



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Aug 20, 2017 – 11:31 AM EDT

PDB ID : 5MQ0
EMDB ID: : EMD-3541
Title : Structure of a spliceosome remodeled for exon ligation
Authors : Fica, S.M.; Oubridge, C.; Galej, W.P.; Wilkinson, M.E.; Newman, A.J.; Bai, X.-C.; Nagai, K.
Deposited on : unknown
Resolution : 4.17 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

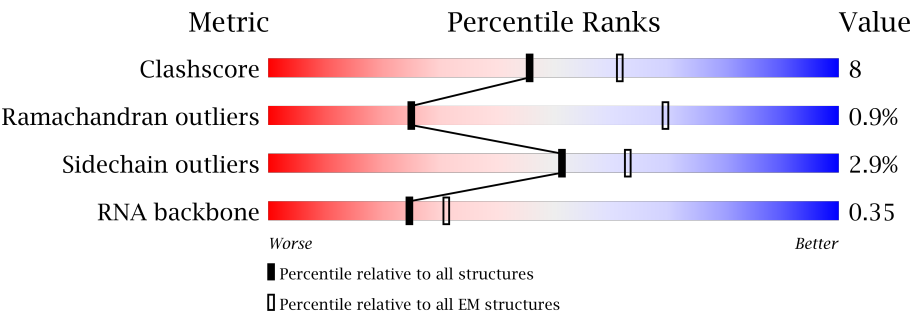
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.17 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.
















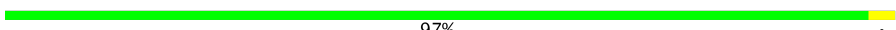











| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Clashscore | 125131 | 1336 |
| Ramachandran outliers | 121729 | 1120 |
| Sidechain outliers | 121581 | 1026 |
| RNA backbone | 3398 | 335 |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------------------------|
| 1 | I | 95 | <div><div>13%19%.64%</div></div> |
| 2 | E | 20 | <div><div>15%50%15%20%</div></div> |
| 3 | 2 | 1175 | <div><div>8%..87%</div></div> |
| 4 | 6 | 112 | <div><div>36%43%10%12%</div></div> |
| 5 | 5 | 179 | <div><div>32%37%9%21%</div></div> |
| 6 | A | 2413 | <div><div>64%15%21%</div></div> |
| 7 | C | 1008 | <div><div>71%16%13%</div></div> |
| 8 | H | 577 | <div><div>52%17%.31%</div></div> |


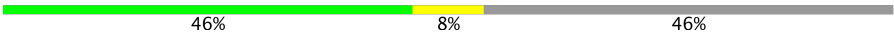






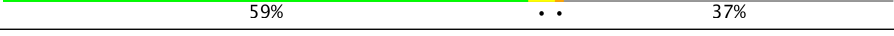
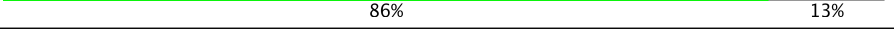
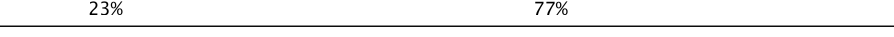


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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 9 | J | 451 |  |
| 10 | K | 379 |  |
| 11 | L | 157 |  |
| 12 | M | 339 |  |
| 13 | N | 364 |  |
| 14 | O | 590 |  |
| 15 | P | 175 |  |
| 16 | R | 135 |  |
| 17 | S | 687 |  |
| 18 | T | 877 |  |
| 19 | a | 251 |  |
| 20 | c | 382 |  |
| 21 | o | 455 |  |
| 22 | X | 68 |  |
| 23 | y | 215 |  |
| 24 | b | 196 |  |
| 24 | k | 196 |  |
| 25 | d | 101 |  |
| 25 | n | 101 |  |
| 26 | e | 94 |  |
| 26 | p | 94 |  |
| 27 | f | 86 |  |
| 27 | q | 86 |  |
| 28 | g | 77 |  |
| 28 | r | 77 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 29 | h | 146 |  |
| 29 | l | 146 |  |
| 30 | j | 110 |  |
| 30 | m | 110 |  |
| 31 | V | 1145 |  |
| 32 | W | 238 |  |
| 33 | Y | 111 |  |
| 34 | 3 | 3 |  |
| 35 | s | 175 |  |
| 36 | t | 503 |  |
| 36 | u | 503 |  |
| 36 | v | 503 |  |
| 36 | w | 503 |  |

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 77441 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 RNA chain called Yeast UBC4 gene for ubiquitin-conjugating enzyme.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 1 | I | 34 | Total | C | N | O | P | 0 | 0 |
| | | | 714 | 321 | 118 | 241 | 34 | | |

- Molecule 2 is a RNA chain called 5'-EXON OF UBC4 PRE-MRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 2 | E | 16 | Total | C | N | O | P | 0 | 0 |
| | | | 346 | 155 | 66 | 109 | 16 | | |

- Molecule 3 is a RNA chain called S.cerevisiae chromosome II reading frame ORF YBR230c.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 3 | 2 | 155 | Total | C | N | O | P | 0 | 0 |
| | | | 3271 | 1462 | 547 | 1107 | 155 | | |

- Molecule 4 is a RNA chain called Saccharomyces cerevisiae strain T.52_2H chromosome XII sequence.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 4 | 6 | 99 | Total | C | N | O | P | 0 | 0 |
| | | | 2108 | 944 | 375 | 690 | 99 | | |

- Molecule 5 is a RNA chain called Saccharomyces cerevisiae strain WI_C_MBSP_4 chromosome VII sequence.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 5 | 5 | 141 | Total | C | N | O | P | 0 | 0 |
| | | | 2999 | 1342 | 530 | 986 | 141 | | |

- Molecule 6 is a protein called Pre-mRNA-splicing factor 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 6 | A | 1914 | Total | C | N | O | S | 0 | 0 |
| | | | 15199 | 9832 | 2669 | 2645 | 53 | | |

- Molecule 7 is a protein called Pre-mRNA-splicing factor SNU114.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 7 | C | 874 | Total | C | N | O | S | 0 | 0 |
| | | | 6562 | 4265 | 1104 | 1168 | 25 | | |

- Molecule 8 is a protein called Pre-mRNA-splicing factor CWC22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8 | H | 401 | Total | C | N | O | S | 0 | 0 |
| | | | 3261 | 2104 | 544 | 595 | 18 | | |

- Molecule 9 is a protein called Pre-mRNA-splicing factor PRP46.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9 | J | 342 | Total | C | N | O | S | 0 | 0 |
| | | | 2690 | 1699 | 475 | 506 | 10 | | |

- Molecule 10 is a protein called Pre-mRNA-processing protein 45.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10 | K | 187 | Total | C | N | O | S | 0 | 0 |
| | | | 1458 | 908 | 269 | 276 | 5 | | |

- Molecule 11 is a protein called Pre-mRNA-splicing factor BUD31.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 11 | L | 155 | Total | C | N | O | S | 0 | 0 |
| | | | 1162 | 737 | 217 | 198 | 10 | | |

- Molecule 12 is a protein called Pre-mRNA-splicing factor CWC2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12 | M | 252 | Total | C | N | O | S | 0 | 0 |
| | | | 2016 | 1281 | 356 | 368 | 11 | | |

- Molecule 13 is a protein called Pre-mRNA-splicing factor SLT11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 13 | N | 227 | Total | C | N | O | S | 0 | 0 |
| | | | 1798 | 1139 | 309 | 335 | 15 | | |

- Molecule 14 is a protein called Pre-mRNA-splicing factor CEF1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14 | O | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1755 | 1102 | 320 | 327 | 6 | | |

- Molecule 15 is a protein called Pre-mRNA-splicing factor CWC15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 15 | P | 69 | Total | C | N | O | S | 0 | 0 |
| | | | 565 | 358 | 112 | 94 | 1 | | |

- Molecule 16 is a protein called Pre-mRNA-splicing factor CWC21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 16 | R | 108 | Total | C | N | O | | 0 | 0 |
| | | | 614 | 369 | 121 | 124 | | | |

- Molecule 17 is a protein called Pre-mRNA-splicing factor CLF1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 17 | S | 468 | Total | C | N | O | S | 0 | 0 |
| | | | 3229 | 2025 | 599 | 598 | 7 | | |

- Molecule 18 is a protein called Pre-mRNA-splicing factor SYF1,PRE-MRNASPLICING FACTOR SYF1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|--|---------|-------|
| 18 | T | 633 | Total | C | N | O | | 0 | 0 |
| | | | 3154 | 1888 | 633 | 633 | | | |

