



Full wwPDB EM Validation Report ⓘ

Nov 17, 2024 – 12:11 am GMT

PDB ID : 6FTJ
EMDB ID : EMD-4317
Title : Cryo-EM Structure of the Mammalian Oligosaccharyltransferase Bound to Sec61 and the Non-programmed 80S Ribosome
Authors : Braunger, K.; Becker, T.; Beckmann, R.
Deposited on : 2018-02-22
Resolution : 4.70 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

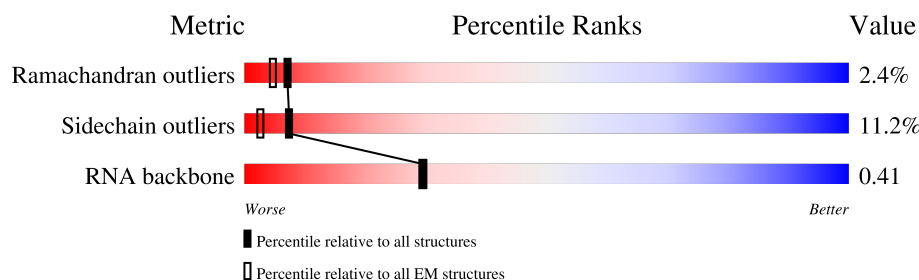
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 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 | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |
| RNA backbone | 6643 | 2191 |

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 244 | <div> <div>57%</div> <div>88%11% .</div> </div> |
| 2 | B | 394 | <div> <div>55%</div> <div>87%12% .</div> </div> |
| 3 | C | 362 | <div> <div>61%</div> <div>84%15% .</div> </div> |
| 4 | D | 292 | <div> <div>58%</div> <div>89%11%</div> </div> |
| 5 | E | 248 | <div> <div>69%</div> <div>78%17%5%</div> </div> |
| 6 | F | 225 | <div> <div>77%</div> <div>87%12% .</div> </div> |
| 7 | G | 241 | <div> <div>76%</div> <div>88%12%</div> </div> |
| 8 | H | 190 | <div> <div>79%</div> <div>87%13%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 9 | I | 213 | |
| 10 | J | 169 | |
| 11 | L | 210 | |
| 12 | M | 138 | |
| 13 | N | 203 | |
| 14 | O | 199 | |
| 15 | P | 153 | |
| 16 | Q | 187 | |
| 17 | R | 180 | |
| 18 | S | 175 | |
| 19 | T | 159 | |
| 20 | U | 99 | |
| 21 | V | 131 | |
| 22 | W | 63 | |
| 23 | X | 119 | |
| 24 | Y | 134 | |
| 25 | Z | 135 | |
| 26 | a | 147 | |
| 27 | b | 75 | |
| 28 | c | 94 | |
| 29 | d | 107 | |
| 30 | e | 128 | |
| 31 | f | 109 | |
| 32 | g | 114 | |
| 33 | h | 122 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 34 | i | 102 | |
| 35 | j | 86 | |
| 36 | k | 69 | |
| 37 | l | 50 | |
| 38 | m | 52 | |
| 39 | n | 23 | |
| 40 | o | 104 | |
| 41 | p | 91 | |
| 42 | r | 136 | |
| 43 | s | 198 | |
| 44 | t | 163 | |
| 45 | u | 3662 | |
| 46 | v | 120 | |
| 47 | w | 156 | |
| 48 | x | 426 | |
| 49 | y | 62 | |
| 50 | z | 29 | |
| 51 | 1 | 162 | |
| 52 | 2 | 60 | |
| 53 | 3 | 120 | |
| 54 | 4 | 34 | |
| 55 | 5 | 696 | |
| 56 | 6 | 97 | |
| 57 | 7 | 25 | |
| 58 | 8 | 80 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 59 | K | 8 | <div> <div>38%</div> <div>25%75%</div> </div> |

2 Entry composition [i](#)

There are 62 unique types of molecules in this entry. The entry contains 152111 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called uL2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1 | A | 244 | Total | C | N | O | S | 0 | 0 |
| | | | 1868 | 1171 | 382 | 309 | 6 | | |

- Molecule 2 is a protein called uL3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2 | B | 394 | Total | C | N | O | S | 0 | 0 |
| | | | 3148 | 2007 | 591 | 537 | 13 | | |

- Molecule 3 is a protein called Ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3 | C | 362 | Total | C | N | O | S | 0 | 0 |
| | | | 2884 | 1814 | 578 | 478 | 14 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| C | 362 | LYS | SER | conflict | UNP G1SVW5 |
| C | 363 | SER | ASP | conflict | UNP G1SVW5 |

- Molecule 4 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4 | D | 292 | Total | C | N | O | S | 0 | 0 |
| | | | 2386 | 1509 | 437 | 426 | 14 | | |

- Molecule 5 is a protein called 60S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5 | E | 236 | Total | C | N | O | S | 0 | 0 |
| | | | 1898 | 1215 | 362 | 318 | 3 | | |

- Molecule 6 is a protein called Ul30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6 | F | 225 | Total | C | N | O | S | 0 | 0 |
| | | | 1870 | 1202 | 358 | 301 | 9 | | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| F | 175 | ALA | THR | conflict | UNP G1SV32 |
| F | 185 | GLY | ASN | conflict | UNP G1SV32 |
| F | 202 | ARG | HIS | conflict | UNP G1SV32 |
| F | 233 | GLU | GLY | conflict | UNP G1SV32 |

- Molecule 7 is a protein called uL8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7 | G | 241 | Total | C | N | O | S | 0 | 0 |
| | | | 1934 | 1233 | 371 | 326 | 4 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| G | 191 | GLY | CYS | conflict | UNP G1STW0 |

- Molecule 8 is a protein called uL6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8 | H | 190 | Total | C | N | O | S | 0 | 0 |
| | | | 1516 | 954 | 284 | 272 | 6 | | |

- Molecule 9 is a protein called Ribosomal protein L10 (Predicted).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9 | I | 204 | Total | C | N | O | S | 0 | 0 |
| | | | 1655 | 1051 | 319 | 272 | 13 | | |

- Molecule 10 is a protein called Ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10 | J | 169 | Total | C | N | O | S | 0 | 0 |
| | | | 1353 | 855 | 252 | 240 | 6 | | |

- Molecule 11 is a protein called eL13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 11 | L | 210 | Total | C | N | O | S | 0 | 0 |
| | | | 1703 | 1065 | 354 | 280 | 4 | | |

- Molecule 12 is a protein called Ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12 | M | 138 | Total | C | N | O | S | 0 | 0 |
| | | | 1137 | 727 | 221 | 182 | 7 | | |

- Molecule 13 is a protein called Ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13 | N | 203 | Total | C | N | O | S | 0 | 0 |
| | | | 1701 | 1072 | 359 | 266 | 4 | | |

- Molecule 14 is a protein called uL13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14 | O | 199 | Total | C | N | O | S | 0 | 0 |
| | | | 1638 | 1056 | 321 | 256 | 5 | | |

- Molecule 15 is a protein called uL22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15 | P | 153 | Total | C | N | O | S | 0 | 0 |
| | | | 1242 | 776 | 241 | 216 | 9 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| P | 54 | GLN | LYS | conflict | UNP G1TVT6 |

- Molecule 16 is a protein called uL14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16 | Q | 187 | Total | C | N | O | S | 0 | 0 |
| | | | 1506 | 941 | 311 | 249 | 5 | | |

- Molecule 17 is a protein called eL19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17 | R | 180 | Total | C | N | O | S | 0 | 0 |
| | | | 1508 | 933 | 328 | 238 | 9 | | |

- Molecule 18 is a protein called eL20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 18 | S | 175 | Total | C | N | O | S | 0 | 0 |
| | | | 1454 | 925 | 284 | 235 | 10 | | |

- Molecule 19 is a protein called eL21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19 | T | 159 | Total | C | N | O | S | 0 | 0 |
| | | | 1298 | 823 | 252 | 217 | 6 | | |

- Molecule 20 is a protein called Ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20 | U | 99 | Total | C | N | O | S | 0 | 0 |
| | | | 808 | 518 | 141 | 147 | 2 | | |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| U | 32 | GLY | ARG | conflict | UNP G1TSG1 |
| U | 36 | ALA | GLU | conflict | UNP G1TSG1 |
| U | 39 | PHE | SER | conflict | UNP G1TSG1 |
| U | 54 | GLY | ARG | conflict | UNP G1TSG1 |
| U | 60 | VAL | ALA | conflict | UNP G1TSG1 |
| U | 97 | ARG | HIS | conflict | UNP G1TSG1 |

- Molecule 21 is a protein called uL14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21 | V | 131 | Total | C | N | O | S | 0 | 0 |
| | | | 979 | 618 | 184 | 172 | 5 | | |

- Molecule 22 is a protein called Ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 22 | W | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 528 | 337 | 103 | 85 | 3 | | |

- Molecule 23 is a protein called uL23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23 | X | 119 | Total | C | N | O | S | 0 | 0 |
| | | | 976 | 624 | 183 | 168 | 1 | | |

- Molecule 24 is a protein called Ribosomal protein L26.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24 | Y | 134 | Total | C | N | O | S | 0 | 0 |
| | | | 1115 | 700 | 226 | 186 | 3 | | |

- Molecule 25 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25 | Z | 135 | Total | C | N | O | S | 0 | 0 |
| | | | 1107 | 714 | 208 | 182 | 3 | | |

- Molecule 26 is a protein called uL15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26 | a | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 1162 | 734 | 239 | 185 | 4 | | |

- Molecule 27 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 27 | b | 75 | Total | C | N | O | S | 0 | 0 |
| | | | 609 | 378 | 130 | 98 | 3 | | |

- Molecule 28 is a protein called eL30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28 | c | 94 | Total | C | N | O | S | 0 | 0 |
| | | | 732 | 465 | 130 | 131 | 6 | | |

- Molecule 29 is a protein called eL31.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29 | d | 107 | Total | C | N | O | S | 0 | 0 |
| | | | 888 | 560 | 171 | 155 | 2 | | |

- Molecule 30 is a protein called eL32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30 | e | 128 | Total | C | N | O | S | 0 | 0 |
| | | | 1053 | 667 | 216 | 165 | 5 | | |

- Molecule 31 is a protein called eL33.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31 | f | 109 | Total | C | N | O | S | 0 | 0 |
| | | | 876 | 555 | 174 | 143 | 4 | | |

- Molecule 32 is a protein called eL34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32 | g | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 906 | 566 | 187 | 147 | 6 | | |

- Molecule 33 is a protein called uL29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33 | h | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 1013 | 640 | 204 | 168 | 1 | | |

- Molecule 34 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34 | i | 102 | Total | C | N | O | S | 0 | 0 |
| | | | 830 | 520 | 176 | 129 | 5 | | |

- Molecule 35 is a protein called Ribosomal protein L37.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35 | j | 86 | Total | C | N | O | S | 0 | 0 |
| | | | 705 | 434 | 155 | 111 | 5 | | |

- Molecule 36 is a protein called eL38.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 36 | k | 69 | Total | C | N | O | S | 0 | 0 |
| | | | 569 | 366 | 103 | 99 | 1 | | |

- Molecule 37 is a protein called eL39.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 37 | l | 50 | Total | C | N | O | S | 0 | 0 |
| | | | 444 | 281 | 98 | 64 | 1 | | |

- Molecule 38 is a protein called eL40.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 38 | m | 52 | Total | C | N | O | S | 0 | 0 |
| | | | 429 | 266 | 90 | 67 | 6 | | |

- Molecule 39 is a protein called 60s ribosomal protein l41.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 39 | n | 23 | Total | C | N | O | S | 0 | 0 |
| | | | 222 | 134 | 61 | 25 | 2 | | |

- Molecule 40 is a protein called eL42.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40 | o | 104 | Total | C | N | O | S | 0 | 0 |
| | | | 851 | 533 | 174 | 138 | 6 | | |

- Molecule 41 is a protein called Ribosomal protein L37a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41 | p | 91 | Total | C | N | O | S | 0 | 0 |
| | | | 708 | 445 | 136 | 120 | 7 | | |

- Molecule 42 is a protein called eL28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42 | r | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1094 | 676 | 229 | 183 | 6 | | |

- Molecule 43 is a protein called 60S acidic ribosomal protein P0.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43 | s | 198 | Total | C | N | O | S | 0 | 0 |
| | | | 1523 | 969 | 265 | 280 | 9 | | |

- Molecule 44 is a protein called Ribosomal protein L12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44 | t | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1238 | 773 | 230 | 230 | 5 | | |

- Molecule 45 is a RNA chain called 28S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 45 | u | 3662 | Total | C | N | O | P | 0 | 0 |
| | | | 78486 | 34947 | 14363 | 25515 | 3661 | | |

- Molecule 46 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 46 | v | 120 | Total | C | N | O | P | 0 | 0 |
| | | | 2558 | 1141 | 456 | 842 | 119 | | |

- Molecule 47 is a RNA chain called 5.8S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 47 | w | 156 | Total | C | N | O | P | 0 | 0 |
| | | | 3314 | 1480 | 585 | 1094 | 155 | | |

- Molecule 48 is a protein called Protein transport protein Sec61 subunit alpha isoform 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 48 | x | 426 | Total | C | N | O | S | 0 | 0 |
| | | | 3313 | 2181 | 535 | 576 | 21 | | |

There are 36 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| x | ? | - | THR | deletion | UNP P38377 |
| x | ? | - | GLY | deletion | UNP P38377 |
| x | ? | - | MET | deletion | UNP P38377 |
| x | ? | - | TYR | deletion | UNP P38377 |
| x | ? | - | GLY | deletion | UNP P38377 |
| x | ? | - | ASP | deletion | UNP P38377 |
| x | ? | - | PRO | deletion | UNP P38377 |
| x | ? | - | SER | deletion | UNP P38377 |
| x | ? | - | GLU | deletion | UNP P38377 |
| x | ? | - | MET | deletion | UNP P38377 |
| x | ? | - | GLY | deletion | UNP P38377 |
| x | 145 | SER | ALA | conflict | UNP P38377 |
| x | ? | - | SER | deletion | UNP P38377 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| x | ? | - | GLY | deletion | UNP P38377 |
| x | ? | - | ASN | deletion | UNP P38377 |
| x | ? | - | LEU | deletion | UNP P38377 |
| x | ? | - | LEU | deletion | UNP P38377 |
| x | ? | - | VAL | deletion | UNP P38377 |
| x | ? | - | SER | deletion | UNP P38377 |
| x | ? | - | LEU | deletion | UNP P38377 |
| x | ? | - | LEU | deletion | UNP P38377 |
| x | ? | - | GLY | deletion | UNP P38377 |
| x | ? | - | THR | deletion | UNP P38377 |
| x | ? | - | TRP | deletion | UNP P38377 |
| x | ? | - | SER | deletion | UNP P38377 |
| x | ? | - | ASP | deletion | UNP P38377 |
| x | ? | - | THR | deletion | UNP P38377 |
| x | ? | - | SER | deletion | UNP P38377 |
| x | ? | - | SER | deletion | UNP P38377 |
| x | ? | - | GLY | deletion | UNP P38377 |
| x | ? | - | GLY | deletion | UNP P38377 |
| x | ? | - | PRO | deletion | UNP P38377 |
| x | ? | - | ALA | deletion | UNP P38377 |
| x | ? | - | ARG | deletion | UNP P38377 |
| x | ? | - | ALA | deletion | UNP P38377 |
| x | ? | - | TYR | deletion | UNP P38377 |

