# Full wwPDB EM Validation Report ⓘ

Nov 26, 2022 – 02:55 PM EST

| | | |
|---|---|---|
| PDB ID | : | 5SVA |
| EMDB ID | : | EMD-8305 |
| Title | : | Mediator-RNA Polymerase II Pre-Initiation Complex |
| Authors | : | Robinson, P.J.; Bushnell, D.A.; Kornberg, R.D. |
| Deposited on | : | 2016-08-05 |
| Resolution | : | 15.30 Å(reported) |

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The following versions of software and data (see references ⓘ) were used in the production of this report:

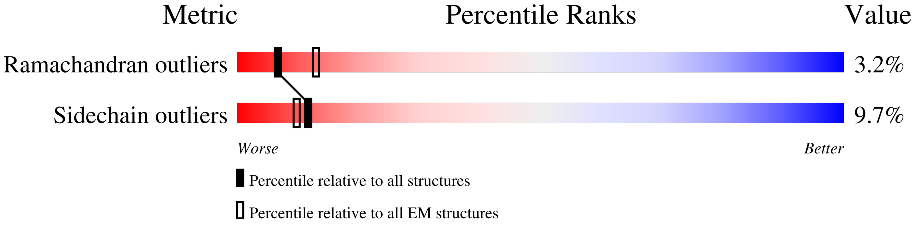
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.31.3 |

# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
*ELECTRON MICROSCOPY*

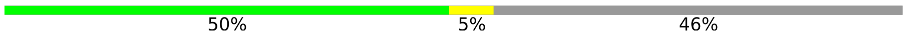
The reported resolution of this entry is 15.30 Å.

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 (#Entries) | EM structures (#Entries) |
|---|---|---|
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

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 >=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 <=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 |  |
| 4 | D | 221 |  |
| 5 | E | 215 |  |
| 6 | F | 155 |  |
| 7 | G | 171 |  |
| 8 | H | 146 |  |
| 9 | I | 122 |  |

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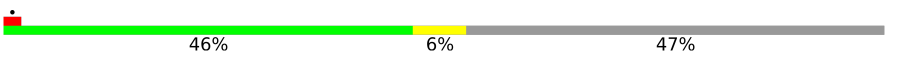
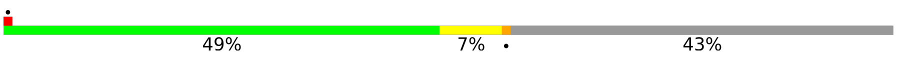
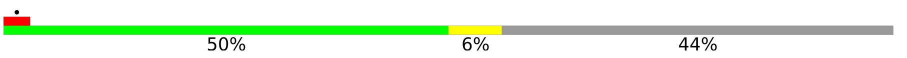
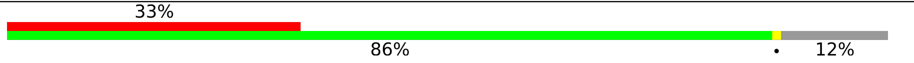
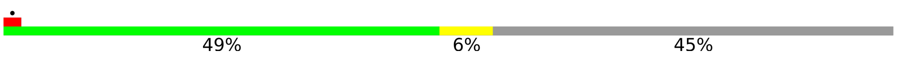
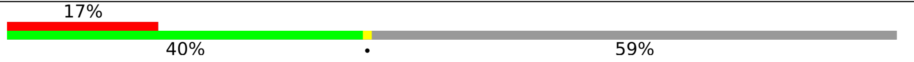
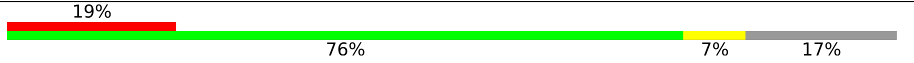
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 10 | J | 70 |  |
| 11 | K | 120 |  |
| 12 | L | 70 |  |
| 13 | M | 295 |  |
| 14 | N | 223 |  |
| 15 | O | 115 |  |
| 16 | P | 687 |  |
| 17 | Q | 307 |  |
| 18 | R | 210 |  |
| 19 | S | 121 |  |
| 20 | T | 284 |  |
| 21 | U | 222 |  |
| 22 | V | 149 |  |
| 23 | W | 140 |  |
| 24 | X | 127 |  |
| 25 | Y | 778 |  |
| 26 | Z | 843 |  |
| 27 | a | 513 |  |
| 28 | b | 72 |  |
| 29 | c | 345 |  |
| 30 | d | 286 |  |
| 31 | e | 122 |  |
| 32 | f | 735 |  |
| 33 | g | 400 |  |
| 34 | h | 482 |  |

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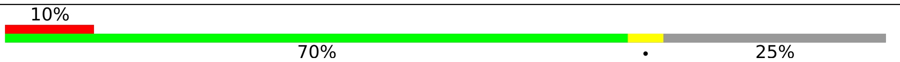
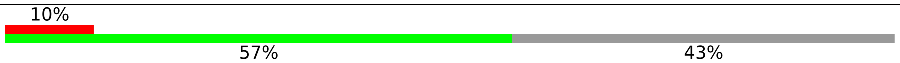
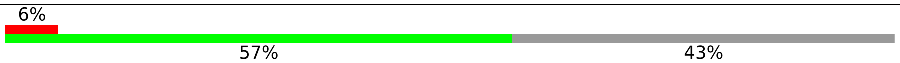
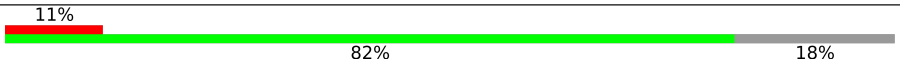
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 35 | i | 328 |  |
| 36 | j | 240 |  |
| 37 | k | 25 |  |
| 38 | l | 108 |  |
| 39 | m | 108 |  |
| 40 | n | 244 |  |

# 2 Entry composition (i)

There are 42 unique types of molecules in this entry. The entry contains 66759 atoms, of which 626 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 |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | A | 1422 | 11174 | 7036 | 1954 | 2122 | 62 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | B | 1156 | 9140 | 5781 | 1606 | 1697 | 56 | 0 | 0 |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | D | 178 | 1434 | 887 | 257 | 288 | 2 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | E | 214 | 1752 | 1111 | 309 | 321 | 11 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | F | 84 | 679 | 434 | 115 | 127 | 3 | 0 | 0 |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 8 | H | 133 | 1068 | 673 | 180 | 211 | 4 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 9 | I | 119 | 971 | 596 | 179 | 186 | 10 | 0 | 0 |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 11 | K | 115 | 920 | 590 | 157 | 171 | 2 | 0 | 1 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 12 | L | 46 | 363 | 224 | 72 | 63 | 4 | 0 | 0 |

- Molecule 13 is a protein called Mediator of RNA polymerase II transcription subunit 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 13 | M | 156 | 777 | 464 | 156 | 156 | 1 | 0 | 0 |

- Molecule 14 is a protein called Mediator of RNA polymerase II transcription subunit 8.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 14 | N | 168 | 891 | 542 | 172 | 177 | 0 | 0 |

- Molecule 15 is a protein called Mediator of RNA polymerase II transcription subunit 11.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 15 | O | 103 | 511 | 305 | 103 | 103 | 0 | 0 |

- Molecule 16 is a protein called Mediator of RNA polymerase II transcription subunit 17.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 16 | P | 487 | 2421 | 1447 | 487 | 487 | 0 | 0 |

- Molecule 17 is a protein called Mediator of RNA polymerase II transcription subunit 18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 17 | Q | 253 | 1979 | 1255 | 330 | 384 | 10 | 0 | 0 |

- Molecule 18 is a protein called Mediator of RNA polymerase II transcription subunit 20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 18 | R | 209 | 1600 | 1011 | 269 | 315 | 5 | 0 | 0 |

- Molecule 19 is a protein called Mediator of RNA polymerase II transcription subunit 22.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 19 | S | 109 | 544 | 326 | 109 | 109 | 0 | 0 |

- Molecule 20 is a protein called Mediator of RNA polymerase II transcription subunit 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 20 | T | 91 | 756 | 475 | 125 | 154 | 2 | 0 | 0 |

- Molecule 21 is a protein called Mediator of RNA polymerase II transcription subunit 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | U | 156 | Total | C | N | O | S | 0 | 0 |
| | | | 1310 | 847 | 220 | 238 | 5 | | |

- Molecule 22 is a protein called Mediator of RNA polymerase II transcription subunit 9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 22 | V | 85 | Total | C | N | O | S | 0 | 0 |
| | | | 720 | 451 | 133 | 135 | 1 | | |

- Molecule 23 is a protein called Mediator of RNA polymerase II transcription subunit 21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 23 | W | 119 | Total | C | N | O | S | 0 | 0 |
| | | | 965 | 608 | 160 | 193 | 4 | | |

- Molecule 24 is a protein called Mediator of RNA polymerase II transcription subunit 31.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 24 | X | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 767 | 506 | 116 | 141 | 4 | | |

- Molecule 25 is a protein called DNA repair helicase RAD3.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 25 | Y | 562 | Total | C | H | N | O | S | 0 | 0 |
| | | | 5175 | 2901 | 626 | 777 | 838 | 33 | | |

- Molecule 26 is a protein called DNA repair helicase RAD25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 26 | Z | 469 | Total | C | N | O | S | 0 | 0 |
| | | | 3769 | 2370 | 660 | 716 | 23 | | |

- Molecule 27 is a protein called RNA polymerase II transcription factor B subunit 2.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 27 | a | 62 | Total | C | N | O | 0 | 0 |
| | | | 518 | 334 | 83 | 101 | | |

- Molecule 28 is a protein called RNA polymerase II transcription factor B subunit 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | b | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 499 | 316 | 88 | 93 | 2 | | |

- Molecule 29 is a protein called Transcription initiation factor IIB.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 29 | c | 189 | Total | C | N | O | S | 0 | 0 |
| | | | 1357 | 838 | 240 | 267 | 12 | | |

- Molecule 30 is a protein called Transcription initiation factor IIA large subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | d | 116 | Total | C | N | O | S | 0 | 0 |
| | | | 956 | 599 | 159 | 195 | 3 | | |

- Molecule 31 is a protein called Transcription initiation factor IIA subunit 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 31 | e | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 792 | 500 | 132 | 156 | 4 | | |

- Molecule 32 is a protein called Transcription initiation factor IIF subunit alpha.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 32 | f | 149 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 788 | 222 | 229 | 4 | | |

- Molecule 33 is a protein called Transcription initiation factor IIF subunit beta.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 33 | g | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1443 | 922 | 248 | 267 | 6 | | |

- Molecule 34 is a protein called Transcription initiation factor IIE subunit alpha.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 34 | h | 118 | Total | C | N | O | S | 0 | 0 |
| | | | 960 | 625 | 158 | 172 | 5 | | |

- Molecule 35 is a protein called Transcription initiation factor IIE subunit beta.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 35 | i | 120 | 987 | 636 | 161 | 187 | 3 | 0 | 0 |

- Molecule 36 is a protein called TATA-box-binding protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 36 | j | 180 | 1416 | 921 | 242 | 247 | 6 | 0 | 0 |

- Molecule 37 is a protein called DNA-directed RNA polymerase II subunit RPB1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 37 | k | 25 | 184 | 116 | 25 | 43 | 0 | 0 |

- Molecule 38 is a DNA chain called 108bp HIS4 Promoter Non-template Strand (-92/+16).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 38 | l | 62 | 1271 | 609 | 222 | 378 | 62 | 0 | 0 |

- Molecule 39 is a DNA chain called 108bp HIS4 Promoter Template Strand (+16/-92).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 39 | m | 62 | 1271 | 607 | 236 | 366 | 62 | 0 | 0 |

- Molecule 40 is a protein called Transcription initiation factor TFIID subunit 14.

| Mol | Chain | Residues | Atoms | | AltConf | Trace |
|---|---|---|---|---|---|---|
| | | | Total | C | | |
| 40 | n | 200 | 200 | 200 | 0 | 200 |

- Molecule 41 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Zn | |
| 41 | A | 2 | 2 | 2 | 0 |
| 41 | B | 1 | 1 | 1 | 0 |
| 41 | C | 1 | 1 | 1 | 0 |

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| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 41 | I | 2 | Total Zn<br>2 2 | 0 |
| 41 | J | 1 | Total Zn<br>1 1 | 0 |
| 41 | L | 1 | Total Zn<br>1 1 | 0 |

- Molecule 42 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

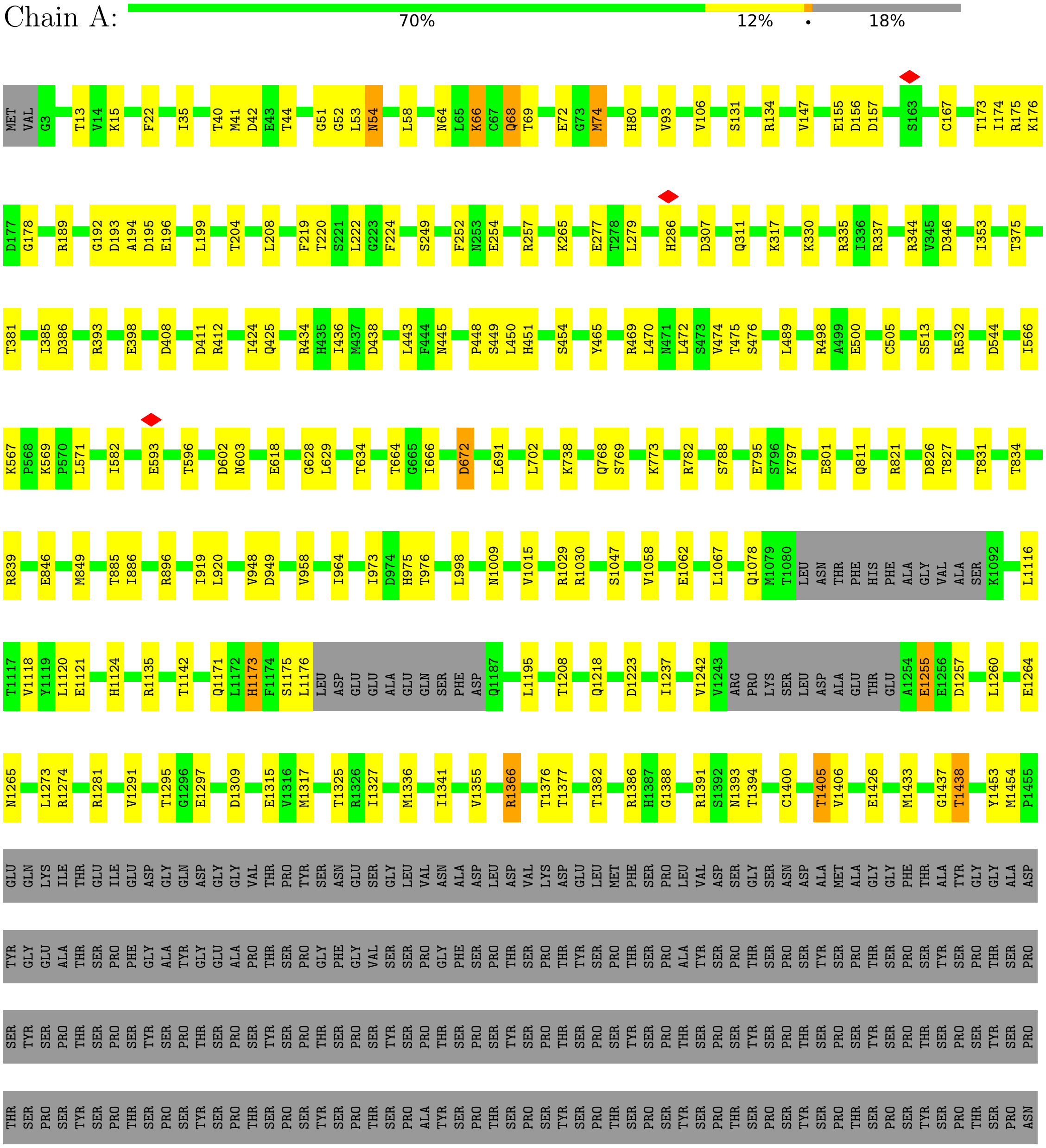
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 42 | A | 1 | Total Mg<br>1 1 | 0 |

# 3 Residue-property plots ⓘ

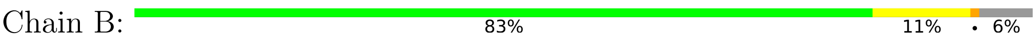
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

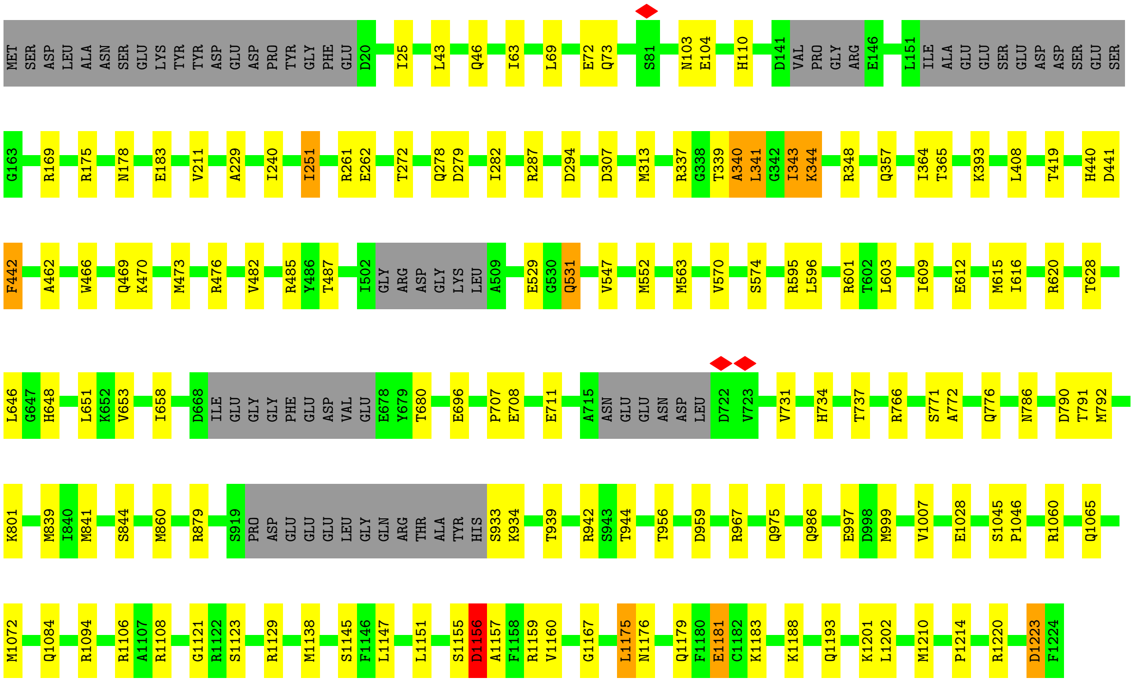
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

Chain A:

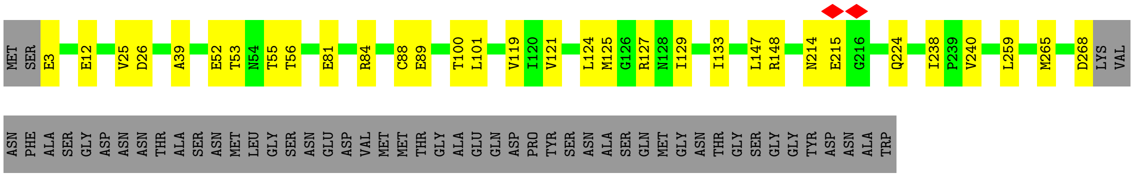


- Molecule 2: DNA-directed RNA polymerase II subunit RPB2

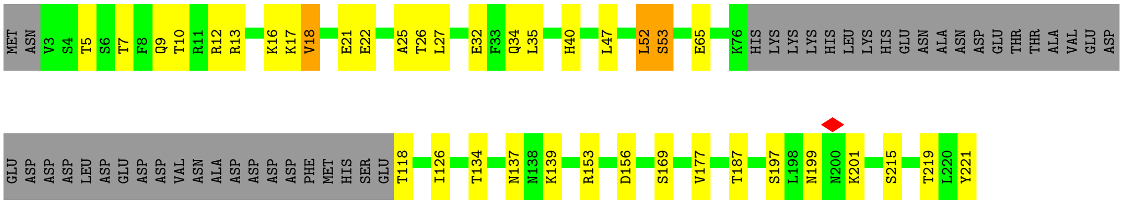




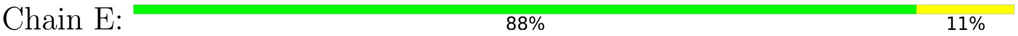
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

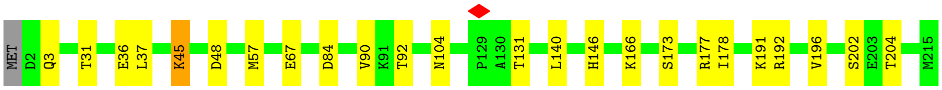


- Molecule 4: DNA-directed RNA polymerase II subunit RPB4



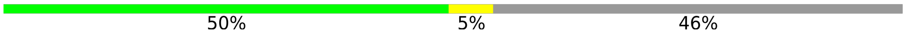
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

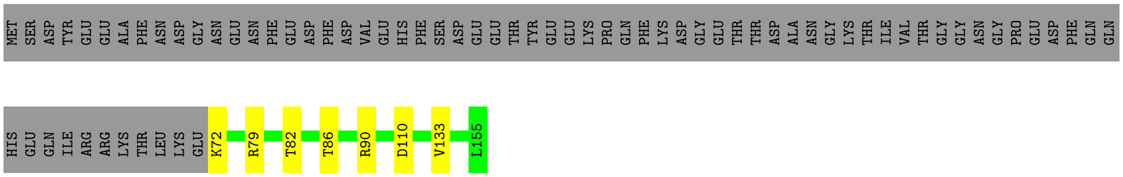




- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

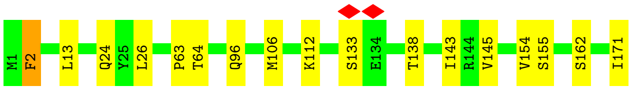
Chain F:





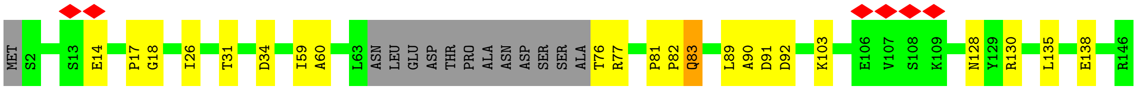
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:



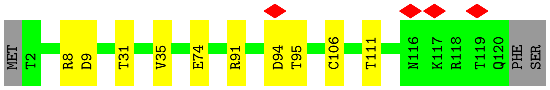
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



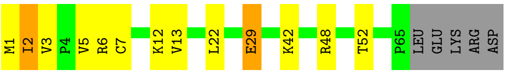
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:



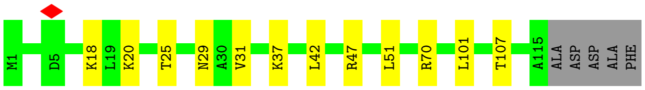
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:

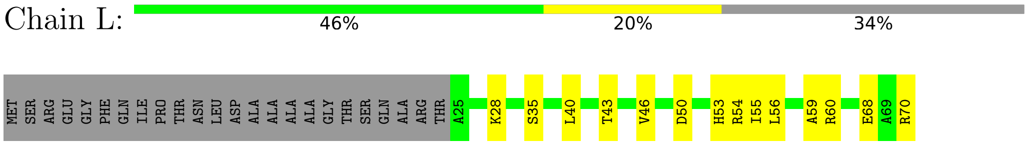


- Molecule 11: DNA-directed RNA polymerase II subunit RPB11

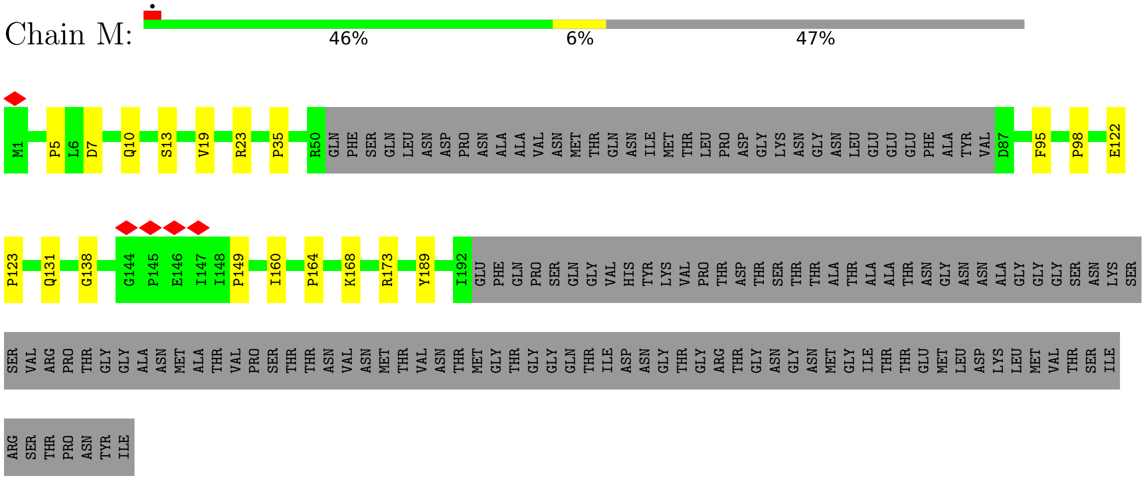
Chain K:



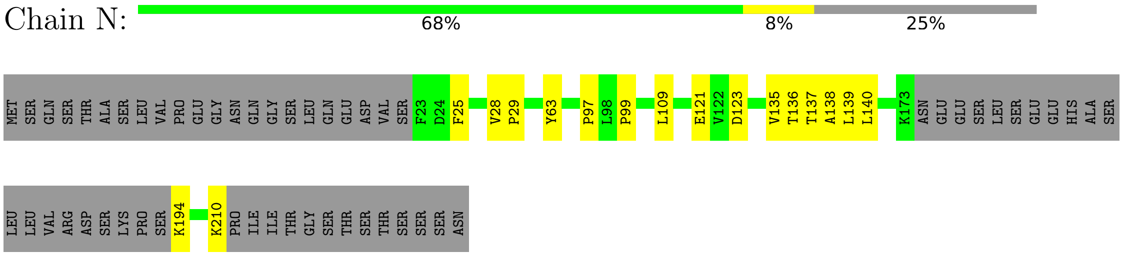
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



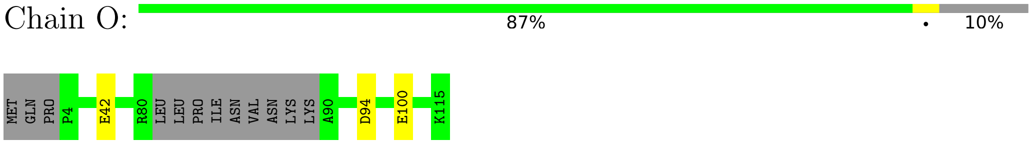
- Molecule 13: Mediator of RNA polymerase II transcription subunit 6



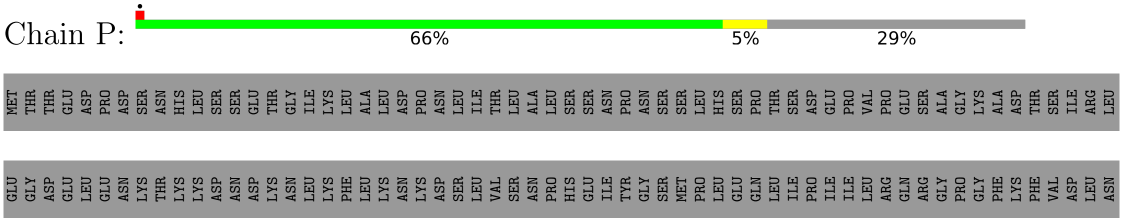
- Molecule 14: Mediator of RNA polymerase II transcription subunit 8

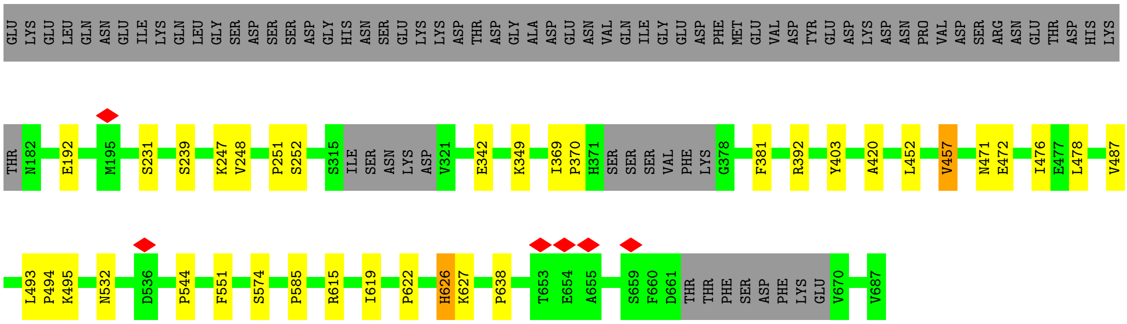


- Molecule 15: Mediator of RNA polymerase II transcription subunit 11



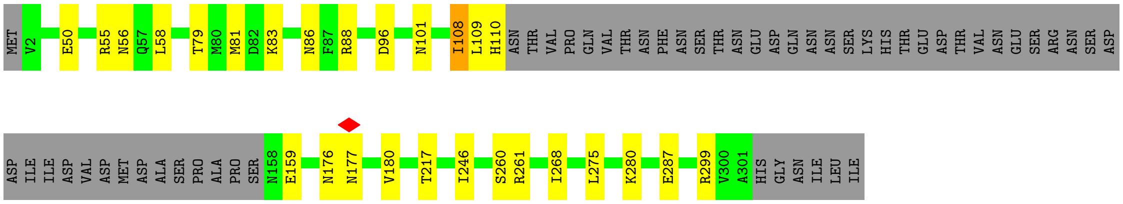
- Molecule 16: Mediator of RNA polymerase II transcription subunit 17





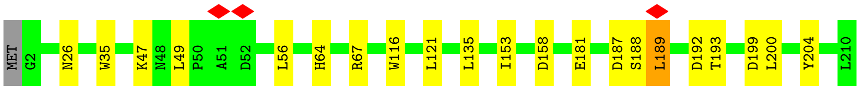
- Molecule 17: Mediator of RNA polymerase II transcription subunit 18

Chain Q:



- Molecule 18: Mediator of RNA polymerase II transcription subunit 20

Chain R:

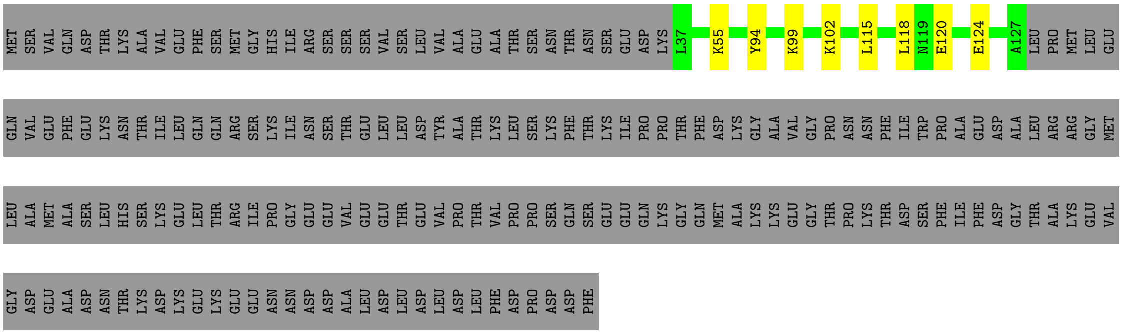


- Molecule 19: Mediator of RNA polymerase II transcription subunit 22

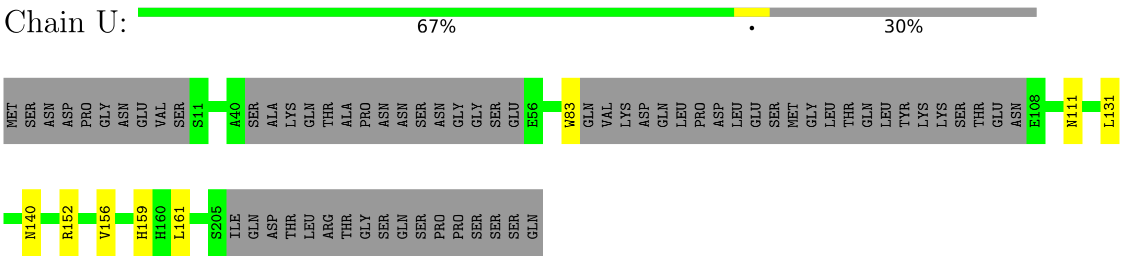
Chain S:

- Molecule 20: Mediator of RNA polymerase II transcription subunit 4

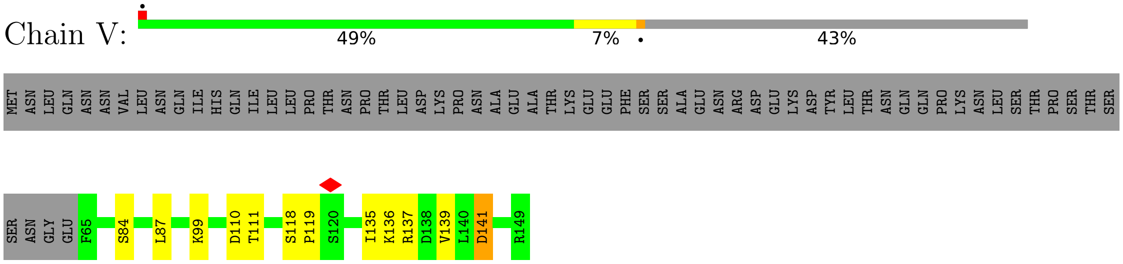
Chain T:



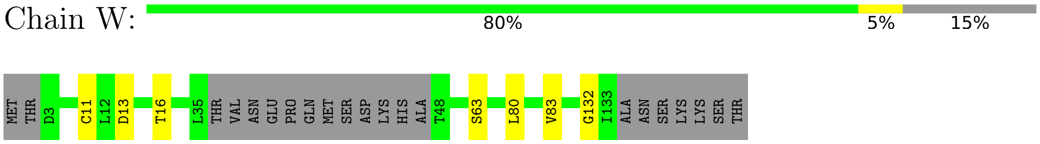
- Molecule 21: Mediator of RNA polymerase II transcription subunit 7



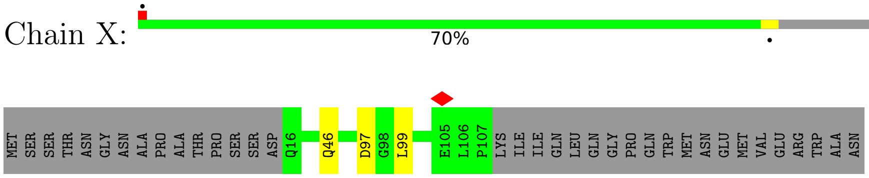
- Molecule 22: Mediator of RNA polymerase II transcription subunit 9



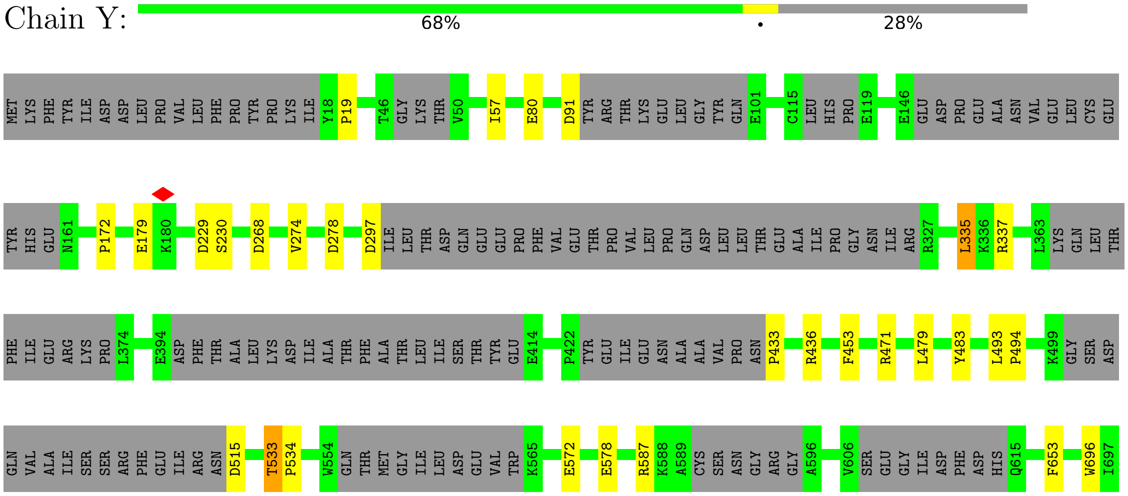
- Molecule 23: Mediator of RNA polymerase II transcription subunit 21