- Molecule 19 is a protein called Pre-mRNA-splicing factor 18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19 | a | 137 | Total | C | N | O | S | 0 | 0 |
| | | | 1119 | 726 | 194 | 196 | 3 | | |

- Molecule 20 is a protein called Pre-mRNA-splicing factor SLU7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20 | c | 103 | Total | C | N | O | S | 0 | 0 |
| | | | 786 | 498 | 142 | 144 | 2 | | |

- Molecule 21 is a protein called Pre-mRNA-processing factor 17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 21 | o | 313 | Total | C | N | O | S | 0 | 0 |
| | | | 2425 | 1537 | 429 | 451 | 8 | | |

- Molecule 22 is a protein called UNKNOWN PROTEIN.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 22 | X | 68 | Total | C | N | O | 0 | 0 |
| | | | 338 | 202 | 68 | 68 | | |

- Molecule 23 is a protein called Pre-mRNA-splicing factor SYF2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23 | y | 83 | Total | C | N | O | S | 0 | 0 |
| | | | 679 | 420 | 125 | 133 | 1 | | |

- Molecule 24 is a protein called Small nuclear ribonucleoprotein-associated protein B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24 | b | 80 | Total | C | N | O | S | 0 | 0 |
| | | | 631 | 403 | 114 | 111 | 3 | | |
| 24 | k | 80 | Total | C | N | O | S | 0 | 0 |
| | | | 631 | 403 | 114 | 111 | 3 | | |

- Molecule 25 is a protein called Small nuclear ribonucleoprotein Sm D3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25 | d | 82 | Total | C | N | O | S | 0 | 0 |
| | | | 625 | 399 | 109 | 115 | 2 | | |
| 25 | n | 82 | Total | C | N | O | S | 0 | 0 |
| | | | 625 | 399 | 109 | 115 | 2 | | |

- Molecule 26 is a protein called Small nuclear ribonucleoprotein E.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 26 | e | 75 | Total | C | N | O | S | 0 | 0 |
| | | | 575 | 379 | 92 | 101 | 3 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 26 | p | 75 | Total | C | N | O | S | 0 | 0 |
| | | | 575 | 379 | 92 | 101 | 3 | | |

- Molecule 27 is a protein called Small nuclear ribonucleoprotein F.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27 | f | 72 | Total | C | N | O | S | 0 | 0 |
| | | | 573 | 368 | 101 | 103 | 1 | | |
| 27 | q | 72 | Total | C | N | O | S | 0 | 0 |
| | | | 573 | 368 | 101 | 103 | 1 | | |

- Molecule 28 is a protein called Small nuclear ribonucleoprotein G.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 28 | g | 69 | Total | C | N | O | S | 0 | 0 |
| | | | 529 | 337 | 93 | 97 | 2 | | |
| 28 | r | 69 | Total | C | N | O | S | 0 | 0 |
| | | | 526 | 336 | 93 | 95 | 2 | | |

- Molecule 29 is a protein called Small nuclear ribonucleoprotein Sm D1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29 | h | 82 | Total | C | N | O | S | 0 | 0 |
| | | | 644 | 409 | 110 | 123 | 2 | | |
| 29 | l | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 618 | 393 | 107 | 116 | 2 | | |

- Molecule 30 is a protein called Small nuclear ribonucleoprotein Sm D2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30 | j | 94 | Total | C | N | O | S | 0 | 0 |
| | | | 741 | 477 | 141 | 119 | 4 | | |
| 30 | m | 93 | Total | C | N | O | S | 0 | 0 |
| | | | 726 | 468 | 136 | 118 | 4 | | |

- Molecule 31 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP22.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 31 | V | 645 | Total | C | N | O | 0 | 0 |
| | | | 3189 | 1899 | 645 | 645 | | |

- Molecule 32 is a protein called U2 small nuclear ribonucleoprotein A'.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 32 | W | 164 | Total | C | N | O | 0 | 0 |
| | | | 816 | 488 | 164 | 164 | | |

- Molecule 33 is a protein called U2 small nuclear ribonucleoprotein B''.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 33 | Y | 84 | Total | C | N | O | 0 | 0 |
| | | | 416 | 248 | 84 | 84 | | |

- Molecule 34 is a RNA chain called 3'-EXON OF UBC4 PRE-MRNA, BOUND BY PRP22 HELICASE.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---|---------|-------|
| 34 | 3 | 3 | Total | C | N | O | P | 0 | 0 |
| | | | 60 | 27 | 6 | 24 | 3 | | |

- Molecule 35 is a protein called Pre-mRNA-splicing factor SNT309.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 35 | s | 110 | Total | C | N | O | 0 | 0 |
| | | | 548 | 328 | 110 | 110 | | |

- Molecule 36 is a protein called Pre-mRNA-processing factor 19.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 36 | t | 438 | Total | C | N | O | 0 | 0 |
| | | | 2171 | 1295 | 438 | 438 | | |
| 36 | u | 116 | Total | C | N | O | 0 | 0 |
| | | | 578 | 346 | 116 | 116 | | |
| 36 | v | 118 | Total | C | N | O | 0 | 0 |
| | | | 588 | 352 | 118 | 118 | | |
| 36 | w | 435 | Total | C | N | O | 0 | 0 |
| | | | 2156 | 1286 | 435 | 435 | | |

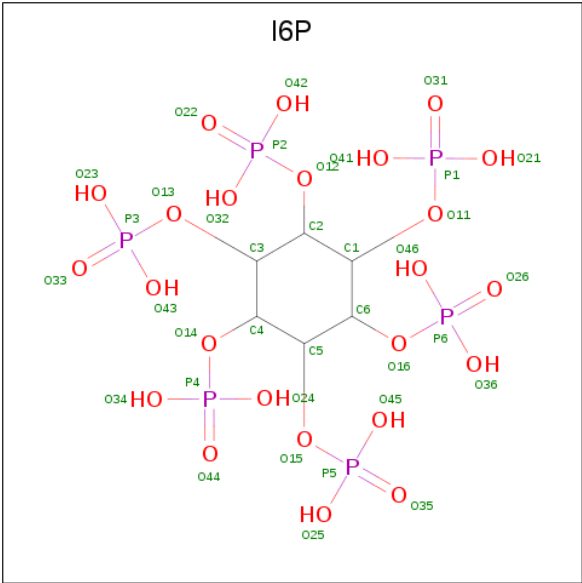
- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 37 | 6 | 3 | Total | Mg | 0 |
| | | | 3 | 3 | |

- Molecule 38 is POTASSIUM ION (three-letter code: K) (formula: K).

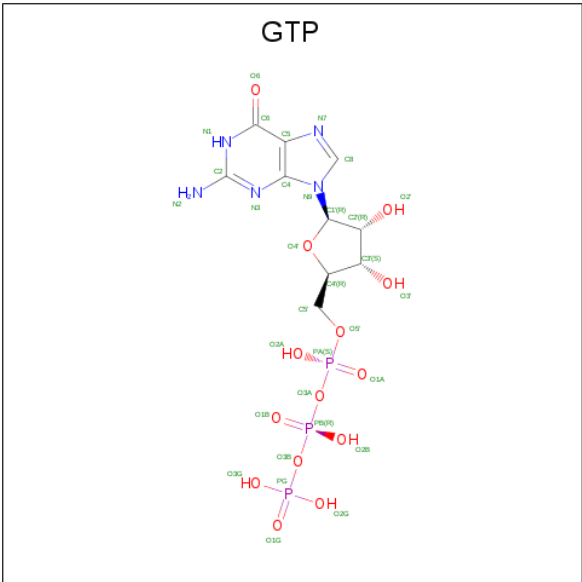
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|---|--|---------|
| 38 | 6 | 2 | Total | K | | 0 |
| | | | 2 | 2 | | |

- Molecule 39 is INOSITOL 1,2,3,4,5,6-HEXAKISPHOSPHATE (three-letter code: I6P) (formula: C₆H₁₈O₂₄P₆).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|---|----|---|---------|
| 39 | A | 1 | Total | C | O | P | 0 |
| | | | 36 | 6 | 24 | 6 | |

- Molecule 40 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 40 | C | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |

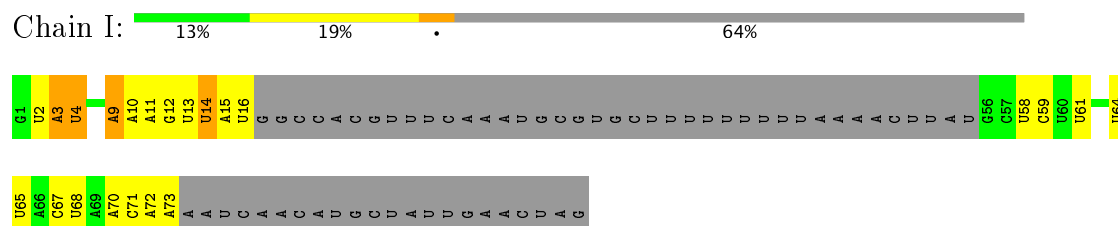
- Molecule 41 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 41 | L | 3 | Total | Zn | 0 |
| | | | 3 | 3 | |
| 41 | N | 2 | Total | Zn | 0 |
| | | | 2 | 2 | |
| 41 | M | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