- Molecule 49 is a protein called Protein transport protein Sec61 subunit gamma.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 49 | y | 62 | Total | C | N | O | S | 0 | 0 |
| | | | 494 | 326 | 86 | 79 | 3 | | |

- Molecule 50 is a protein called Protein transport protein Sec61 subunit beta.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 50 | z | 29 | Total | C | N | O | S | 0 | 0 |
| | | | 229 | 157 | 36 | 34 | 2 | | |

- Molecule 51 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 1,RPN1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 51 | 1 | 162 | Total | C | N | O | | 0 | 0 |
| | | | 882 | 550 | 165 | 167 | | | |

- Molecule 52 is a protein called TMEM258.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 52 | 2 | 60 | Total | C | N | O | 0 | 0 |
| | | | 300 | 180 | 60 | 60 | | |

- Molecule 53 is a protein called Oligosaccharyltransferase complex subunit OSTC.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53 | 3 | 120 | Total | C | N | O | S | 0 | 0 |
| | | | 802 | 529 | 130 | 136 | 7 | | |

- Molecule 54 is a protein called OST4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 54 | 4 | 34 | Total | C | N | O | S | 0 | 0 |
| | | | 268 | 180 | 41 | 45 | 2 | | |

- Molecule 55 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 55 | 5 | 644 | Total | C | N | O | S | 0 | 0 |
| | | | 5090 | 3331 | 819 | 904 | 36 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| 5 | 88 | LEU | ILE | conflict | UNP F1PJP5 |

- Molecule 56 is a protein called DAD1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 56 | 6 | 97 | Total | C | N | O | 0 | 0 |
| | | | 485 | 291 | 97 | 97 | | |

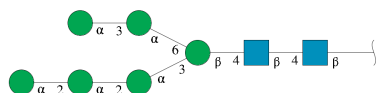
- Molecule 57 is a protein called OST48.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 57 | 7 | 25 | Total | C | N | O | 0 | 0 |
| | | | 125 | 75 | 25 | 25 | | |

- Molecule 58 is a protein called RPN2.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 58 | 8 | 80 | Total | C | N | O | 0 | 0 |
| | | | 400 | 240 | 80 | 80 | | |

- Molecule 59 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 59 | K | 8 | Total | C | N | O | 0 | 0 |
| | | | 94 | 52 | 2 | 40 | | |

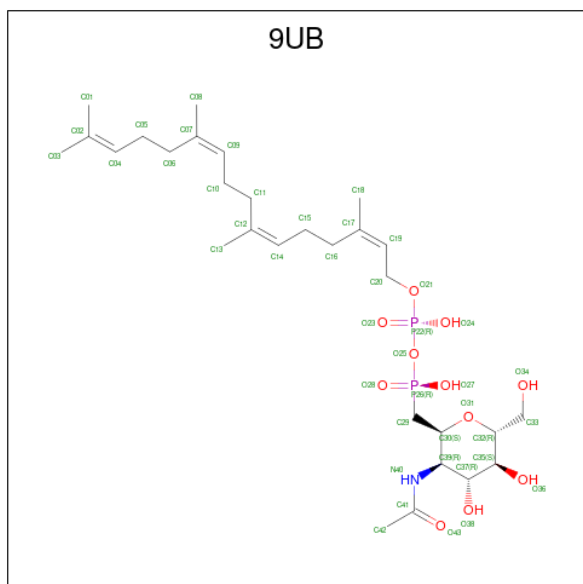
- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|-----|---------|
| 60 | B | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 60 | I | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 60 | P | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 60 | V | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 60 | a | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 60 | e | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 60 | g | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 60 | u | 145 | Total | Mg | 0 |
| | | | 145 | 145 | |
| 60 | v | 5 | Total | Mg | 0 |
| | | | 5 | 5 | |
| 60 | w | 2 | Total | Mg | 0 |
| | | | 2 | 2 | |

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 61 | g | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 61 | j | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 61 | m | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 61 | o | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 61 | p | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

- Molecule 62 is [(2 {S},3 {R},4 {R},5 {S},6 {R})-3-acetamido-6-(hydroxymethyl)-4,5-bis(oxidanyl)oxan-2-yl]methyl-[oxidanyl-[(2 {Z},6 {Z},10 {Z})-3,7,11,15-tetramethylhexadeca-2,6,10,14-tetraenoxy]phosphoryl]oxy-phosphinic acid (three-letter code: 9UB) (formula: $C_{29}H_{51}NO_{11}P_2$).

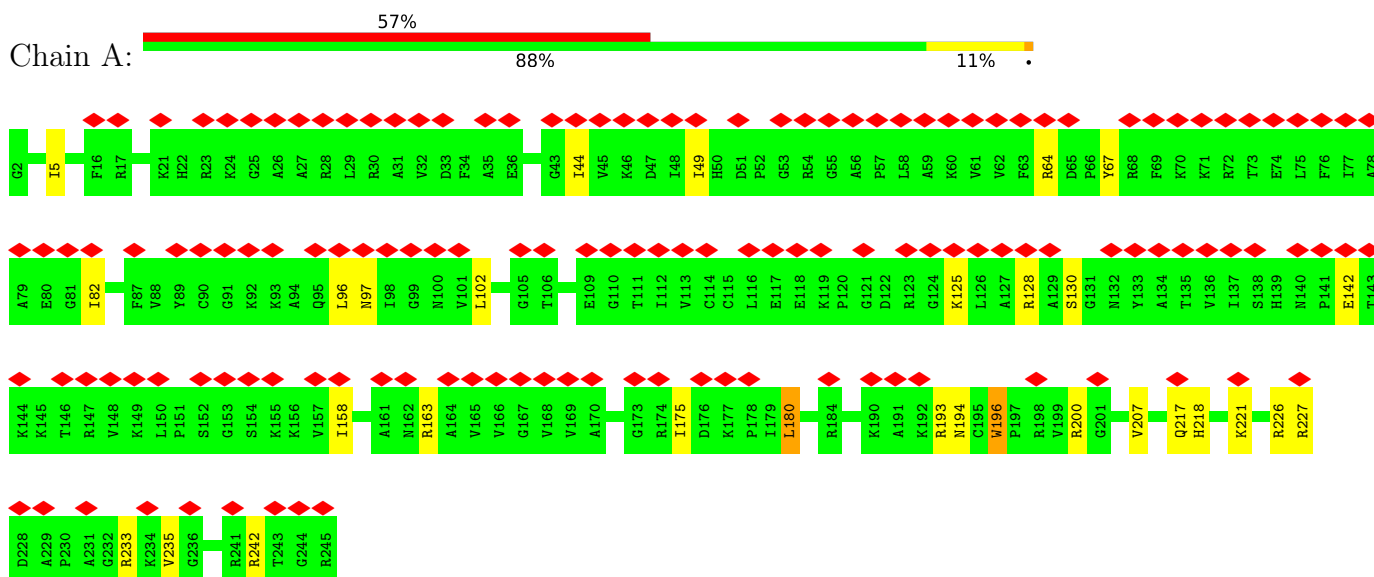


| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 62 | 5 | 1 | Total | C | N | O | P | 0 |
| | | | 43 | 29 | 1 | 11 | 2 | |

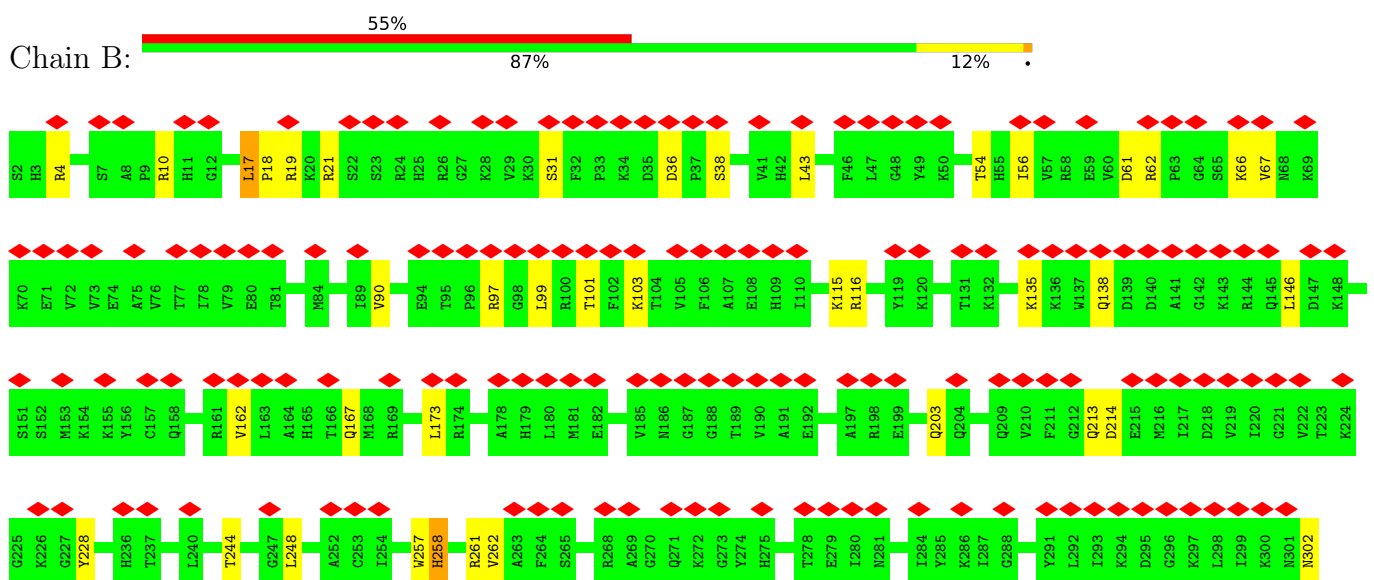
3 Residue-property plots

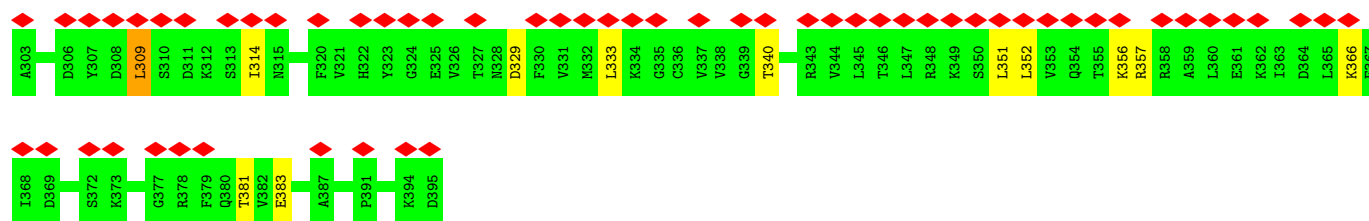
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: uL2

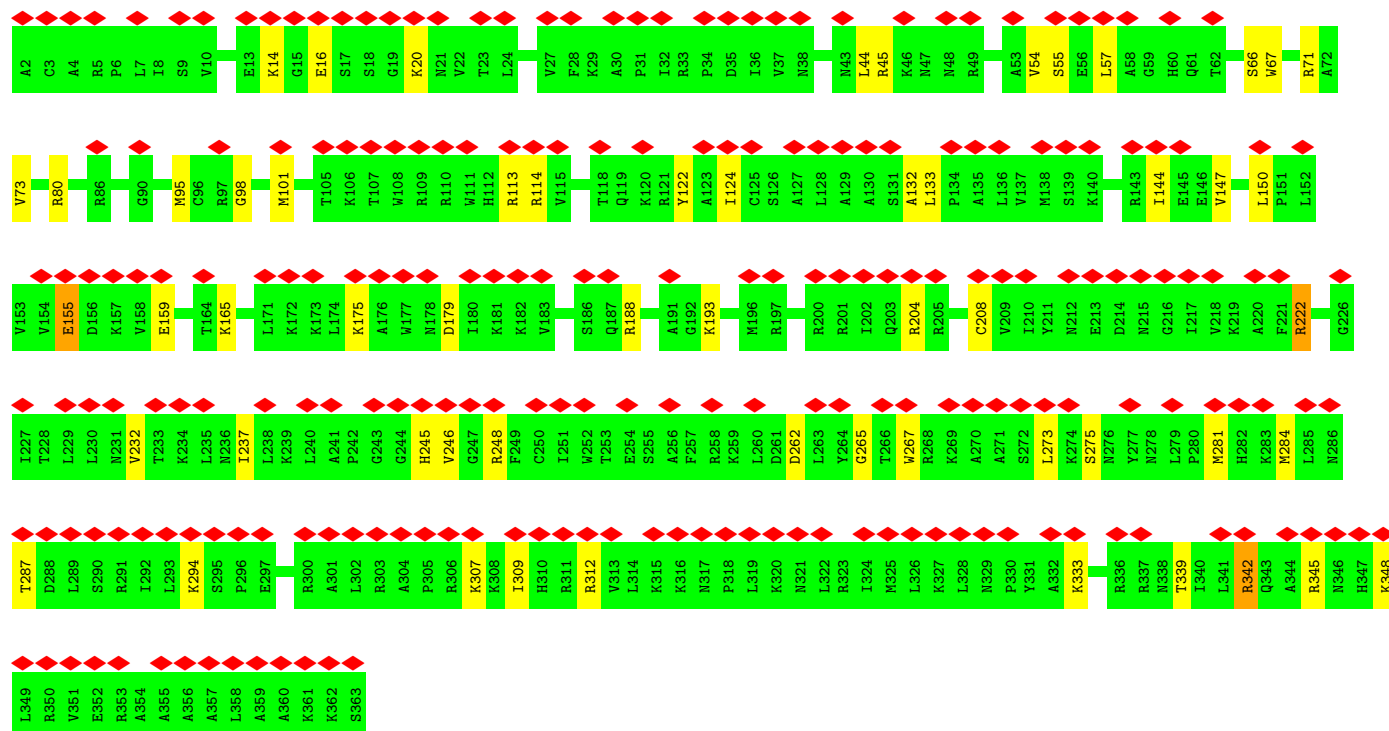
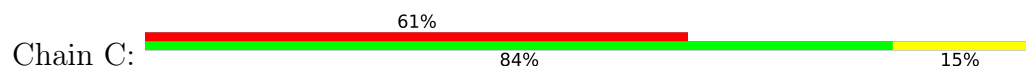


