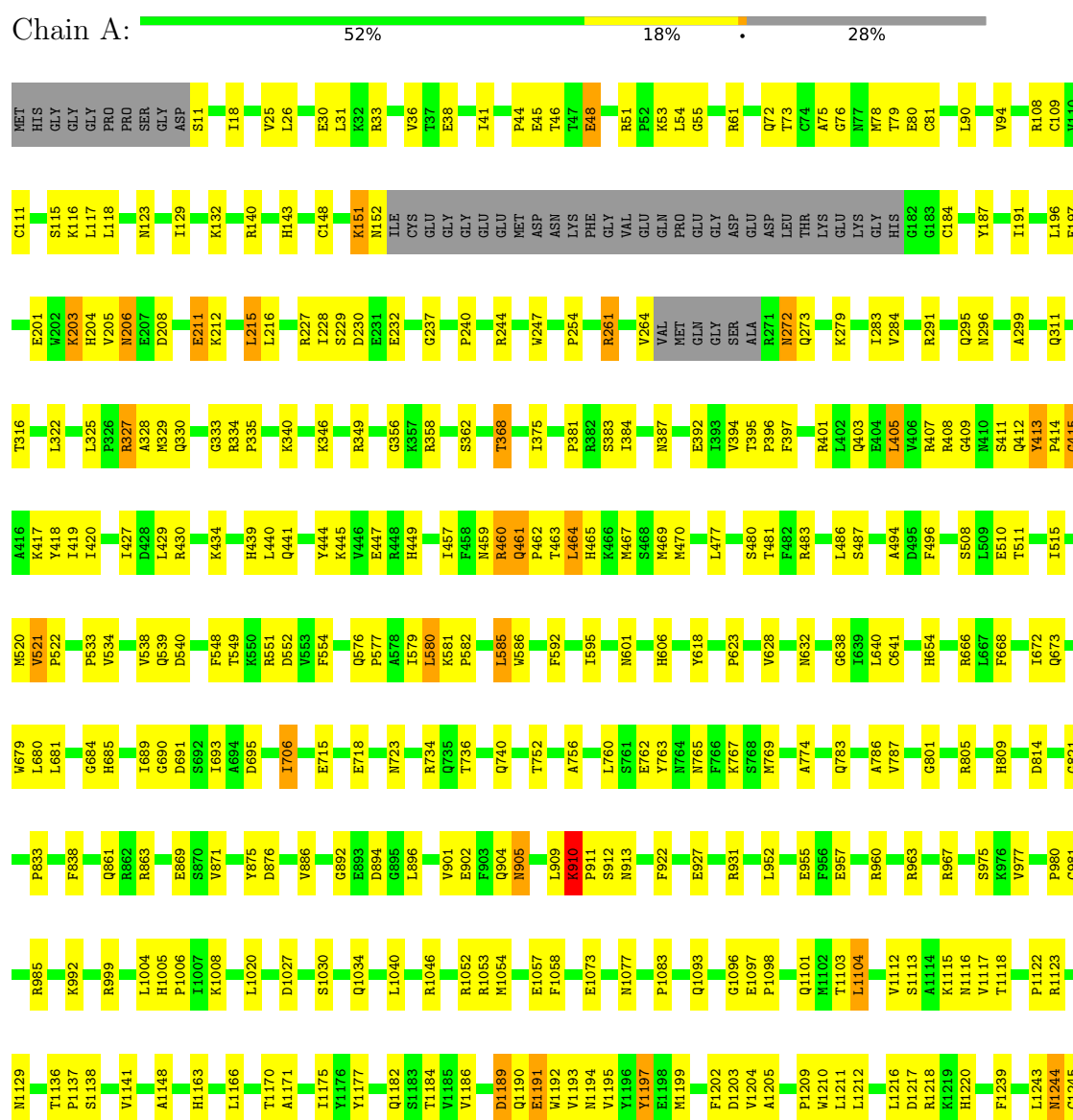
| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 25  | P     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |



### 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 subunit







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

Chain C: 80% 15% 5%



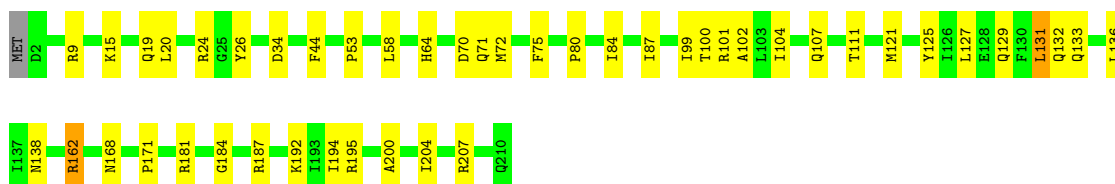
- Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D: 80% 11% 10%



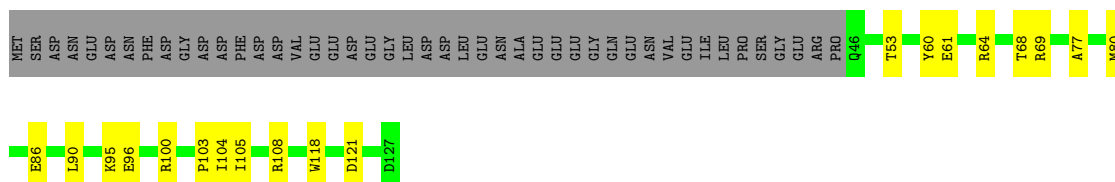
- Molecule 5: DNA-directed RNA polymerase II subunit E

Chain E: 78% 21% 1%




- Molecule 6: DNA-directed RNA polymerase II subunit F

Chain F: 50% 15% 35%



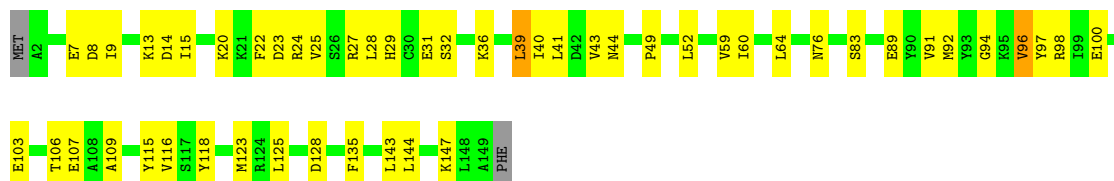
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:  79% 19% ..



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

Chain H:  65% 33% ..




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

Chain I:  73% 19% • 6%




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

Chain J:  81% 18% •



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

Chain K:  81% 16% ..

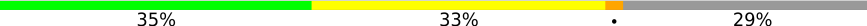


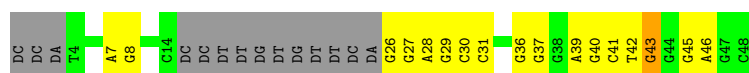
- Molecule 12: RPB12

Chain L:  59% 21% 21%

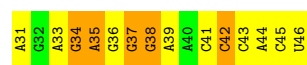
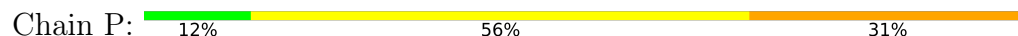


- Molecule 13: DNA (36-MER)

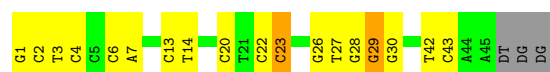
Chain N:  35% 33% • 29%



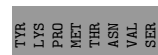
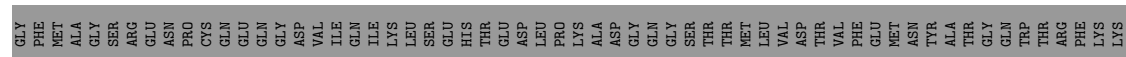
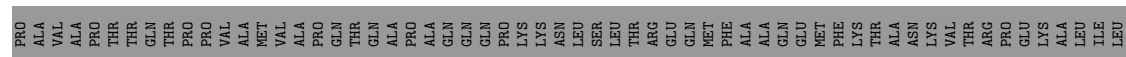
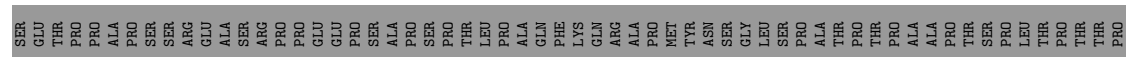
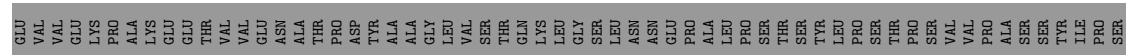
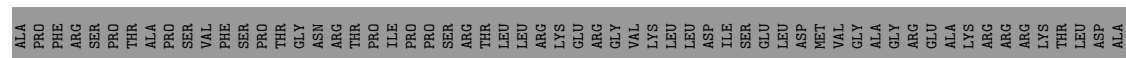
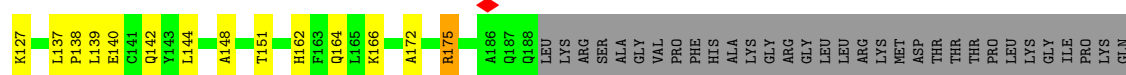
- Molecule 14: RNA (5'-D<sup>\*</sup>(GTP))-R(P<sup>\*</sup>AP<sup>\*</sup>GP<sup>\*</sup>AP<sup>\*</sup>GP<sup>\*</sup>AP<sup>\*</sup>GP<sup>\*</sup>GP<sup>\*</sup>GP<sup>\*</sup>AP<sup>\*</sup>AP<sup>\*</sup>CP<sup>\*</sup>CP<sup>\*</sup>CP<sup>\*</sup>AP<sup>\*</sup>AP<sup>\*</sup>CP<sup>\*</sup>U)-3')