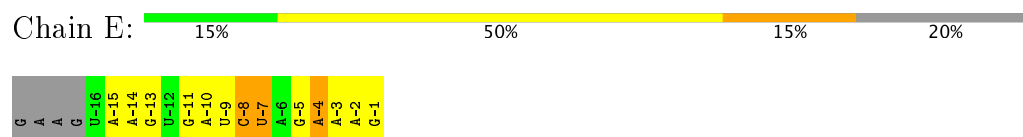
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

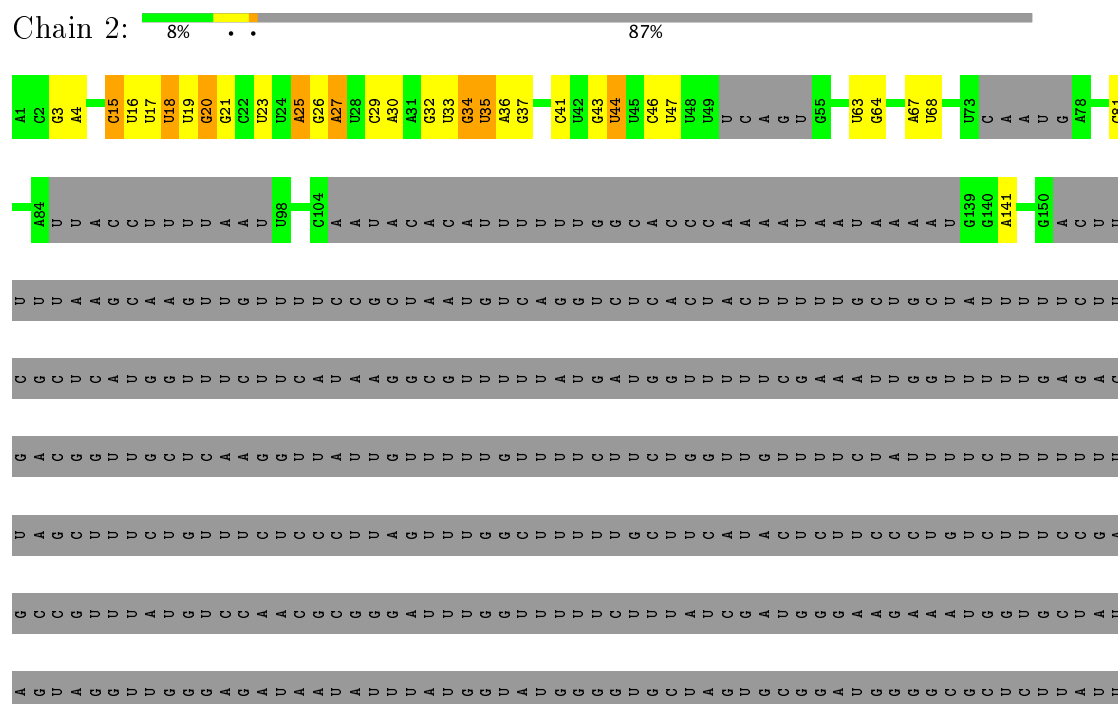
- Molecule 1: Yeast UBC4 gene for ubiquitin-conjugating enzyme



- Molecule 2: 5'-EXON OF UBC4 PRE-MRNA



- Molecule 3: *S.cerevisiae* chromosome II reading frame ORF YBR230c



Chain A:

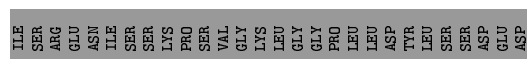
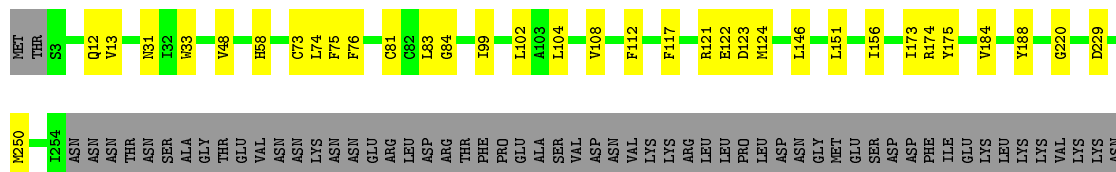
[illegible]





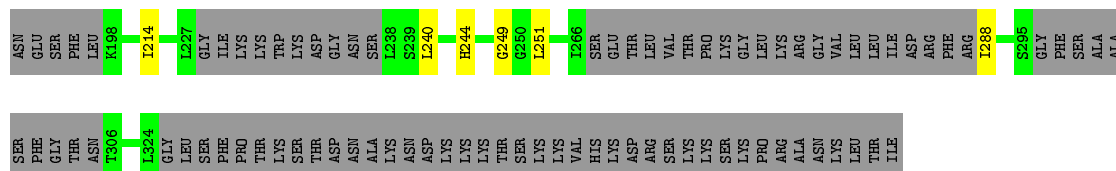
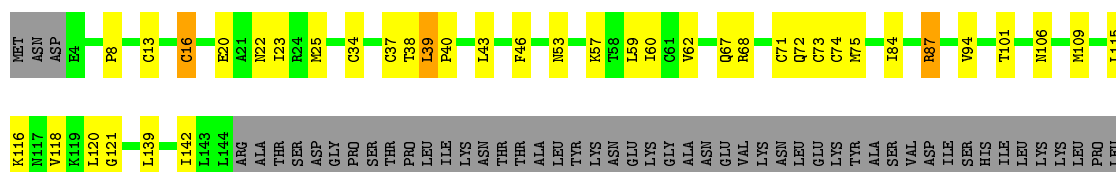
- Molecule 12: Pre-mRNA-splicing factor CWC2

Chain M:



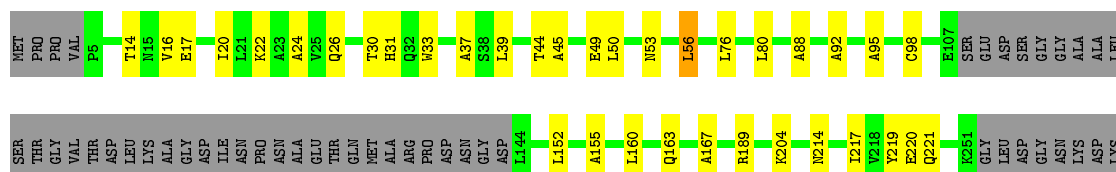
- Molecule 13: Pre-mRNA-splicing factor SLT11

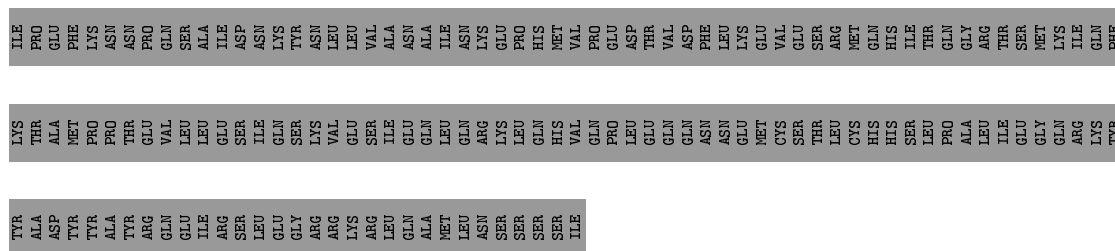
Chain N:



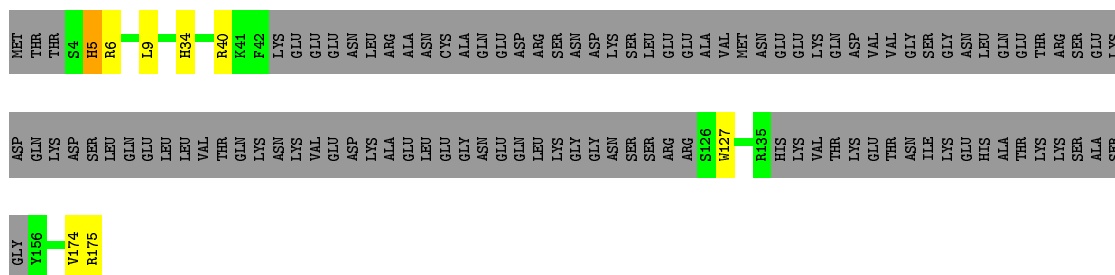
- Molecule 14: Pre-mRNA-splicing factor CEF1