• Molecule 2: uL3

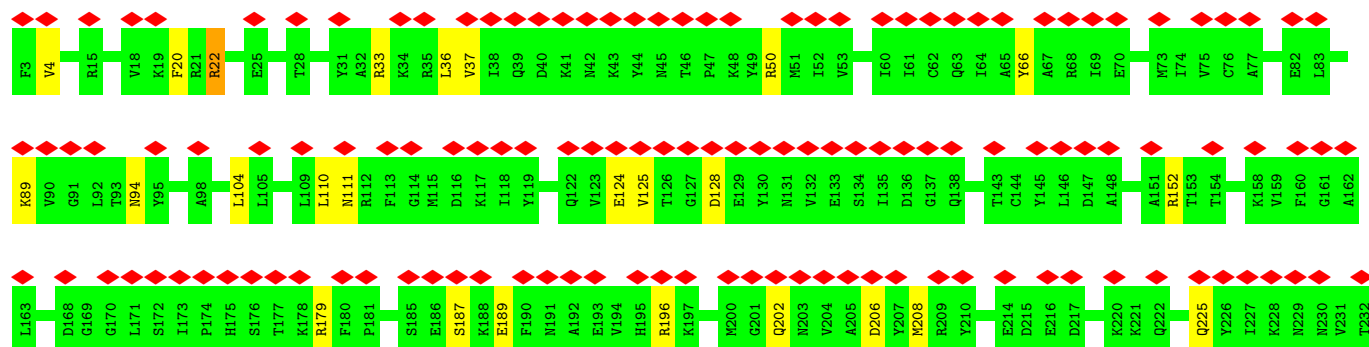
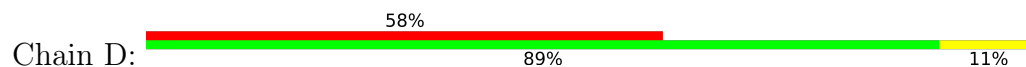


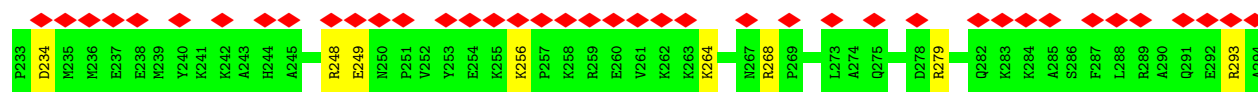


• Molecule 3: Ribosomal protein L4

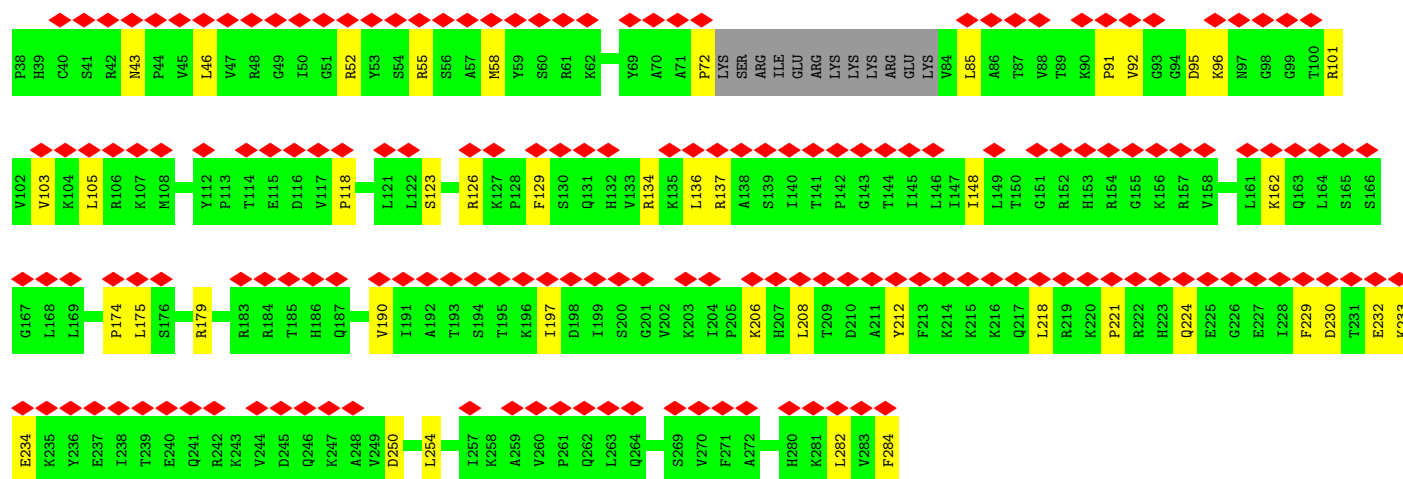
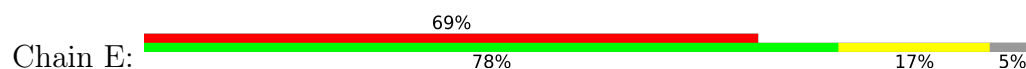


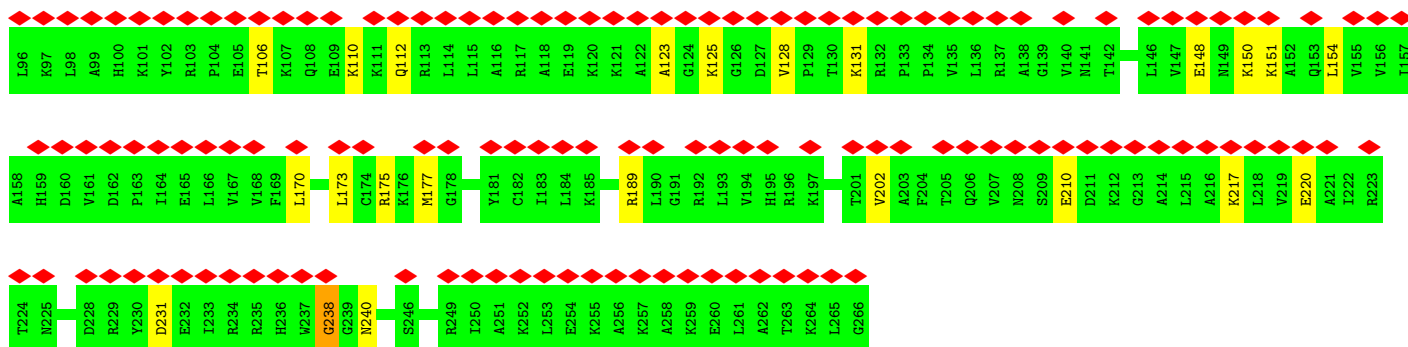
• Molecule 4: 60S ribosomal protein L5



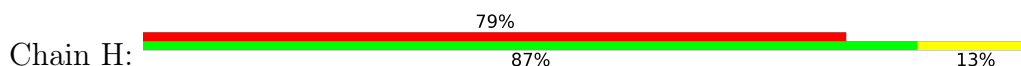


• Molecule 5: 60S ribosomal protein L6

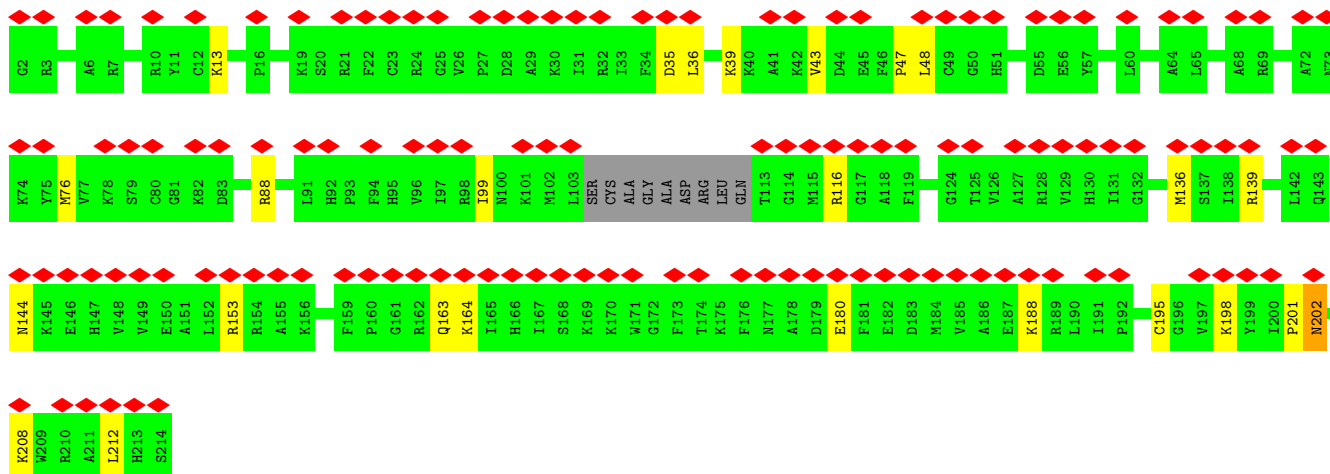
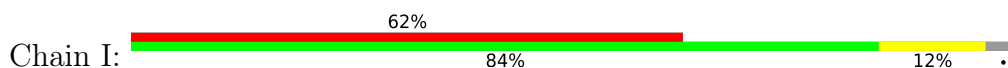




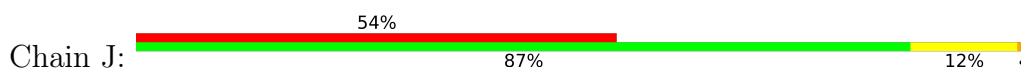
- Molecule 8: uL6

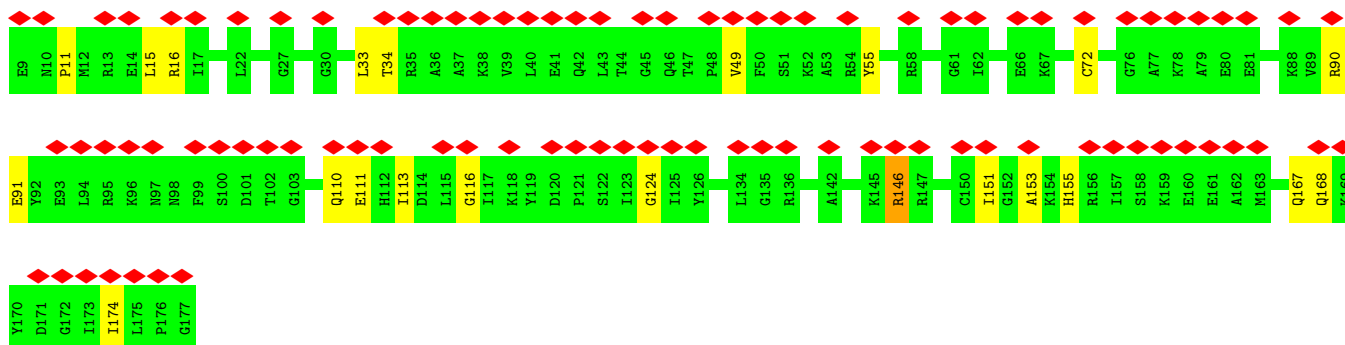


- Molecule 9: Ribosomal protein L10 (Predicted)

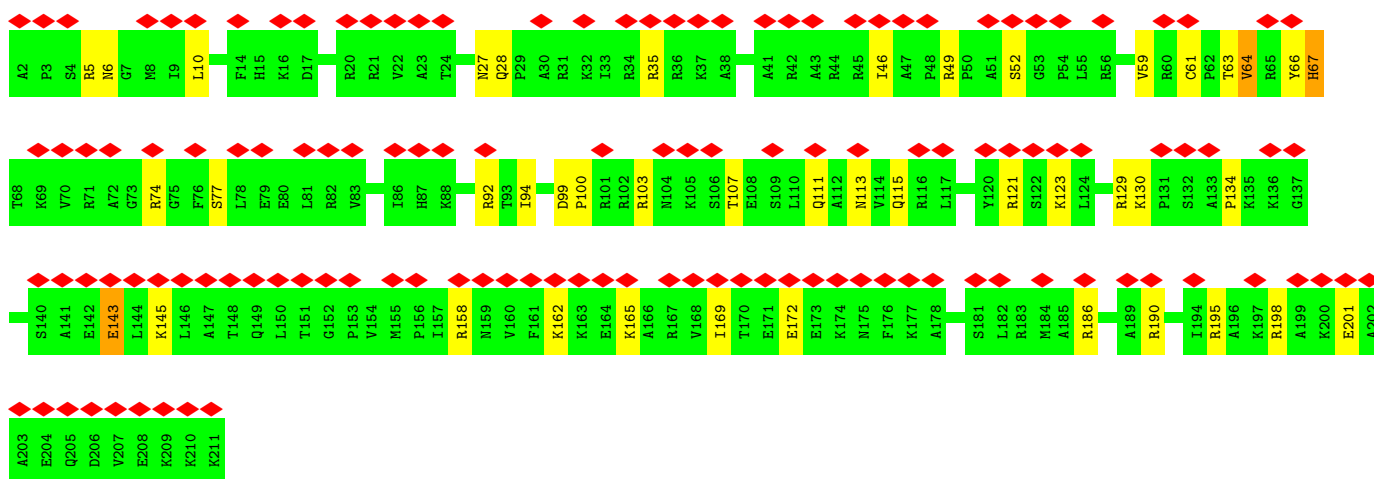


- Molecule 10: Ribosomal protein L11

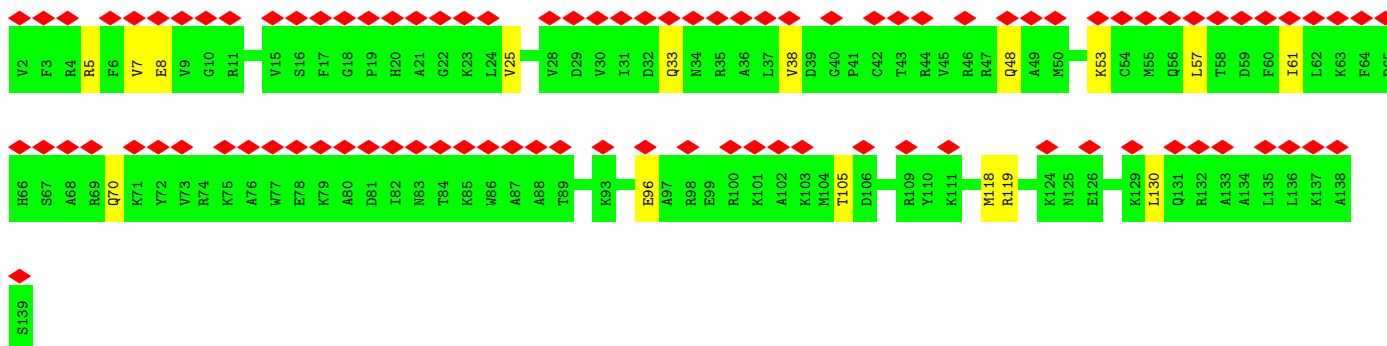
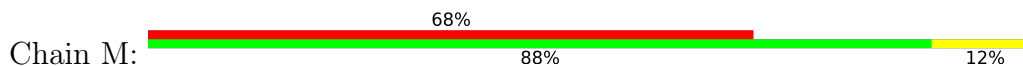