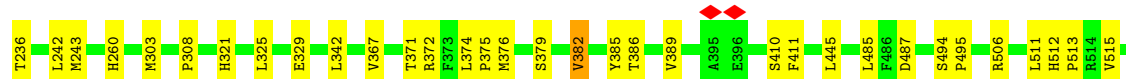
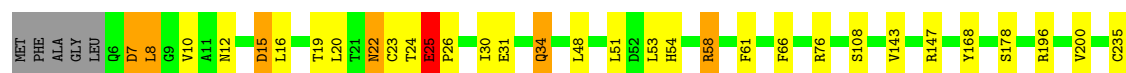
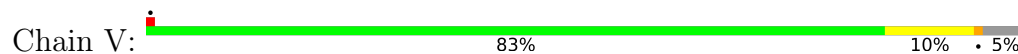
- Molecule 15: DNA (45-MER)



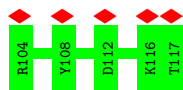
- Molecule 16: Negative elongation factor A



- Molecule 17: Negative elongation factor B

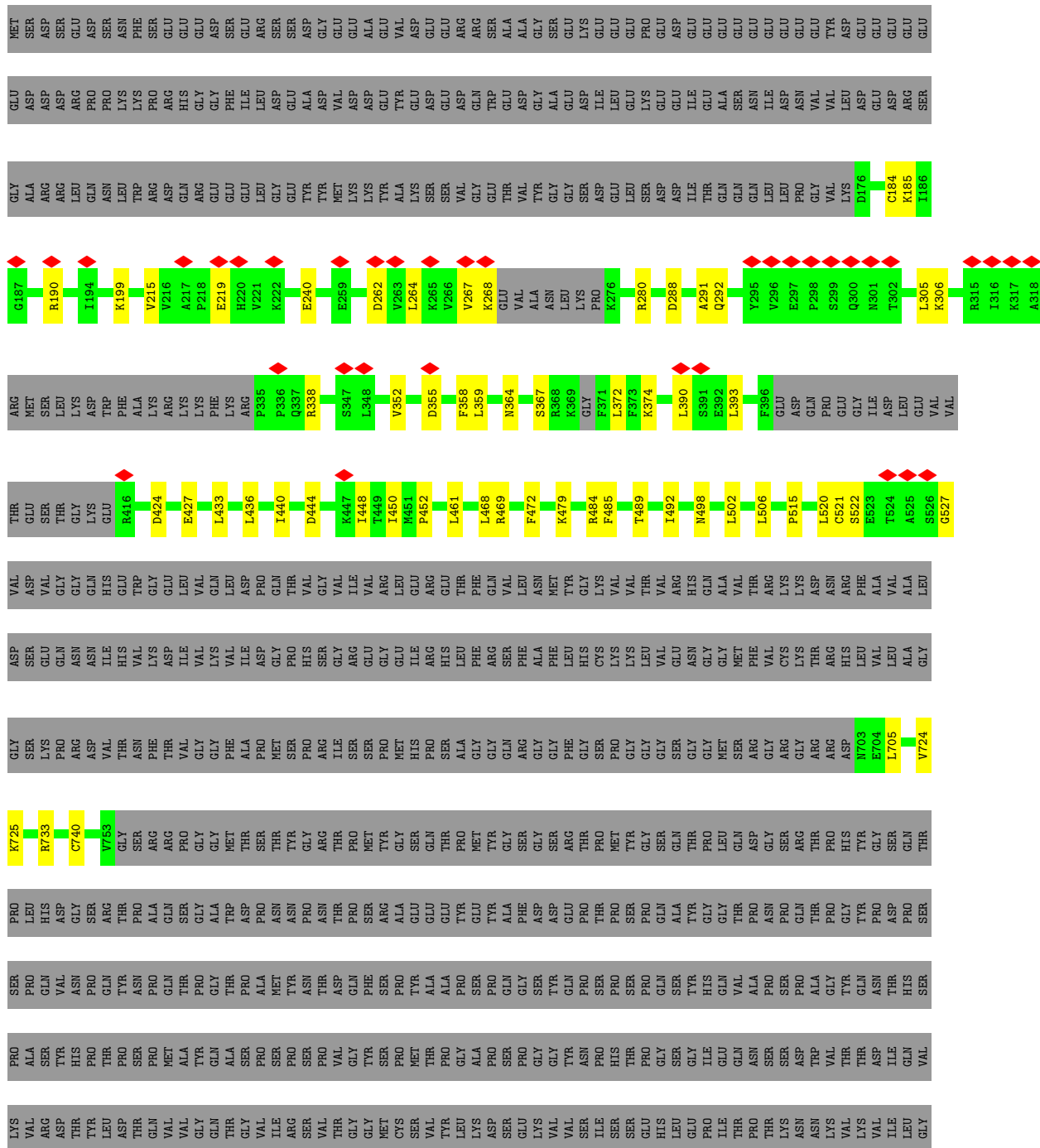






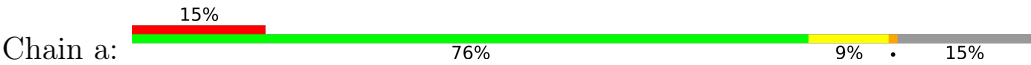
- Molecule 21: Transcription elongation factor SPT5

Chain Z:  28% 5% 67%



GLU ASP  
ASP ARG  
GLU HIS  
GLU ASN  
THR  
ALA  
THR  
GLY  
VAL  
LEU  
LEU  
SER  
ILE  
ASP  
GLY  
GLU  
ASP  
GLY  
ILE  
VAL  
ARG  
MET  
ASP  
LEU  
ASP  
GLU  
GLN  
LEU  
LEU  
LEU  
ILE  
LEU  
ASN  
LEU  
ARG  
PHE  
GLY  
LYS  
LEU  
LEU  
GLU  
ALA

● Molecule 22: mRNA-capping enzyme



MET  
ALA  
HIS  
ASN  
K5  
I6  
R9  
W10  
L11  
N12  
S37  
Q38  
V39  
A40  
E41  
M43  
R44  
K55  
S56  
L57  
K58  
V59  
K60  
M61  
G62  
L63  
E80  
C97  
F113  
ASN  
GLU  
ARG  
ASN  
PRO  
P119  
K144  
M145  
I164  
L188  
W192  
C193  
F194  
E198  
ASP  
GLU  
ASP  
GLU  
ASP

GLU  
ASP  
GLY  
LYS  
LYS  
GLU  
SER  
GLU  
PRO  
GLY  
SER  
SER  
ALA  
SER  
PHE  
GLY  
LYS  
ARG  
ARG  
LYS  
GLU  
ARG  
LEU  
LYS  
G229  
A230  
I231  
F232  
L233  
E234  
G235  
V236  
T237  
V238  
K239  
L250  
H258  
S275  
M276  
D277  
K278  
Q279  
N280  
I281  
K282  
L283  
L284  
D285  
L286  
K287  
P288  
D305  
G306  
T307  
N308

E509  
E326  
F327  
P328  
F329  
K330  
K331  
D332  
L333  
R334  
M335  
H336  
L337  
S338  
V351  
N352  
G353  
Q354  
A355  
R358  
Y362  
N368  
S369  
Q370  
P371  
D374  
G375  
D376  
F377  
N378  
L381  
Q382  
R386  
E387  
I388  
I389  
S390  
P391  
R392  
H393  
E394  
K395  
M396  
K397  
T398  
G399  
L400  
I401  
D402  
K403  
T404  
Q405

F416  
C419  
R422  
E426  
GLY  
ASN  
PHE  
ALA  
ALA  
GLU  
VAL  
SER  
H435  
D454  
P461  
P462  
S463  
L464  
N465  
S466  
V467  
D468  
F469  
R470  
R475  
E479  
G480  
L481  
L482  
P483  
V503  
Y510  
T514  
T515  
R528  
Q529  
R530  
F535  
P536  
I549  
S550  
N551  
P552  
V553  
THR  
LYS

GLU  
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ARG  
CYS  
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ALA  
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THR  
GLU  
LEU  
MET  
PRO  
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PRO  
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LYS  
ARG  
PRO  
ARG  
PRO  
LEU  
THR



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 69000                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | 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                    | 2.963                                   | Depositor |
| Minimum map value                    | -1.420                                  | Depositor |
| Average map value                    | 0.008                                   | Depositor |
| Map value standard deviation         | 0.077                                   | Depositor |
| Recommended contour level            | 0.22                                    | Depositor |
| Map size (Å)                         | 426.88, 426.88, 426.88                  | wwPDB     |
| Map dimensions                       | 320, 320, 320                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.334, 1.334, 1.334                     | 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: GTP, ZN, MG