Chain O:





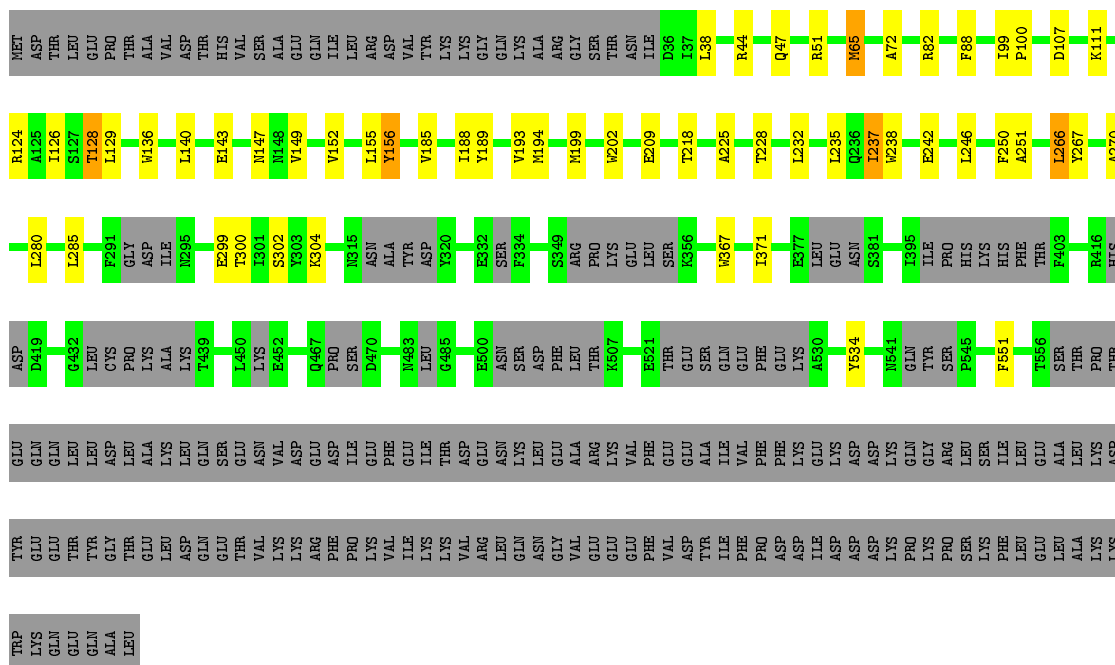
- Molecule 15: Pre-mRNA-splicing factor CWC15




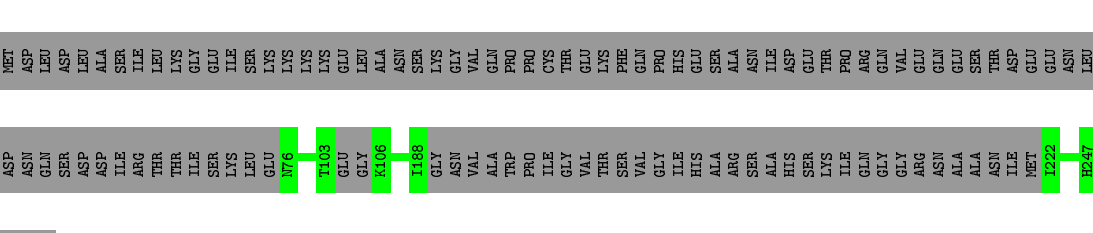
- Molecule 16: Pre-mRNA-splicing factor CWC21




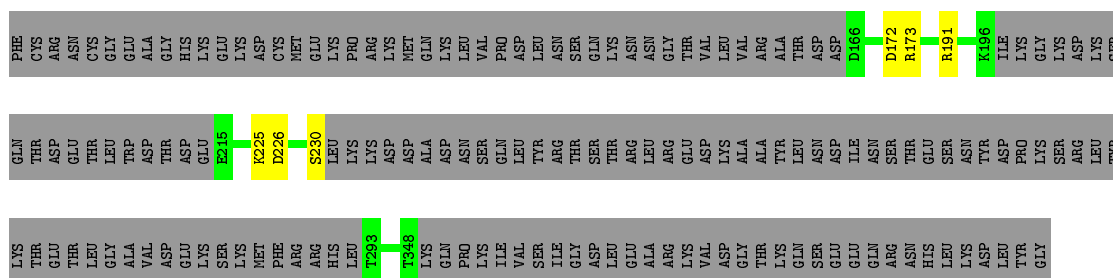
- Molecule 17: Pre-mRNA-splicing factor CLF1



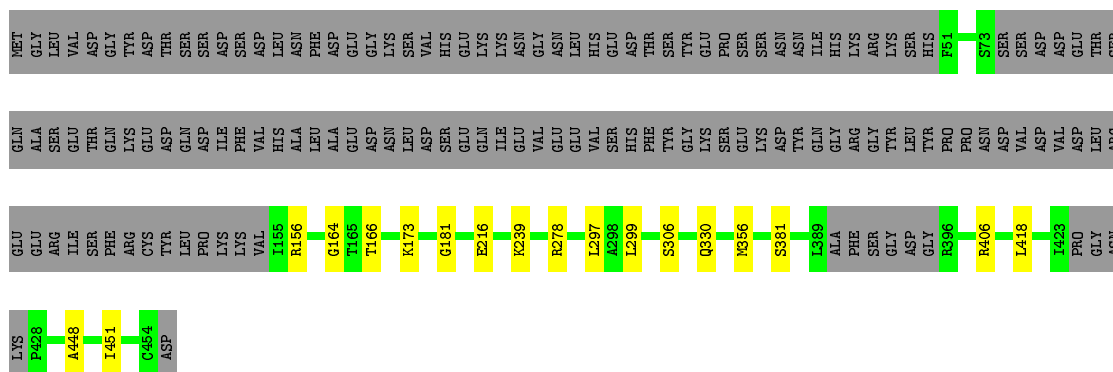
- [illegible]

- Chain a: 
- 

- Chain c: 



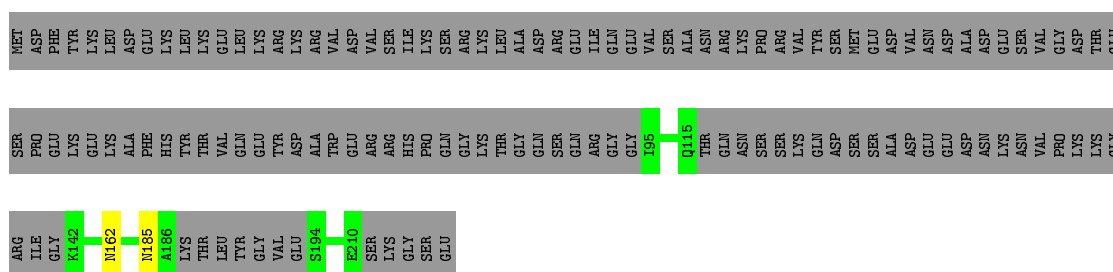
- Molecule 21: Pre-mRNA-processing factor 17



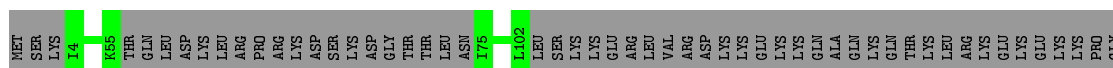
- Molecule 22: UNKNOWN PROTEIN

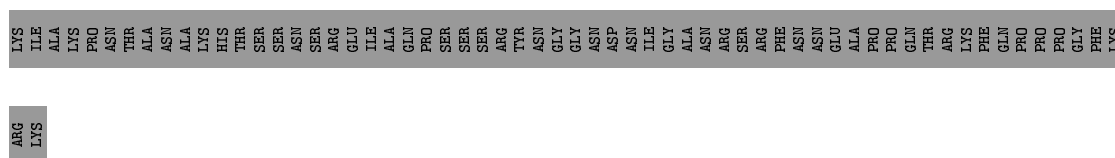


- Molecule 23: Pre-mRNA-splicing factor SYF2

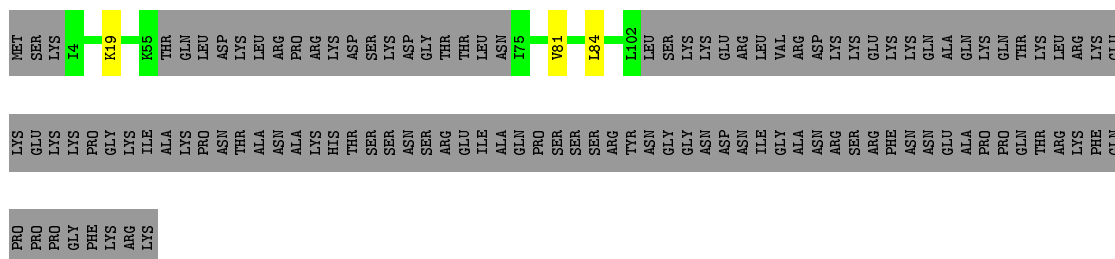


- Molecule 24: Small nuclear ribonucleoprotein-associated protein B

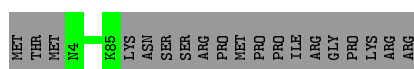
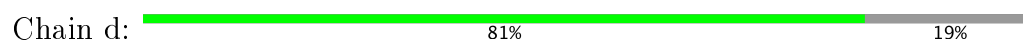