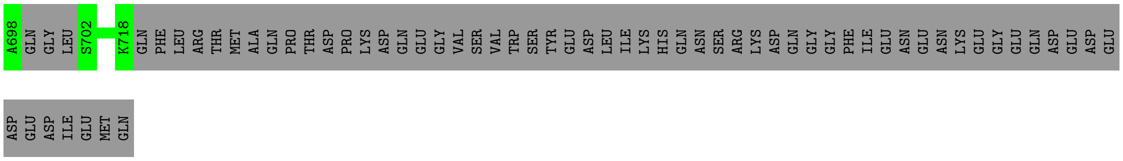


- Molecule 24: Mediator of RNA polymerase II transcription subunit 31

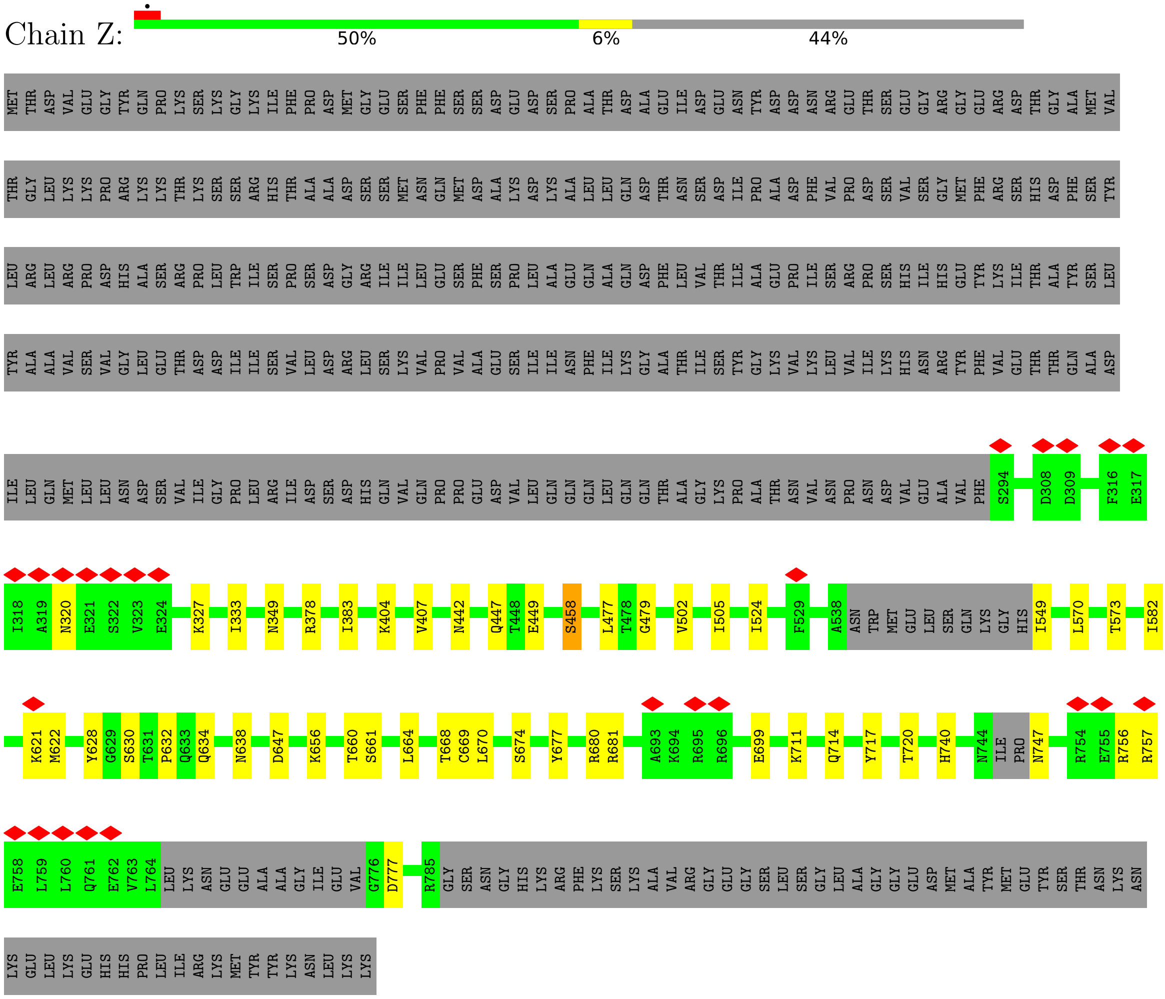


- Molecule 25: DNA repair helicase RAD3

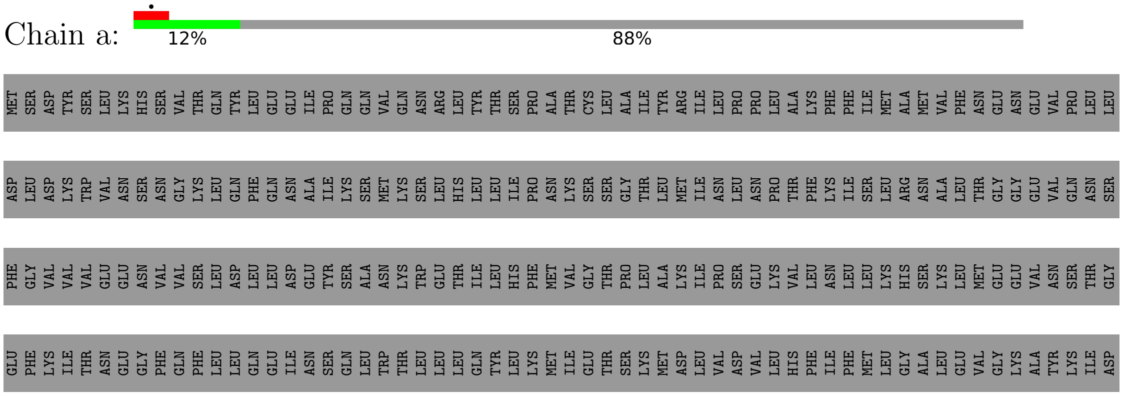


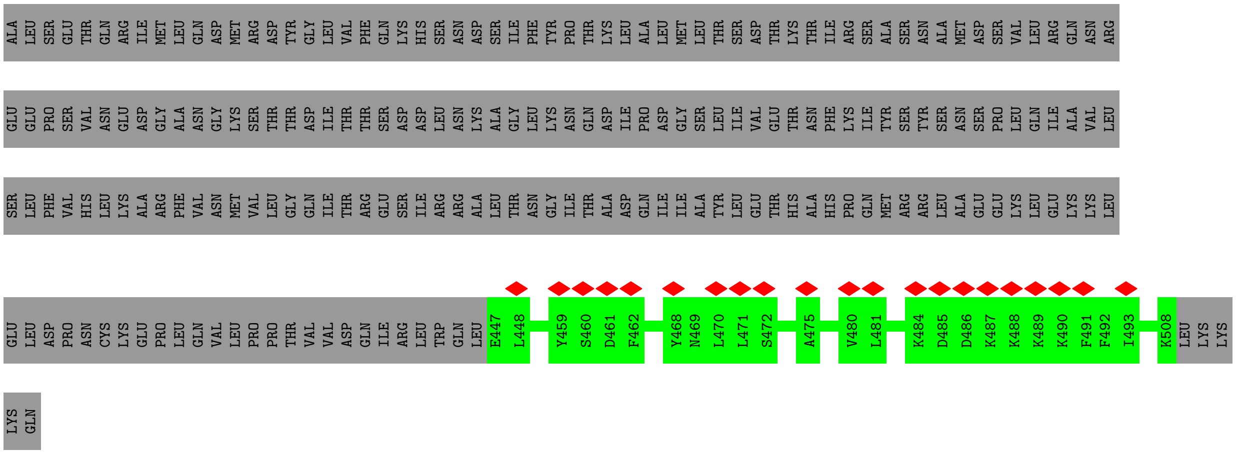


- Molecule 26: DNA repair helicase RAD25

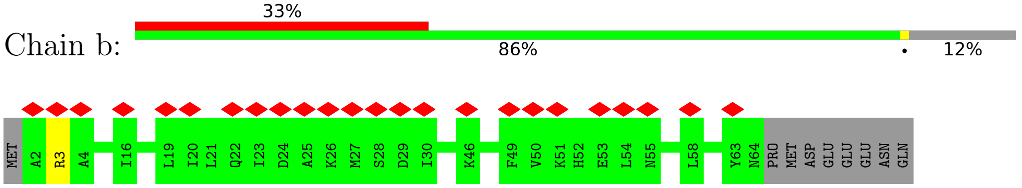


- Molecule 27: RNA polymerase II transcription factor B subunit 2

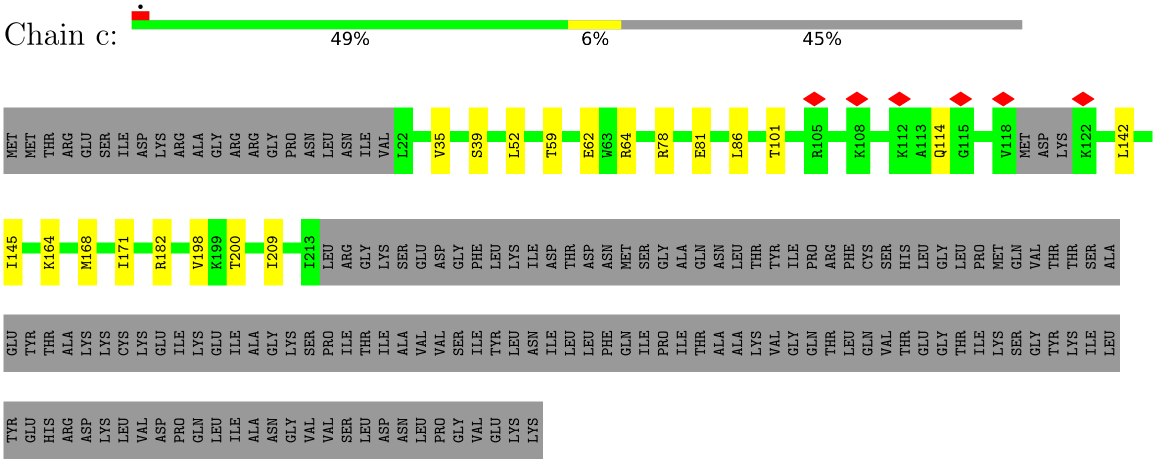




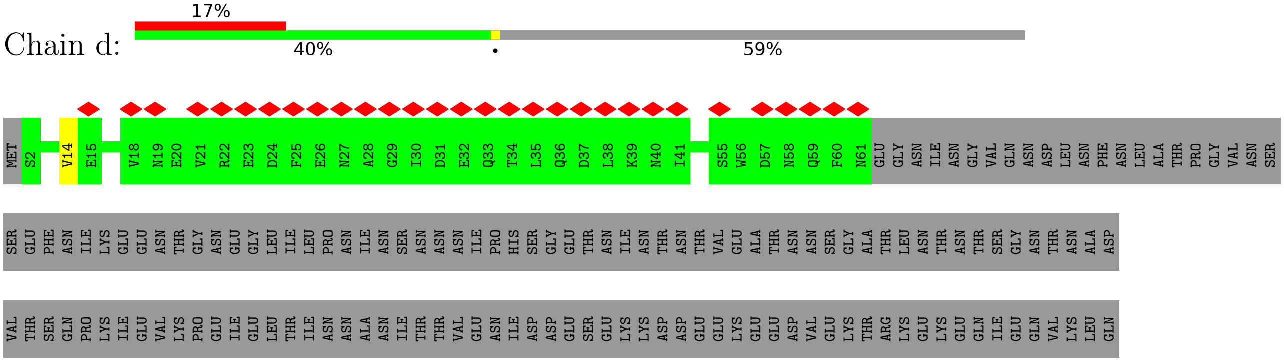
- Molecule 28: RNA polymerase II transcription factor B subunit 5

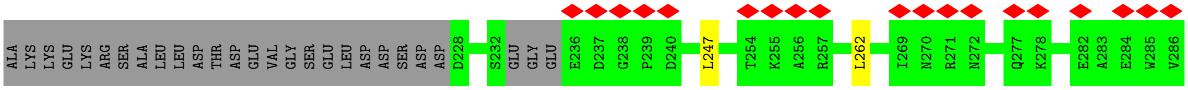


- Molecule 29: Transcription initiation factor IIB



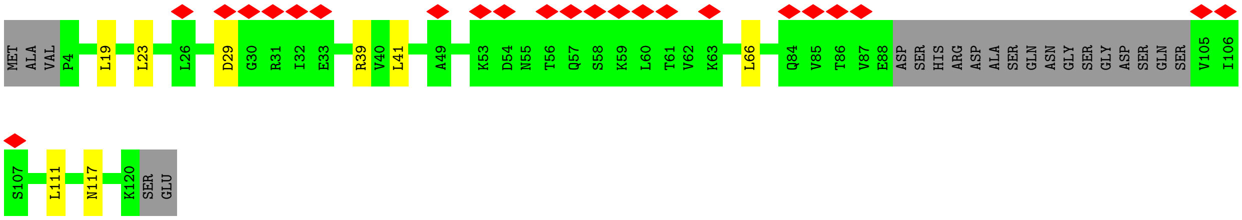
- Molecule 30: Transcription initiation factor IIA large subunit





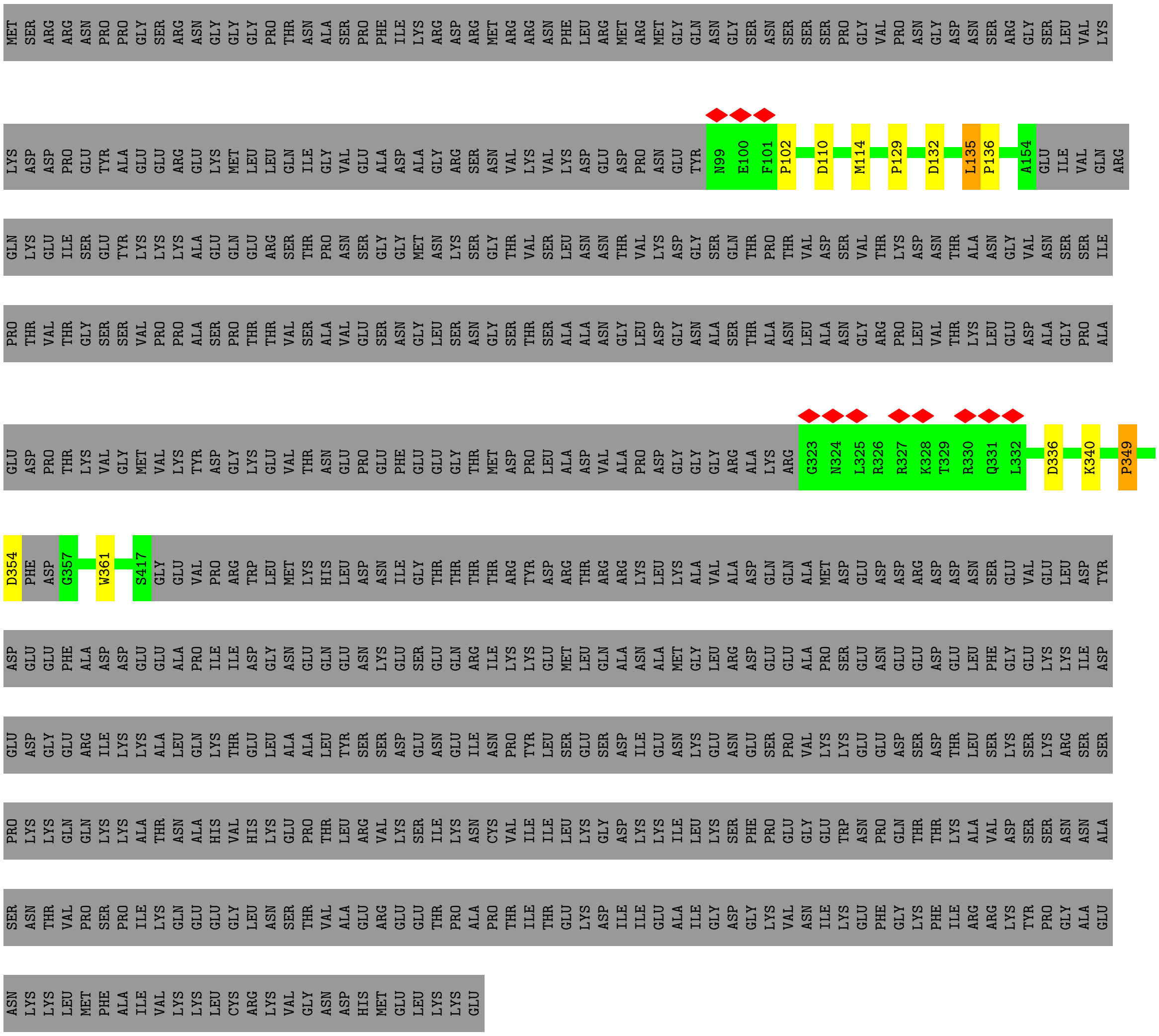
- Molecule 31: Transcription initiation factor IIA subunit 2

Chain e:

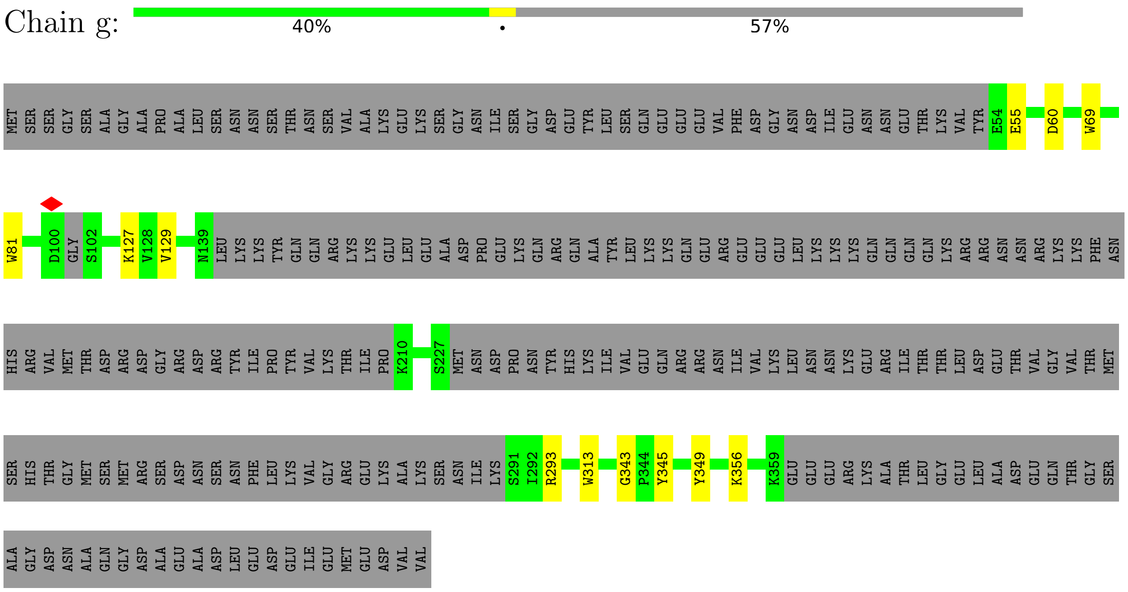


- Molecule 32: Transcription initiation factor IIF subunit alpha

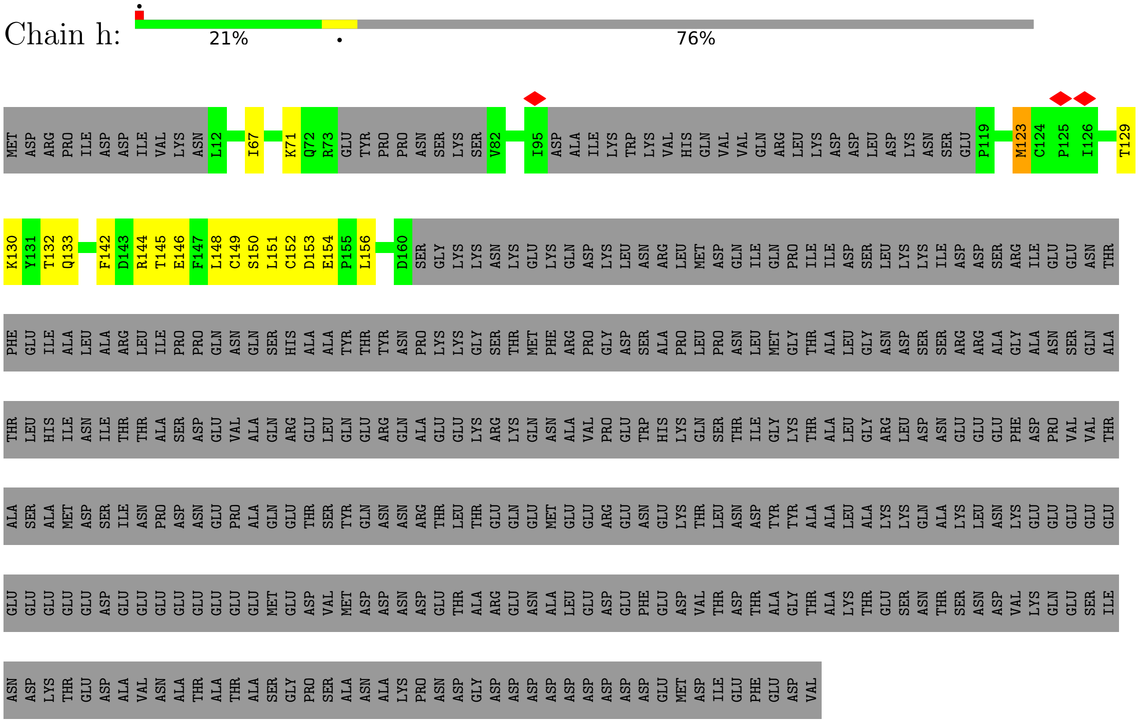
Chain f:



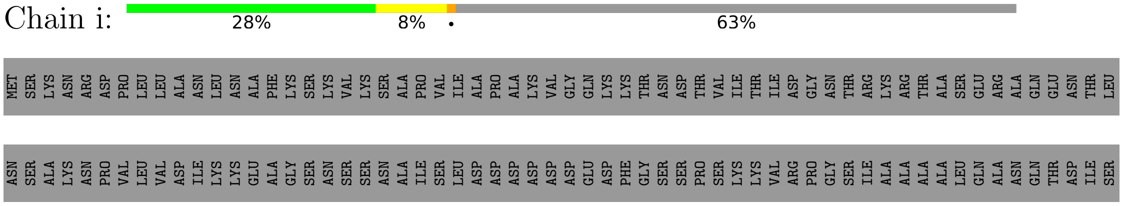
- Molecule 33: Transcription initiation factor IIF subunit beta

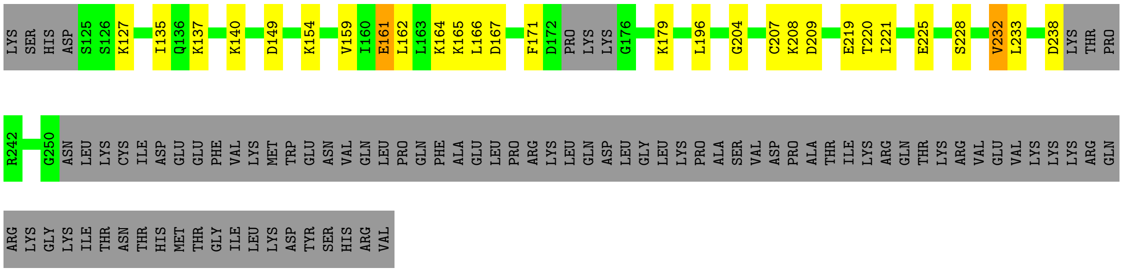


• Molecule 34: Transcription initiation factor IIE subunit alpha



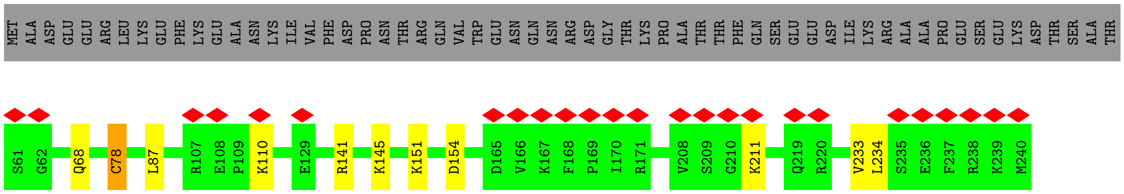
• Molecule 35: Transcription initiation factor IIE subunit beta





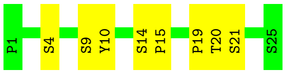
- Molecule 36: TATA-box-binding protein

Chain j:



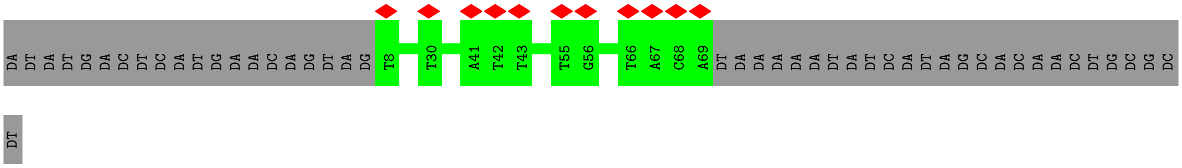
- Molecule 37: DNA-directed RNA polymerase II subunit RPB1

Chain k:



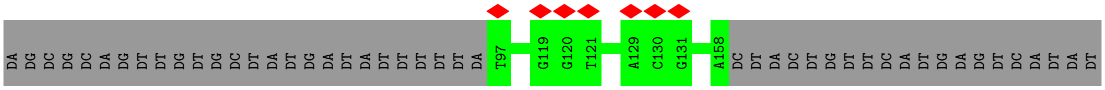
- Molecule 38: 108bp HIS4 Promoter Non-template Strand (-92/+16)

Chain l:



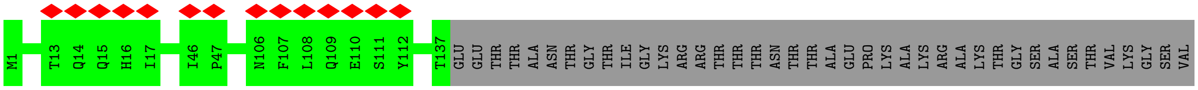
- Molecule 39: 108bp HIS4 Promoter Template Strand (+16/-92)

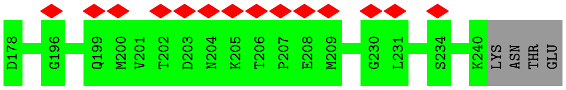
Chain m:



- Molecule 40: Transcription initiation factor TFIID subunit 14

Chain n:




D178
G196
Q199
M200
V201
T202
D203
N204
K205
T206
P207
E208
M209
G230
L231
S234
K240
LYS
ASN
THR
GLU

# 4 Experimental information

| **Property** | **Value** | **Source** |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 170600 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | NONE | Depositor |
| Microscope | FEI TECNAI 20 | Depositor |
| Voltage (kV) | 200 | Depositor |
| Electron dose $(e^-/\text{Å}^2)$ | 15 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN ULTRASCAN 4000 (4k x 4k) | Depositor |
| Maximum map value | 0.153 | Depositor |
| Minimum map value | -0.044 | Depositor |
| Average map value | 0.002 | Depositor |
| Map value standard deviation | 0.010 | Depositor |
| Recommended contour level | 0.025 | Depositor |
| Map size (Å) | 503.8, 503.8, 503.8 | wwPDB |
| Map dimensions | 220, 220, 220 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 2.29, 2.29, 2.29 | Depositor |

# 5 Model quality ⓘ

## 5.1 Standard geometry ⓘ

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

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 | 0.51 | 1/11374 (0.0%) | 0.79 | 5/15384 (0.0%) |
| 2 | B | 0.48 | 0/9317 | 0.74 | 4/12567 (0.0%) |
| 3 | C | 0.49 | 0/2133 | 0.78 | 2/2891 (0.1%) |
| 4 | D | 0.51 | 0/1444 | 0.83 | 2/1935 (0.1%) |
| 5 | E | 0.48 | 0/1788 | 0.72 | 0/2406 |
| 6 | F | 0.58 | 0/691 | 0.79 | 0/933 |
| 7 | G | 0.51 | 0/1368 | 0.81 | 0/1844 |
| 8 | H | 0.51 | 0/1086 | 0.80 | 0/1470 |
| 9 | I | 0.47 | 0/989 | 0.78 | 0/1331 |
| 10 | J | 0.54 | 0/541 | 0.88 | 1/727 (0.1%) |
| 11 | K | 0.48 | 0/938 | 0.71 | 0/1267 |
| 12 | L | 0.54 | 0/365 | 0.79 | 0/485 |
| 13 | M | 0.61 | 0/775 | 0.83 | 0/1077 |
| 14 | N | 0.53 | 0/893 | 0.76 | 0/1237 |
| 15 | O | 0.52 | 0/509 | 0.67 | 0/707 |
| 16 | P | 0.58 | 0/2417 | 0.79 | 2/3369 (0.1%) |
| 17 | Q | 0.56 | 0/2014 | 0.75 | 0/2728 |
| 18 | R | 0.50 | 2/1626 (0.1%) | 0.66 | 0/2205 |
| 19 | S | 0.57 | 0/542 | 0.73 | 0/755 |
| 20 | T | 0.69 | 0/763 | 1.10 | 2/1025 (0.2%) |
| 21 | U | 0.43 | 0/1339 | 0.60 | 0/1808 |
| 22 | V | 0.73 | 0/732 | 1.01 | 4/984 (0.4%) |
| 23 | W | 0.47 | 0/973 | 0.64 | 0/1308 |
| 24 | X | 0.39 | 0/789 | 0.53 | 0/1077 |
| 25 | Y | 0.55 | 2/4616 (0.0%) | 0.79 | 13/6196 (0.2%) |
| 26 | Z | 0.78 | 0/3837 | 0.98 | 8/5177 (0.2%) |
| 27 | a | 0.67 | 0/527 | 0.68 | 0/704 |
| 28 | b | 0.60 | 0/504 | 0.69 | 1/679 (0.1%) |
| 29 | c | 0.29 | 0/1373 | 0.47 | 0/1863 |
| 30 | d | 0.40 | 0/970 | 0.57 | 0/1310 |
| 31 | e | 0.42 | 0/800 | 0.63 | 0/1080 |
| 32 | f | 0.33 | 0/1267 | 0.82 | 9/1700 (0.5%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 33 | g | 0.66 | 0/1469 | 0.73 | 3/1972 (0.2%) |
| 34 | h | 0.96 | 0/978 | 1.11 | 1/1321 (0.1%) |
| 35 | i | 0.37 | 0/1003 | 0.61 | 0/1345 |
| 36 | j | 0.41 | 0/1443 | 0.62 | 0/1942 |
| 37 | k | 0.77 | 0/194 | 0.69 | 0/270 |
| 38 | l | 0.43 | 0/1423 | 0.89 | 0/2195 |
| 39 | m | 0.47 | 0/1427 | 0.89 | 0/2199 |
| All | All | 0.54 | 5/67237 (0.0%) | 0.78 | 57/91473 (0.1%) |

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 |
|---|---|---|---|
| 2 | B | 0 | 1 |
| 13 | M | 0 | 2 |
| 16 | P | 0 | 3 |
| 17 | Q | 0 | 1 |
| 25 | Y | 0 | 1 |
| 26 | Z | 0 | 1 |
| All | All | 0 | 9 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1394 | THR | C-N | -6.29 | 1.21 | 1.33 |
| 25 | Y | 172 | PRO | N-CD | 5.61 | 1.55 | 1.47 |
| 25 | Y | 19 | PRO | N-CD | 5.51 | 1.55 | 1.47 |
| 18 | R | 35 | TRP | CD2-CE2 | 5.06 | 1.47 | 1.41 |
| 18 | R | 116 | TRP | CD2-CE2 | 5.04 | 1.47 | 1.41 |

All (57) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | Y | 493 | LEU | C-N-CD | -13.71 | 90.45 | 120.60 |
| 25 | Y | 533 | THR | C-N-CD | -13.65 | 90.57 | 120.60 |
| 32 | f | 135 | LEU | C-N-CD | -11.09 | 96.21 | 120.60 |
| 26 | Z | 505 | ILE | CB-CA-C | -9.99 | 91.62 | 111.60 |
| 25 | Y | 433 | PRO | CA-N-CD | -9.03 | 98.86 | 111.50 |
| 32 | f | 129 | PRO | CA-N-CD | -8.28 | 99.90 | 111.50 |
| 32 | f | 349 | PRO | CA-N-CD | -7.96 | 100.35 | 111.50 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 32 | f | 102 | PRO | CA-N-CD | -7.60 | 100.86 | 111.50 |
| 1 | A | 346 | ASP | O-C-N | -7.53 | 110.65 | 122.70 |
| 34 | h | 123 | MET | CG-SD-CE | -7.14 | 88.78 | 100.20 |
| 25 | Y | 471 | ARG | NE-CZ-NH2 | 6.60 | 123.60 | 120.30 |
| 25 | Y | 436 | ARG | NE-CZ-NH2 | 6.55 | 123.58 | 120.30 |
| 25 | Y | 337 | ARG | NE-CZ-NH2 | 6.55 | 123.57 | 120.30 |
| 26 | Z | 477 | LEU | C-N-CA | -6.26 | 106.04 | 121.70 |
| 22 | V | 87 | LEU | CB-CA-C | -6.13 | 98.54 | 110.20 |
| 20 | T | 115 | LEU | CB-CA-C | -6.12 | 98.57 | 110.20 |
| 4 | D | 25 | ALA | C-N-CA | 6.11 | 136.98 | 121.70 |
| 26 | Z | 670 | LEU | CB-CG-CD1 | -6.10 | 100.63 | 111.00 |
| 25 | Y | 453 | PHE | N-CA-C | -5.91 | 95.05 | 111.00 |
| 20 | T | 94 | TYR | CA-CB-CG | -5.81 | 102.36 | 113.40 |
| 22 | V | 136 | LYS | N-CA-CB | -5.77 | 100.22 | 110.60 |
| 25 | Y | 696 | TRP | CZ3-CH2-CZ2 | 5.71 | 128.46 | 121.60 |
| 1 | A | 58 | LEU | CA-CB-CG | 5.70 | 128.40 | 115.30 |
| 1 | A | 194 | ALA | C-N-CA | 5.66 | 135.86 | 121.70 |
| 33 | g | 69 | TRP | CZ3-CH2-CZ2 | 5.65 | 128.38 | 121.60 |
| 2 | B | 340 | ALA | C-N-CA | 5.65 | 135.83 | 121.70 |
| 33 | g | 81 | TRP | CZ3-CH2-CZ2 | 5.64 | 128.37 | 121.60 |
| 32 | f | 361 | TRP | CZ3-CH2-CZ2 | 5.62 | 128.35 | 121.60 |
| 33 | g | 313 | TRP | CZ3-CH2-CZ2 | 5.57 | 128.28 | 121.60 |
| 26 | Z | 632 | PRO | N-CA-CB | 5.55 | 109.96 | 103.30 |
| 22 | V | 141 | ASP | CB-CG-OD1 | 5.50 | 123.25 | 118.30 |
| 4 | D | 26 | THR | N-CA-C | -5.49 | 96.19 | 111.00 |
| 2 | B | 628 | THR | C-N-CA | 5.47 | 135.36 | 121.70 |
| 3 | C | 39 | ALA | N-CA-C | 5.46 | 125.75 | 111.00 |
| 3 | C | 89 | GLU | N-CA-C | -5.29 | 96.70 | 111.00 |
| 1 | A | 1394 | THR | C-N-CA | 5.29 | 133.40 | 122.30 |
| 25 | Y | 229 | ASP | CB-CG-OD2 | 5.24 | 123.02 | 118.30 |
| 32 | f | 354 | ASP | CB-CG-OD2 | 5.24 | 123.01 | 118.30 |
| 32 | f | 336 | ASP | CB-CG-OD2 | 5.23 | 123.01 | 118.30 |
| 25 | Y | 91 | ASP | CB-CG-OD2 | 5.21 | 122.99 | 118.30 |
| 25 | Y | 515 | ASP | CB-CG-OD2 | 5.21 | 122.99 | 118.30 |
| 25 | Y | 297 | ASP | CB-CG-OD2 | 5.21 | 122.99 | 118.30 |
| 26 | Z | 777 | ASP | CB-CG-OD2 | 5.21 | 122.99 | 118.30 |
| 32 | f | 110 | ASP | CB-CG-OD2 | 5.21 | 122.99 | 118.30 |
| 32 | f | 132 | ASP | CB-CG-OD2 | 5.21 | 122.99 | 118.30 |
| 2 | B | 1181 | GLU | N-CA-C | 5.14 | 124.88 | 111.00 |
| 26 | Z | 458 | SER | N-CA-CB | 5.13 | 118.20 | 110.50 |
| 26 | Z | 479 | GLY | N-CA-C | 5.13 | 125.91 | 113.10 |
| 25 | Y | 278 | ASP | CB-CG-OD2 | 5.11 | 122.90 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 26 | Z | 502 | VAL | CB-CA-C | -5.10 | 101.71 | 111.40 |
| 16 | P | 457 | VAL | N-CA-C | 5.09 | 124.75 | 111.00 |
| 16 | P | 342 | GLU | N-CA-C | 5.08 | 124.71 | 111.00 |
| 22 | V | 139 | VAL | CA-CB-CG1 | -5.04 | 103.34 | 110.90 |
| 28 | b | 3 | ARG | NE-CZ-NH1 | 5.04 | 122.82 | 120.30 |
| 1 | A | 346 | ASP | CA-C-N | 5.02 | 128.24 | 117.20 |
| 2 | B | 1156 | ASP | N-CA-C | 5.01 | 124.52 | 111.00 |
| 10 | J | 5 | VAL | N-CA-C | -5.01 | 97.48 | 111.00 |

There are no chirality outliers.

All (9) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | B | 43 | LEU | Mainchain |
| 13 | M | 10 | GLN | Peptide |
| 13 | M | 138 | GLY | Peptide |
| 16 | P | 471 | ASN | Peptide |
| 16 | P | 532 | ASN | Peptide |
| 16 | P | 626 | HIS | Peptide |
| 17 | Q | 101 | ASN | Peptide |
| 25 | Y | 335 | LEU | Peptide |
| 26 | Z | 661 | SER | Peptide |

## 5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | A | 1414/1733 (82%) | 1254 (89%) | 112 (8%) | 48 (3%) | 3 26 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 2 | B | 1142/1224 (93%) | 1022 (90%) | 84 (7%) | 36 (3%) | 4 | 26 |
| 3 | C | 264/318 (83%) | 242 (92%) | 20 (8%) | 2 (1%) | 19 | 60 |
| 4 | D | 174/221 (79%) | 149 (86%) | 17 (10%) | 8 (5%) | 2 | 21 |
| 5 | E | 212/215 (99%) | 195 (92%) | 13 (6%) | 4 (2%) | 8 | 38 |
| 6 | F | 82/155 (53%) | 75 (92%) | 7 (8%) | 0 | 100 | 100 |
| 7 | G | 169/171 (99%) | 157 (93%) | 9 (5%) | 3 (2%) | 8 | 40 |
| 8 | H | 129/146 (88%) | 106 (82%) | 14 (11%) | 9 (7%) | 1 | 14 |
| 9 | I | 117/122 (96%) | 98 (84%) | 16 (14%) | 3 (3%) | 5 | 31 |
| 10 | J | 63/70 (90%) | 51 (81%) | 9 (14%) | 3 (5%) | 2 | 21 |
| 11 | K | 113/120 (94%) | 109 (96%) | 4 (4%) | 0 | 100 | 100 |
| 12 | L | 44/70 (63%) | 19 (43%) | 14 (32%) | 11 (25%) | 0 | 1 |
| 13 | M | 152/295 (52%) | 115 (76%) | 20 (13%) | 17 (11%) | 0 | 7 |
| 14 | N | 164/223 (74%) | 133 (81%) | 16 (10%) | 15 (9%) | 1 | 11 |
| 15 | O | 99/115 (86%) | 92 (93%) | 4 (4%) | 3 (3%) | 4 | 28 |
| 16 | P | 479/687 (70%) | 385 (80%) | 61 (13%) | 33 (7%) | 1 | 15 |
| 17 | Q | 249/307 (81%) | 217 (87%) | 25 (10%) | 7 (3%) | 5 | 30 |
| 18 | R | 207/210 (99%) | 190 (92%) | 12 (6%) | 5 (2%) | 6 | 33 |
| 19 | S | 105/121 (87%) | 91 (87%) | 7 (7%) | 7 (7%) | 1 | 15 |
| 20 | T | 89/284 (31%) | 69 (78%) | 20 (22%) | 0 | 100 | 100 |
| 21 | U | 150/222 (68%) | 127 (85%) | 22 (15%) | 1 (1%) | 22 | 63 |
| 22 | V | 83/149 (56%) | 73 (88%) | 5 (6%) | 5 (6%) | 1 | 17 |
| 23 | W | 115/140 (82%) | 95 (83%) | 18 (16%) | 2 (2%) | 9 | 42 |
| 24 | X | 90/127 (71%) | 86 (96%) | 4 (4%) | 0 | 100 | 100 |
| 25 | Y | 534/778 (69%) | 503 (94%) | 23 (4%) | 8 (2%) | 10 | 46 |
| 26 | Z | 461/843 (55%) | 430 (93%) | 26 (6%) | 5 (1%) | 14 | 52 |
| 27 | a | 60/513 (12%) | 60 (100%) | 0 | 0 | 100 | 100 |
| 28 | b | 61/72 (85%) | 58 (95%) | 3 (5%) | 0 | 100 | 100 |
| 29 | c | 185/345 (54%) | 164 (89%) | 19 (10%) | 2 (1%) | 14 | 52 |
| 30 | d | 110/286 (38%) | 103 (94%) | 7 (6%) | 0 | 100 | 100 |
| 31 | e | 97/122 (80%) | 93 (96%) | 4 (4%) | 0 | 100 | 100 |
| 32 | f | 143/735 (20%) | 130 (91%) | 9 (6%) | 4 (3%) | 5 | 30 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 33 | g | 164/400 (41%) | 148 (90%) | 12 (7%) | 4 (2%) | 6 | 33 |
| 34 | h | 112/482 (23%) | 100 (89%) | 10 (9%) | 2 (2%) | 8 | 40 |
| 35 | i | 114/328 (35%) | 102 (90%) | 9 (8%) | 3 (3%) | 5 | 31 |
| 36 | j | 178/240 (74%) | 170 (96%) | 5 (3%) | 3 (2%) | 9 | 42 |
| 37 | k | 23/25 (92%) | 9 (39%) | 6 (26%) | 8 (35%) | 0 | 0 |
| All | All | 8147/12614 (65%) | 7220 (89%) | 666 (8%) | 261 (3%) | 7 | 26 |