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     | 0.25         | 0/11509        | 0.51        | 1/15542 (0.0%) |
| 2   | B     | 0.25         | 0/9226         | 0.51        | 1/12451 (0.0%) |
| 3   | C     | 0.24         | 0/2115         | 0.48        | 0/2873         |
| 4   | D     | 0.24         | 0/1011         | 0.45        | 0/1364         |
| 5   | E     | 0.24         | 0/1752         | 0.50        | 0/2366         |
| 6   | F     | 0.23         | 0/668          | 0.50        | 0/901          |
| 7   | G     | 0.25         | 0/1336         | 0.46        | 0/1820         |
| 8   | H     | 0.25         | 0/1207         | 0.52        | 0/1628         |
| 9   | I     | 0.24         | 0/973          | 0.48        | 0/1316         |
| 10  | J     | 0.24         | 0/542          | 0.46        | 0/730          |
| 11  | K     | 0.25         | 0/939          | 0.46        | 0/1271         |
| 12  | L     | 0.24         | 0/395          | 0.58        | 0/524          |
| 13  | N     | 0.57         | 1/804 (0.1%)   | 0.91        | 0/1240         |
| 14  | P     | 0.25         | 0/389          | 0.85        | 0/605          |
| 15  | T     | 0.56         | 0/1015         | 1.06        | 2/1562 (0.1%)  |
| 16  | U     | 0.23         | 0/1434         | 0.47        | 0/1948         |
| 17  | V     | 0.25         | 0/4496         | 0.46        | 0/6074         |
| 18  | W     | 0.26         | 0/3891         | 0.48        | 0/5307         |
| 19  | X     | 0.27         | 0/295          | 0.53        | 0/388          |
| 20  | Y     | 0.23         | 0/927          | 0.48        | 0/1250         |
| 21  | Z     | 0.24         | 0/2928         | 0.48        | 0/3940         |
| 22  | a     | 0.28         | 0/4213         | 0.57        | 4/5687 (0.1%)  |
| All | All   | 0.27         | 1/52065 (0.0%) | 0.53        | 8/70787 (0.0%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 13  | N     | 43  | DG   | N9-C4 | -5.88 | 1.33        | 1.38     |

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

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 22  | a     | 535 | PHE  | CB-CA-C   | 7.84  | 126.08      | 110.40   |
| 1   | A     | 415 | GLY  | C-N-CA    | 6.13  | 137.04      | 121.70   |
| 2   | B     | 631 | GLN  | C-N-CA    | -6.04 | 106.61      | 121.70   |
| 15  | T     | 23  | DC   | O5'-P-OP1 | -5.81 | 100.47      | 105.70   |
| 22  | a     | 284 | LEU  | CA-CB-CG  | 5.70  | 128.40      | 115.30   |

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     | 11299 | 0        | 11416    | 272     | 0            |
| 2   | B     | 9046  | 0        | 9078     | 206     | 0            |
| 3   | C     | 2072  | 0        | 2016     | 35      | 0            |
| 4   | D     | 997   | 0        | 953      | 11      | 0            |
| 5   | E     | 1721  | 0        | 1737     | 31      | 0            |
| 6   | F     | 658   | 0        | 684      | 13      | 0            |
| 7   | G     | 1305  | 0        | 1267     | 22      | 0            |
| 8   | H     | 1186  | 0        | 1147     | 40      | 0            |
| 9   | I     | 950   | 0        | 880      | 18      | 0            |
| 10  | J     | 533   | 0        | 557      | 9       | 0            |
| 11  | K     | 920   | 0        | 942      | 15      | 0            |
| 12  | L     | 389   | 0        | 395      | 10      | 0            |
| 13  | N     | 714   | 0        | 379      | 22      | 0            |
| 14  | P     | 347   | 0        | 175      | 10      | 0            |
| 15  | T     | 910   | 0        | 507      | 21      | 0            |
| 16  | U     | 1410  | 0        | 1455     | 36      | 0            |
| 17  | V     | 4411  | 0        | 4503     | 67      | 0            |
| 18  | W     | 3823  | 0        | 3520     | 89      | 0            |
| 19  | X     | 293   | 0        | 340      | 17      | 0            |
| 20  | Y     | 911   | 0        | 905      | 12      | 0            |
| 21  | Z     | 2880  | 0        | 2925     | 38      | 0            |
| 22  | a     | 4096  | 0        | 4076     | 0       | 0            |
| 23  | A     | 1     | 0        | 0        | 0       | 0            |
| 24  | A     | 2     | 0        | 0        | 0       | 0            |
| 24  | B     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 24  | C     | 1     | 0        | 0        | 0       | 0            |
| 24  | I     | 2     | 0        | 0        | 0       | 0            |
| 24  | L     | 1     | 0        | 0        | 0       | 0            |
| 24  | Y     | 1     | 0        | 0        | 0       | 0            |
| 25  | P     | 32    | 0        | 11       | 0       | 0            |
| All | All   | 50912 | 0        | 49868    | 819     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 819 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) |
|------------------|------------------|--------------------------|-------------------|
| 18:W:404:ALA:HB1 | 18:W:407:LEU:HB3 | 1.30                     | 1.06              |
| 17:V:54:HIS:HA   | 18:W:129:PRO:HG2 | 1.40                     | 1.02              |
| 2:B:630:LYS:C    | 2:B:632:LYS:H    | 1.64                     | 1.00              |
| 13:N:43:DG:N2    | 15:T:6:DC:N3     | 2.11                     | 0.96              |
| 1:A:1115:LYS:HE3 | 1:A:1339:ASP:HA  | 1.47                     | 0.96              |

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     | 1418/1970 (72%) | 1308 (92%) | 106 (8%) | 4 (0%)   | 41          | 75  |
| 2   | B     | 1123/1174 (96%) | 1054 (94%) | 68 (6%)  | 1 (0%)   | 51          | 84  |
| 3   | C     | 254/271 (94%)   | 248 (98%)  | 6 (2%)   | 0        | 100         | 100 |
| 4   | D     | 126/142 (89%)   | 121 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 5   | E     | 207/210 (99%)   | 199 (96%)  | 8 (4%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 6   | F     | 80/127 (63%)    | 79 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 7   | G     | 169/172 (98%)   | 163 (96%)  | 6 (4%)   | 0        | 100         | 100 |
| 8   | H     | 146/150 (97%)   | 138 (94%)  | 8 (6%)   | 0        | 100         | 100 |
| 9   | I     | 115/125 (92%)   | 108 (94%)  | 7 (6%)   | 0        | 100         | 100 |
| 10  | J     | 65/67 (97%)     | 64 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 11  | K     | 113/117 (97%)   | 110 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 12  | L     | 44/58 (76%)     | 42 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 16  | U     | 181/528 (34%)   | 178 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 17  | V     | 548/580 (94%)   | 529 (96%)  | 18 (3%)  | 1 (0%)   | 47          | 79  |
| 18  | W     | 530/584 (91%)   | 462 (87%)  | 62 (12%) | 6 (1%)   | 14          | 51  |
| 19  | X     | 35/380 (9%)     | 35 (100%)  | 0        | 0        | 100         | 100 |
| 20  | Y     | 114/121 (94%)   | 113 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 21  | Z     | 348/1087 (32%)  | 335 (96%)  | 13 (4%)  | 0        | 100         | 100 |
| 22  | a     | 503/597 (84%)   | 457 (91%)  | 42 (8%)  | 4 (1%)   | 19          | 57  |
| All | All   | 6119/8460 (72%) | 5743 (94%) | 360 (6%) | 16 (0%)  | 44          | 75  |

5 of 16 Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 910  | LYS  |
| 1   | A     | 1205 | ALA  |
| 17  | V     | 25   | GLU  |
| 18  | W     | 400  | GLU  |
| 18  | W     | 401  | ASN  |

### 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     | 1255/1749 (72%) | 1193 (95%) | 62 (5%)  | 25          | 54 |
| 2   | B     | 989/1027 (96%)  | 956 (97%)  | 33 (3%)  | 38          | 63 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 3   | C     | 235/248 (95%)   | 232 (99%)  | 3 (1%)   | 69          | 82  |
| 4   | D     | 104/126 (82%)   | 104 (100%) | 0        | 100         | 100 |
| 5   | E     | 191/192 (100%)  | 186 (97%)  | 5 (3%)   | 46          | 68  |
| 6   | F     | 71/111 (64%)    | 70 (99%)   | 1 (1%)   | 67          | 81  |
| 7   | G     | 138/153 (90%)   | 130 (94%)  | 8 (6%)   | 20          | 50  |
| 8   | H     | 129/131 (98%)   | 124 (96%)  | 5 (4%)   | 32          | 59  |
| 9   | I     | 105/112 (94%)   | 101 (96%)  | 4 (4%)   | 33          | 59  |
| 10  | J     | 56/56 (100%)    | 54 (96%)   | 2 (4%)   | 35          | 61  |
| 11  | K     | 104/106 (98%)   | 101 (97%)  | 3 (3%)   | 42          | 65  |
| 12  | L     | 43/55 (78%)     | 43 (100%)  | 0        | 100         | 100 |
| 16  | U     | 158/451 (35%)   | 156 (99%)  | 2 (1%)   | 69          | 82  |
| 17  | V     | 493/515 (96%)   | 483 (98%)  | 10 (2%)  | 55          | 74  |
| 18  | W     | 359/511 (70%)   | 347 (97%)  | 12 (3%)  | 38          | 63  |
| 19  | X     | 33/331 (10%)    | 29 (88%)   | 4 (12%)  | 5           | 24  |
| 20  | Y     | 102/105 (97%)   | 102 (100%) | 0        | 100         | 100 |
| 21  | Z     | 319/940 (34%)   | 318 (100%) | 1 (0%)   | 92          | 95  |
| 22  | a     | 456/534 (85%)   | 405 (89%)  | 51 (11%) | 6           | 27  |
| All | All   | 5340/7453 (72%) | 5134 (96%) | 206 (4%) | 36          | 59  |

5 of 206 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | H     | 96  | VAL  |
| 18  | W     | 264 | GLU  |
| 22  | a     | 510 | TYR  |
| 9   | I     | 119 | CYS  |
| 17  | V     | 15  | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | V     | 22  | ASN  |
| 22  | a     | 465 | ASN  |
| 17  | V     | 119 | HIS  |
| 20  | Y     | 12  | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1457 | ASN  |