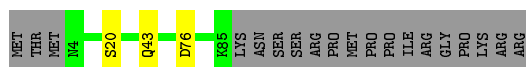
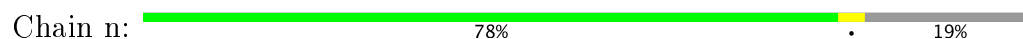
- Molecule 24: Small nuclear ribonucleoprotein-associated protein B



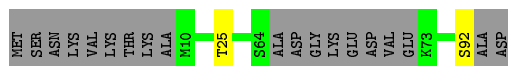
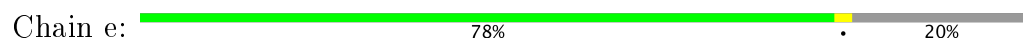
- Molecule 25: Small nuclear ribonucleoprotein Sm D3



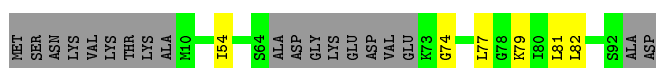
- Molecule 25: Small nuclear ribonucleoprotein Sm D3



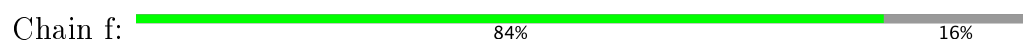
- Molecule 26: Small nuclear ribonucleoprotein E

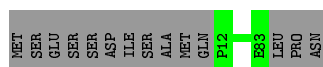


- Molecule 26: Small nuclear ribonucleoprotein E



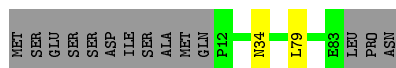
- Molecule 27: Small nuclear ribonucleoprotein F





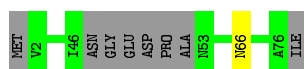
- Molecule 27: Small nuclear ribonucleoprotein F

Chain q: 81% 16%



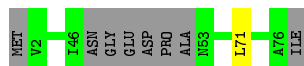
- Molecule 28: Small nuclear ribonucleoprotein G

Chain g: 88% 10%



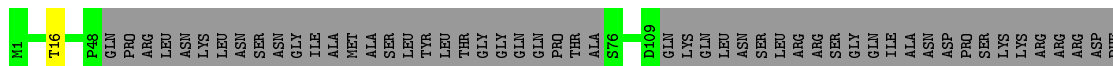
- Molecule 28: Small nuclear ribonucleoprotein G

Chain r: 88% 10%



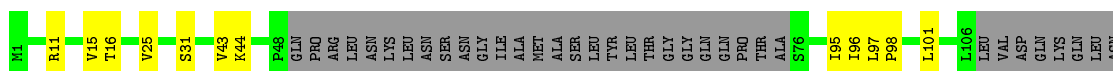
- Molecule 29: Small nuclear ribonucleoprotein Sm D1

Chain h: 55% 44%



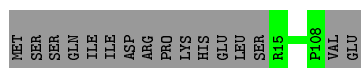
- Molecule 29: Small nuclear ribonucleoprotein Sm D1

Chain l: 46% 8% 46%



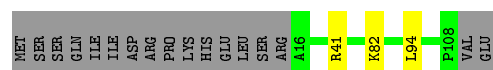
- Molecule 30: Small nuclear ribonucleoprotein Sm D2

Chain j: 85% 15%



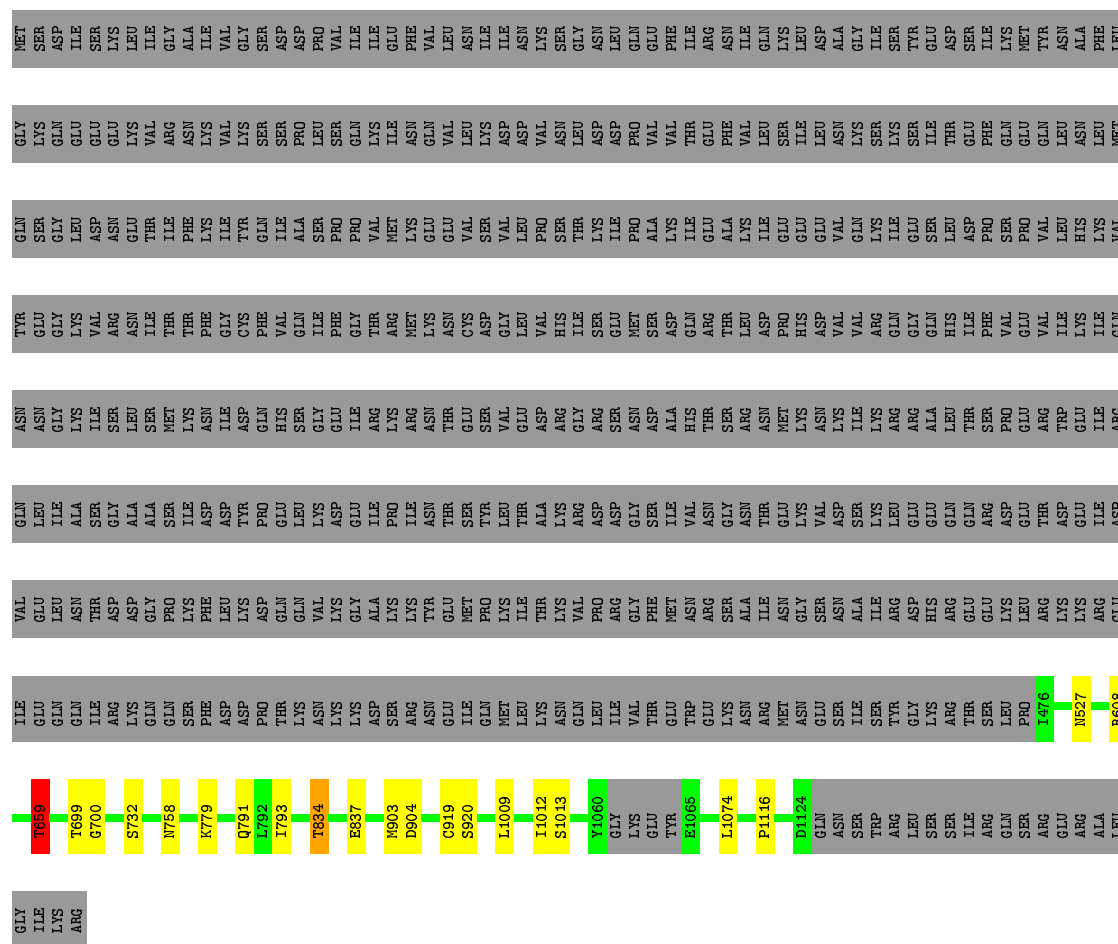
- Molecule 30: Small nuclear ribonucleoprotein Sm D2

Chain m: 82% • 15%



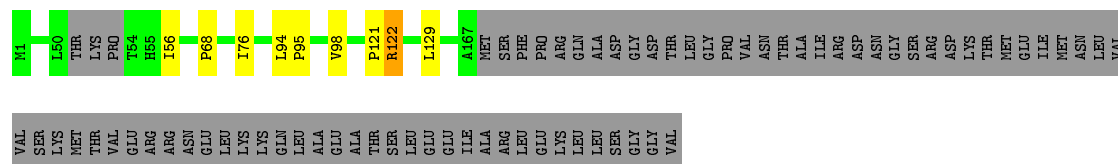
- Molecule 31: Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP22

Chain V:  54% . 44%



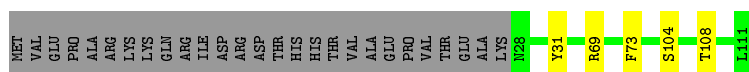
- Molecule 32: U2 small nuclear ribonucleoprotein A'