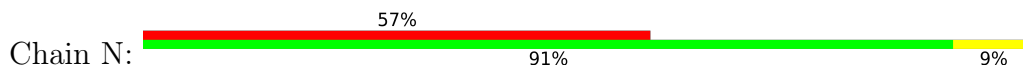
• Molecule 11: eL13

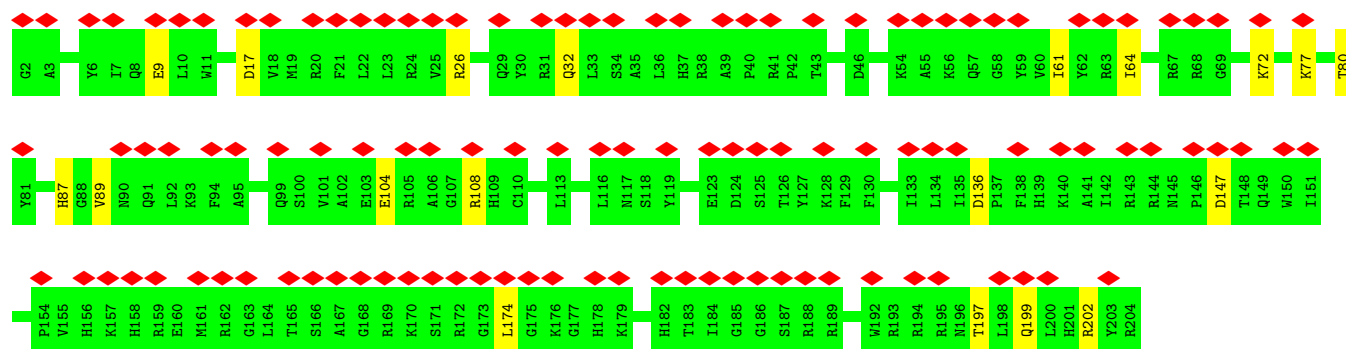


• Molecule 12: Ribosomal protein L14

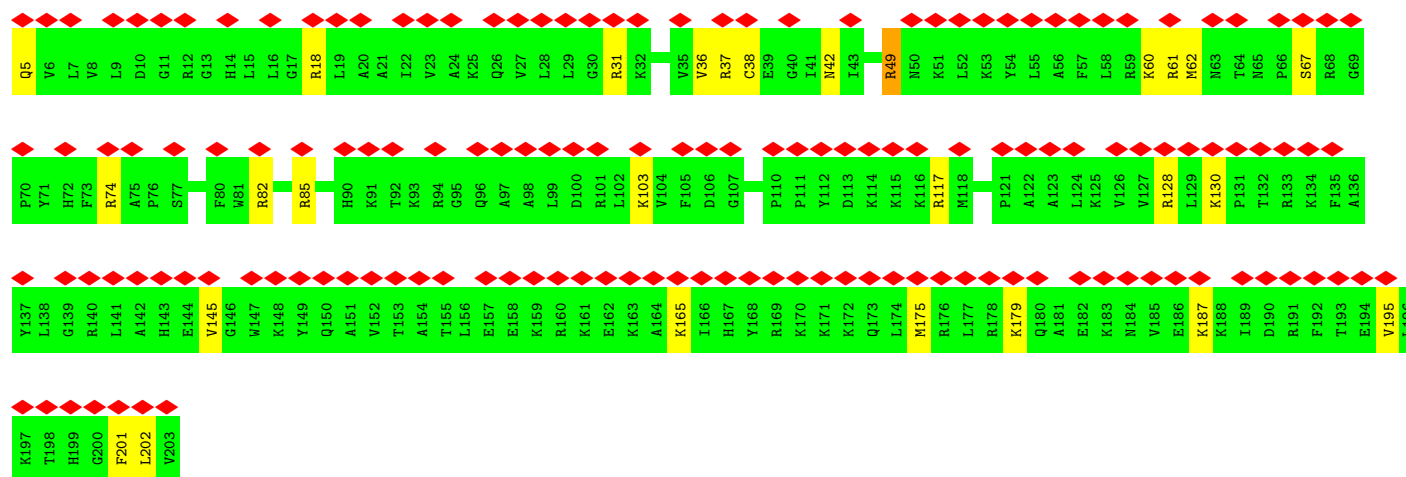
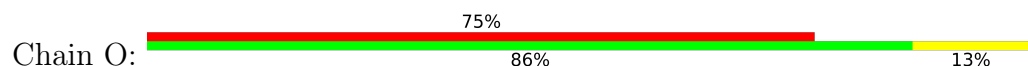


• Molecule 13: Ribosomal protein L15

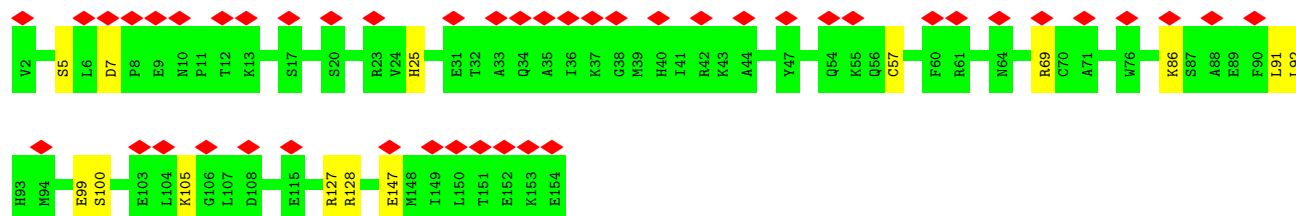
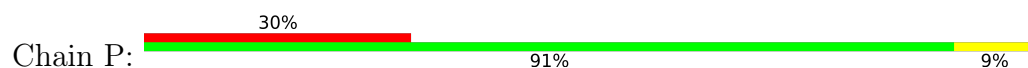




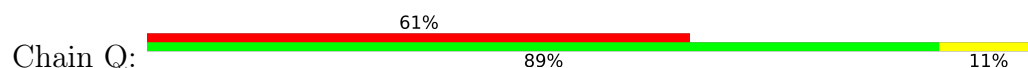
• Molecule 14: uL13

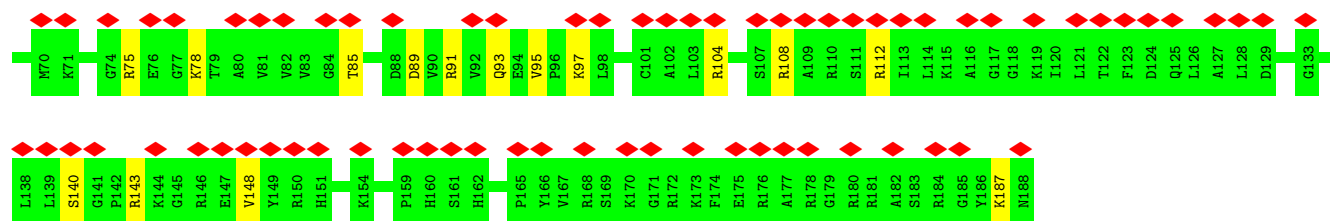


• Molecule 15: uL22

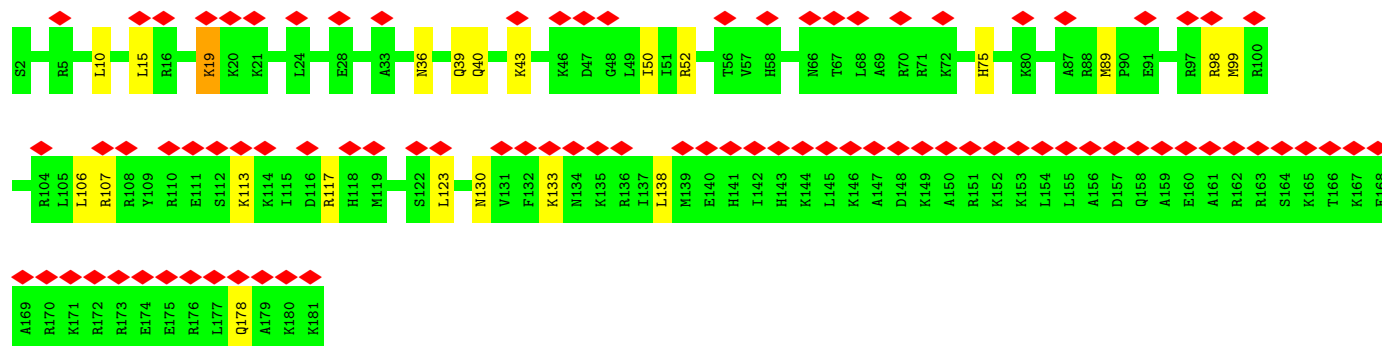
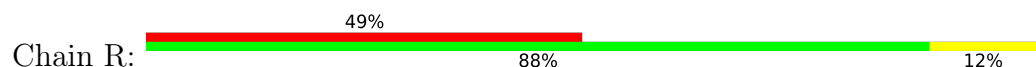


• Molecule 16: uL14

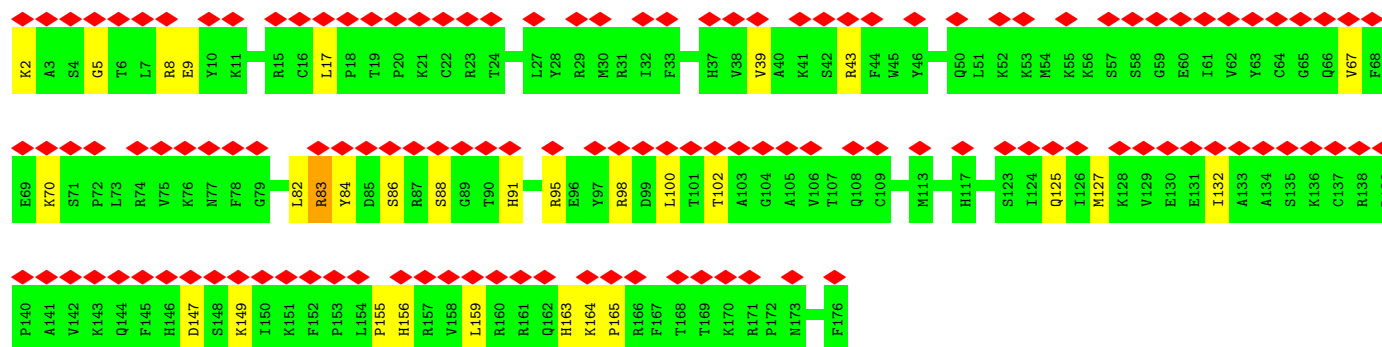
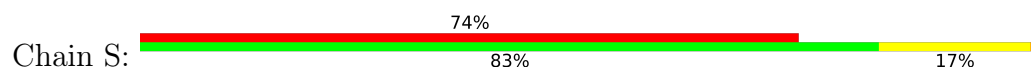




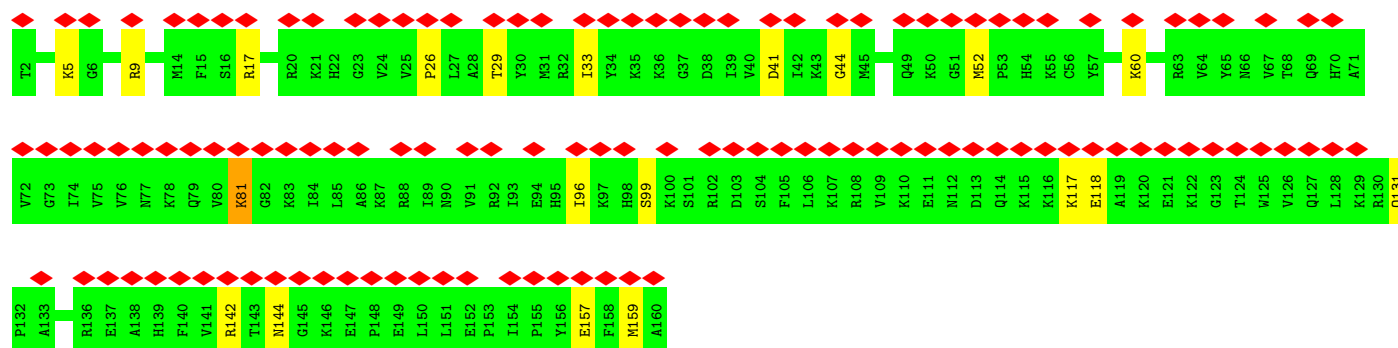
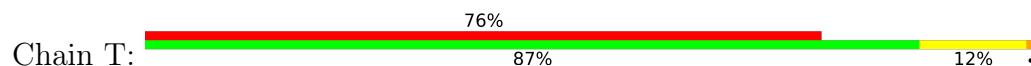
• Molecule 17: eL19