### 5.3.3 RNA [i](#)

| Mol | Chain | Analysed    | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 14  | P     | 15/16 (93%) | 10 (66%)          | 0               |

5 of 10 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | P     | 33  | A    |
| 14  | P     | 34  | G    |
| 14  | P     | 35  | A    |
| 14  | P     | 36  | G    |
| 14  | P     | 37  | G    |

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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 |
| 25  | GTP  | P     | 101 | 14   | 26,34,34     | 1.12 | 2 (7%)   | 32,54,54    | 1.85 | 7 (21%)  |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 25  | GTP  | P     | 101 | 14   | -       | 5/18/38/38 | 0/3/3/3 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 25  | P     | 101 | GTP  | C5-C6 | -3.98 | 1.39        | 1.47     |
| 25  | P     | 101 | GTP  | C2-N3 | 2.15  | 1.38        | 1.33     |

The worst 5 of 7 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 25  | P     | 101 | GTP  | PA-O3A-PB | -5.42 | 114.23      | 132.83   |
| 25  | P     | 101 | GTP  | PB-O3B-PG | -4.87 | 116.11      | 132.83   |
| 25  | P     | 101 | GTP  | C5-C6-N1  | 3.16  | 119.53      | 113.95   |
| 25  | P     | 101 | GTP  | C8-N7-C5  | 3.04  | 108.78      | 102.99   |
| 25  | P     | 101 | GTP  | C2-N1-C6  | -2.79 | 119.97      | 125.10   |

There are no chirality outliers.

All (5) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | P     | 101 | GTP  | C5'-O5'-PA-O1A  |
| 25  | P     | 101 | GTP  | C5'-O5'-PA-O2A  |
| 25  | P     | 101 | GTP  | O4'-C4'-C5'-O5' |
| 25  | P     | 101 | GTP  | C3'-C4'-C5'-O5' |
| 25  | P     | 101 | GTP  | C5'-O5'-PA-O3A  |

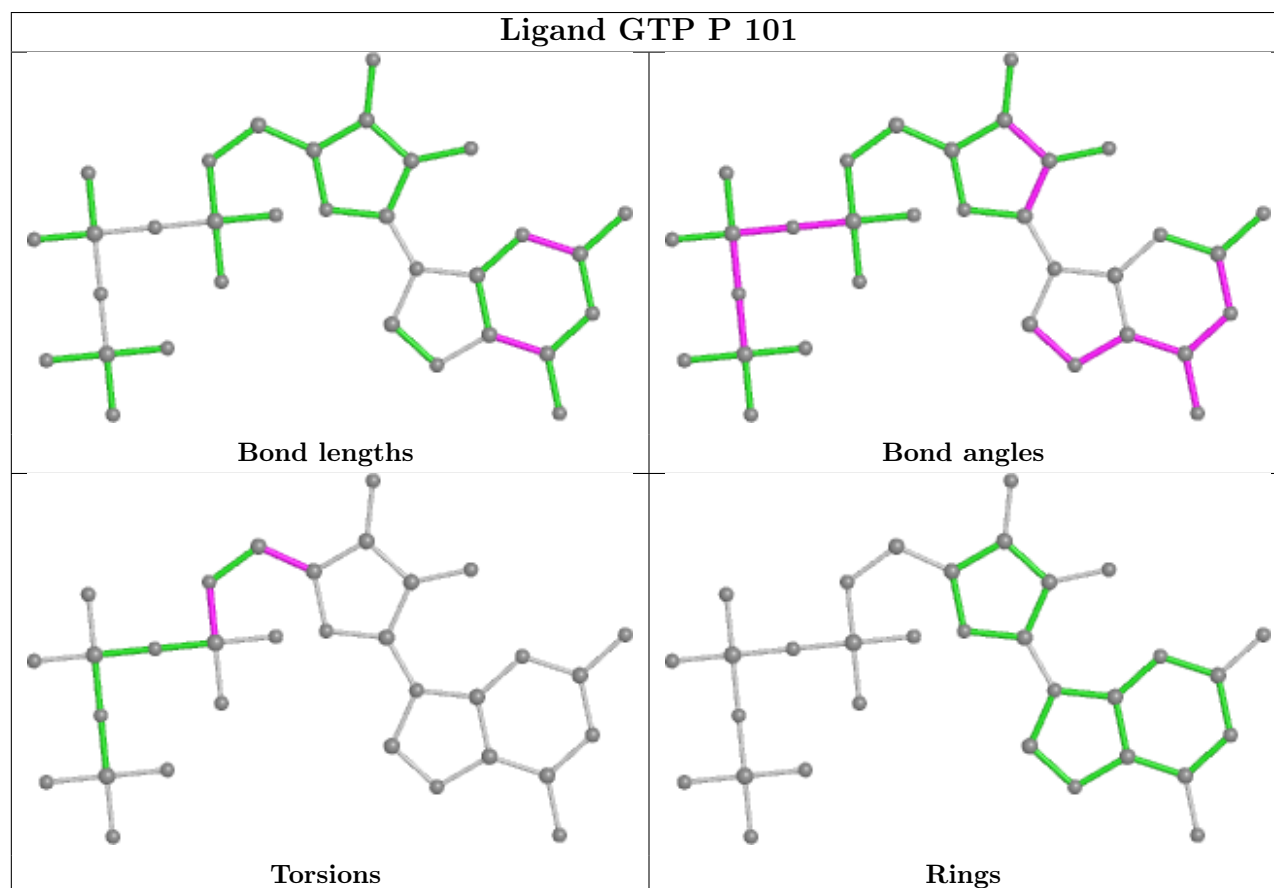
There are no ring outliers.

No monomer is involved in short contacts.

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.

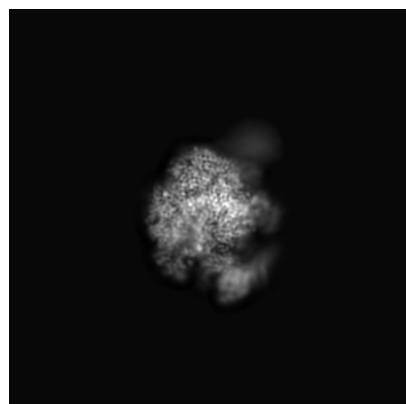
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37352. These allow visual inspection of the internal detail of the map and identification of artifacts.

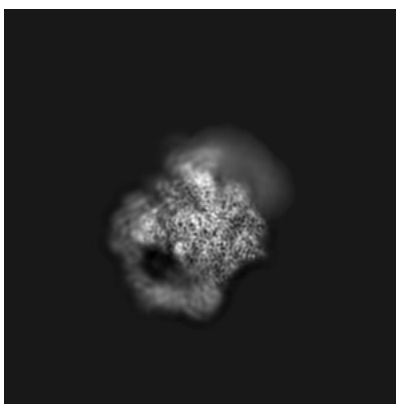
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

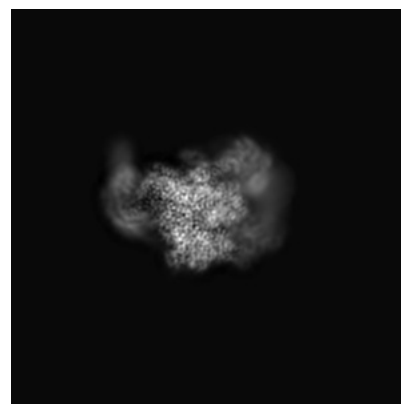
#### 6.1.1 Primary map



X

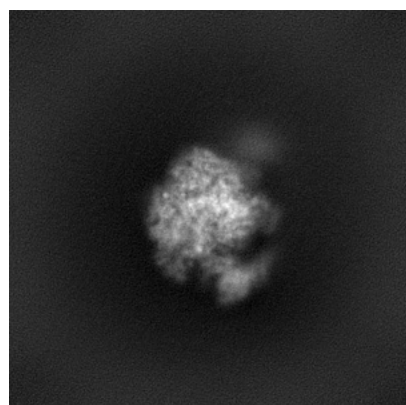


Y

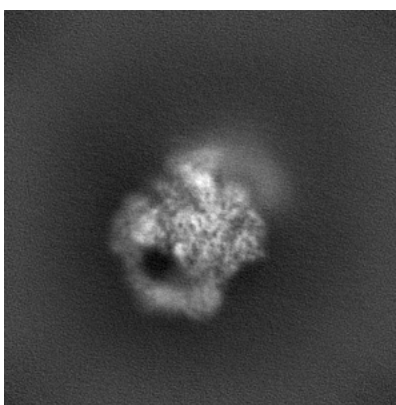


Z

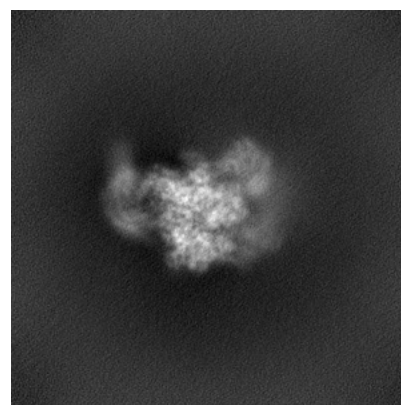
#### 6.1.2 Raw map



X



Y

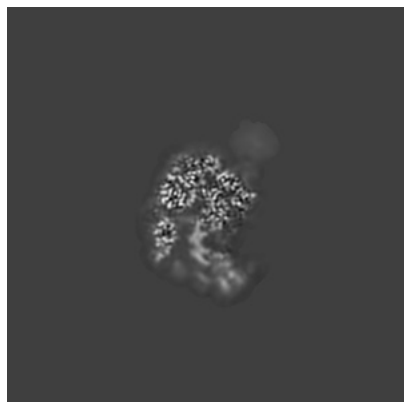


Z

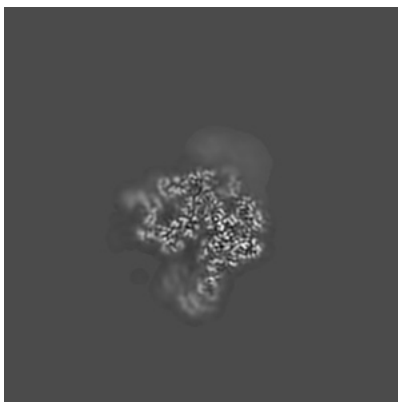
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