All (261) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 74 | MET |
| 1 | A | 189 | ARG |
| 1 | A | 195 | ASP |
| 1 | A | 286 | HIS |
| 1 | A | 317 | LYS |
| 1 | A | 449 | SER |
| 1 | A | 628 | GLY |
| 1 | A | 1377 | THR |
| 1 | A | 1405 | THR |
| 2 | B | 229 | ALA |
| 2 | B | 307 | ASP |
| 2 | B | 344 | LYS |
| 2 | B | 442 | PHE |
| 2 | B | 466 | TRP |
| 2 | B | 473 | MET |
| 2 | B | 531 | GLN |
| 2 | B | 772 | ALA |
| 2 | B | 1046 | PRO |
| 2 | B | 1181 | GLU |
| 4 | D | 18 | VAL |
| 4 | D | 53 | SER |
| 4 | D | 199 | ASN |
| 9 | I | 9 | ASP |
| 9 | I | 95 | THR |
| 12 | L | 50 | ASP |
| 12 | L | 53 | HIS |
| 12 | L | 59 | ALA |
| 13 | M | 5 | PRO |
| 13 | M | 7 | ASP |
| 13 | M | 13 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | M | 23 | ARG |
| 13 | M | 35 | PRO |
| 13 | M | 98 | PRO |
| 13 | M | 123 | PRO |
| 13 | M | 164 | PRO |
| 13 | M | 173 | ARG |
| 14 | N | 25 | PHE |
| 14 | N | 29 | PRO |
| 14 | N | 99 | PRO |
| 14 | N | 109 | LEU |
| 14 | N | 121 | GLU |
| 14 | N | 135 | VAL |
| 14 | N | 140 | LEU |
| 15 | O | 94 | ASP |
| 16 | P | 231 | SER |
| 16 | P | 251 | PRO |
| 16 | P | 252 | SER |
| 16 | P | 349 | LYS |
| 16 | P | 369 | ILE |
| 16 | P | 370 | PRO |
| 16 | P | 381 | PHE |
| 16 | P | 476 | ILE |
| 16 | P | 487 | VAL |
| 16 | P | 494 | PRO |
| 16 | P | 495 | LYS |
| 16 | P | 544 | PRO |
| 16 | P | 615 | ARG |
| 16 | P | 619 | ILE |
| 16 | P | 622 | PRO |
| 16 | P | 626 | HIS |
| 17 | Q | 56 | ASN |
| 17 | Q | 108 | ILE |
| 17 | Q | 177 | ASN |
| 17 | Q | 299 | ARG |
| 18 | R | 204 | TYR |
| 19 | S | 19 | VAL |
| 19 | S | 47 | GLU |
| 19 | S | 102 | LYS |
| 19 | S | 104 | ILE |
| 22 | V | 84 | SER |
| 25 | Y | 494 | PRO |
| 25 | Y | 534 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 25 | Y | 572 | GLU |
| 26 | Z | 447 | GLN |
| 26 | Z | 458 | SER |
| 26 | Z | 699 | GLU |
| 29 | c | 200 | THR |
| 32 | f | 136 | PRO |
| 32 | f | 349 | PRO |
| 33 | g | 129 | VAL |
| 34 | h | 149 | CYS |
| 35 | i | 232 | VAL |
| 36 | j | 154 | ASP |
| 37 | k | 4 | SER |
| 37 | k | 14 | SER |
| 37 | k | 21 | SER |
| 1 | A | 40 | THR |
| 1 | A | 44 | THR |
| 1 | A | 51 | GLY |
| 1 | A | 52 | GLY |
| 1 | A | 66 | LYS |
| 1 | A | 68 | GLN |
| 1 | A | 167 | CYS |
| 1 | A | 178 | GLY |
| 1 | A | 193 | ASP |
| 1 | A | 224 | PHE |
| 1 | A | 252 | PHE |
| 1 | A | 254 | GLU |
| 1 | A | 330 | LYS |
| 1 | A | 672 | ASP |
| 1 | A | 1175 | SER |
| 1 | A | 1281 | ARG |
| 1 | A | 1437 | GLY |
| 2 | B | 262 | GLU |
| 2 | B | 282 | ILE |
| 2 | B | 339 | THR |
| 2 | B | 341 | LEU |
| 2 | B | 707 | PRO |
| 2 | B | 731 | VAL |
| 2 | B | 792 | MET |
| 2 | B | 1175 | LEU |
| 2 | B | 1176 | ASN |
| 4 | D | 16 | LYS |
| 4 | D | 52 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | D | 169 | SER |
| 5 | E | 36 | GLU |
| 7 | G | 2 | PHE |
| 8 | H | 17 | PRO |
| 8 | H | 81 | PRO |
| 8 | H | 82 | PRO |
| 8 | H | 83 | GLN |
| 8 | H | 90 | ALA |
| 10 | J | 6 | ARG |
| 12 | L | 35 | SER |
| 13 | M | 19 | VAL |
| 13 | M | 95 | PHE |
| 13 | M | 131 | GLN |
| 13 | M | 149 | PRO |
| 13 | M | 189 | TYR |
| 14 | N | 137 | THR |
| 14 | N | 138 | ALA |
| 15 | O | 42 | GLU |
| 16 | P | 420 | ALA |
| 16 | P | 457 | VAL |
| 16 | P | 472 | GLU |
| 16 | P | 493 | LEU |
| 16 | P | 585 | PRO |
| 16 | P | 638 | PRO |
| 17 | Q | 109 | LEU |
| 17 | Q | 261 | ARG |
| 18 | R | 187 | ASP |
| 22 | V | 110 | ASP |
| 25 | Y | 268 | ASP |
| 26 | Z | 378 | ARG |
| 26 | Z | 449 | GLU |
| 34 | h | 153 | ASP |
| 36 | j | 78 | CYS |
| 37 | k | 10 | TYR |
| 37 | k | 15 | PRO |
| 37 | k | 19 | PRO |
| 37 | k | 20 | THR |
| 1 | A | 54 | ASN |
| 1 | A | 975 | HIS |
| 1 | A | 1173 | HIS |
| 2 | B | 340 | ALA |
| 2 | B | 343 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 711 | GLU |
| 2 | B | 1155 | SER |
| 2 | B | 1156 | ASP |
| 2 | B | 1157 | ALA |
| 2 | B | 1167 | GLY |
| 4 | D | 22 | GLU |
| 5 | E | 45 | LYS |
| 5 | E | 48 | ASP |
| 7 | G | 154 | VAL |
| 8 | H | 18 | GLY |
| 12 | L | 40 | LEU |
| 12 | L | 54 | ARG |
| 13 | M | 160 | ILE |
| 14 | N | 63 | TYR |
| 14 | N | 139 | LEU |
| 16 | P | 239 | SER |
| 16 | P | 392 | ARG |
| 16 | P | 403 | TYR |
| 16 | P | 478 | LEU |
| 16 | P | 627 | LYS |
| 18 | R | 56 | LEU |
| 25 | Y | 230 | SER |
| 25 | Y | 274 | VAL |
| 25 | Y | 483 | TYR |
| 32 | f | 114 | MET |
| 32 | f | 135 | LEU |
| 35 | i | 204 | GLY |
| 37 | k | 9 | SER |
| 1 | A | 69 | THR |
| 1 | A | 72 | GLU |
| 1 | A | 465 | TYR |
| 1 | A | 569 | LYS |
| 1 | A | 846 | GLU |
| 1 | A | 958 | VAL |
| 1 | A | 1255 | GLU |
| 1 | A | 1438 | THR |
| 2 | B | 441 | ASP |
| 2 | B | 648 | HIS |
| 2 | B | 1108 | ARG |
| 3 | C | 88 | CYS |
| 9 | I | 91 | ARG |
| 10 | J | 29 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 12 | L | 43 | THR |
| 12 | L | 56 | LEU |
| 12 | L | 60 | ARG |
| 13 | M | 168 | LYS |
| 14 | N | 136 | THR |
| 16 | P | 192 | GLU |
| 16 | P | 247 | LYS |
| 16 | P | 248 | VAL |
| 16 | P | 452 | LEU |
| 16 | P | 574 | SER |
| 18 | R | 189 | LEU |
| 33 | g | 60 | ASP |
| 35 | i | 161 | GLU |
| 36 | j | 110 | LYS |
| 1 | A | 156 | ASP |
| 1 | A | 567 | LYS |
| 1 | A | 1171 | GLN |
| 1 | A | 1366 | ARG |
| 2 | B | 251 | ILE |
| 2 | B | 462 | ALA |
| 2 | B | 469 | GLN |
| 2 | B | 1223 | ASP |
| 4 | D | 21 | GLU |
| 8 | H | 60 | ALA |
| 8 | H | 128 | ASN |
| 10 | J | 2 | ILE |
| 14 | N | 123 | ASP |
| 15 | O | 100 | GLU |
| 16 | P | 551 | PHE |
| 18 | R | 135 | LEU |
| 19 | S | 32 | ASP |
| 19 | S | 100 | ASP |
| 22 | V | 111 | THR |
| 22 | V | 118 | SER |
| 22 | V | 119 | PRO |
| 33 | g | 345 | TYR |
| 1 | A | 35 | ILE |
| 1 | A | 155 | GLU |
| 1 | A | 885 | THR |
| 3 | C | 214 | ASN |
| 12 | L | 28 | LYS |
| 12 | L | 46 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 21 | U | 111 | ASN |
| 23 | W | 132 | GLY |
| 29 | c | 164 | LYS |
| 1 | A | 196 | GLU |
| 1 | A | 1388 | GLY |
| 5 | E | 90 | VAL |
| 7 | G | 63 | PRO |
| 2 | B | 364 | ILE |
| 13 | M | 122 | GLU |
| 23 | W | 83 | VAL |
| 1 | A | 192 | GLY |
| 1 | A | 448 | PRO |
| 2 | B | 1121 | GLY |
| 14 | N | 28 | VAL |
| 14 | N | 97 | PRO |
| 25 | Y | 533 | THR |
| 2 | B | 1214 | PRO |
| 8 | H | 59 | ILE |
| 19 | S | 58 | VAL |
| 17 | Q | 83 | LYS |
| 33 | g | 343 | GLY |

### 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 | 1240/1520 (82%) | 1071 (86%) | 169 (14%) | 3 | 17 |
| 2 | B | 985/1061 (93%) | 868 (88%) | 117 (12%) | 5 | 20 |
| 3 | C | 234/274 (85%) | 206 (88%) | 28 (12%) | 5 | 20 |
| 4 | D | 160/200 (80%) | 129 (81%) | 31 (19%) | 1 | 8 |
| 5 | E | 196/197 (100%) | 175 (89%) | 21 (11%) | 6 | 23 |
| 6 | F | 74/137 (54%) | 67 (90%) | 7 (10%) | 8 | 27 |
| 7 | G | 152/152 (100%) | 137 (90%) | 15 (10%) | 8 | 26 |
| 8 | H | 117/128 (91%) | 103 (88%) | 14 (12%) | 5 | 20 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 9 | I | 113/116 (97%) | 106 (94%) | 7 (6%) | 18 | 43 |
| 10 | J | 60/65 (92%) | 49 (82%) | 11 (18%) | 1 | 10 |
| 11 | K | 99/102 (97%) | 87 (88%) | 12 (12%) | 5 | 20 |
| 12 | L | 40/57 (70%) | 37 (92%) | 3 (8%) | 13 | 38 |
| 13 | M | 1/259 (0%) | 1 (100%) | 0 | 100 | 100 |
| 14 | N | 16/207 (8%) | 14 (88%) | 2 (12%) | 4 | 19 |
| 17 | Q | 226/280 (81%) | 206 (91%) | 20 (9%) | 10 | 31 |
| 18 | R | 177/178 (99%) | 162 (92%) | 15 (8%) | 10 | 33 |
| 20 | T | 87/258 (34%) | 81 (93%) | 6 (7%) | 15 | 40 |
| 21 | U | 149/208 (72%) | 142 (95%) | 7 (5%) | 26 | 51 |
| 22 | V | 84/144 (58%) | 80 (95%) | 4 (5%) | 25 | 51 |
| 23 | W | 113/132 (86%) | 108 (96%) | 5 (4%) | 28 | 53 |
| 24 | X | 87/117 (74%) | 84 (97%) | 3 (3%) | 37 | 60 |
| 25 | Y | 512/707 (72%) | 504 (98%) | 8 (2%) | 62 | 79 |
| 26 | Z | 412/737 (56%) | 375 (91%) | 37 (9%) | 9 | 30 |
| 27 | a | 57/468 (12%) | 57 (100%) | 0 | 100 | 100 |
| 28 | b | 57/66 (86%) | 57 (100%) | 0 | 100 | 100 |
| 29 | c | 136/299 (46%) | 118 (87%) | 18 (13%) | 4 | 18 |
| 30 | d | 107/260 (41%) | 104 (97%) | 3 (3%) | 43 | 65 |
| 31 | e | 91/108 (84%) | 83 (91%) | 8 (9%) | 10 | 31 |
| 32 | f | 136/641 (21%) | 135 (99%) | 1 (1%) | 84 | 90 |
| 33 | g | 162/363 (45%) | 157 (97%) | 5 (3%) | 40 | 62 |
| 34 | h | 108/429 (25%) | 91 (84%) | 17 (16%) | 2 | 14 |
| 35 | i | 113/295 (38%) | 86 (76%) | 27 (24%) | 0 | 4 |
| 36 | j | 152/205 (74%) | 143 (94%) | 9 (6%) | 19 | 45 |
| 37 | k | 25/25 (100%) | 25 (100%) | 0 | 100 | 100 |
| All | All | 6478/10395 (62%) | 5848 (90%) | 630 (10%) | 12 | 27 |