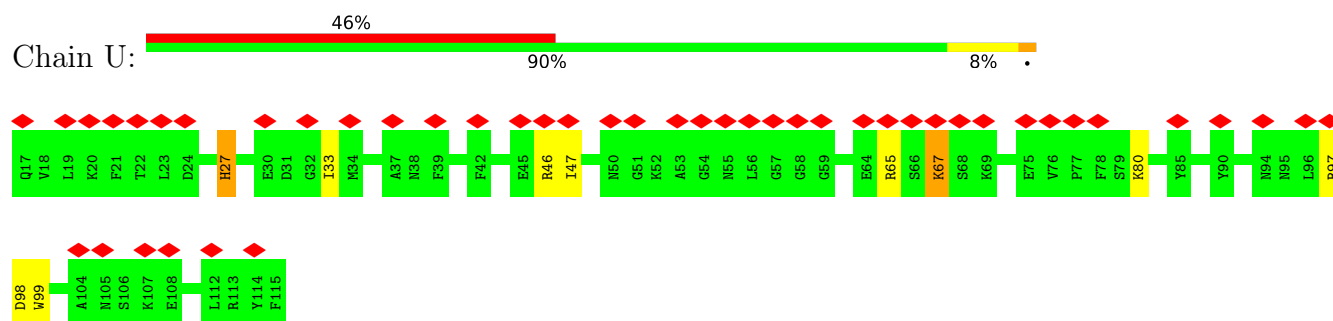
• Molecule 18: eL20



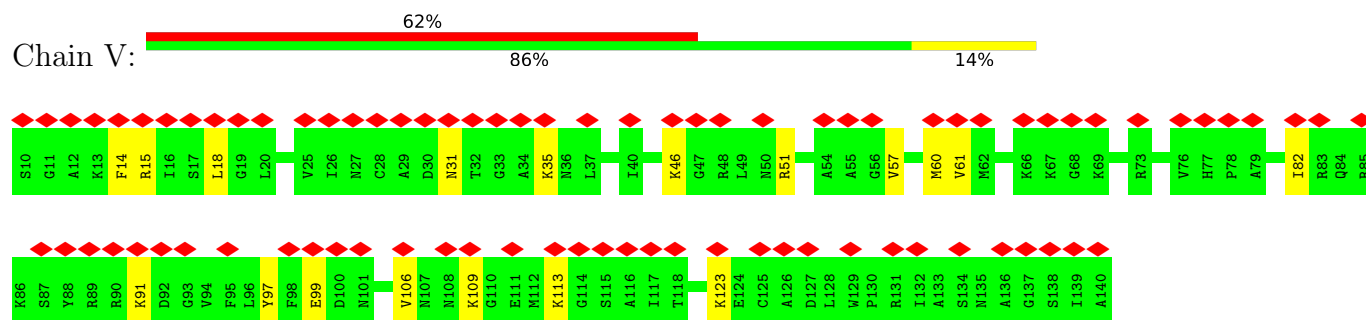
• Molecule 19: eL21



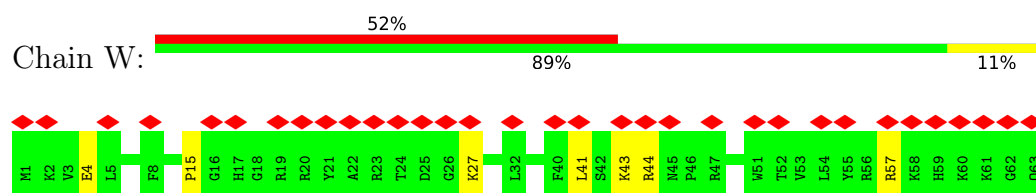
• Molecule 20: Ribosomal protein L22



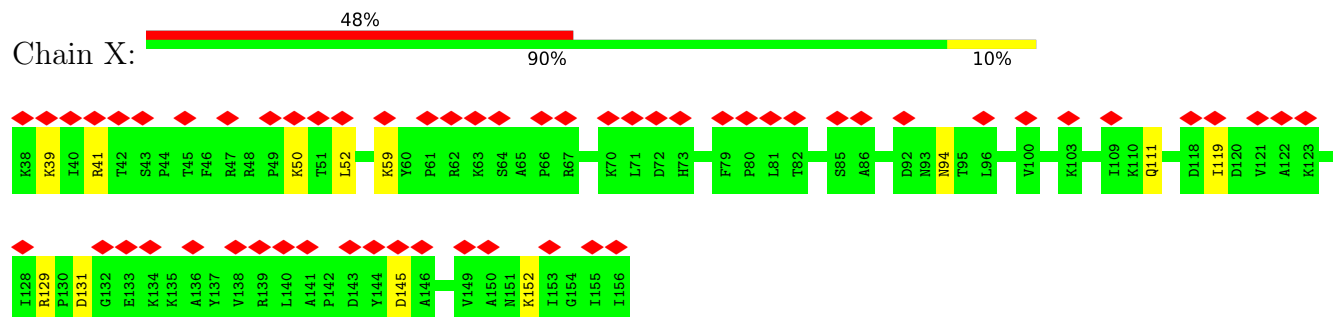
• Molecule 21: uL14



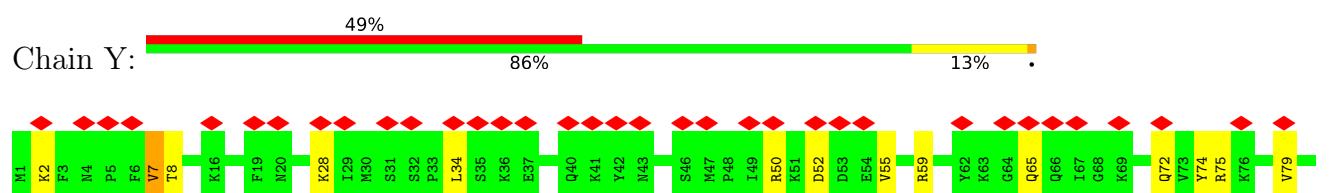
• Molecule 22: Ribosomal protein L24

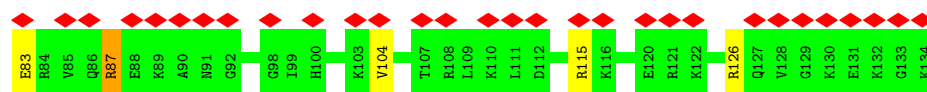


• Molecule 23: uL23

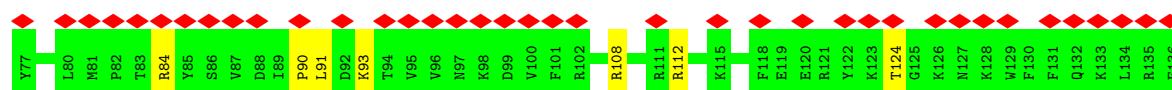
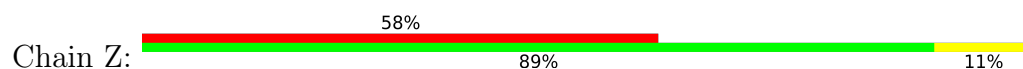


• Molecule 24: Ribosomal protein L26

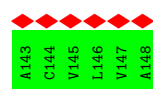
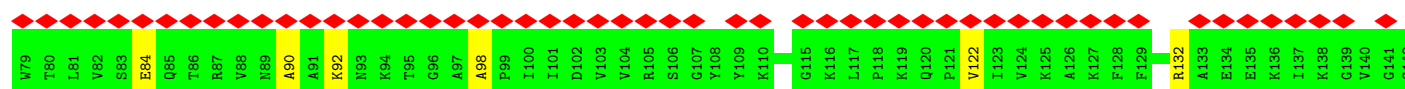
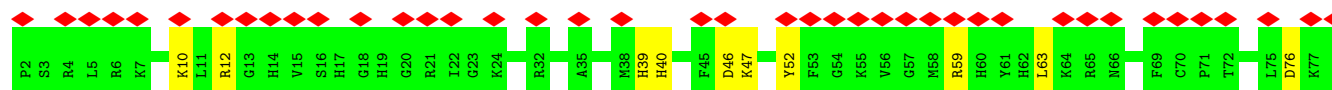
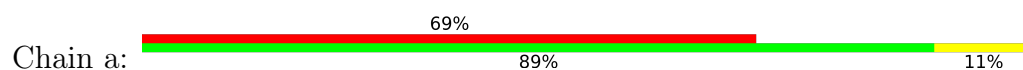




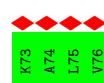
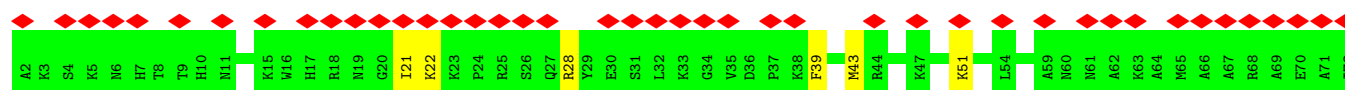
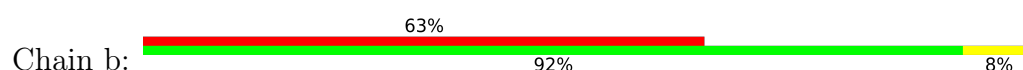
• Molecule 25: 60S ribosomal protein L27



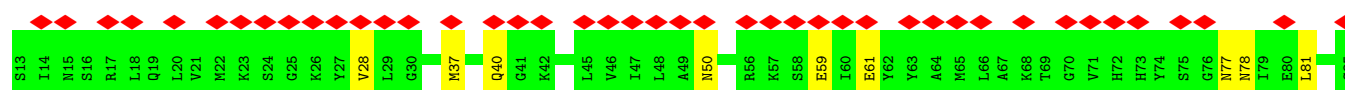
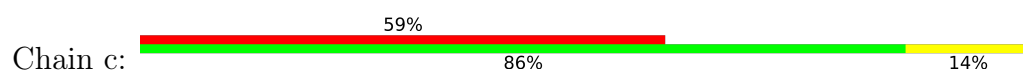
• Molecule 26: uL15

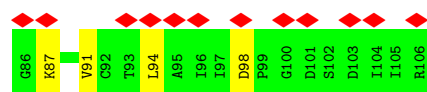


• Molecule 27: 60S ribosomal protein L29

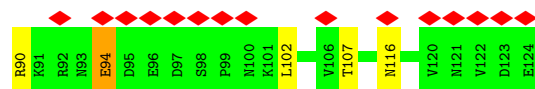
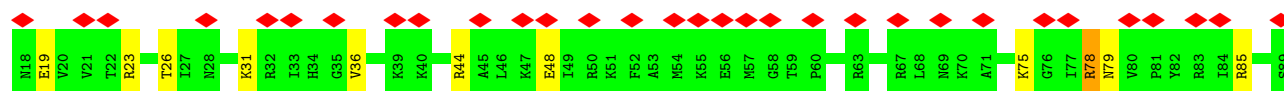
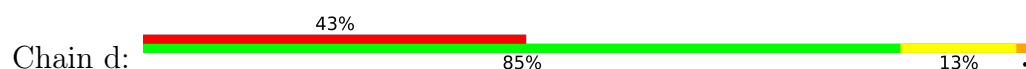


• Molecule 28: eL30

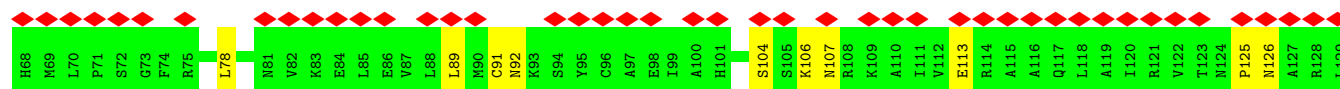
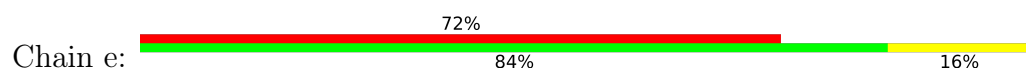




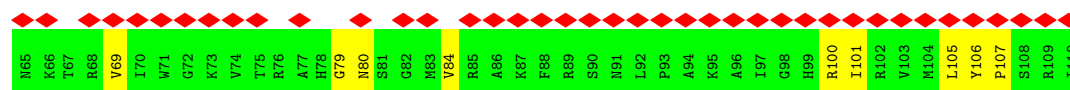
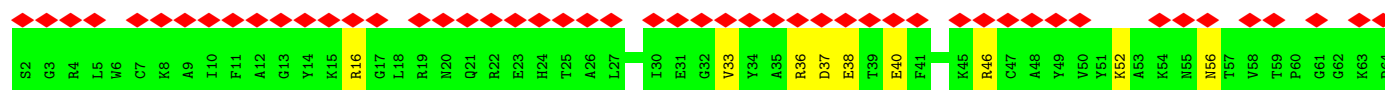
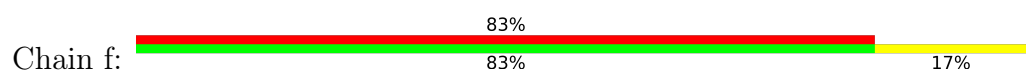
• Molecule 29: eL31



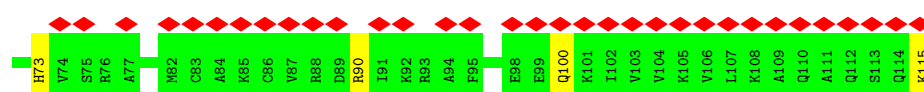
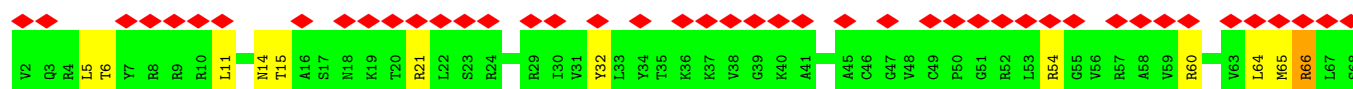
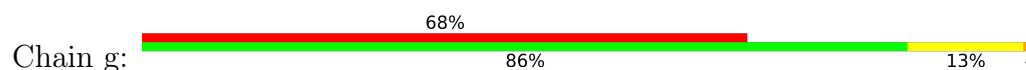
• Molecule 30: eL32



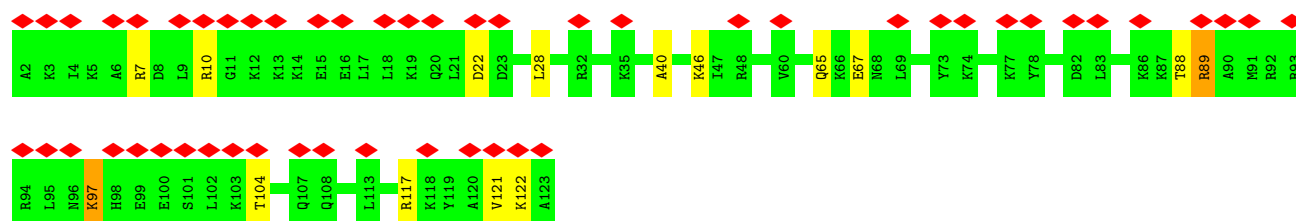
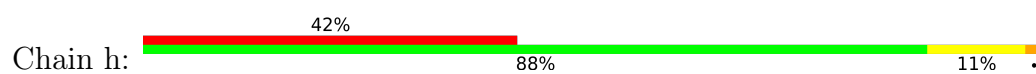
• Molecule 31: eL33