Chain W:  65% . 31%



- Molecule 33: U2 small nuclear ribonucleoprotein B''

Chain Y:  71% 5% 24%



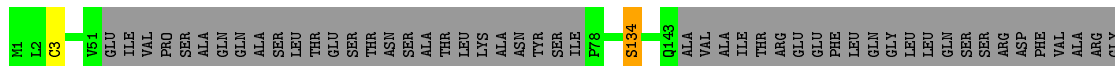
- Molecule 34: 3'-EXON OF UBC4 PRE-MRNA, BOUND BY PRP22 HELICASE



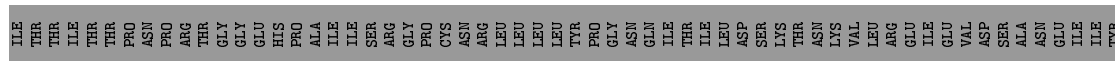
- Molecule 35: Pre-mRNA-splicing factor SNT309



- Molecule 36: Pre-mRNA-processing factor 19



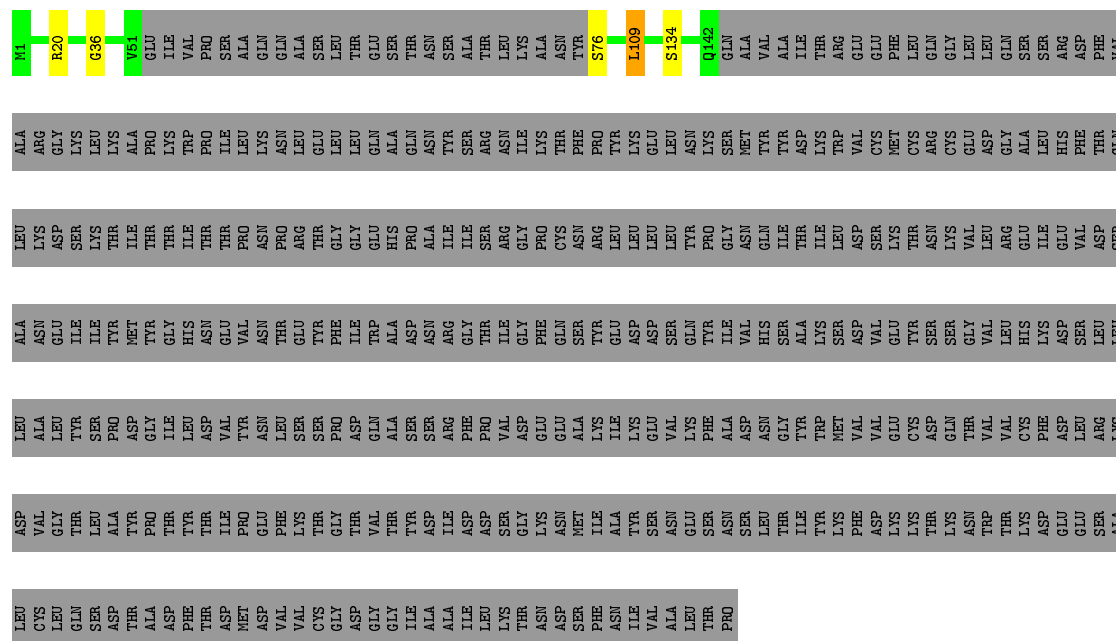
- Molecule 36: Pre-mRNA-processing factor 19



THR ALA ASP PHE THR ASP MET ASP VAL VAL CYS GLY ASP GLY GLY ILE ALA ALA ILE LEU LYS THR THR ASN ASP SER PHE ASN ILE VAL ALA LEU THR PRO

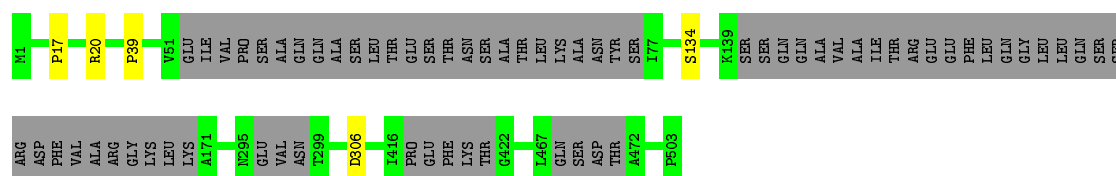
- Molecule 36: Pre-mRNA-processing factor 19

Chain v: 22% . 77%



- Molecule 36: Pre-mRNA-processing factor 19

Chain w: 85% • 14%



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 29527 | 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 ($e^-/\text{\AA}^2$) | 2 | Depositor |
| Minimum defocus (nm) | 500 | Depositor |
| Maximum defocus (nm) | 4500 | Depositor |
| Magnification | 81000 | Depositor |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG, K, I6P, 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 > 2$ | RMSZ | # $ Z > 2$ |
| 1 | I | 0.33 | 0/795 | 0.83 | 1/1231 (0.1%) |
| 10 | K | 0.44 | 0/1480 | 0.75 | 0/2000 |
| 11 | L | 0.46 | 0/1186 | 0.72 | 0/1606 |
| 12 | M | 0.41 | 0/2062 | 0.66 | 0/2772 |
| 13 | N | 0.41 | 0/1823 | 0.71 | 0/2456 |
| 14 | O | 0.46 | 0/1781 | 0.78 | 0/2385 |
| 15 | P | 0.39 | 0/580 | 0.66 | 0/776 |
| 16 | R | 0.41 | 0/617 | 0.68 | 0/848 |
| 17 | S | 0.47 | 0/3269 | 0.76 | 0/4446 |
| 18 | T | 0.42 | 0/3036 | 0.71 | 0/4197 |
| 19 | a | 0.38 | 0/1141 | 0.61 | 0/1546 |
| 2 | E | 0.34 | 0/388 | 0.78 | 0/603 |
| 20 | c | 0.45 | 1/798 (0.1%) | 0.60 | 0/1074 |
| 21 | o | 0.41 | 0/2491 | 0.64 | 0/3384 |
| 23 | y | 0.34 | 0/681 | 0.54 | 0/902 |
| 24 | b | 0.36 | 0/636 | 0.63 | 0/856 |
| 24 | k | 0.35 | 0/636 | 0.58 | 0/856 |
| 25 | d | 0.35 | 0/634 | 0.56 | 0/859 |
| 25 | n | 0.37 | 0/634 | 0.53 | 0/859 |
| 26 | e | 0.41 | 0/585 | 0.61 | 0/795 |
| 26 | p | 0.40 | 0/585 | 0.56 | 0/795 |
| 27 | f | 0.40 | 0/585 | 0.57 | 0/791 |
| 27 | q | 0.40 | 0/585 | 0.61 | 0/791 |
| 28 | g | 0.50 | 0/532 | 0.61 | 0/715 |
| 28 | r | 0.35 | 0/529 | 0.50 | 0/711 |
| 29 | h | 0.38 | 0/649 | 0.54 | 0/880 |
| 29 | l | 0.40 | 0/623 | 0.64 | 0/844 |
| 3 | 2 | 0.27 | 0/3639 | 0.72 | 0/5643 |
| 30 | j | 0.36 | 0/753 | 0.57 | 0/1013 |
| 30 | m | 0.37 | 0/738 | 0.61 | 0/995 |
| 31 | V | 0.57 | 2/3186 (0.1%) | 1.53 | 9/4434 (0.2%) |
| 32 | W | 0.31 | 0/814 | 0.53 | 0/1134 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | # Z >2 | RMSZ | # Z >2 |
| 33 | Y | 0.32 | 0/415 | 0.55 | 0/577 |
| 34 | 3 | 0.19 | 0/65 | 0.65 | 0/98 |
| 35 | s | 0.57 | 0/546 | 0.80 | 0/760 |
| 36 | t | 0.46 | 0/2165 | 0.71 | 3/3010 (0.1%) |
| 36 | u | 0.57 | 0/576 | 0.78 | 0/802 |
| 36 | v | 0.59 | 0/586 | 0.89 | 3/816 (0.4%) |
| 36 | w | 0.47 | 0/2150 | 0.68 | 2/2989 (0.1%) |
| 4 | 6 | 0.33 | 0/2357 | 0.72 | 1/3667 (0.0%) |
| 5 | 5 | 0.32 | 0/3351 | 0.73 | 0/5213 |
| 6 | A | 0.46 | 0/15598 | 0.73 | 0/21212 |
| 7 | C | 0.42 | 0/6703 | 0.69 | 0/9138 |
| 8 | H | 0.48 | 0/3314 | 0.77 | 0/4463 |
| 9 | J | 0.47 | 0/2749 | 0.74 | 0/3735 |
| All | All | 0.43 | 3/79046 (0.0%) | 0.76 | 19/109677 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 15 | P | 0 | 1 |
| 21 | o | 0 | 1 |
| 24 | k | 0 | 1 |
| 31 | V | 0 | 3 |
| 35 | s | 0 | 2 |
| 36 | t | 0 | 2 |
| 36 | v | 0 | 1 |
| 36 | w | 0 | 1 |
| 7 | C | 0 | 1 |
| 9 | J | 0 | 1 |
| All | All | 0 | 14 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 31 | V | 1009 | LEU | C-N | 7.26 | 1.50 | 1.34 |
| 20 | c | 230 | SER | C-O | 6.14 | 1.35 | 1.23 |
| 31 | V | 834 | THR | C-N | -5.27 | 1.22 | 1.34 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 31 | V | 834 | THR | C-N-CA | -46.64 | 5.11 | 121.70 |
| 31 | V | 834 | THR | CA-C-N | -38.77 | 31.91 | 117.20 |
| 31 | V | 1009 | LEU | O-C-N | 27.39 | 166.52 | 122.70 |
| 31 | V | 1009 | LEU | CA-C-N | -22.51 | 67.67 | 117.20 |
| 31 | V | 1009 | LEU | C-N-CA | -18.95 | 74.32 | 121.70 |