All (630) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 13 | THR |
| 1 | A | 15 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 22 | PHE |
| 1 | A | 41 | MET |
| 1 | A | 42 | ASP |
| 1 | A | 53 | LEU |
| 1 | A | 54 | ASN |
| 1 | A | 64 | ASN |
| 1 | A | 66 | LYS |
| 1 | A | 68 | GLN |
| 1 | A | 74 | MET |
| 1 | A | 80 | HIS |
| 1 | A | 93 | VAL |
| 1 | A | 106 | VAL |
| 1 | A | 131 | SER |
| 1 | A | 134 | ARG |
| 1 | A | 147 | VAL |
| 1 | A | 157 | ASP |
| 1 | A | 173 | THR |
| 1 | A | 174 | ILE |
| 1 | A | 175 | ARG |
| 1 | A | 176 | LYS |
| 1 | A | 199 | LEU |
| 1 | A | 204 | THR |
| 1 | A | 208 | LEU |
| 1 | A | 219 | PHE |
| 1 | A | 220 | THR |
| 1 | A | 222 | LEU |
| 1 | A | 249 | SER |
| 1 | A | 257 | ARG |
| 1 | A | 265 | LYS |
| 1 | A | 277 | GLU |
| 1 | A | 279 | LEU |
| 1 | A | 307 | ASP |
| 1 | A | 311 | GLN |
| 1 | A | 335 | ARG |
| 1 | A | 337 | ARG |
| 1 | A | 344 | ARG |
| 1 | A | 353 | ILE |
| 1 | A | 375 | THR |
| 1 | A | 381 | THR |
| 1 | A | 385 | ILE |
| 1 | A | 386 | ASP |
| 1 | A | 393 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 398 | GLU |
| 1 | A | 408 | ASP |
| 1 | A | 411 | ASP |
| 1 | A | 412 | ARG |
| 1 | A | 424 | ILE |
| 1 | A | 425 | GLN |
| 1 | A | 434 | ARG |
| 1 | A | 436 | ILE |
| 1 | A | 438 | ASP |
| 1 | A | 443 | LEU |
| 1 | A | 445 | ASN |
| 1 | A | 450 | LEU |
| 1 | A | 451 | HIS |
| 1 | A | 454 | SER |
| 1 | A | 469 | ARG |
| 1 | A | 470 | LEU |
| 1 | A | 472 | LEU |
| 1 | A | 474 | VAL |
| 1 | A | 475 | THR |
| 1 | A | 476 | SER |
| 1 | A | 489 | LEU |
| 1 | A | 498 | ARG |
| 1 | A | 500 | GLU |
| 1 | A | 505 | CYS |
| 1 | A | 513 | SER |
| 1 | A | 532 | ARG |
| 1 | A | 544 | ASP |
| 1 | A | 566 | ILE |
| 1 | A | 571 | LEU |
| 1 | A | 582 | ILE |
| 1 | A | 593 | GLU |
| 1 | A | 596 | THR |
| 1 | A | 602 | ASP |
| 1 | A | 603 | ASN |
| 1 | A | 618 | GLU |
| 1 | A | 629 | LEU |
| 1 | A | 634 | THR |
| 1 | A | 664 | THR |
| 1 | A | 666 | ILE |
| 1 | A | 672 | ASP |
| 1 | A | 691 | LEU |
| 1 | A | 702 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 738 | LYS |
| 1 | A | 768 | GLN |
| 1 | A | 769 | SER |
| 1 | A | 773 | LYS |
| 1 | A | 782 | ARG |
| 1 | A | 788 | SER |
| 1 | A | 795 | GLU |
| 1 | A | 797 | LYS |
| 1 | A | 801 | GLU |
| 1 | A | 811 | GLN |
| 1 | A | 821 | ARG |
| 1 | A | 826 | ASP |
| 1 | A | 827 | THR |
| 1 | A | 831 | THR |
| 1 | A | 834 | THR |
| 1 | A | 839 | ARG |
| 1 | A | 849 | MET |
| 1 | A | 886 | ILE |
| 1 | A | 896 | ARG |
| 1 | A | 919 | ILE |
| 1 | A | 920 | LEU |
| 1 | A | 948 | VAL |
| 1 | A | 949 | ASP |
| 1 | A | 964 | ILE |
| 1 | A | 973 | ILE |
| 1 | A | 976 | THR |
| 1 | A | 998 | LEU |
| 1 | A | 1009 | ASN |
| 1 | A | 1015 | VAL |
| 1 | A | 1029 | ARG |
| 1 | A | 1030 | ARG |
| 1 | A | 1047 | SER |
| 1 | A | 1058 | VAL |
| 1 | A | 1062 | GLU |
| 1 | A | 1067 | LEU |
| 1 | A | 1078 | GLN |
| 1 | A | 1116 | LEU |
| 1 | A | 1118 | VAL |
| 1 | A | 1120 | LEU |
| 1 | A | 1121 | GLU |
| 1 | A | 1124 | HIS |
| 1 | A | 1135 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1142 | THR |
| 1 | A | 1173 | HIS |
| 1 | A | 1176 | LEU |
| 1 | A | 1195 | LEU |
| 1 | A | 1208 | THR |
| 1 | A | 1218 | GLN |
| 1 | A | 1223 | ASP |
| 1 | A | 1237 | ILE |
| 1 | A | 1242 | VAL |
| 1 | A | 1255 | GLU |
| 1 | A | 1257 | ASP |
| 1 | A | 1260 | LEU |
| 1 | A | 1264 | GLU |
| 1 | A | 1265 | ASN |
| 1 | A | 1273 | LEU |
| 1 | A | 1274 | ARG |
| 1 | A | 1291 | VAL |
| 1 | A | 1295 | THR |
| 1 | A | 1297 | GLU |
| 1 | A | 1309 | ASP |
| 1 | A | 1315 | GLU |
| 1 | A | 1317 | MET |
| 1 | A | 1325 | THR |
| 1 | A | 1327 | ILE |
| 1 | A | 1336 | MET |
| 1 | A | 1341 | ILE |
| 1 | A | 1355 | VAL |
| 1 | A | 1366 | ARG |
| 1 | A | 1376 | THR |
| 1 | A | 1382 | THR |
| 1 | A | 1386 | ARG |
| 1 | A | 1391 | ARG |
| 1 | A | 1393 | ASN |
| 1 | A | 1400 | CYS |
| 1 | A | 1405 | THR |
| 1 | A | 1406 | VAL |
| 1 | A | 1426 | GLU |
| 1 | A | 1433 | MET |
| 1 | A | 1438 | THR |
| 1 | A | 1453 | TYR |
| 1 | A | 1454 | MET |
| 2 | B | 25 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 46 | GLN |
| 2 | B | 63 | ILE |
| 2 | B | 69 | LEU |
| 2 | B | 72 | GLU |
| 2 | B | 73 | GLN |
| 2 | B | 103 | ASN |
| 2 | B | 104 | GLU |
| 2 | B | 110 | HIS |
| 2 | B | 169 | ARG |
| 2 | B | 175 | ARG |
| 2 | B | 178 | ASN |
| 2 | B | 183 | GLU |
| 2 | B | 211 | VAL |
| 2 | B | 240 | ILE |
| 2 | B | 251 | ILE |
| 2 | B | 261 | ARG |
| 2 | B | 272 | THR |
| 2 | B | 278 | GLN |
| 2 | B | 279 | ASP |
| 2 | B | 287 | ARG |
| 2 | B | 294 | ASP |
| 2 | B | 313 | MET |
| 2 | B | 337 | ARG |
| 2 | B | 341 | LEU |
| 2 | B | 343 | ILE |
| 2 | B | 344 | LYS |
| 2 | B | 348 | ARG |
| 2 | B | 357 | GLN |
| 2 | B | 365 | THR |
| 2 | B | 393 | LYS |
| 2 | B | 408 | LEU |
| 2 | B | 419 | THR |
| 2 | B | 440 | HIS |
| 2 | B | 442 | PHE |
| 2 | B | 470 | LYS |
| 2 | B | 476 | ARG |
| 2 | B | 482 | VAL |
| 2 | B | 485 | ARG |
| 2 | B | 487 | THR |
| 2 | B | 529 | GLU |
| 2 | B | 531 | GLN |
| 2 | B | 547 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 552 | MET |
| 2 | B | 563 | MET |
| 2 | B | 570 | VAL |
| 2 | B | 574 | SER |
| 2 | B | 595 | ARG |
| 2 | B | 596 | LEU |
| 2 | B | 601 | ARG |
| 2 | B | 603 | LEU |
| 2 | B | 609 | ILE |
| 2 | B | 612 | GLU |
| 2 | B | 615 | MET |
| 2 | B | 616 | ILE |
| 2 | B | 620 | ARG |
| 2 | B | 646 | LEU |
| 2 | B | 651 | LEU |
| 2 | B | 653 | VAL |
| 2 | B | 658 | ILE |
| 2 | B | 680 | THR |
| 2 | B | 696 | GLU |
| 2 | B | 708 | GLU |
| 2 | B | 734 | HIS |
| 2 | B | 737 | THR |
| 2 | B | 766 | ARG |
| 2 | B | 771 | SER |
| 2 | B | 776 | GLN |
| 2 | B | 786 | ASN |
| 2 | B | 790 | ASP |
| 2 | B | 791 | THR |
| 2 | B | 801 | LYS |
| 2 | B | 839 | MET |
| 2 | B | 841 | MET |
| 2 | B | 844 | SER |
| 2 | B | 860 | MET |
| 2 | B | 879 | ARG |
| 2 | B | 933 | SER |
| 2 | B | 934 | LYS |
| 2 | B | 939 | THR |
| 2 | B | 942 | ARG |
| 2 | B | 944 | THR |
| 2 | B | 956 | THR |
| 2 | B | 959 | ASP |
| 2 | B | 967 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 975 | GLN |
| 2 | B | 986 | GLN |
| 2 | B | 997 | GLU |
| 2 | B | 999 | MET |
| 2 | B | 1007 | VAL |
| 2 | B | 1028 | GLU |
| 2 | B | 1045 | SER |
| 2 | B | 1060 | ARG |
| 2 | B | 1065 | GLN |
| 2 | B | 1072 | MET |
| 2 | B | 1084 | GLN |
| 2 | B | 1094 | ARG |
| 2 | B | 1106 | ARG |
| 2 | B | 1123 | SER |
| 2 | B | 1129 | ARG |
| 2 | B | 1138 | MET |
| 2 | B | 1145 | SER |
| 2 | B | 1147 | LEU |
| 2 | B | 1151 | LEU |
| 2 | B | 1156 | ASP |
| 2 | B | 1159 | ARG |
| 2 | B | 1160 | VAL |
| 2 | B | 1175 | LEU |
| 2 | B | 1179 | GLN |
| 2 | B | 1183 | LYS |
| 2 | B | 1188 | LYS |
| 2 | B | 1193 | GLN |
| 2 | B | 1201 | LYS |
| 2 | B | 1202 | LEU |
| 2 | B | 1210 | MET |
| 2 | B | 1220 | ARG |
| 2 | B | 1223 | ASP |
| 3 | C | 3 | GLU |
| 3 | C | 12 | GLU |
| 3 | C | 25 | VAL |
| 3 | C | 26 | ASP |
| 3 | C | 52 | GLU |
| 3 | C | 53 | THR |
| 3 | C | 55 | THR |
| 3 | C | 56 | THR |
| 3 | C | 81 | GLU |
| 3 | C | 84 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | C | 100 | THR |
| 3 | C | 101 | LEU |
| 3 | C | 119 | VAL |
| 3 | C | 121 | VAL |
| 3 | C | 124 | LEU |
| 3 | C | 125 | MET |
| 3 | C | 127 | ARG |
| 3 | C | 129 | ILE |
| 3 | C | 133 | ILE |
| 3 | C | 147 | LEU |
| 3 | C | 148 | ARG |
| 3 | C | 215 | GLU |
| 3 | C | 224 | GLN |
| 3 | C | 238 | ILE |
| 3 | C | 240 | VAL |
| 3 | C | 259 | LEU |
| 3 | C | 265 | MET |
| 3 | C | 268 | ASP |
| 4 | D | 5 | THR |
| 4 | D | 7 | THR |
| 4 | D | 9 | GLN |
| 4 | D | 10 | THR |
| 4 | D | 12 | ARG |
| 4 | D | 13 | ARG |
| 4 | D | 17 | LYS |
| 4 | D | 18 | VAL |
| 4 | D | 27 | LEU |
| 4 | D | 32 | GLU |
| 4 | D | 34 | GLN |
| 4 | D | 35 | LEU |
| 4 | D | 40 | HIS |
| 4 | D | 47 | LEU |
| 4 | D | 52 | LEU |
| 4 | D | 53 | SER |
| 4 | D | 65 | GLU |
| 4 | D | 118 | THR |
| 4 | D | 126 | ILE |
| 4 | D | 134 | THR |
| 4 | D | 137 | ASN |
| 4 | D | 139 | LYS |
| 4 | D | 153 | ARG |
| 4 | D | 156 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | D | 177 | VAL |
| 4 | D | 187 | THR |
| 4 | D | 197 | SER |
| 4 | D | 201 | LYS |
| 4 | D | 215 | SER |
| 4 | D | 219 | THR |
| 4 | D | 221 | TYR |
| 5 | E | 3 | GLN |
| 5 | E | 31 | THR |
| 5 | E | 37 | LEU |
| 5 | E | 45 | LYS |
| 5 | E | 57 | MET |
| 5 | E | 67 | GLU |
| 5 | E | 84 | ASP |
| 5 | E | 92 | THR |
| 5 | E | 104 | ASN |
| 5 | E | 131 | THR |
| 5 | E | 140 | LEU |
| 5 | E | 146 | HIS |
| 5 | E | 166 | LYS |
| 5 | E | 173 | SER |
| 5 | E | 177 | ARG |
| 5 | E | 178 | ILE |
| 5 | E | 191 | LYS |
| 5 | E | 192 | ARG |
| 5 | E | 196 | VAL |
| 5 | E | 202 | SER |
| 5 | E | 204 | THR |
| 6 | F | 72 | LYS |
| 6 | F | 79 | ARG |
| 6 | F | 82 | THR |
| 6 | F | 86 | THR |
| 6 | F | 90 | ARG |
| 6 | F | 110 | ASP |
| 6 | F | 133 | VAL |
| 7 | G | 2 | PHE |
| 7 | G | 13 | LEU |
| 7 | G | 24 | GLN |
| 7 | G | 26 | LEU |
| 7 | G | 64 | THR |
| 7 | G | 96 | GLN |
| 7 | G | 106 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | G | 112 | LYS |
| 7 | G | 133 | SER |
| 7 | G | 138 | THR |
| 7 | G | 143 | ILE |
| 7 | G | 145 | VAL |
| 7 | G | 155 | SER |
| 7 | G | 162 | SER |
| 7 | G | 171 | ILE |
| 8 | H | 14 | GLU |
| 8 | H | 26 | ILE |
| 8 | H | 31 | THR |
| 8 | H | 34 | ASP |
| 8 | H | 76 | THR |
| 8 | H | 77 | ARG |
| 8 | H | 83 | GLN |
| 8 | H | 89 | LEU |
| 8 | H | 91 | ASP |
| 8 | H | 92 | ASP |
| 8 | H | 103 | LYS |
| 8 | H | 130 | ARG |
| 8 | H | 135 | LEU |
| 8 | H | 138 | GLU |
| 9 | I | 8 | ARG |
| 9 | I | 31 | THR |
| 9 | I | 35 | VAL |
| 9 | I | 74 | GLU |
| 9 | I | 94 | ASP |
| 9 | I | 106 | CYS |
| 9 | I | 111 | THR |
| 10 | J | 1 | MET |
| 10 | J | 2 | ILE |
| 10 | J | 3 | VAL |
| 10 | J | 7 | CYS |
| 10 | J | 12 | LYS |
| 10 | J | 13 | VAL |
| 10 | J | 22 | LEU |
| 10 | J | 29 | GLU |
| 10 | J | 42 | LYS |
| 10 | J | 48 | ARG |
| 10 | J | 52 | THR |
| 11 | K | 18 | LYS |
| 11 | K | 20 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | K | 25 | THR |
| 11 | K | 29 | ASN |
| 11 | K | 31 | VAL |
| 11 | K | 37 | LYS |
| 11 | K | 42 | LEU |
| 11 | K | 47 | ARG |
| 11 | K | 51 | LEU |
| 11 | K | 70 | ARG |
| 11 | K | 101 | LEU |
| 11 | K | 107 | THR |
| 12 | L | 55 | ILE |
| 12 | L | 68 | GLU |
| 12 | L | 70 | ARG |
| 14 | N | 194 | LYS |
| 14 | N | 210 | LYS |
| 17 | Q | 50 | GLU |
| 17 | Q | 55 | ARG |
| 17 | Q | 58 | LEU |
| 17 | Q | 79 | THR |
| 17 | Q | 81 | MET |
| 17 | Q | 86 | ASN |
| 17 | Q | 88 | ARG |
| 17 | Q | 96 | ASP |
| 17 | Q | 108 | ILE |
| 17 | Q | 110 | HIS |
| 17 | Q | 159 | GLU |
| 17 | Q | 176 | ASN |
| 17 | Q | 180 | VAL |
| 17 | Q | 217 | THR |
| 17 | Q | 246 | ILE |
| 17 | Q | 260 | SER |
| 17 | Q | 268 | ILE |
| 17 | Q | 275 | LEU |
| 17 | Q | 280 | LYS |
| 17 | Q | 287 | GLU |
| 18 | R | 26 | ASN |
| 18 | R | 47 | LYS |
| 18 | R | 49 | LEU |
| 18 | R | 64 | HIS |
| 18 | R | 67 | ARG |
| 18 | R | 121 | LEU |
| 18 | R | 153 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 18 | R | 158 | ASP |
| 18 | R | 181 | GLU |
| 18 | R | 188 | SER |
| 18 | R | 189 | LEU |
| 18 | R | 192 | ASP |
| 18 | R | 193 | THR |
| 18 | R | 199 | ASP |
| 18 | R | 200 | LEU |
| 20 | T | 55 | LYS |
| 20 | T | 99 | LYS |
| 20 | T | 102 | LYS |
| 20 | T | 118 | LEU |
| 20 | T | 120 | GLU |
| 20 | T | 124 | GLU |
| 21 | U | 83 | TRP |
| 21 | U | 131 | LEU |
| 21 | U | 140 | ASN |
| 21 | U | 152 | ARG |
| 21 | U | 156 | VAL |
| 21 | U | 159 | HIS |
| 21 | U | 161 | LEU |
| 22 | V | 99 | LYS |
| 22 | V | 135 | ILE |
| 22 | V | 137 | ARG |
| 22 | V | 141 | ASP |
| 23 | W | 11 | CYS |
| 23 | W | 13 | ASP |
| 23 | W | 16 | THR |
| 23 | W | 63 | SER |
| 23 | W | 80 | LEU |
| 24 | X | 46 | GLN |
| 24 | X | 97 | ASP |
| 24 | X | 99 | LEU |
| 25 | Y | 57 | ILE |
| 25 | Y | 80 | GLU |
| 25 | Y | 179 | GLU |
| 25 | Y | 335 | LEU |
| 25 | Y | 479 | LEU |
| 25 | Y | 578 | GLU |
| 25 | Y | 587 | ARG |
| 25 | Y | 653 | PHE |
| 26 | Z | 320 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 26 | Z | 327 | LYS |
| 26 | Z | 333 | ILE |
| 26 | Z | 349 | ASN |
| 26 | Z | 383 | ILE |
| 26 | Z | 404 | LYS |
| 26 | Z | 407 | VAL |
| 26 | Z | 442 | ASN |
| 26 | Z | 524 | ILE |
| 26 | Z | 549 | ILE |
| 26 | Z | 570 | LEU |
| 26 | Z | 573 | THR |
| 26 | Z | 582 | ILE |
| 26 | Z | 621 | LYS |
| 26 | Z | 622 | MET |
| 26 | Z | 628 | TYR |
| 26 | Z | 630 | SER |
| 26 | Z | 634 | GLN |
| 26 | Z | 638 | ASN |
| 26 | Z | 647 | ASP |
| 26 | Z | 656 | LYS |
| 26 | Z | 660 | THR |
| 26 | Z | 664 | LEU |
| 26 | Z | 668 | THR |
| 26 | Z | 669 | CYS |
| 26 | Z | 674 | SER |
| 26 | Z | 677 | TYR |
| 26 | Z | 680 | ARG |
| 26 | Z | 681 | ARG |
| 26 | Z | 711 | LYS |
| 26 | Z | 714 | GLN |
| 26 | Z | 717 | TYR |
| 26 | Z | 720 | THR |
| 26 | Z | 740 | HIS |
| 26 | Z | 747 | ASN |
| 26 | Z | 756 | ARG |
| 26 | Z | 757 | ARG |
| 29 | c | 35 | VAL |
| 29 | c | 39 | SER |
| 29 | c | 52 | LEU |
| 29 | c | 59 | THR |
| 29 | c | 62 | GLU |
| 29 | c | 64 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 29 | c | 78 | ARG |
| 29 | c | 81 | GLU |
| 29 | c | 86 | LEU |
| 29 | c | 101 | THR |
| 29 | c | 114 | GLN |
| 29 | c | 142 | LEU |
| 29 | c | 145 | ILE |
| 29 | c | 168 | MET |
| 29 | c | 171 | ILE |
| 29 | c | 182 | ARG |
| 29 | c | 198 | VAL |
| 29 | c | 209 | ILE |
| 30 | d | 14 | VAL |
| 30 | d | 247 | LEU |
| 30 | d | 262 | LEU |
| 31 | e | 19 | LEU |
| 31 | e | 23 | LEU |
| 31 | e | 29 | ASP |
| 31 | e | 39 | ARG |
| 31 | e | 41 | LEU |
| 31 | e | 66 | LEU |
| 31 | e | 111 | LEU |
| 31 | e | 117 | ASN |
| 32 | f | 340 | LYS |
| 33 | g | 55 | GLU |
| 33 | g | 127 | LYS |
| 33 | g | 293 | ARG |
| 33 | g | 349 | TYR |
| 33 | g | 356 | LYS |
| 34 | h | 67 | ILE |
| 34 | h | 71 | LYS |
| 34 | h | 123 | MET |
| 34 | h | 129 | THR |
| 34 | h | 130 | LYS |
| 34 | h | 132 | THR |
| 34 | h | 133 | GLN |
| 34 | h | 142 | PHE |
| 34 | h | 144 | ARG |
| 34 | h | 145 | THR |
| 34 | h | 146 | GLU |
| 34 | h | 148 | LEU |
| 34 | h | 150 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | h | 151 | LEU |
| 34 | h | 152 | CYS |
| 34 | h | 154 | GLU |
| 34 | h | 156 | LEU |
| 35 | i | 127 | LYS |
| 35 | i | 135 | ILE |
| 35 | i | 137 | LYS |
| 35 | i | 140 | LYS |
| 35 | i | 149 | ASP |
| 35 | i | 154 | LYS |
| 35 | i | 159 | VAL |
| 35 | i | 161 | GLU |
| 35 | i | 162 | LEU |
| 35 | i | 164 | LYS |
| 35 | i | 165 | LYS |
| 35 | i | 166 | LEU |
| 35 | i | 167 | ASP |
| 35 | i | 171 | PHE |
| 35 | i | 179 | LYS |
| 35 | i | 196 | LEU |
| 35 | i | 207 | CYS |
| 35 | i | 208 | LYS |
| 35 | i | 209 | ASP |
| 35 | i | 219 | GLU |
| 35 | i | 220 | THR |
| 35 | i | 221 | ILE |
| 35 | i | 225 | GLU |
| 35 | i | 228 | SER |
| 35 | i | 232 | VAL |
| 35 | i | 233 | LEU |
| 35 | i | 238 | ASP |
| 36 | j | 68 | GLN |
| 36 | j | 78 | CYS |
| 36 | j | 87 | LEU |
| 36 | j | 141 | ARG |
| 36 | j | 145 | LYS |
| 36 | j | 151 | LYS |
| 36 | j | 211 | LYS |
| 36 | j | 233 | VAL |
| 36 | j | 234 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (114) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 425 | GLN |
| 1 | A | 545 | GLN |
| 1 | A | 548 | ASN |
| 1 | A | 603 | ASN |
| 1 | A | 966 | ASN |
| 1 | A | 994 | GLN |
| 1 | A | 1106 | ASN |
| 1 | A | 1140 | HIS |
| 1 | A | 1173 | HIS |
| 1 | A | 1270 | ASN |
| 1 | A | 1393 | ASN |
| 2 | B | 110 | HIS |
| 2 | B | 300 | HIS |
| 2 | B | 325 | GLN |
| 2 | B | 350 | GLN |
| 2 | B | 357 | GLN |
| 2 | B | 449 | ASN |
| 2 | B | 842 | ASN |
| 2 | B | 975 | GLN |
| 2 | B | 1025 | HIS |
| 2 | B | 1193 | GLN |
| 2 | B | 1195 | HIS |
| 3 | C | 184 | ASN |
| 4 | D | 37 | GLN |
| 4 | D | 143 | ASN |
| 4 | D | 165 | GLN |
| 5 | E | 3 | GLN |
| 7 | G | 71 | ASN |
| 7 | G | 102 | GLN |
| 8 | H | 35 | GLN |
| 8 | H | 83 | GLN |
| 9 | I | 83 | ASN |
| 9 | I | 89 | GLN |
| 9 | I | 108 | HIS |
| 17 | Q | 4 | GLN |
| 17 | Q | 53 | ASN |
| 17 | Q | 57 | GLN |
| 17 | Q | 86 | ASN |
| 17 | Q | 176 | ASN |
| 17 | Q | 205 | ASN |
| 17 | Q | 243 | ASN |
| 17 | Q | 258 | ASN |
| 17 | Q | 269 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 18 | R | 26 | ASN |
| 18 | R | 68 | GLN |
| 18 | R | 118 | GLN |
| 20 | T | 66 | ASN |
| 21 | U | 74 | GLN |
| 21 | U | 75 | GLN |
| 21 | U | 168 | HIS |
| 21 | U | 169 | GLN |
| 21 | U | 198 | GLN |
| 22 | V | 108 | ASN |
| 23 | W | 74 | ASN |
| 24 | X | 95 | ASN |
| 25 | Y | 60 | GLN |
| 25 | Y | 62 | HIS |
| 25 | Y | 138 | ASN |
| 25 | Y | 242 | ASN |
| 25 | Y | 362 | HIS |
| 25 | Y | 628 | GLN |
| 25 | Y | 661 | HIS |
| 25 | Y | 707 | ASN |
| 26 | Z | 320 | ASN |
| 26 | Z | 331 | GLN |
| 26 | Z | 349 | ASN |
| 26 | Z | 361 | GLN |
| 26 | Z | 366 | GLN |
| 26 | Z | 423 | GLN |
| 26 | Z | 426 | GLN |
| 26 | Z | 434 | ASN |
| 26 | Z | 447 | GLN |
| 26 | Z | 471 | GLN |
| 26 | Z | 491 | HIS |
| 26 | Z | 508 | HIS |
| 26 | Z | 528 | ASN |
| 26 | Z | 551 | ASN |
| 26 | Z | 589 | GLN |
| 26 | Z | 596 | GLN |
| 26 | Z | 638 | ASN |
| 26 | Z | 648 | GLN |
| 26 | Z | 676 | HIS |
| 26 | Z | 738 | HIS |
| 26 | Z | 740 | HIS |
| 26 | Z | 747 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 26 | Z | 761 | GLN |
| 28 | b | 11 | GLN |
| 28 | b | 22 | GLN |
| 29 | c | 208 | ASN |
| 30 | d | 3 | ASN |
| 30 | d | 40 | ASN |
| 30 | d | 43 | GLN |
| 30 | d | 59 | GLN |
| 30 | d | 270 | ASN |
| 30 | d | 272 | ASN |
| 31 | e | 57 | GLN |
| 31 | e | 84 | GLN |
| 31 | e | 117 | ASN |
| 33 | g | 86 | ASN |
| 33 | g | 98 | ASN |
| 33 | g | 118 | HIS |
| 33 | g | 131 | ASN |
| 33 | g | 220 | HIS |
| 33 | g | 328 | HIS |
| 34 | h | 50 | ASN |
| 34 | h | 133 | GLN |
| 34 | h | 141 | ASN |
| 35 | i | 199 | GLN |
| 35 | i | 216 | GLN |
| 36 | j | 68 | GLN |
| 36 | j | 88 | HIS |
| 36 | j | 144 | GLN |
| 36 | j | 158 | GLN |
| 36 | j | 219 | GLN |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8305. 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