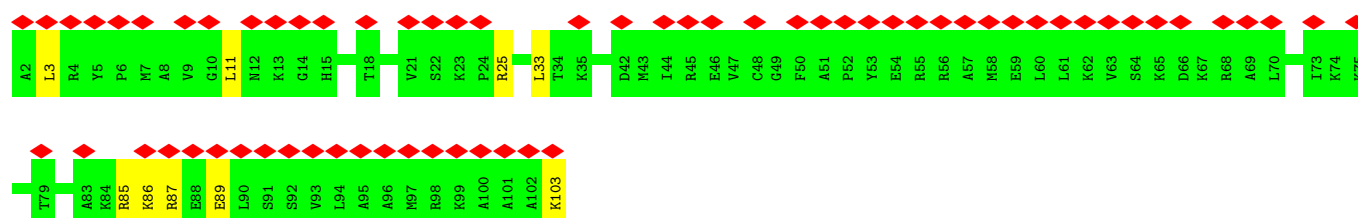
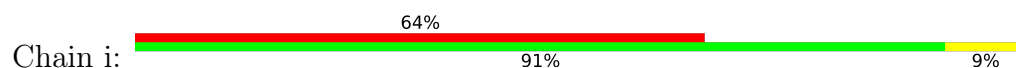
• Molecule 32: eL34



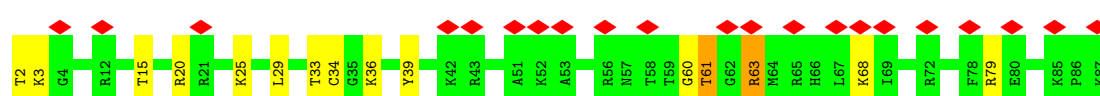
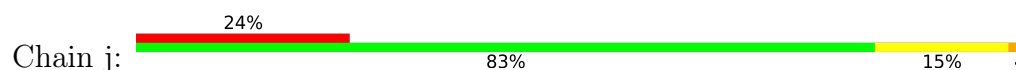
• Molecule 33: uL29



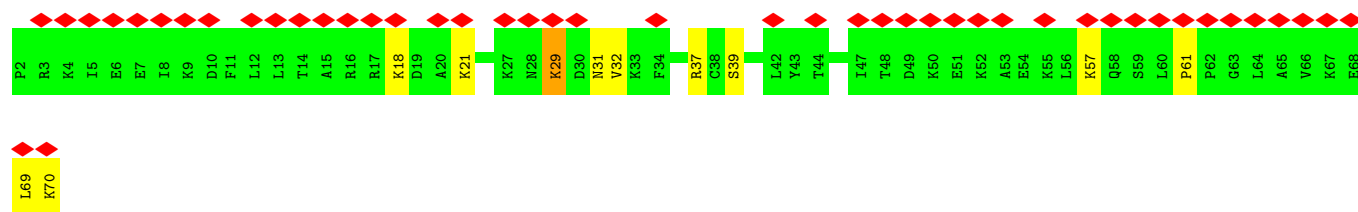
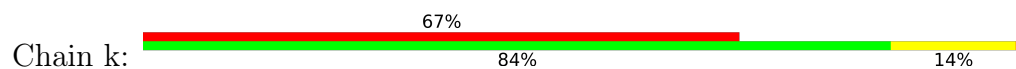
• Molecule 34: 60S ribosomal protein L36



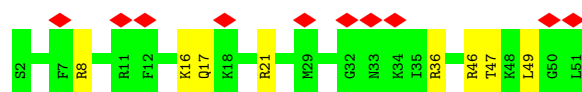
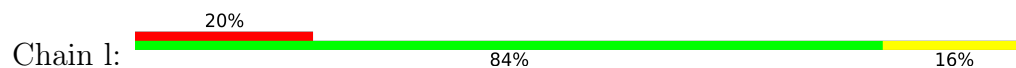
• Molecule 35: Ribosomal protein L37



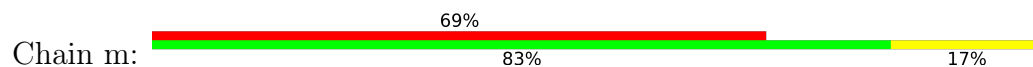
• Molecule 36: eL38

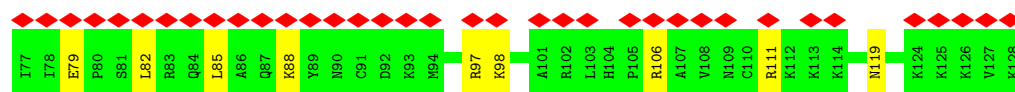


• Molecule 37: eL39

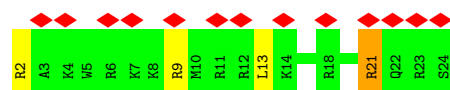
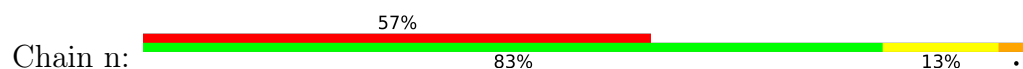


• Molecule 38: eL40

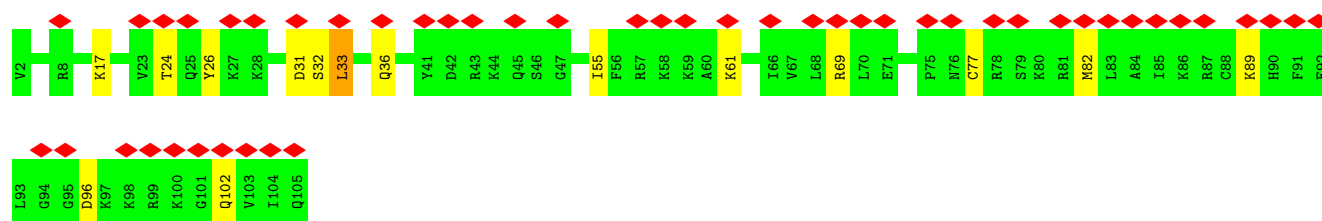
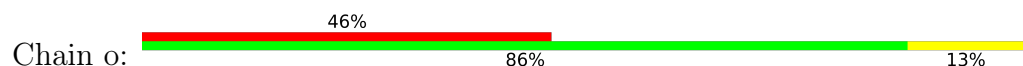




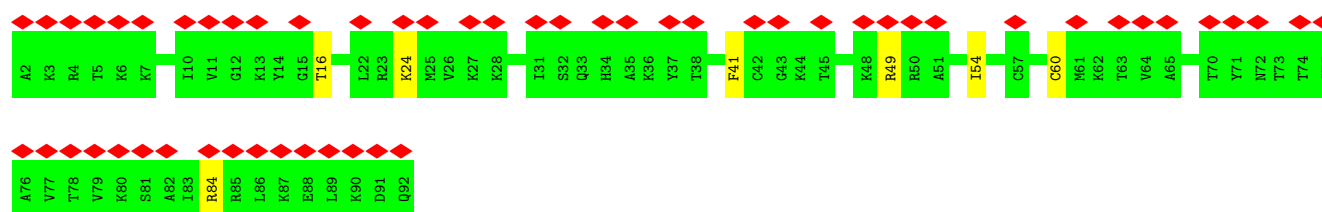
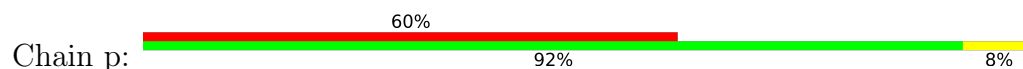
- Molecule 39: 60s ribosomal protein l41



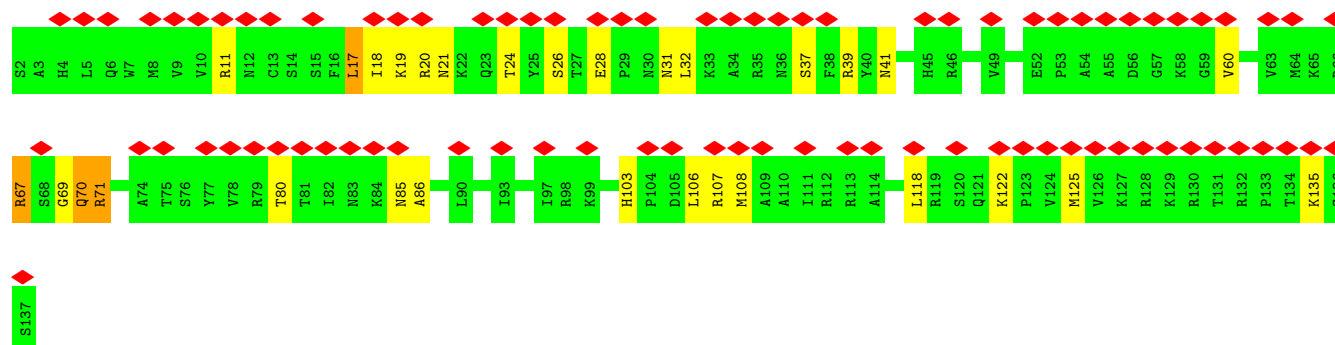
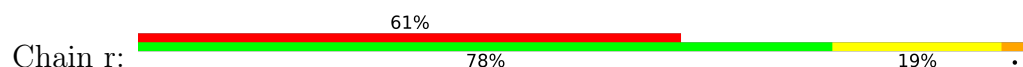
- Molecule 40: eL42