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 7 | C | 105 | ILE | Peptide |
| 9 | J | 194 | HIS | Peptide |
| 15 | P | 5 | HIS | Peptide |
| 31 | V | 659 | THR | Mainchain |
| 21 | o | 239 | LYS | Peptide |

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 | I | 714 | 0 | 361 | 6 | 0 |
| 2 | E | 346 | 0 | 173 | 11 | 0 |
| 3 | 2 | 3271 | 0 | 1660 | 26 | 0 |
| 4 | 6 | 2108 | 0 | 1063 | 29 | 0 |
| 5 | 5 | 2999 | 0 | 1515 | 34 | 0 |
| 6 | A | 15199 | 0 | 14954 | 262 | 0 |
| 7 | C | 6562 | 0 | 6486 | 105 | 0 |
| 8 | H | 3261 | 0 | 3323 | 91 | 0 |
| 9 | J | 2690 | 0 | 2690 | 85 | 0 |
| 10 | K | 1458 | 0 | 1468 | 20 | 0 |
| 11 | L | 1162 | 0 | 1111 | 19 | 0 |
| 12 | M | 2016 | 0 | 1985 | 32 | 0 |
| 13 | N | 1798 | 0 | 1842 | 38 | 0 |
| 14 | O | 1755 | 0 | 1794 | 24 | 0 |
| 15 | P | 565 | 0 | 555 | 7 | 0 |
| 16 | R | 614 | 0 | 390 | 8 | 0 |
| 17 | S | 3229 | 0 | 2573 | 37 | 0 |
| 18 | T | 3154 | 0 | 1331 | 94 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 19 | a | 1119 | 0 | 1164 | 0 | 0 |
| 20 | c | 786 | 0 | 719 | 0 | 0 |
| 21 | o | 2425 | 0 | 2253 | 0 | 0 |
| 22 | X | 338 | 0 | 70 | 1 | 0 |
| 23 | y | 679 | 0 | 706 | 0 | 0 |
| 24 | b | 631 | 0 | 670 | 0 | 0 |
| 24 | k | 631 | 0 | 665 | 0 | 0 |
| 25 | d | 625 | 0 | 647 | 0 | 0 |
| 25 | n | 625 | 0 | 647 | 0 | 0 |
| 26 | e | 575 | 0 | 597 | 0 | 0 |
| 26 | p | 575 | 0 | 597 | 0 | 0 |
| 27 | f | 573 | 0 | 572 | 0 | 0 |
| 27 | q | 573 | 0 | 572 | 0 | 0 |
| 28 | g | 529 | 0 | 557 | 0 | 0 |
| 28 | r | 526 | 0 | 555 | 0 | 0 |
| 29 | h | 644 | 0 | 686 | 0 | 0 |
| 29 | l | 618 | 0 | 660 | 0 | 0 |
| 30 | j | 741 | 0 | 778 | 0 | 0 |
| 30 | m | 726 | 0 | 754 | 0 | 0 |
| 31 | V | 3189 | 0 | 1412 | 12 | 0 |
| 32 | W | 816 | 0 | 340 | 1 | 0 |
| 33 | Y | 416 | 0 | 182 | 14 | 0 |
| 34 | 3 | 60 | 0 | 31 | 10 | 0 |
| 35 | s | 548 | 0 | 219 | 0 | 0 |
| 36 | t | 2171 | 0 | 945 | 0 | 0 |
| 36 | u | 578 | 0 | 246 | 0 | 0 |
| 36 | v | 588 | 0 | 250 | 0 | 0 |
| 36 | w | 2156 | 0 | 938 | 0 | 0 |
| 37 | 6 | 3 | 0 | 0 | 0 | 0 |
| 38 | 6 | 2 | 0 | 0 | 0 | 0 |
| 39 | A | 36 | 0 | 6 | 0 | 0 |
| 40 | C | 32 | 0 | 12 | 0 | 0 |
| 41 | L | 3 | 0 | 0 | 0 | 0 |
| 41 | M | 1 | 0 | 0 | 0 | 0 |
| 41 | N | 2 | 0 | 0 | 0 | 0 |
| All | All | 77441 | 0 | 63724 | 846 | 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 8.

The worst 5 of 846 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:T:119:ALA:HB2 | 18:T:131:ALA:CB | 1.25 | 1.63 |
| 18:T:119:ALA:CB | 18:T:131:ALA:HB3 | 1.40 | 1.48 |
| 18:T:237:THR:N | 18:T:240:ASN:N | 1.73 | 1.34 |
| 18:T:300:ASP:CB | 18:T:303:LEU:CB | 2.06 | 1.33 |
| 18:T:119:ALA:HB1 | 18:T:128:ILE:CA | 1.58 | 1.33 |

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 | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 6 | A | 1906/2413 (79%) | 1733 (91%) | 161 (8%) | 12 (1%) | 28 | 70 |
| 7 | C | 864/1008 (86%) | 771 (89%) | 87 (10%) | 6 (1%) | 25 | 68 |
| 8 | H | 393/577 (68%) | 353 (90%) | 36 (9%) | 4 (1%) | 18 | 61 |
| 9 | J | 340/451 (75%) | 295 (87%) | 39 (12%) | 6 (2%) | 10 | 50 |
| 10 | K | 183/379 (48%) | 163 (89%) | 17 (9%) | 3 (2%) | 11 | 52 |
| 11 | L | 153/157 (98%) | 136 (89%) | 16 (10%) | 1 (1%) | 25 | 68 |
| 12 | M | 250/339 (74%) | 236 (94%) | 12 (5%) | 2 (1%) | 22 | 66 |
| 13 | N | 217/364 (60%) | 191 (88%) | 22 (10%) | 4 (2%) | 10 | 50 |
| 14 | O | 207/590 (35%) | 193 (93%) | 11 (5%) | 3 (1%) | 13 | 54 |
| 15 | P | 63/175 (36%) | 56 (89%) | 7 (11%) | 0 | 100 | 100 |
| 16 | R | 104/135 (77%) | 91 (88%) | 12 (12%) | 1 (1%) | 18 | 61 |
| 17 | S | 438/687 (64%) | 415 (95%) | 20 (5%) | 3 (1%) | 25 | 68 |
| 18 | T | 557/877 (64%) | 532 (96%) | 22 (4%) | 3 (0%) | 32 | 73 |
| 19 | a | 131/251 (52%) | 123 (94%) | 8 (6%) | 0 | 100 | 100 |
| 20 | c | 97/382 (25%) | 87 (90%) | 8 (8%) | 2 (2%) | 8 | 46 |
| 21 | o | 305/455 (67%) | 251 (82%) | 46 (15%) | 8 (3%) | 6 | 42 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 23 | y | 77/215 (36%) | 76 (99%) | 1 (1%) | 0 | 100 | 100 |
| 24 | b | 76/196 (39%) | 74 (97%) | 2 (3%) | 0 | 100 | 100 |
| 24 | k | 76/196 (39%) | 68 (90%) | 7 (9%) | 1 (1%) | 14 | 56 |
| 25 | d | 80/101 (79%) | 73 (91%) | 7 (9%) | 0 | 100 | 100 |
| 25 | n | 80/101 (79%) | 74 (92%) | 6 (8%) | 0 | 100 | 100 |
| 26 | e | 71/94 (76%) | 62 (87%) | 9 (13%) | 0 | 100 | 100 |
| 26 | p | 71/94 (76%) | 66 (93%) | 4 (6%) | 1 (1%) | 13 | 54 |
| 27 | f | 70/86 (81%) | 61 (87%) | 9 (13%) | 0 | 100 | 100 |
| 27 | q | 70/86 (81%) | 65 (93%) | 5 (7%) | 0 | 100 | 100 |
| 28 | g | 65/77 (84%) | 63 (97%) | 2 (3%) | 0 | 100 | 100 |
| 28 | r | 65/77 (84%) | 57 (88%) | 8 (12%) | 0 | 100 | 100 |
| 29 | h | 78/146 (53%) | 71 (91%) | 7 (9%) | 0 | 100 | 100 |
| 29 | l | 75/146 (51%) | 65 (87%) | 8 (11%) | 2 (3%) | 6 | 41 |
| 30 | j | 92/110 (84%) | 83 (90%) | 9 (10%) | 0 | 100 | 100 |
| 30 | m | 91/110 (83%) | 84 (92%) | 7 (8%) | 0 | 100 | 100 |
| 31 | V | 639/1145 (56%) | 602 (94%) | 34 (5%) | 3 (0%) | 32 | 73 |
| 32 | W | 160/238 (67%) | 117 (73%) | 35 (22%) | 8 (5%) | 2 | 28 |
| 33 | Y | 82/111 (74%) | 76 (93%) | 6 (7%) | 0 | 100 | 100 |
| 35 | s | 106/175 (61%) | 92 (87%) | 8 (8%) | 6 (6%) | 2 | 25 |
| 36 | t | 426/503 (85%) | 417 (98%) | 9 (2%) | 0 | 100 | 100 |
| 36 | u | 112/503 (22%) | 104 (93%) | 8 (7%) | 0 | 100 | 100 |
| 36 | v | 114/503 (23%) | 108 (95%) | 3 (3%) | 3 (3%) | 6 | 42 |
| 36 | w | 423/503 (84%) | 414 (98%) | 7 (2%) | 2 (0%) | 32 | 73 |
| All | All | 9407/14756 (64%) | 8598 (91%) | 725 (8%) | 84 (1%) | 25 | 63 |