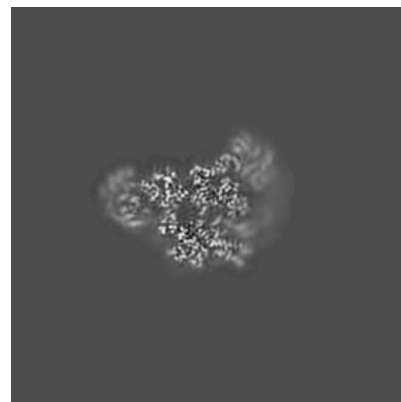
### 6.2.1 Primary map



X Index: 160

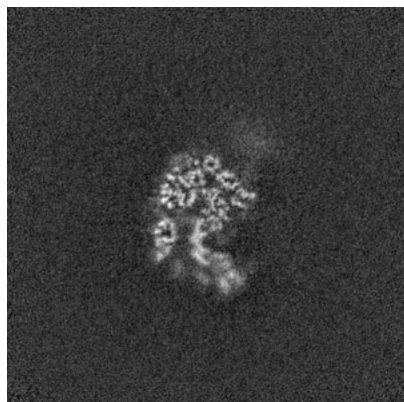


Y Index: 160

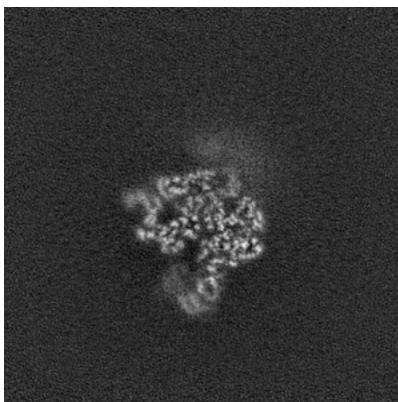


Z Index: 160

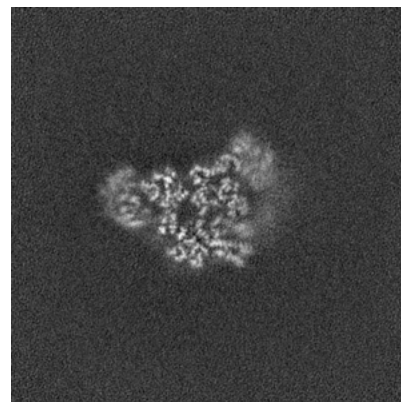
### 6.2.2 Raw map



X Index: 160



Y Index: 160

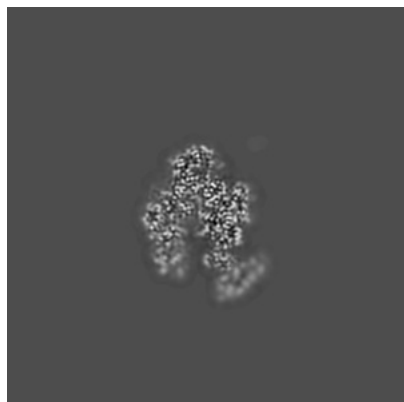


Z Index: 160

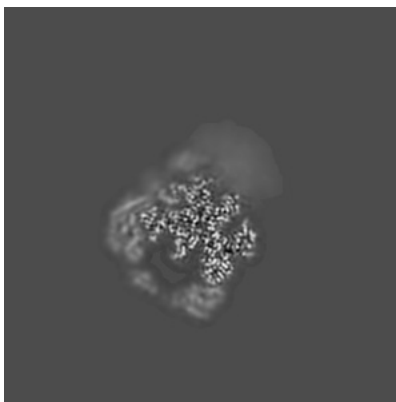
The images above show central slices of the map in three orthogonal directions.

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

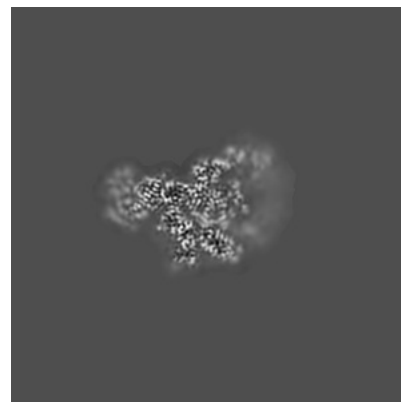
### 6.3.1 Primary map



X Index: 150

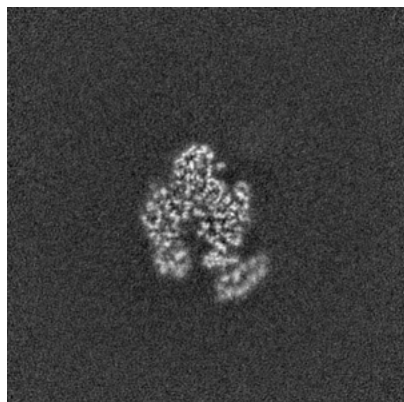


Y Index: 173

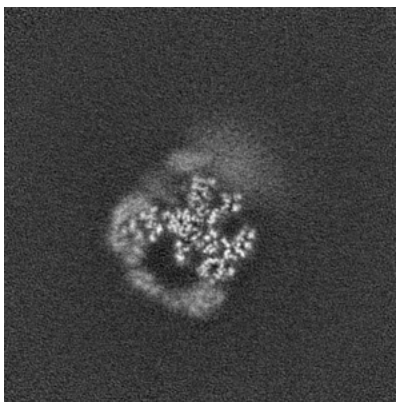


Z Index: 166

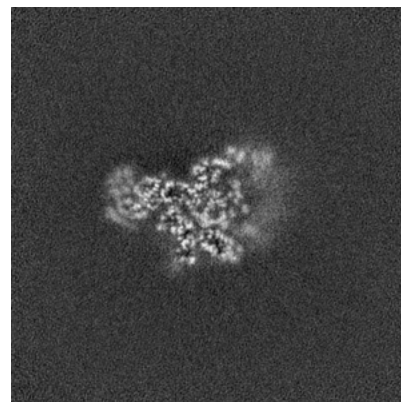
### 6.3.2 Raw map



X Index: 148



Y Index: 176

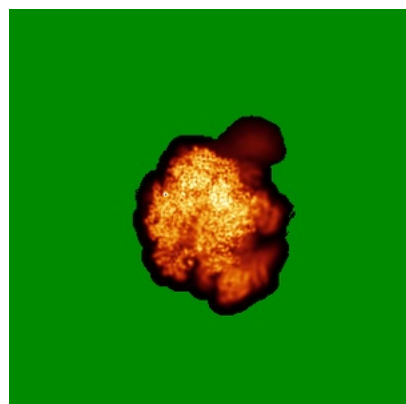


Z Index: 166

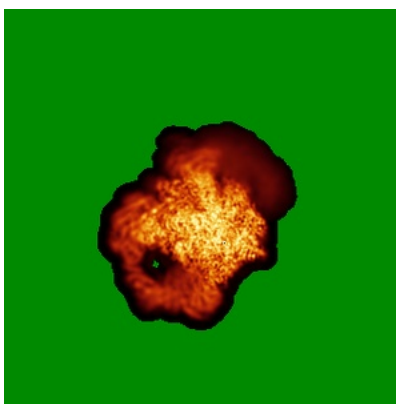
The images above show the largest variance slices of the map in three orthogonal directions.

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

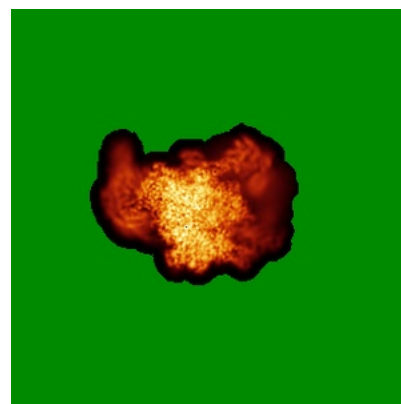
### 6.4.1 Primary map



X

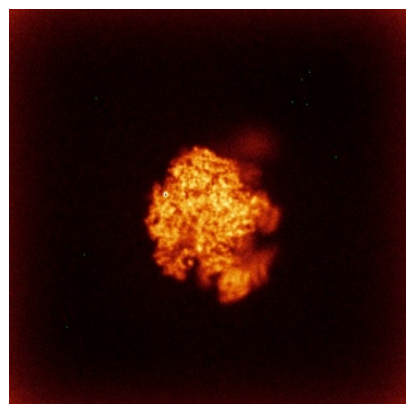


Y

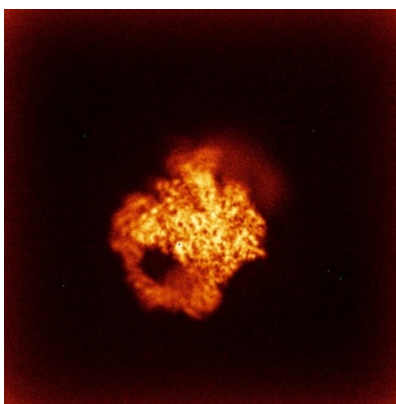


Z

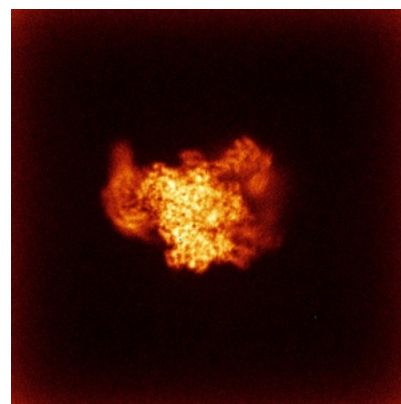
### 6.4.2 Raw map



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.