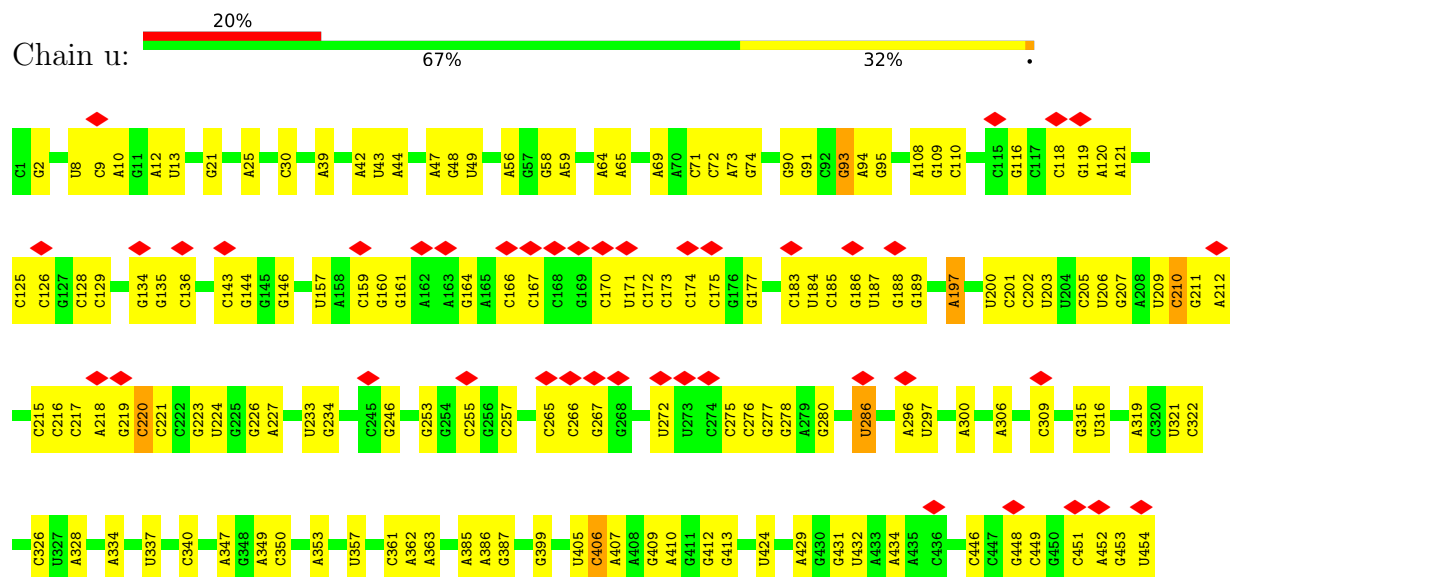
- Molecule 41: Ribosomal protein L37a



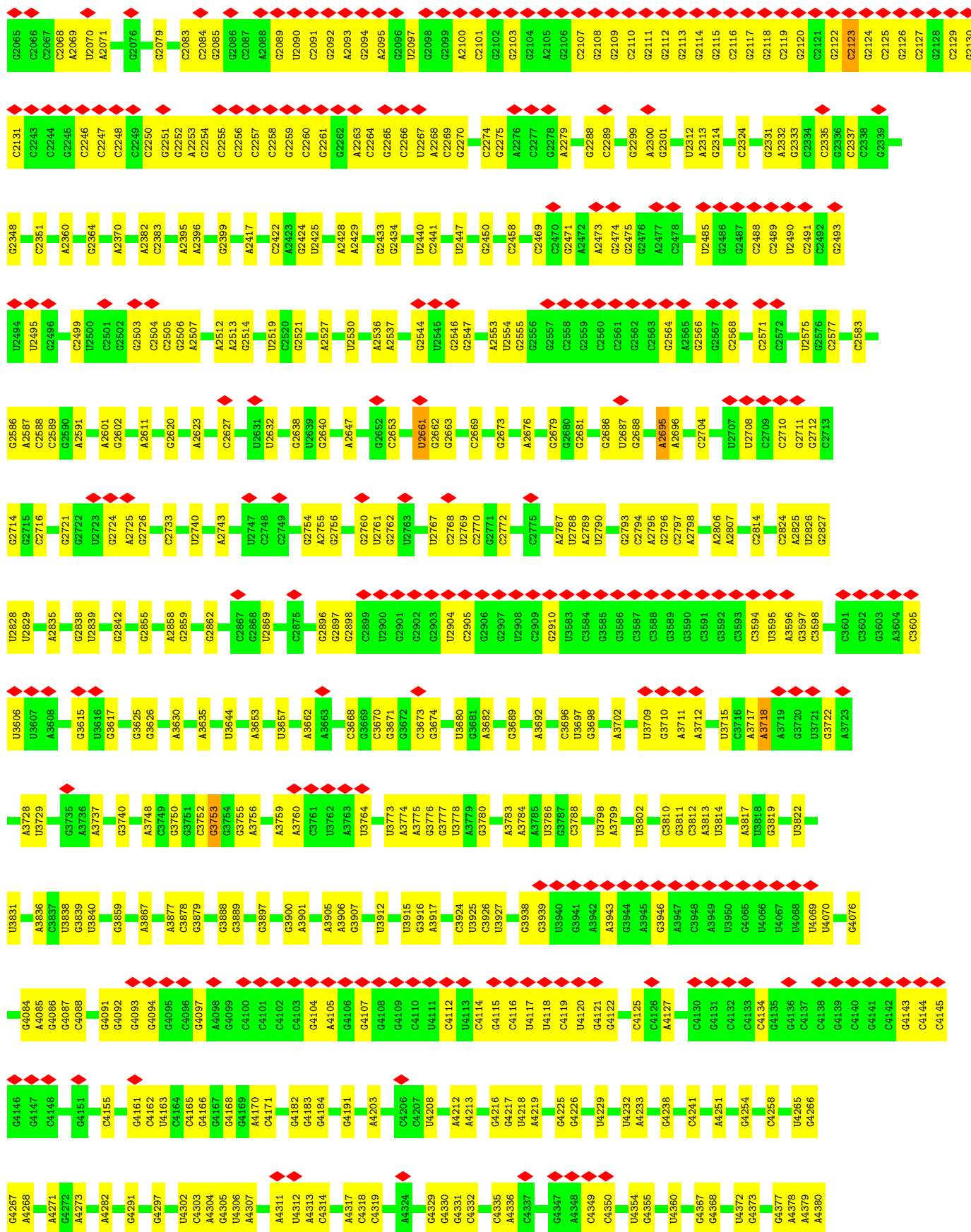
- Molecule 42: eL28

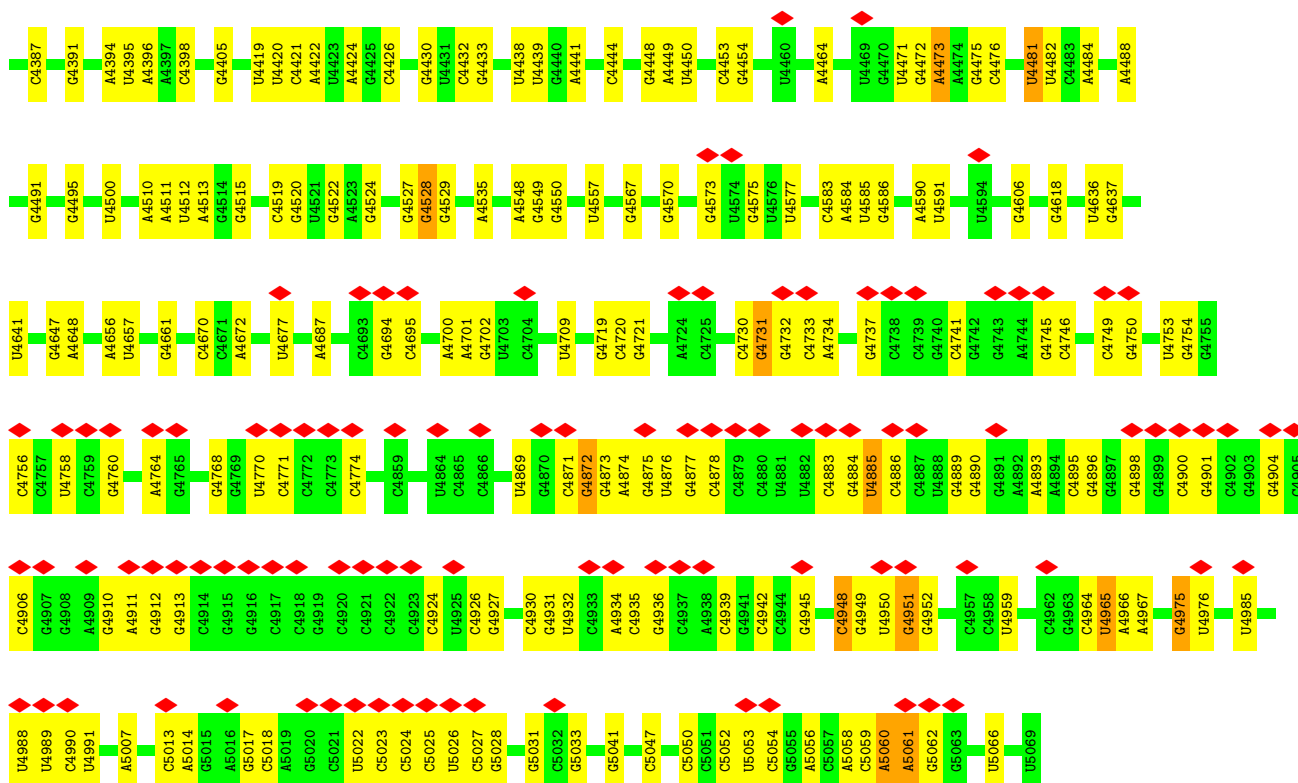


- Molecule 43: 60S acidic ribosomal protein P0

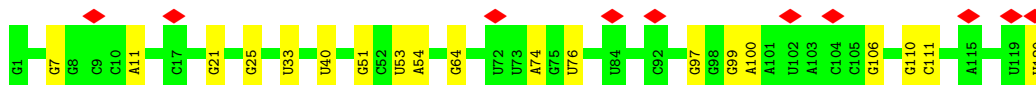
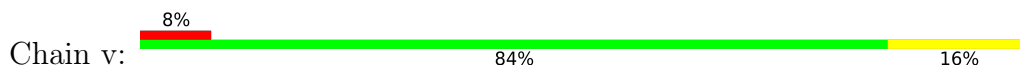




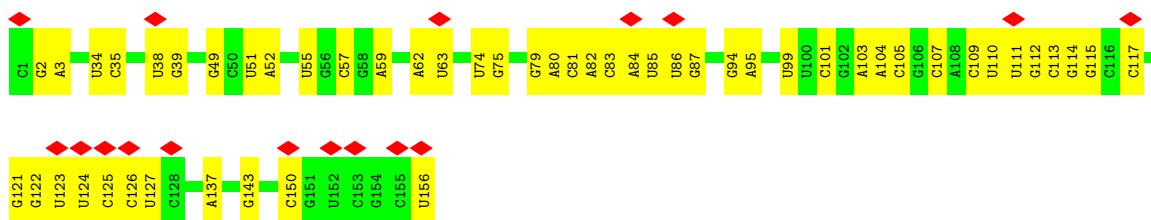




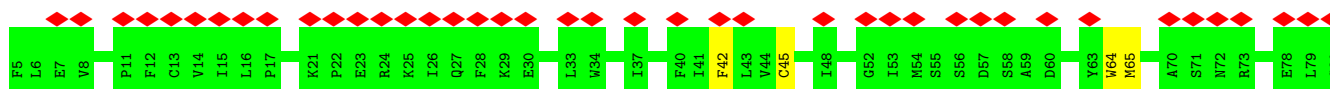
• Molecule 46: 5S ribosomal RNA

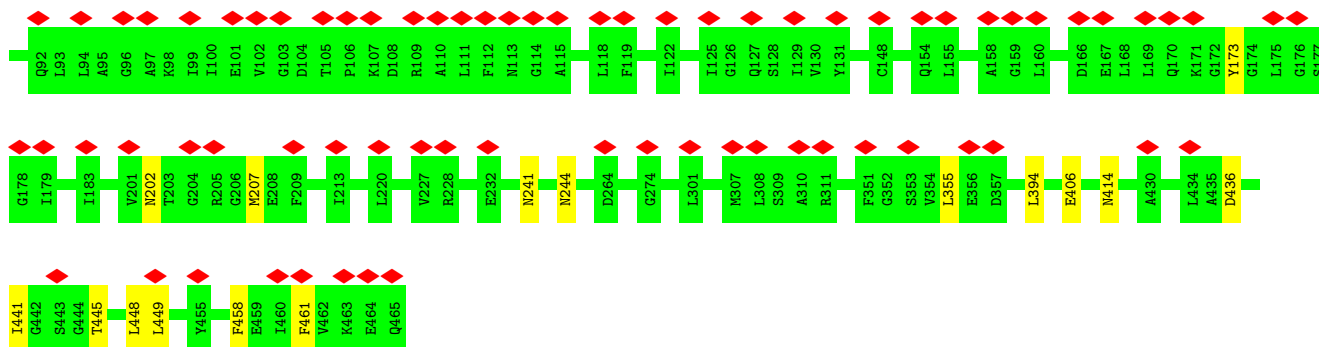


• Molecule 47: 5.8S ribosomal RNA

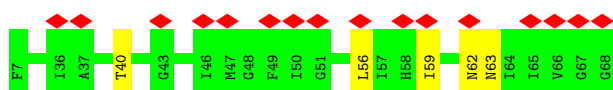
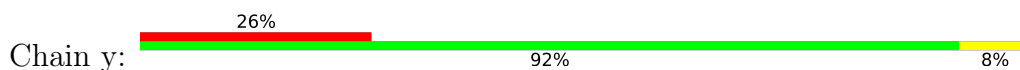


• Molecule 48: Protein transport protein Sec61 subunit alpha isoform 1

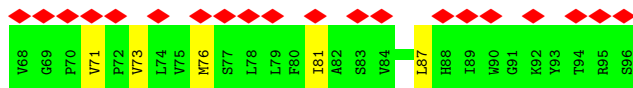
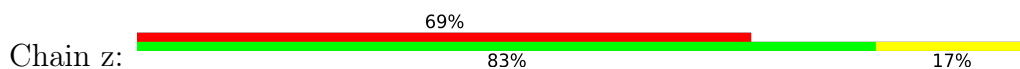




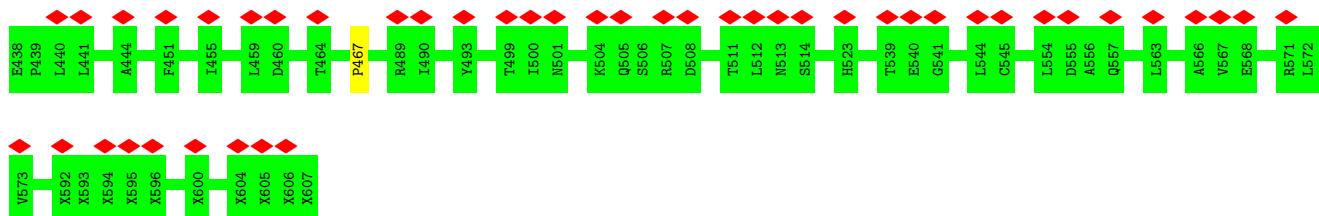
- Molecule 49: Protein transport protein Sec61 subunit gamma



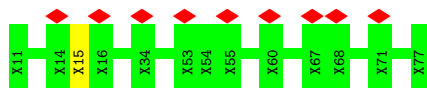
- Molecule 50: Protein transport protein Sec61 subunit beta



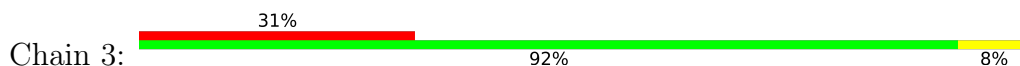
- Molecule 51: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 1, RPN1

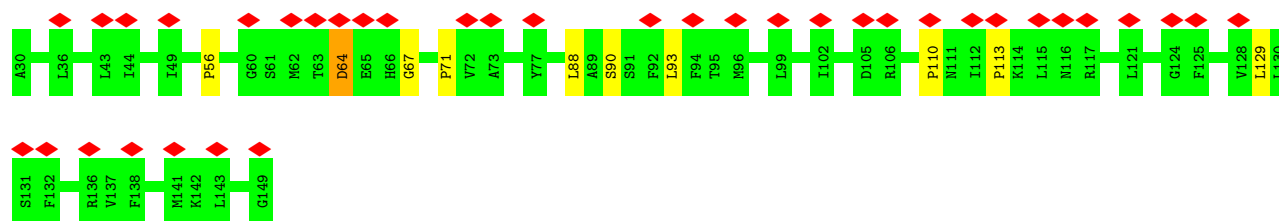


- Molecule 52: TMEM258

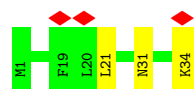
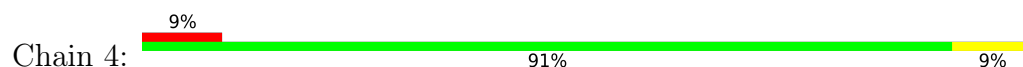


- Molecule 53: Oligosaccharyltransferase complex subunit OSTC

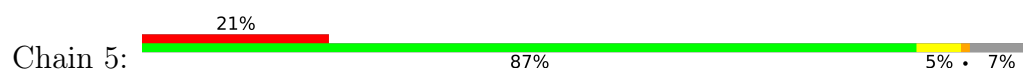




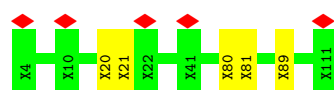
• Molecule 54: OST4



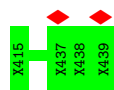
• Molecule 55: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3A



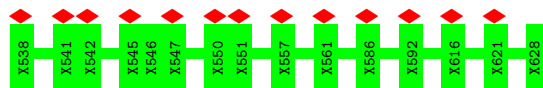
• Molecule 56: DAD1



• Molecule 57: OST48



- Molecule 58: RPN2



- Molecule 59: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 90895 | 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 ($e^-/\text{\AA}^2$) | 28 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | FEI FALCON III (4k x 4k) | Depositor |
| Maximum map value | 0.291 | Depositor |
| Minimum map value | -0.169 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.008 | Depositor |
| Recommended contour level | 0.04 | Depositor |
| Map size (Å) | 596.2, 596.2, 596.2 | wwPDB |
| Map dimensions | 500, 500, 500 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.1924, 1.1924, 1.1924 | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, NAG, ZN, MG, 9UB