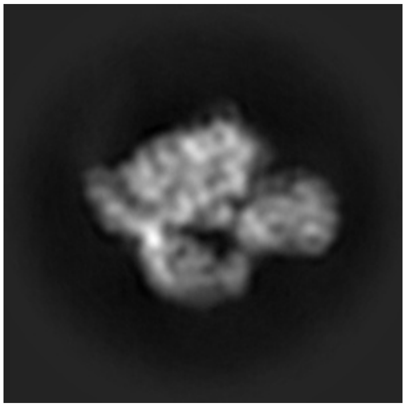
### 6.1.1 Primary map

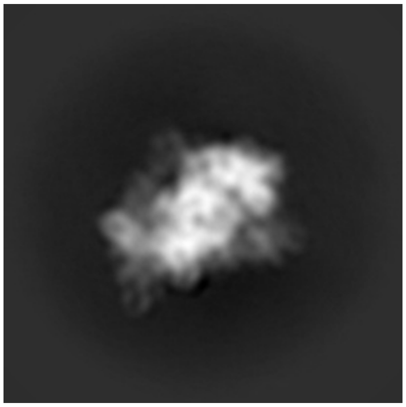

X

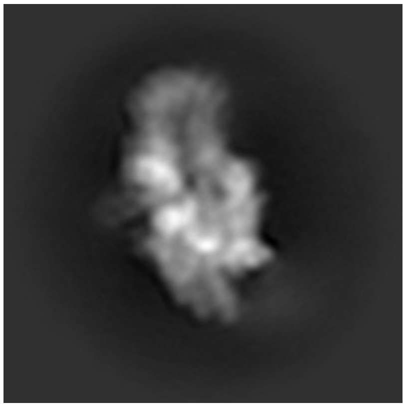

Y


Z

### 6.1.2 Raw map


X


Y


Z

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

## 6.2 Central slices ⓘ

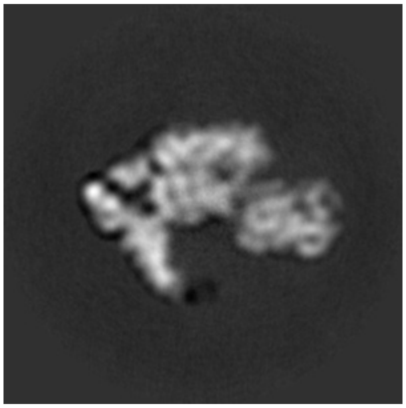
### 6.2.1 Primary map

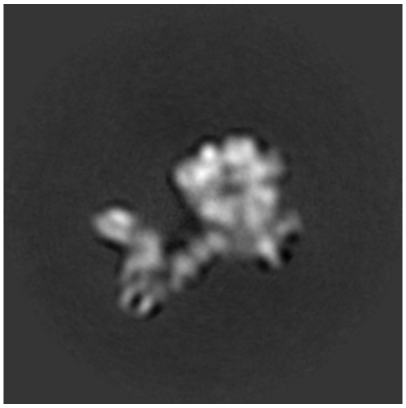

X Index: 110

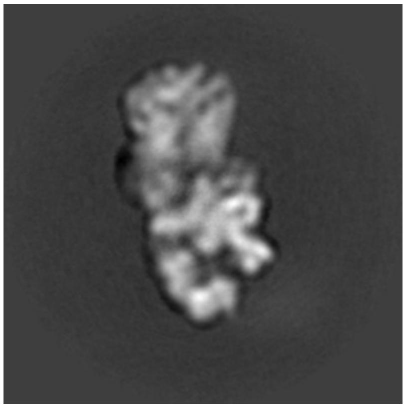

Y Index: 110


Z Index: 110

### 6.2.2 Raw map


X Index: 110


Y Index: 110


Z Index: 110

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

## 6.3 Largest variance slices

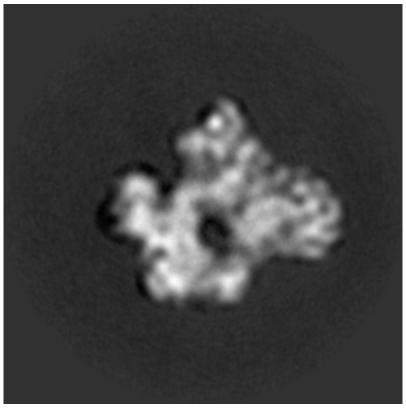
### 6.3.1 Primary map

X Index: 90

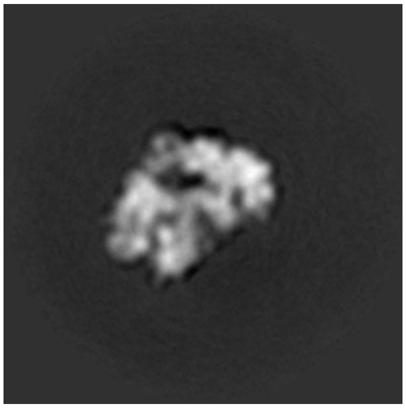
Y Index: 86

Z Index: 103

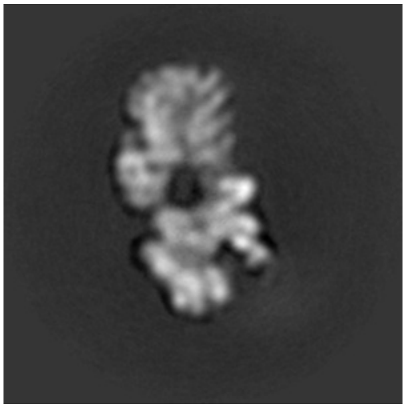
### 6.3.2 Raw map



X Index: 90



Y Index: 86

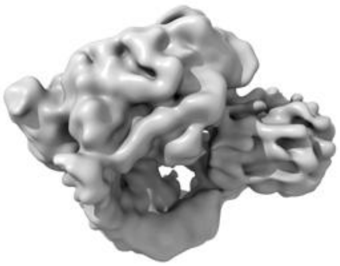


Z Index: 103

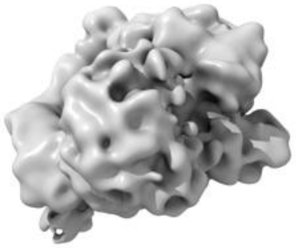
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views ⓘ

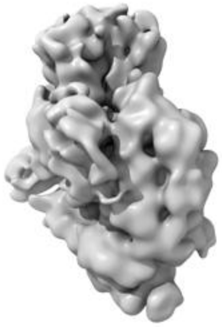
### 6.4.1 Primary map



X



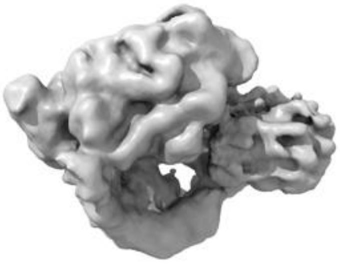
Y



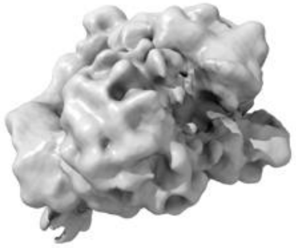
Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



X



Y

Z

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

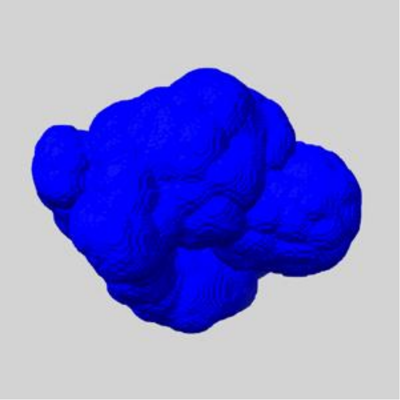
## 6.5 Mask visualisation

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

A mask typically either:

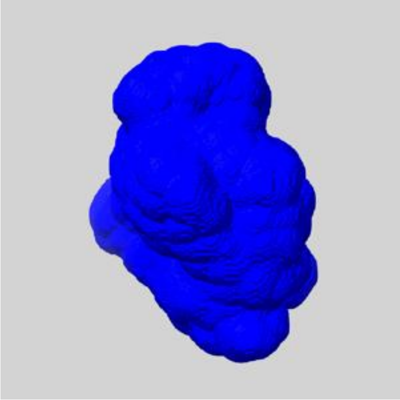
- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

### 6.5.1 emd_8305_msk_1.map



X

Y

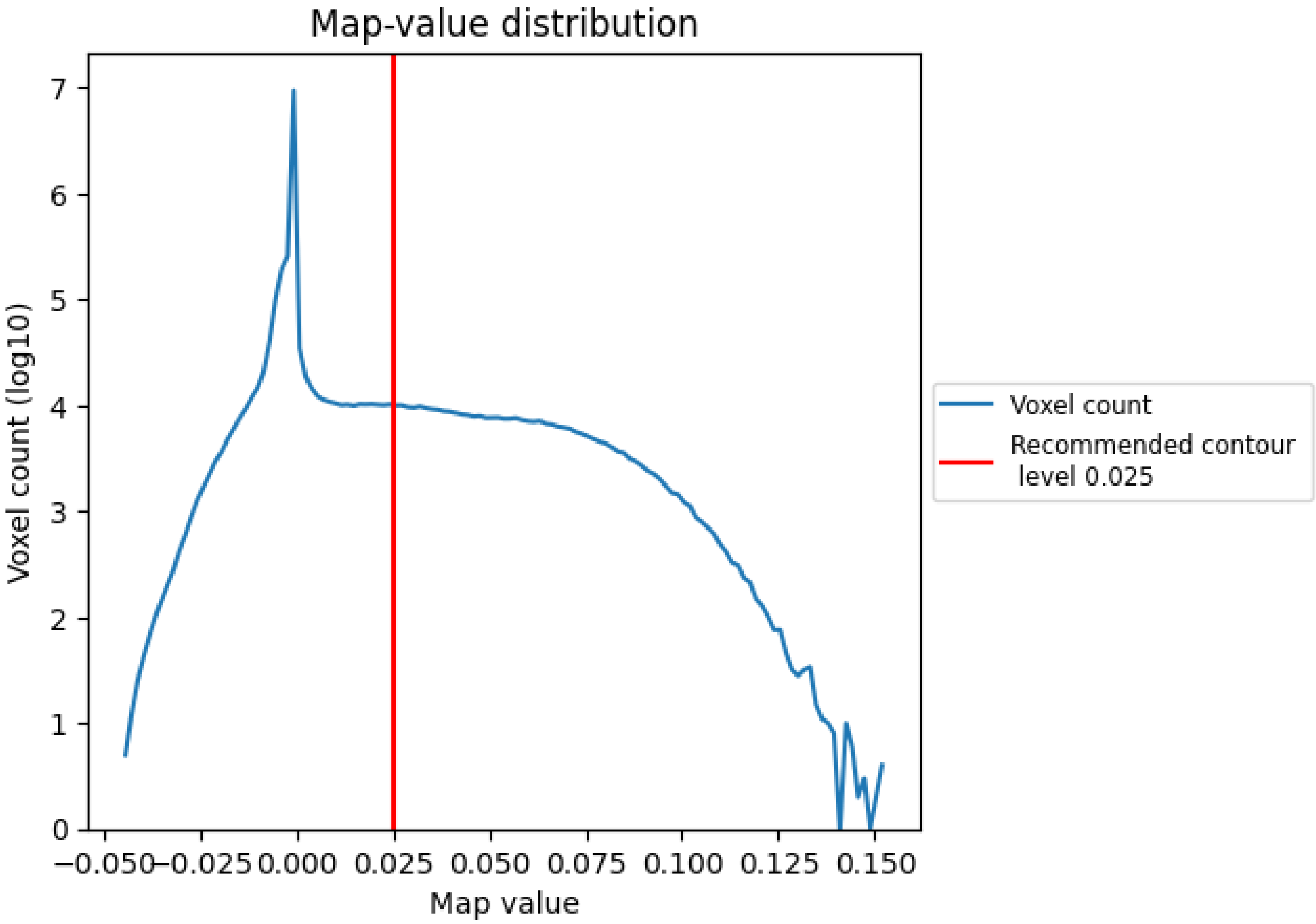


Z

# 7 Map analysis ⓘ

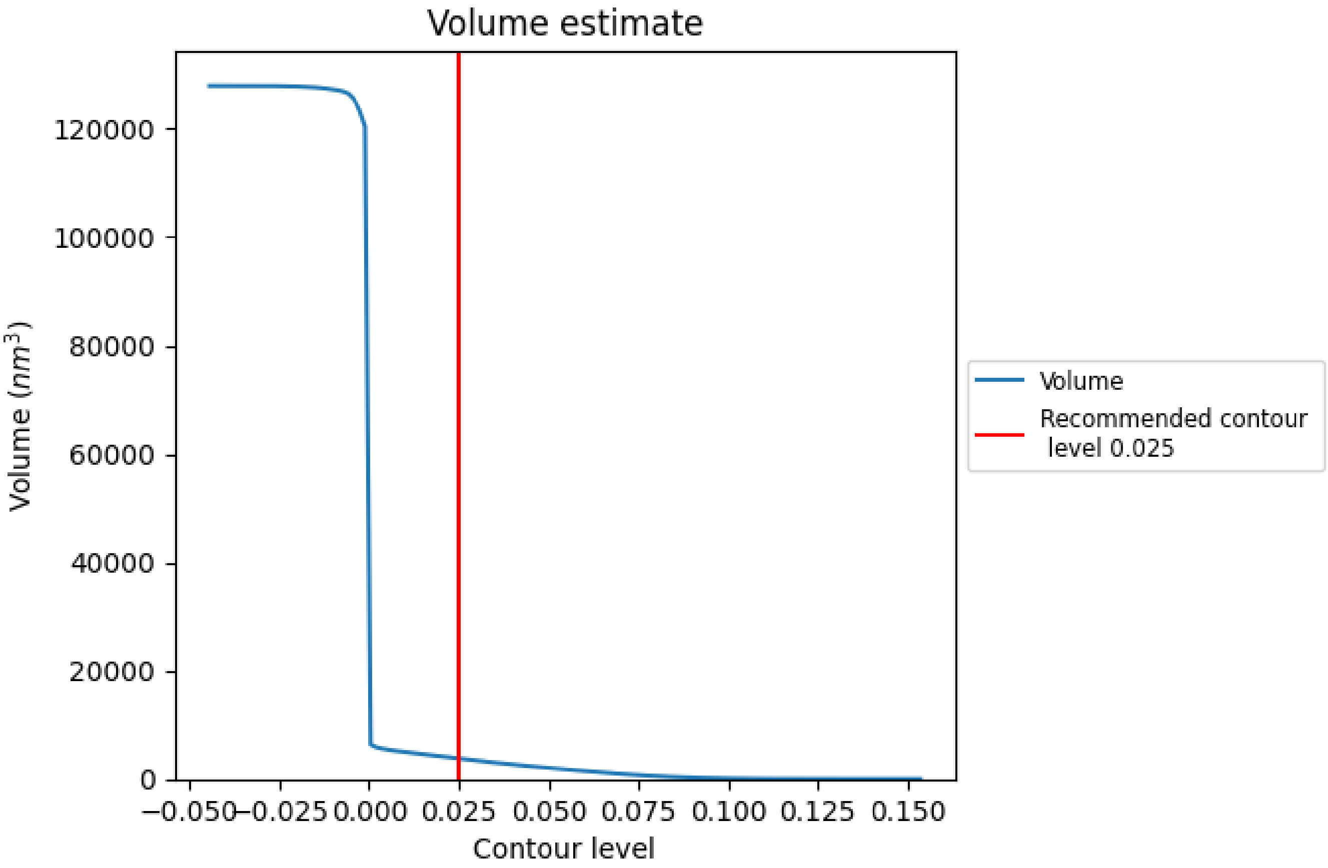
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution ⓘ



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.