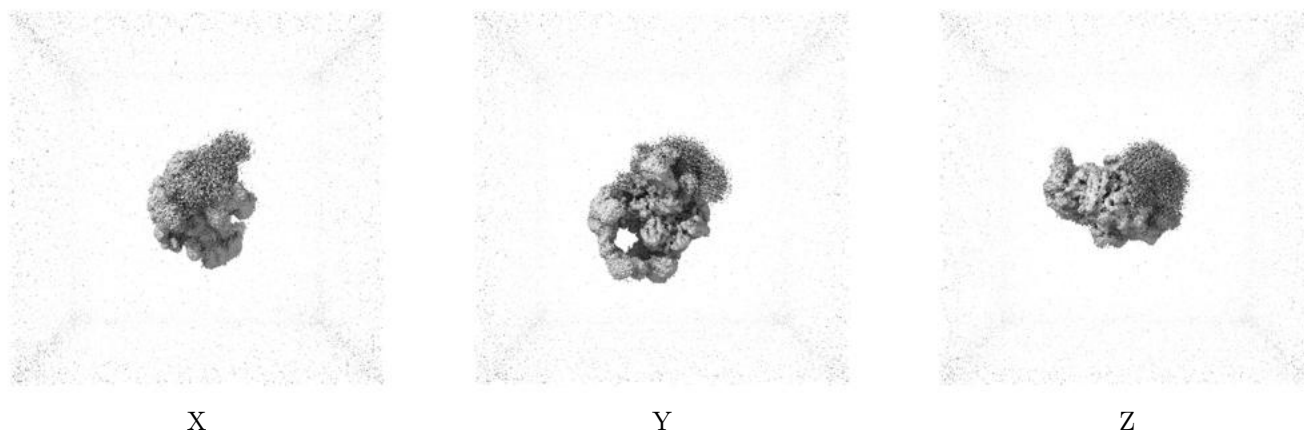
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.22. 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](#)

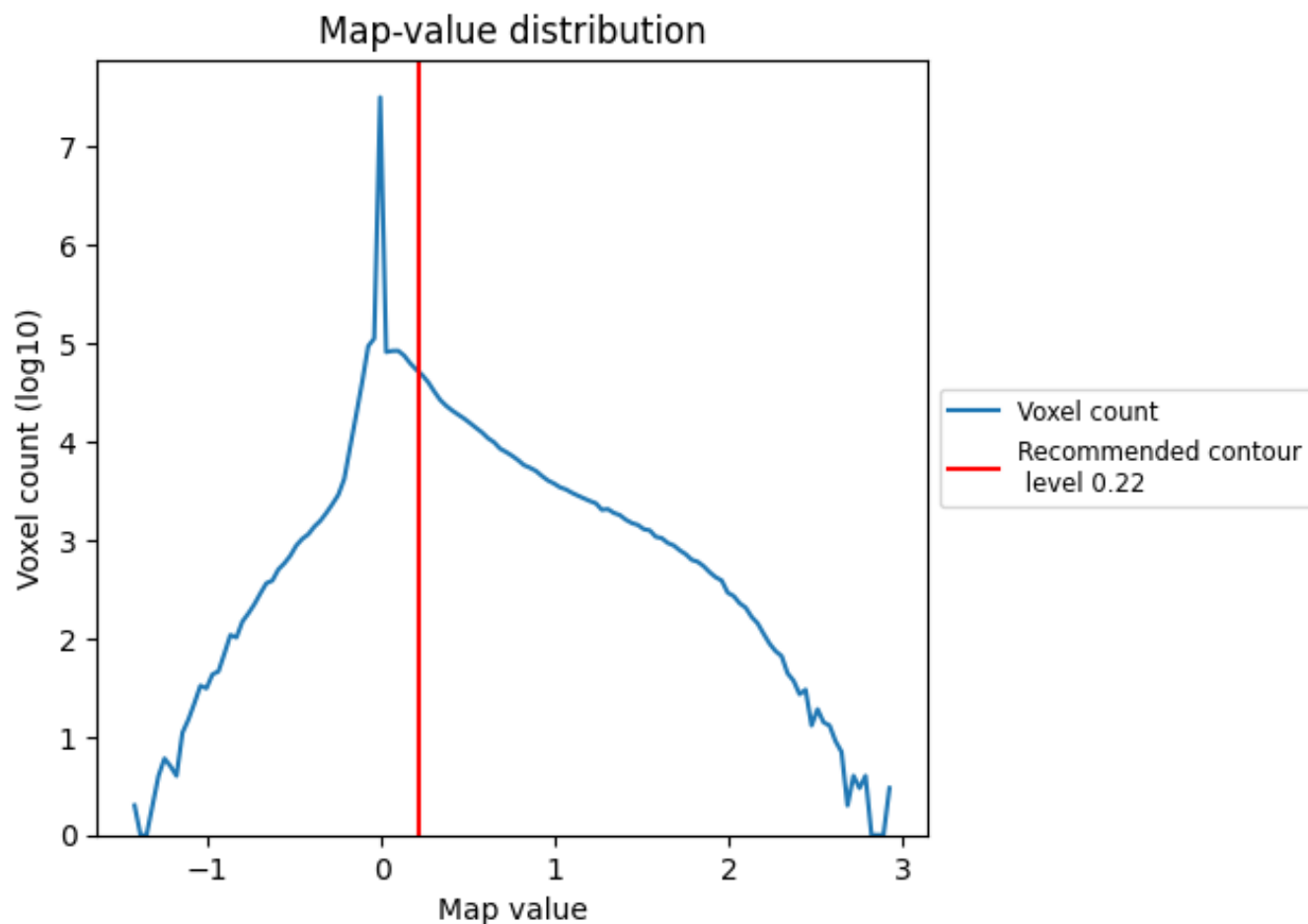
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

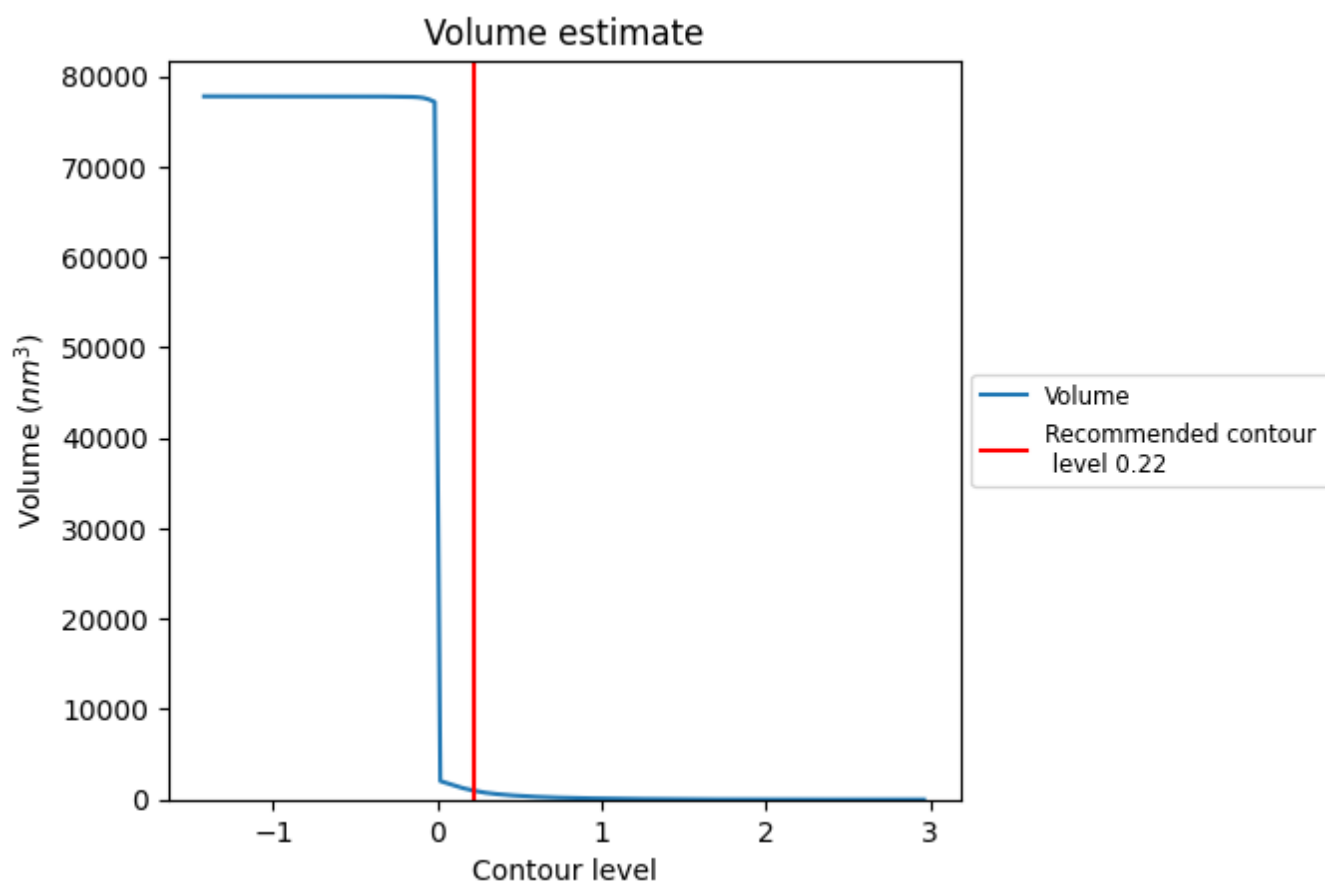
This section contains the results of statistical analysis of the map.