5 of 84 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 6 | A | 487 | ASN |
| 6 | A | 742 | VAL |
| 6 | A | 1620 | TYR |
| 7 | C | 568 | SER |
| 7 | C | 901 | GLU |

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 | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 6 | A | 1577/2182 (72%) | 1549 (98%) | 28 (2%) | 64 | 84 |
| 7 | C | 681/910 (75%) | 662 (97%) | 19 (3%) | 49 | 74 |
| 8 | H | 366/538 (68%) | 357 (98%) | 9 (2%) | 53 | 77 |
| 9 | J | 299/397 (75%) | 280 (94%) | 19 (6%) | 20 | 55 |
| 10 | K | 159/328 (48%) | 152 (96%) | 7 (4%) | 33 | 66 |
| 11 | L | 112/141 (79%) | 105 (94%) | 7 (6%) | 21 | 56 |
| 12 | M | 214/296 (72%) | 210 (98%) | 4 (2%) | 62 | 83 |
| 13 | N | 211/332 (64%) | 205 (97%) | 6 (3%) | 49 | 74 |
| 14 | O | 187/525 (36%) | 181 (97%) | 6 (3%) | 44 | 72 |
| 15 | P | 56/151 (37%) | 54 (96%) | 2 (4%) | 40 | 70 |
| 16 | R | 25/121 (21%) | 24 (96%) | 1 (4%) | 36 | 67 |
| 17 | S | 230/633 (36%) | 221 (96%) | 9 (4%) | 37 | 68 |
| 18 | T | 1/786 (0%) | 1 (100%) | 0 | 100 | 100 |
| 19 | a | 125/225 (56%) | 125 (100%) | 0 | 100 | 100 |
| 20 | c | 71/346 (20%) | 68 (96%) | 3 (4%) | 34 | 67 |
| 21 | o | 256/413 (62%) | 247 (96%) | 9 (4%) | 41 | 71 |
| 23 | y | 76/193 (39%) | 74 (97%) | 2 (3%) | 51 | 76 |
| 24 | b | 70/176 (40%) | 70 (100%) | 0 | 100 | 100 |
| 24 | k | 70/176 (40%) | 69 (99%) | 1 (1%) | 71 | 86 |
| 25 | d | 69/89 (78%) | 69 (100%) | 0 | 100 | 100 |
| 25 | n | 69/89 (78%) | 66 (96%) | 3 (4%) | 33 | 66 |
| 26 | e | 65/83 (78%) | 63 (97%) | 2 (3%) | 45 | 73 |
| 26 | p | 65/83 (78%) | 60 (92%) | 5 (8%) | 15 | 50 |
| 27 | f | 63/77 (82%) | 63 (100%) | 0 | 100 | 100 |
| 27 | q | 63/77 (82%) | 61 (97%) | 2 (3%) | 44 | 72 |
| 28 | g | 58/66 (88%) | 57 (98%) | 1 (2%) | 66 | 85 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|-------------|
| 28 | r | 57/66 (86%) | 56 (98%) | 1 (2%) | 64 84 |
| 29 | h | 77/129 (60%) | 76 (99%) | 1 (1%) | 73 87 |
| 29 | l | 73/129 (57%) | 63 (86%) | 10 (14%) | 4 26 |
| 30 | j | 79/103 (77%) | 79 (100%) | 0 | 100 100 |
| 30 | m | 77/103 (75%) | 74 (96%) | 3 (4%) | 37 68 |
| All | All | 5601/9963 (56%) | 5441 (97%) | 160 (3%) | 51 74 |

5 of 160 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | J | 443 | ASN |
| 12 | M | 13 | VAL |
| 30 | m | 82 | LYS |
| 9 | J | 450 | ARG |
| 10 | K | 202 | MET |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | C | 830 | ASN |
| 10 | K | 195 | ASN |
| 29 | l | 14 | GLN |
| 8 | H | 320 | ASN |
| 9 | J | 443 | ASN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|----------------|-------------------|-----------------|
| 1 | I | 32/95 (33%) | 14 (43%) | 4 (12%) |
| 2 | E | 15/20 (75%) | 5 (33%) | 1 (6%) |
| 3 | 2 | 146/1175 (12%) | 49 (33%) | 5 (3%) |
| 34 | 3 | 2/3 (66%) | 2 (100%) | 0 |
| 4 | 6 | 98/112 (87%) | 37 (37%) | 3 (3%) |
| 5 | 5 | 138/179 (77%) | 61 (44%) | 3 (2%) |
| All | All | 431/1584 (27%) | 168 (38%) | 16 (3%) |

5 of 168 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 2 | U |
| 1 | I | 3 | A |
| 1 | I | 4 | U |
| 1 | I | 10 | A |
| 1 | I | 11 | A |

5 of 16 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | 2 | 1123 | C |
| 3 | 2 | 1124 | U |
| 4 | 6 | 92 | C |
| 3 | 2 | 17 | U |
| 5 | 5 | 27 | G |

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 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 | $\# Z > 2$ |
| 39 | I6P | A | 3001 | - | 36,36,36 | 0.64 | 0 | 54,60,60 | 1.06 | 3 (5%) |
| 40 | GTP | C | 1101 | - | 27,34,34 | 1.05 | 2 (7%) | 27,54,54 | 2.07 | 8 (29%) |

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 |
|-----|------|-------|------|------|---------|------------|---------|
| 39 | I6P | A | 3001 | - | - | 0/30/54/54 | 0/1/1/1 |
| 40 | GTP | C | 1101 | - | - | 0/18/38/38 | 0/3/3/3 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 40 | C | 1101 | GTP | C5-C4 | 2.68 | 1.46 | 1.40 |
| 40 | C | 1101 | GTP | C6-C5 | 3.52 | 1.48 | 1.41 |

The worst 5 of 11 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 40 | C | 1101 | GTP | C6-C5-C4 | -4.33 | 116.54 | 120.84 |
| 40 | C | 1101 | GTP | N3-C2-N1 | -3.39 | 122.51 | 127.46 |
| 40 | C | 1101 | GTP | C5-C6-N1 | -3.18 | 118.96 | 123.48 |
| 40 | C | 1101 | GTP | C4-C5-N7 | -2.66 | 106.84 | 109.41 |
| 40 | C | 1101 | GTP | C1'-N9-C4 | -2.42 | 122.45 | 126.64 |

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 22 | X | 1 |
| 18 | T | 1 |
| 31 | V | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | X | 27:UNK | C | 86:UNK | N | 8.48 |
| 1 | V | 903:MET | C | 904:ASP | N | 2.35 |
| 1 | T | 300:ASP | C | 301:LYS | N | 2.16 |