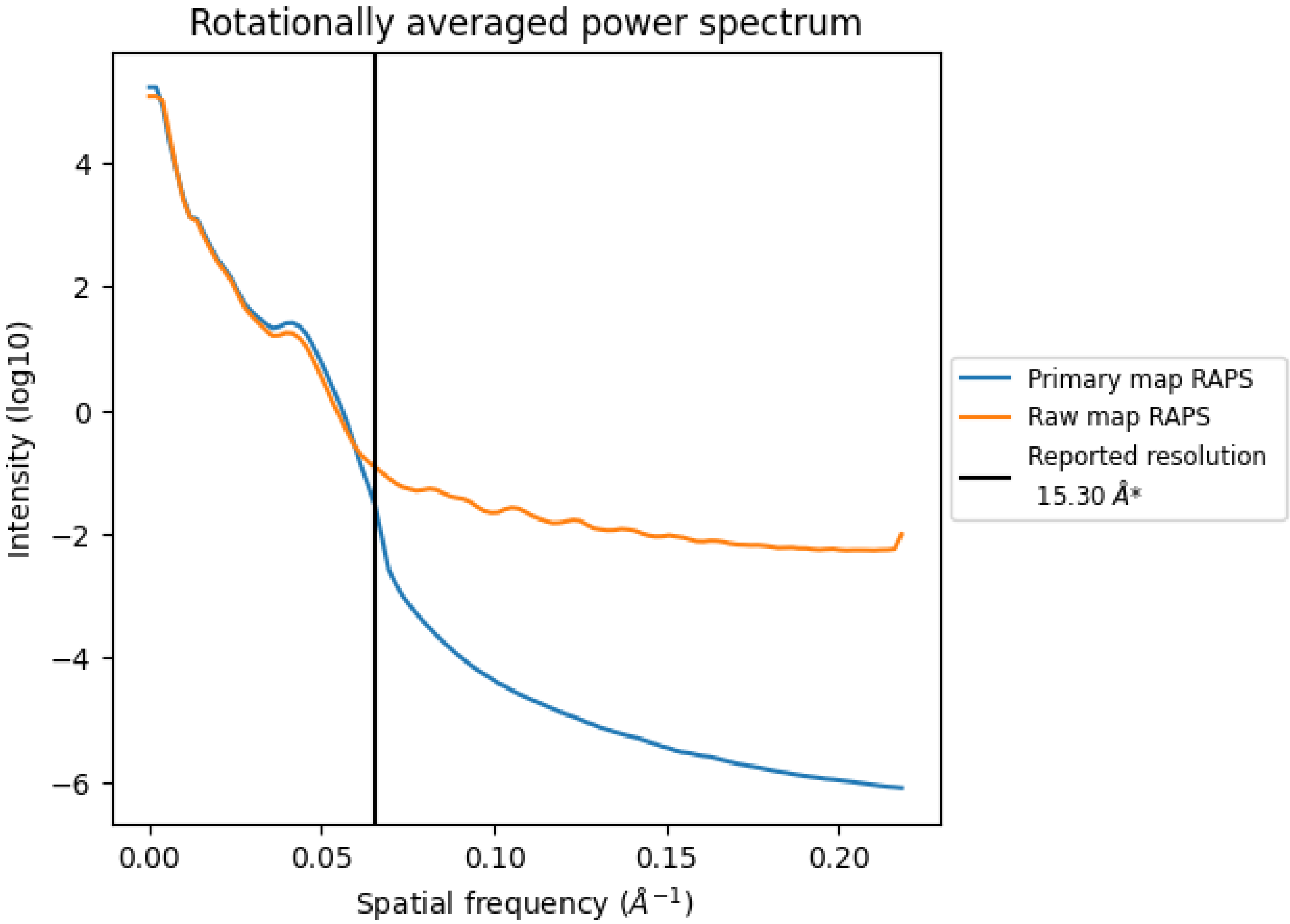
## 7.2 Volume estimate ⓘ



The volume at the recommended contour level is 3796 nm$^3$; this corresponds to an approximate mass of 3429 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 ⓘ

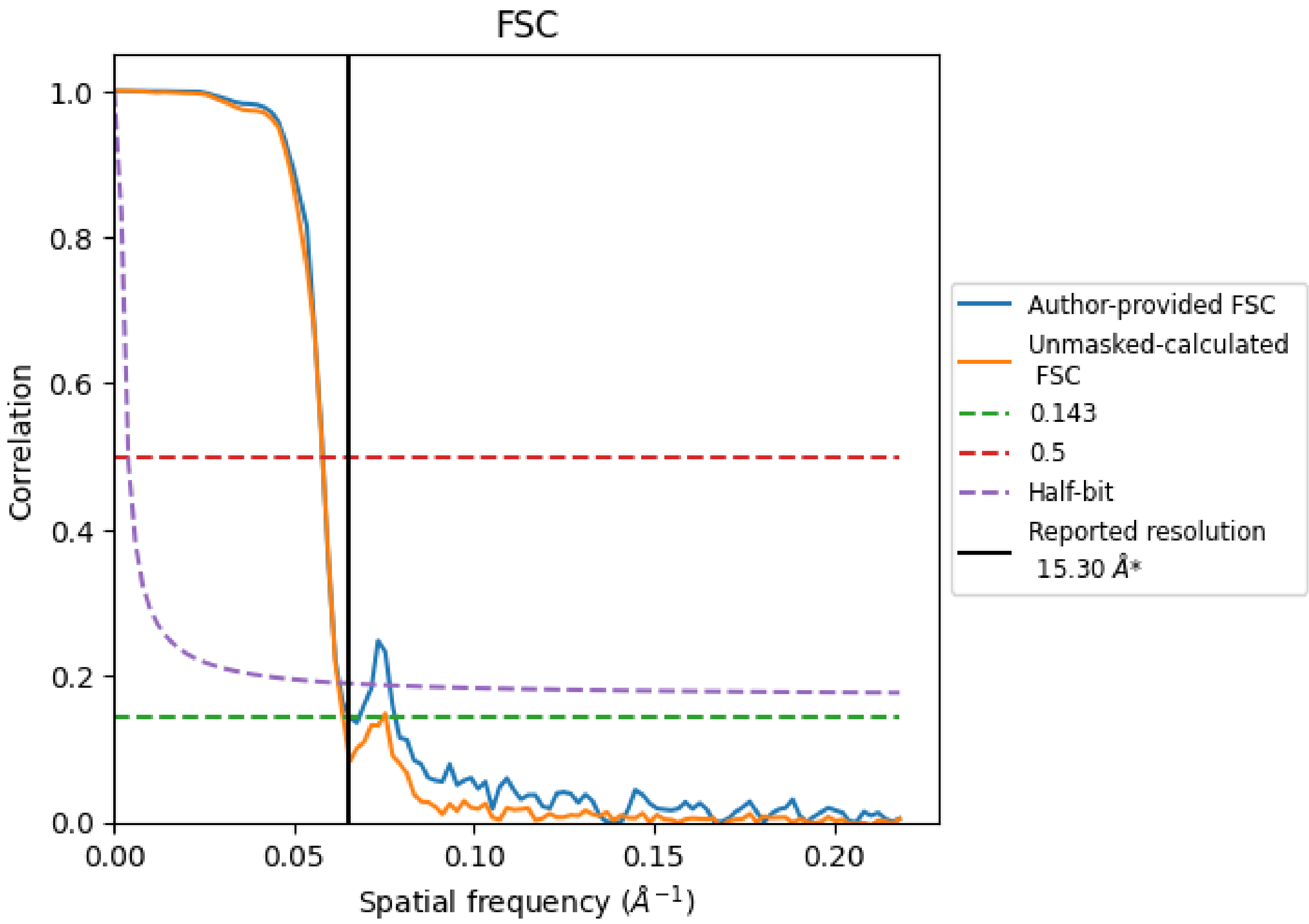


*Reported resolution corresponds to spatial frequency of 0.065 $\AA^{-1}$

# 8 Fourier-Shell correlation ⓘ

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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.065 Å$^{-1}$

## 8.2 Resolution estimates

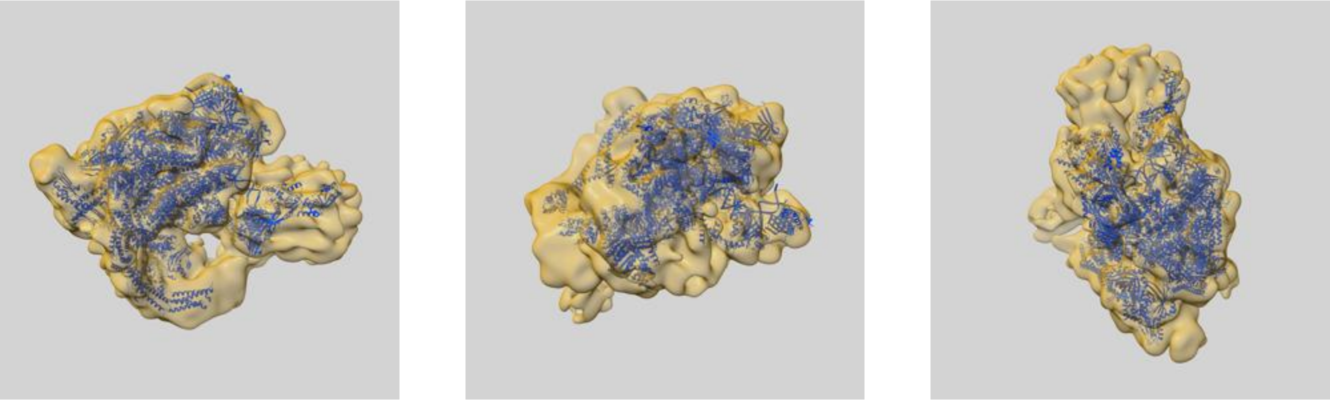
| **Resolution estimate (Å)** | **Estimation criterion (FSC cut-off)** | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 15.30 | - | - |
| Author-provided FSC curve | 15.27 | 17.24 | 15.97 |
| Unmasked-calculated* | 15.70 | 17.27 | 16.05 |

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

# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8305 and PDB model 5SVA. Per-residue inclusion information can be found in section 3 on page 12.

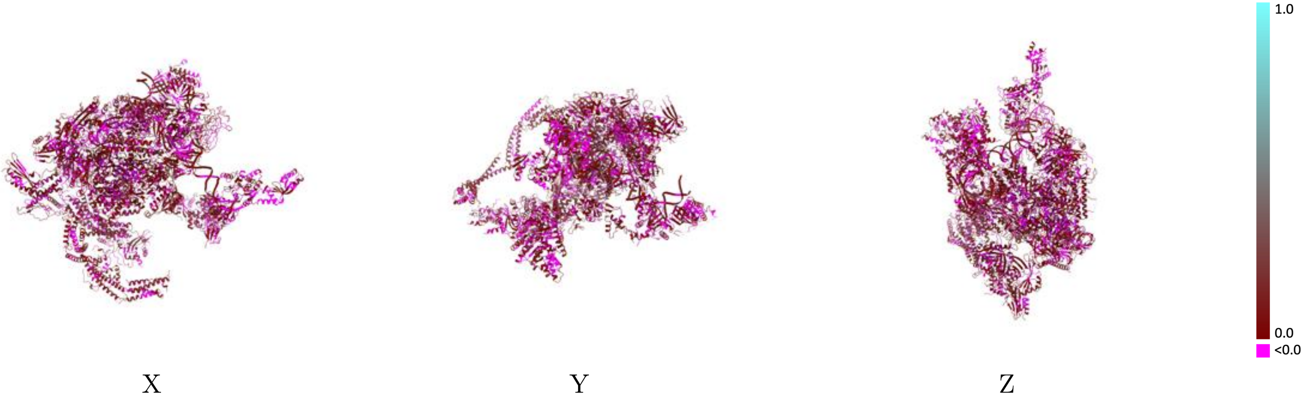
## 9.1 Map-model overlay (i)



X Y Z

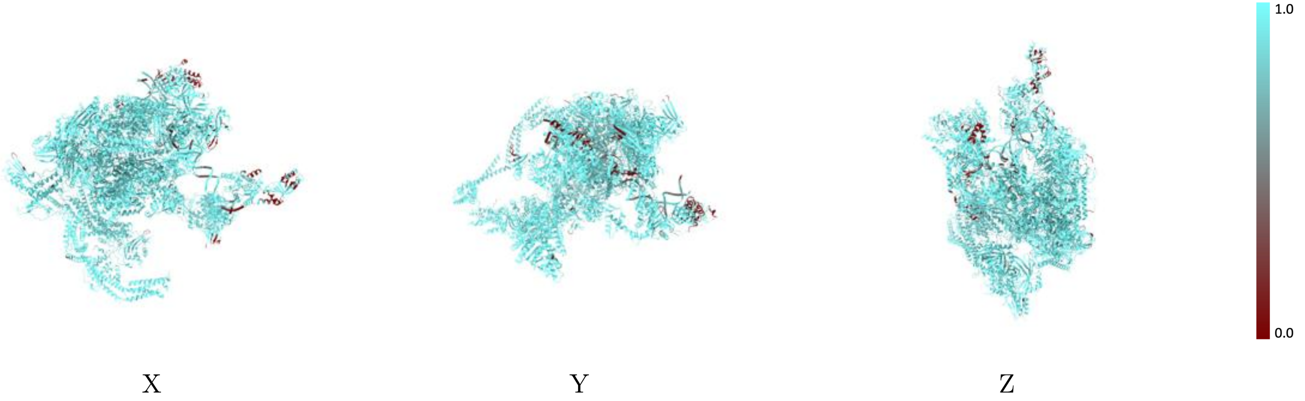
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model ⓘ



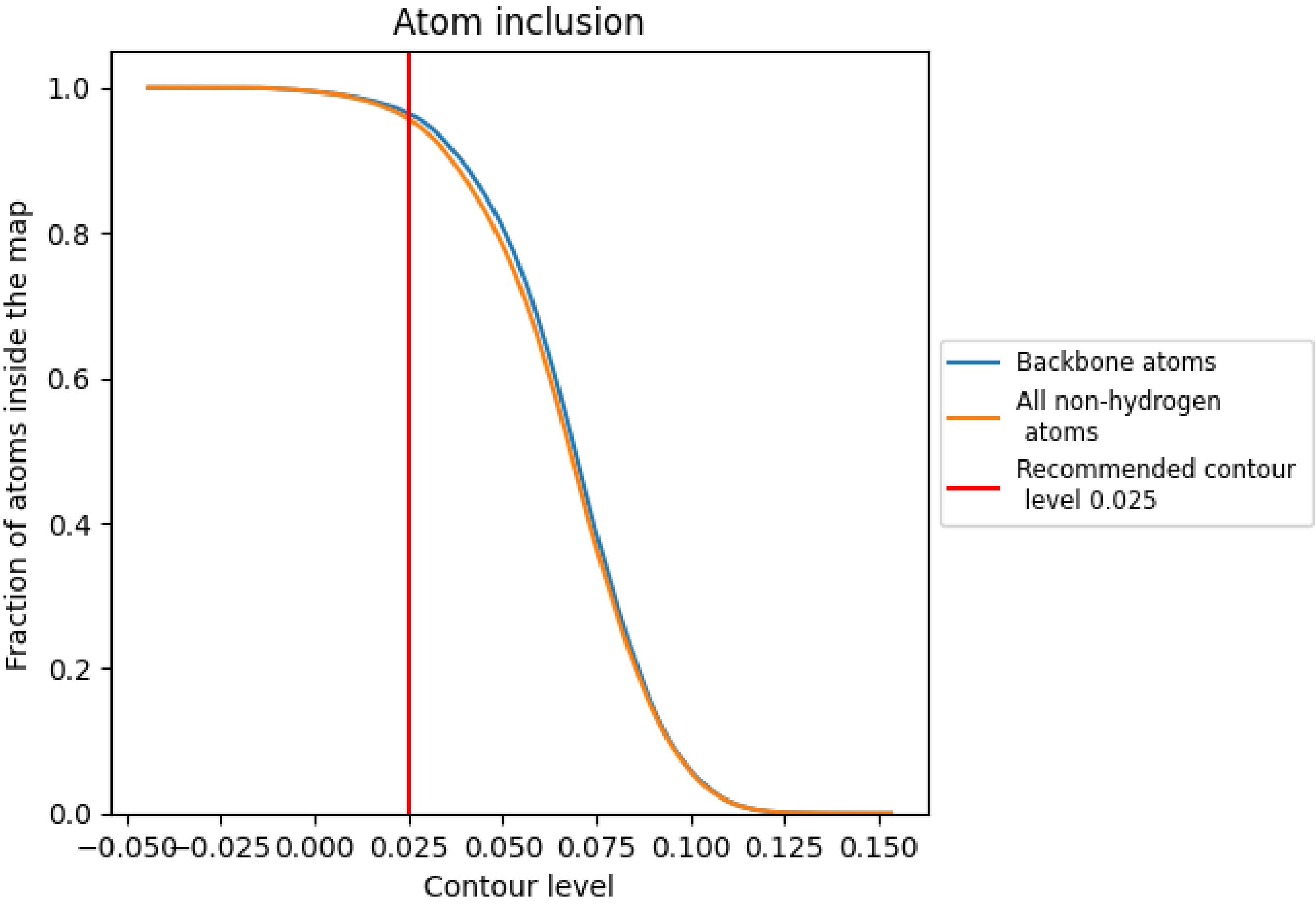
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.025).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 96% of all backbone atoms, 96% 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 (0.025) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.9567 | 0.0490 |
| A | 0.9933 | 0.0610 |
| B | 0.9962 | 0.0400 |
| C | 0.9898 | 0.0500 |
| D | 0.9780 | 0.0630 |
| E | 0.9930 | 0.0720 |
| F | 0.9970 | 0.0640 |
| G | 0.9758 | 0.0570 |
| H | 0.9510 | 0.0380 |
| I | 0.9440 | 0.0490 |
| J | 1.0000 | 0.0810 |
| K | 0.9746 | 0.0720 |
| L | 1.0000 | 0.0570 |
| M | 0.9665 | 0.0290 |
| N | 0.9989 | 0.0450 |
| O | 1.0000 | 0.0700 |
| P | 0.9851 | 0.0610 |
| Q | 0.9923 | 0.0460 |
| R | 0.9810 | 0.0630 |
| S | 1.0000 | 0.0330 |
| T | 0.9798 | 0.0460 |
| U | 0.9961 | 0.0700 |
| V | 0.9772 | 0.1040 |
| W | 0.9958 | 0.0940 |
| X | 0.9854 | 0.0070 |
| Y | 0.9923 | 0.0450 |
| Z | 0.9340 | 0.0360 |
| a | 0.6090 | -0.0120 |
| b | 0.6037 | 0.0000 |
| c | 0.9679 | 0.0260 |
| d | 0.5480 | 0.0070 |
| e | 0.7375 | 0.0220 |
| f | 0.9133 | 0.0170 |
| g | 0.9823 | 0.0240 |
| h | 0.9606 | 0.0620 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| i | 🟦 1.0000 | 🟥 0.0750 |
| j | 🟦 0.8256 | 🟥 0.0390 |
| k | 🟦 1.0000 | 🟪 -0.0140 |
| l | 🟦 0.7679 | 🟥 0.0630 |
| m | 🟦 0.8253 | 🟥 0.0540 |
| n | 🟦 0.8600 | 🟥 0.0390 |