### 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](#)

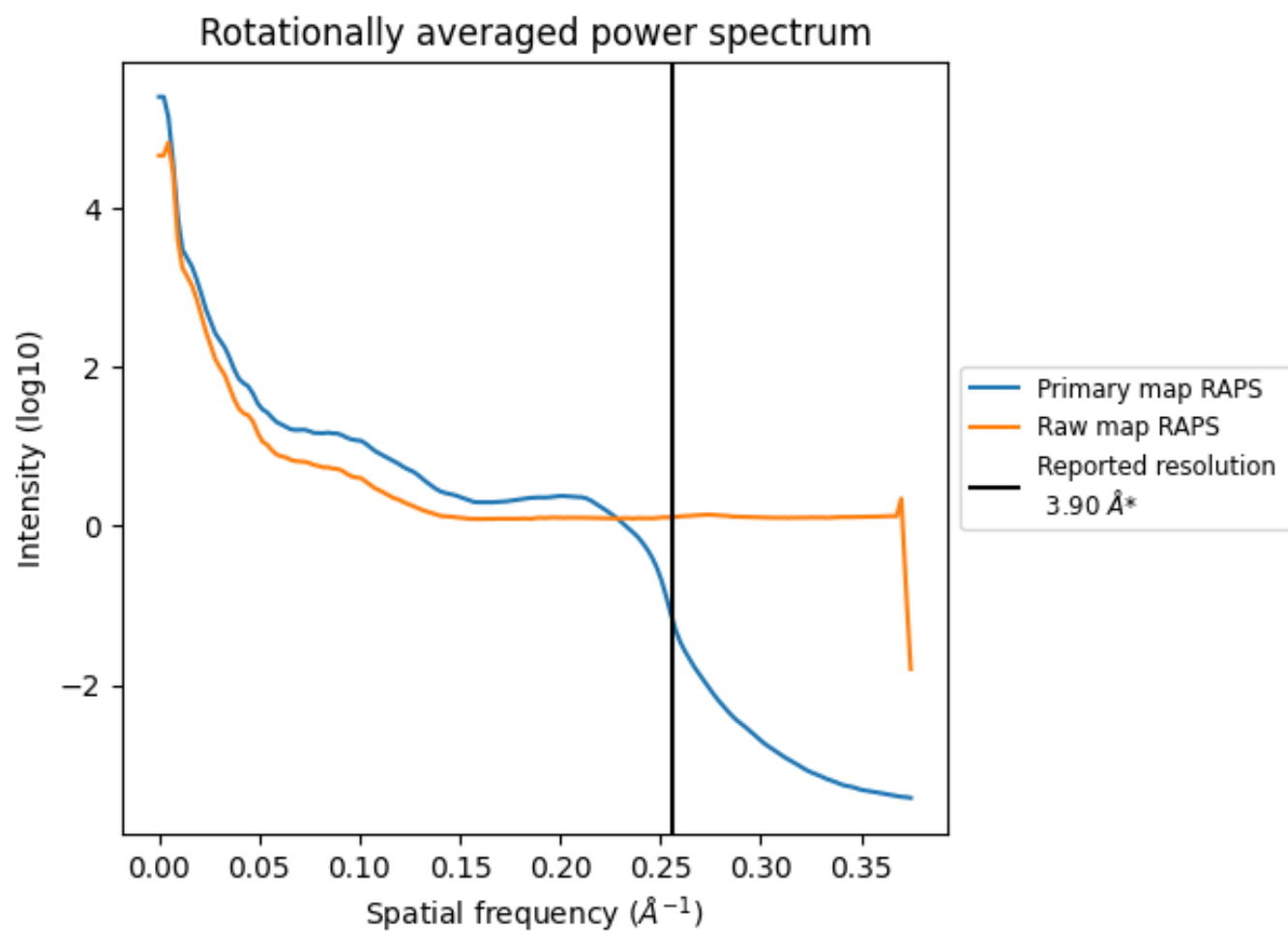


The volume at the recommended contour level is 991  $\text{nm}^3$ ; this corresponds to an approximate mass of 896 kDa.

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 ⓘ

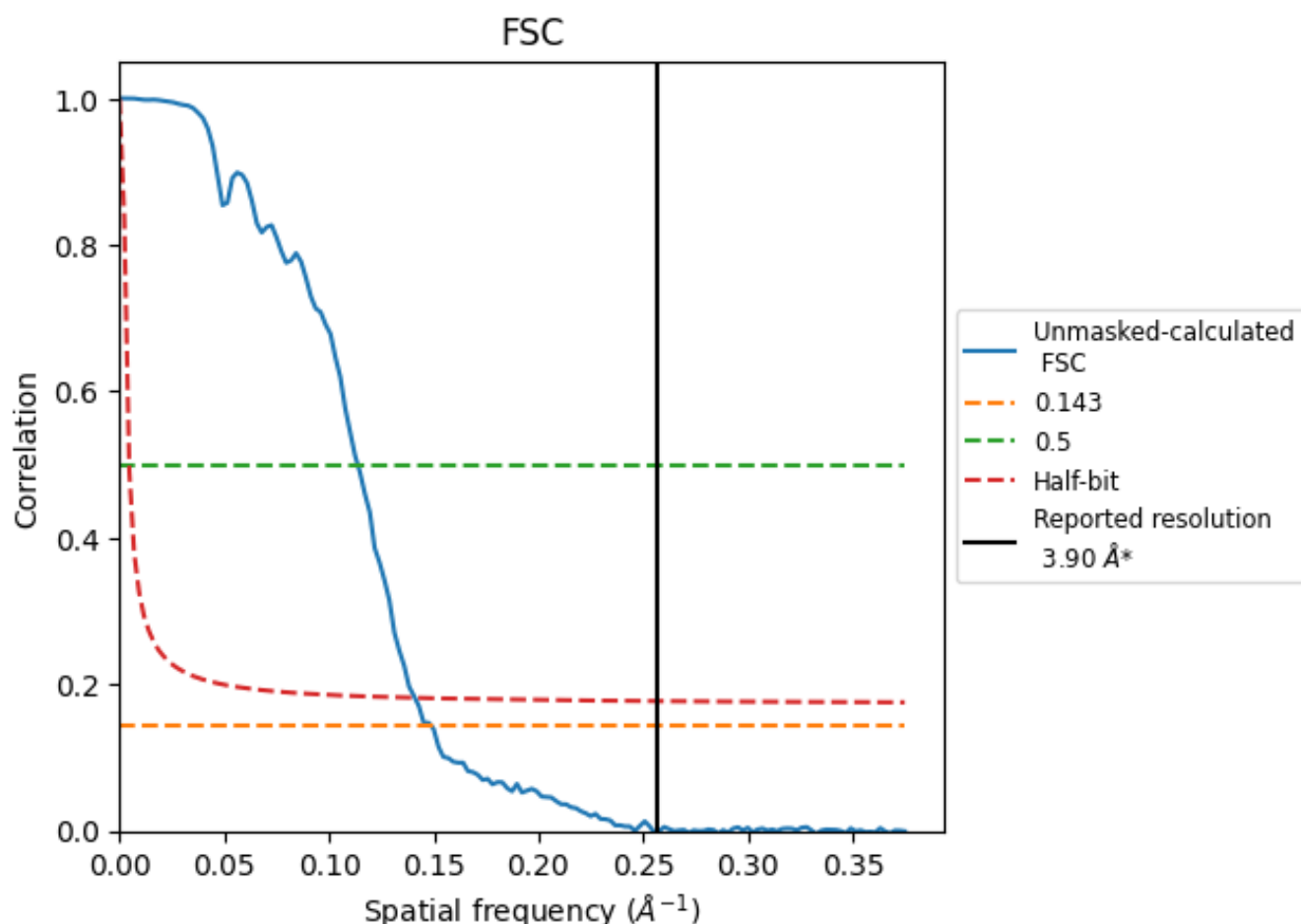


\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>

## 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 0.256 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

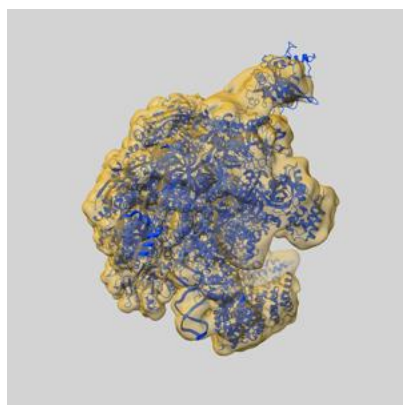
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.90                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 6.72                               | 8.80 | 7.10     |

\*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 6.72 differs from the reported value 3.9 by more than 10 %

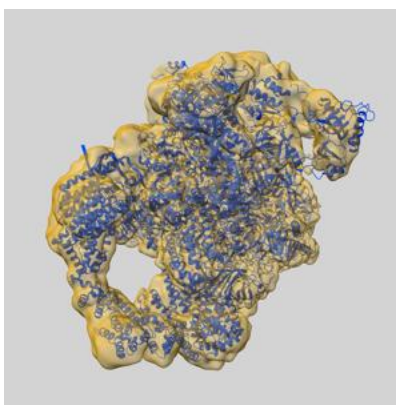
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37352 and PDB model 8W8E. Per-residue inclusion information can be found in section [3](#) on page [9](#).

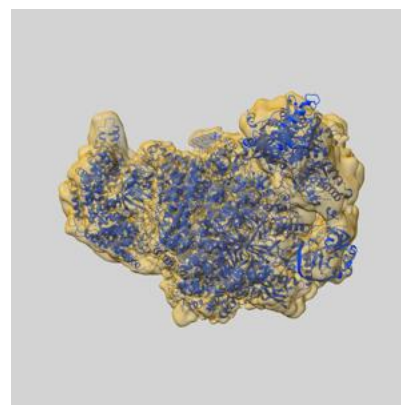
### 9.1 Map-model overlay [i](#)



X



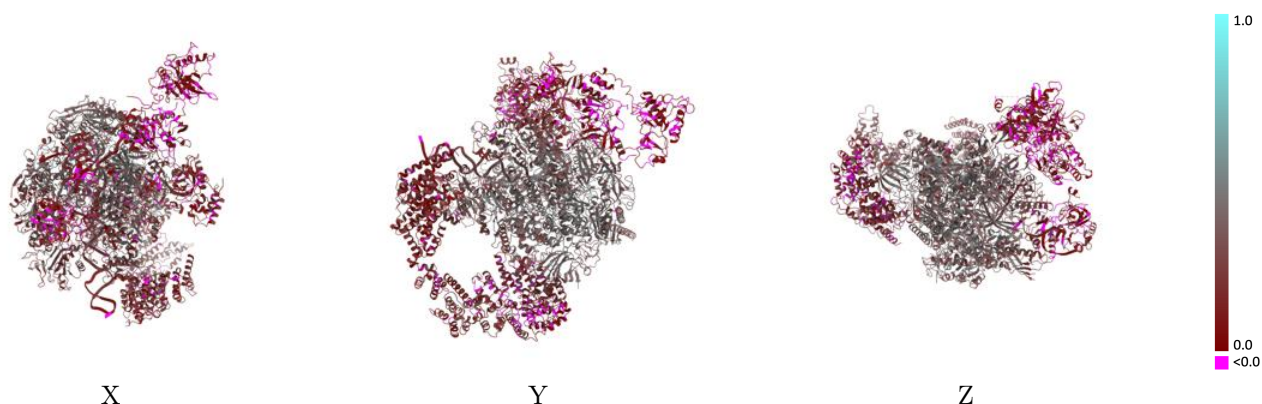
Y



Z

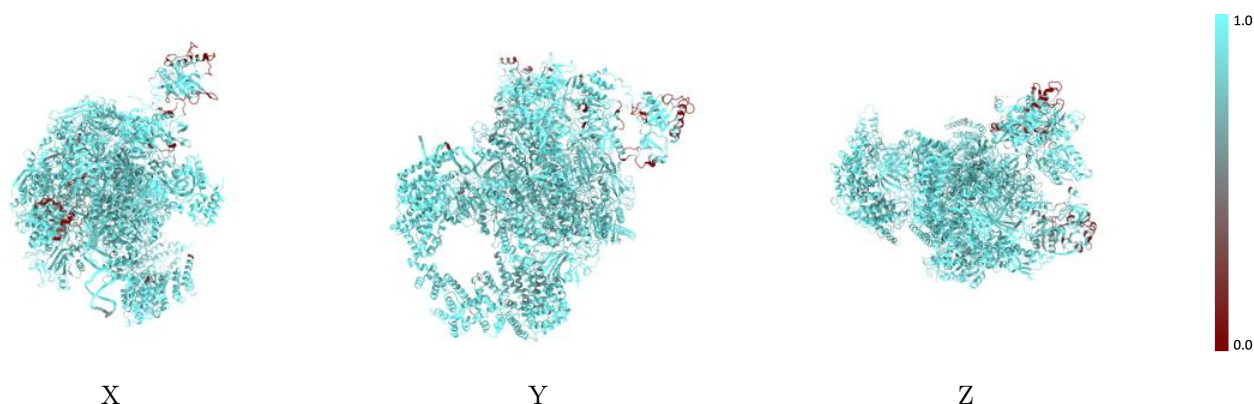
The images above show the 3D surface view of the map at the recommended contour level 0.22 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



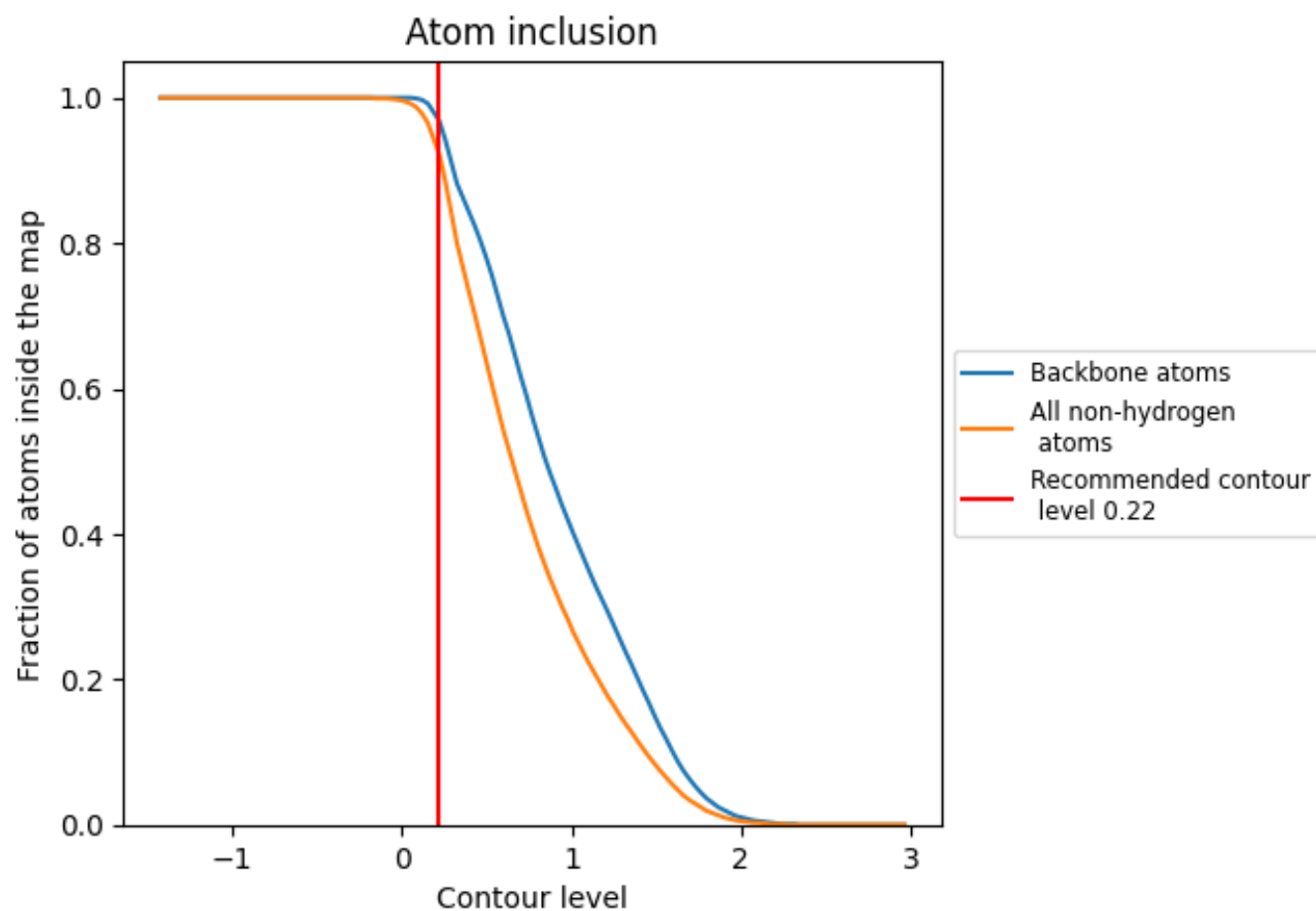
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.22).















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 92% 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 (0.22) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.9240   |  0.2650   |
| A     |  0.9410   |  0.3600   |
| B     |  0.9550   |  0.3700   |
| C     |  0.9640   |  0.3770   |
| D     |  0.9690   |  0.1650   |
| E     |  0.9530   |  0.3450   |
| F     |  0.9300   |  0.3680   |
| G     |  0.9640   |  0.2120   |
| H     |  0.9580   |  0.3910   |
| I     |  0.9650   |  0.3180   |
| J     |  0.9460   |  0.3840   |
| K     |  0.9560   |  0.3890   |
| L     |  0.9810   |  0.3530   |
| N     |  0.9230   |  0.2000   |
| P     |  0.9840  |  0.2490  |
| T     |  0.9570 |  0.2330 |
| U     |  0.9420 |  0.1020 |
| V     |  0.9480 |  0.1600 |
| W     |  0.9310 |  0.1380 |
| X     |  0.9730 |  0.1600 |
| Y     |  0.6420 |  0.0910 |
| Z     |  0.8380 |  0.1200 |
| a     |  0.7870 |  0.0560 |