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 | 0.46 | 0/1906 | 0.79 | 0/2556 |
| 2 | B | 0.40 | 0/3216 | 0.78 | 1/4311 (0.0%) |
| 3 | C | 0.43 | 0/2938 | 0.80 | 5/3946 (0.1%) |
| 4 | D | 0.37 | 0/2432 | 0.70 | 1/3257 (0.0%) |
| 5 | E | 0.46 | 0/1936 | 0.82 | 2/2600 (0.1%) |
| 6 | F | 0.40 | 0/1905 | 0.75 | 1/2539 (0.0%) |
| 7 | G | 0.38 | 0/1967 | 0.73 | 1/2647 (0.0%) |
| 8 | H | 0.37 | 0/1535 | 0.71 | 0/2063 |
| 9 | I | 0.41 | 0/1693 | 0.69 | 0/2260 |
| 10 | J | 0.38 | 0/1376 | 0.73 | 0/1841 |
| 11 | L | 0.41 | 0/1734 | 0.79 | 0/2317 |
| 12 | M | 0.38 | 0/1158 | 0.74 | 0/1547 |
| 13 | N | 0.43 | 0/1746 | 0.83 | 0/2338 |
| 14 | O | 0.40 | 0/1671 | 0.77 | 0/2234 |
| 15 | P | 0.42 | 0/1268 | 0.75 | 0/1701 |
| 16 | Q | 0.41 | 0/1530 | 0.81 | 1/2041 (0.0%) |
| 17 | R | 0.41 | 0/1524 | 0.79 | 0/2013 |
| 18 | S | 0.40 | 0/1493 | 0.85 | 3/2002 (0.1%) |
| 19 | T | 0.41 | 0/1326 | 0.72 | 0/1770 |
| 20 | U | 0.41 | 0/822 | 0.68 | 0/1103 |
| 21 | V | 0.40 | 0/993 | 0.73 | 0/1332 |
| 22 | W | 0.48 | 0/541 | 0.83 | 1/720 (0.1%) |
| 23 | X | 0.42 | 0/993 | 0.74 | 0/1334 |
| 24 | Y | 0.37 | 0/1132 | 0.80 | 2/1504 (0.1%) |
| 25 | Z | 0.40 | 0/1130 | 0.72 | 0/1507 |
| 26 | a | 0.40 | 0/1191 | 0.79 | 0/1590 |
| 27 | b | 0.44 | 0/619 | 0.73 | 0/818 |
| 28 | c | 0.36 | 0/742 | 0.69 | 0/996 |
| 29 | d | 0.38 | 0/903 | 0.81 | 1/1216 (0.1%) |
| 30 | e | 0.47 | 0/1071 | 0.85 | 0/1429 |
| 31 | f | 0.52 | 0/895 | 0.87 | 0/1198 |
| 32 | g | 0.42 | 0/916 | 0.81 | 1/1220 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 33 | h | 0.36 | 0/1021 | 0.77 | 1/1348 (0.1%) |
| 34 | i | 0.40 | 0/841 | 0.82 | 2/1112 (0.2%) |
| 35 | j | 0.46 | 0/720 | 0.94 | 1/952 (0.1%) |
| 36 | k | 0.37 | 0/575 | 0.69 | 0/761 |
| 37 | l | 0.50 | 0/454 | 0.84 | 0/599 |
| 38 | m | 0.37 | 0/435 | 0.76 | 0/575 |
| 39 | n | 0.41 | 0/223 | 0.92 | 1/284 (0.4%) |
| 40 | o | 0.39 | 0/864 | 0.75 | 0/1140 |
| 41 | p | 0.42 | 0/718 | 0.71 | 0/953 |
| 42 | r | 0.46 | 0/1110 | 0.77 | 1/1484 (0.1%) |
| 43 | s | 0.38 | 0/1547 | 0.58 | 0/2088 |
| 44 | t | 0.41 | 0/1257 | 0.69 | 0/1697 |
| 45 | u | 0.41 | 11/87790 (0.0%) | 0.80 | 94/136937 (0.1%) |
| 46 | v | 0.31 | 0/2858 | 0.69 | 0/4455 |
| 47 | w | 0.36 | 0/3701 | 0.74 | 0/5766 |
| 48 | x | 0.52 | 0/3383 | 0.79 | 3/4584 (0.1%) |
| 49 | y | 0.49 | 0/504 | 0.76 | 1/673 (0.1%) |
| 50 | z | 0.42 | 0/236 | 0.74 | 0/321 |
| 51 | 1 | 0.39 | 0/757 | 0.53 | 1/1052 (0.1%) |
| 53 | 3 | 0.57 | 0/815 | 0.89 | 5/1107 (0.5%) |
| 54 | 4 | 0.52 | 0/273 | 0.66 | 0/371 |
| 55 | 5 | 0.66 | 5/5224 (0.1%) | 0.86 | 17/7093 (0.2%) |
| All | All | 0.42 | 16/161608 (0.0%) | 0.79 | 147/237302 (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 |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 1 |
| 2 | B | 0 | 4 |
| 3 | C | 0 | 2 |
| 4 | D | 0 | 1 |
| 5 | E | 0 | 1 |
| 7 | G | 0 | 1 |
| 9 | I | 0 | 2 |
| 11 | L | 0 | 3 |
| 17 | R | 0 | 1 |
| 18 | S | 0 | 2 |
| 19 | T | 0 | 1 |
| 20 | U | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 24 | Y | 0 | 1 |
| 31 | f | 0 | 1 |
| 42 | r | 0 | 2 |
| 45 | u | 0 | 1 |
| 48 | x | 0 | 2 |
| 52 | 2 | 0 | 1 |
| 53 | 3 | 0 | 2 |
| 55 | 5 | 0 | 6 |
| 56 | 6 | 0 | 5 |
| All | All | 0 | 41 |

All (16) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 45 | u | 680 | G | O3'-P | -33.63 | 1.20 | 1.61 |
| 45 | u | 692 | A | O3'-P | 32.98 | 2.00 | 1.61 |
| 45 | u | 1965 | G | O3'-P | -23.04 | 1.33 | 1.61 |
| 45 | u | 472 | C | O3'-P | -19.63 | 1.37 | 1.61 |
| 55 | 5 | 545 | ASN | C-N | -18.35 | 0.91 | 1.34 |
| 55 | 5 | 550 | THR | C-N | -16.38 | 0.96 | 1.34 |
| 45 | u | 197 | A | O3'-P | 13.18 | 1.76 | 1.61 |
| 55 | 5 | 513 | ARG | C-N | 10.49 | 1.58 | 1.34 |
| 45 | u | 462 | G | O3'-P | -9.24 | 1.50 | 1.61 |
| 55 | 5 | 194 | TRP | CB-CG | -7.09 | 1.37 | 1.50 |
| 45 | u | 223 | G | O3'-P | -6.55 | 1.53 | 1.61 |
| 45 | u | 207 | G | O3'-P | -6.23 | 1.53 | 1.61 |
| 45 | u | 1847 | C | O3'-P | -6.12 | 1.53 | 1.61 |
| 45 | u | 957 | G | O3'-P | 5.59 | 1.67 | 1.61 |
| 55 | 5 | 477 | TRP | CB-CG | -5.33 | 1.40 | 1.50 |
| 45 | u | 1358 | G | O3'-P | 5.09 | 1.67 | 1.61 |

All (147) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 55 | 5 | 545 | ASN | C-N-CA | -16.91 | 79.43 | 121.70 |
| 45 | u | 462 | G | P-O3'-C3' | -16.27 | 100.18 | 119.70 |
| 55 | 5 | 545 | ASN | O-C-N | 14.89 | 146.53 | 122.70 |
| 45 | u | 680 | G | O3'-P-O5' | 14.37 | 131.31 | 104.00 |
| 55 | 5 | 545 | ASN | CA-C-N | -13.11 | 88.36 | 117.20 |
| 45 | u | 3753 | G | N9-C1'-C2' | -11.93 | 98.49 | 114.00 |
| 45 | u | 197 | A | P-O3'-C3' | 11.51 | 133.51 | 119.70 |
| 45 | u | 220 | C | N1-C1'-C2' | -11.09 | 99.58 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 45 | u | 3718 | A | N9-C1'-C2' | -10.28 | 100.64 | 114.00 |
| 55 | 5 | 550 | THR | O-C-N | -10.25 | 106.30 | 122.70 |
| 45 | u | 1358 | G | C4'-C3'-O3' | 10.20 | 133.39 | 113.00 |
| 45 | u | 1357 | C | C4'-C3'-O3' | 9.69 | 132.38 | 113.00 |
| 55 | 5 | 513 | ARG | O-C-N | -9.14 | 108.08 | 122.70 |
| 24 | Y | 87 | ARG | NE-CZ-NH2 | 9.13 | 124.86 | 120.30 |
| 45 | u | 223 | G | P-O3'-C3' | 9.04 | 130.55 | 119.70 |
| 45 | u | 692 | A | P-O3'-C3' | 8.98 | 130.48 | 119.70 |
| 48 | x | 449 | LEU | CA-CB-CG | -8.96 | 94.69 | 115.30 |
| 45 | u | 4975 | G | C2'-C3'-O3' | 8.96 | 129.20 | 109.50 |
| 22 | W | 44 | ARG | NE-CZ-NH1 | 8.60 | 124.60 | 120.30 |
| 45 | u | 90 | G | C2'-C3'-O3' | 8.39 | 127.95 | 109.50 |
| 45 | u | 4528 | G | C2'-C3'-O3' | 8.35 | 127.88 | 109.50 |
| 45 | u | 3888 | G | C2'-C3'-O3' | 8.31 | 127.78 | 109.50 |
| 45 | u | 1969 | G | N9-C1'-C2' | -8.26 | 102.91 | 112.00 |
| 45 | u | 4948 | C | C2'-C3'-O3' | 8.05 | 127.22 | 109.50 |
| 18 | S | 83 | ARG | NE-CZ-NH2 | 7.99 | 124.30 | 120.30 |
| 45 | u | 220 | C | C2'-C3'-O3' | 7.99 | 127.08 | 109.50 |
| 45 | u | 1211 | G | C2'-C3'-O3' | 7.96 | 127.00 | 109.50 |
| 45 | u | 3697 | U | C2'-C3'-O3' | 7.91 | 126.91 | 109.50 |
| 35 | j | 63 | ARG | NE-CZ-NH1 | 7.88 | 124.24 | 120.30 |
| 45 | u | 1455 | G | C2'-C3'-O3' | 7.77 | 126.59 | 109.50 |
| 45 | u | 2858 | A | N9-C1'-C2' | -7.63 | 103.60 | 112.00 |
| 3 | C | 342 | ARG | NE-CZ-NH1 | 7.62 | 124.11 | 120.30 |
| 45 | u | 2858 | A | C4'-C3'-O3' | 7.62 | 128.24 | 113.00 |
| 45 | u | 1292 | C | C2'-C3'-O3' | 7.53 | 126.06 | 109.50 |
| 45 | u | 3718 | A | C4'-C3'-O3' | 7.50 | 127.99 | 113.00 |
| 55 | 5 | 532 | ILE | O-C-N | -7.49 | 110.72 | 122.70 |
| 45 | u | 275 | C | C2'-C3'-O3' | 7.35 | 125.66 | 109.50 |
| 45 | u | 5060 | A | C2'-C3'-O3' | 7.33 | 125.62 | 109.50 |
| 45 | u | 125 | C | C2'-C3'-O3' | 7.33 | 125.61 | 109.50 |
| 45 | u | 2797 | C | N1-C1'-C2' | -7.28 | 103.99 | 112.00 |
| 45 | u | 1477 | C | C2'-C3'-O3' | 7.28 | 125.52 | 109.50 |
| 45 | u | 5061 | A | C2'-C3'-O3' | 7.20 | 125.34 | 109.50 |
| 45 | u | 47 | A | C4'-C3'-O3' | 7.19 | 127.38 | 113.00 |
| 45 | u | 2027 | U | N1-C1'-C2' | -7.16 | 104.12 | 112.00 |
| 45 | u | 2695 | A | C2'-C3'-O3' | 7.15 | 125.22 | 109.50 |
| 45 | u | 5059 | C | C2'-C3'-O3' | 7.15 | 125.22 | 109.50 |
| 45 | u | 406 | C | C2'-C3'-O3' | 7.14 | 125.20 | 109.50 |
| 55 | 5 | 550 | THR | C-N-CA | 7.04 | 139.30 | 121.70 |
| 55 | 5 | 550 | THR | CA-C-N | 7.02 | 132.65 | 117.20 |
| 55 | 5 | 350 | SER | C-N-CA | -7.01 | 104.18 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 45 | u | 209 | U | O4'-C1'-N1 | 6.97 | 113.78 | 108.20 |
| 45 | u | 1485 | C | C2'-C3'-O3' | 6.93 | 124.78 | 113.70 |
| 45 | u | 462 | G | OP1-P-O3' | -6.80 | 90.23 | 105.20 |
| 45 | u | 1279 | A | C2'-C3'-O3' | 6.79 | 124.57 | 113.70 |
| 45 | u | 2046 | G | C2'-C3'-O3' | 6.78 | 124.54 | 113.70 |
| 45 | u | 1236 | C | C2'-C3'-O3' | 6.71 | 124.43 | 113.70 |
| 45 | u | 977 | C | C2'-C3'-O3' | 6.68 | 124.39 | 113.70 |
| 45 | u | 692 | A | OP1-P-O3' | 6.67 | 119.88 | 105.20 |
| 55 | 5 | 257 | VAL | N-CA-C | -6.67 | 93.01 | 111.00 |
| 45 | u | 4885 | U | C2'-C3'-O3' | 6.66 | 124.36 | 113.70 |
| 45 | u | 93 | G | C4'-C3'-O3' | 6.65 | 126.30 | 113.00 |
| 45 | u | 1818 | G | C2'-C3'-O3' | 6.54 | 124.16 | 113.70 |
| 34 | i | 25 | ARG | NE-CZ-NH1 | 6.50 | 123.55 | 120.30 |
| 45 | u | 209 | U | C4'-C3'-O3' | 6.44 | 125.89 | 113.00 |
| 45 | u | 2083 | C | C4'-C3'-O3' | 6.42 | 125.85 | 113.00 |
| 4 | D | 22 | ARG | NE-CZ-NH1 | 6.41 | 123.51 | 120.30 |
| 45 | u | 93 | G | N9-C1'-C2' | -6.39 | 104.97 | 112.00 |
| 45 | u | 3657 | U | C2'-C3'-O3' | 6.38 | 123.90 | 113.70 |
| 45 | u | 680 | G | OP2-P-O3' | -6.33 | 91.28 | 105.20 |
| 5 | E | 208 | LEU | CA-CB-CG | 6.33 | 129.85 | 115.30 |
| 45 | u | 1474 | C | C2'-C3'-O3' | 6.31 | 123.80 | 113.70 |
| 48 | x | 448 | LEU | CA-CB-CG | 6.30 | 129.78 | 115.30 |
| 45 | u | 1398 | A | C2'-C3'-O3' | 6.28 | 123.74 | 113.70 |
| 45 | u | 1500 | A | C2'-C3'-O3' | 6.26 | 123.72 | 113.70 |
| 45 | u | 1969 | G | C4'-C3'-O3' | 6.24 | 125.48 | 113.00 |
| 45 | u | 2123 | C | C2'-C3'-O3' | 6.23 | 123.67 | 113.70 |
| 45 | u | 1380 | G | N9-C1'-C2' | 6.20 | 122.06 | 114.00 |
| 45 | u | 1239 | C | C2'-C3'-O3' | 6.20 | 123.61 | 113.70 |
| 45 | u | 2632 | U | N1-C1'-C2' | 6.17 | 122.02 | 114.00 |
| 45 | u | 1072 | C | N1-C1'-C2' | 6.08 | 121.90 | 114.00 |
| 55 | 5 | 349 | VAL | N-CA-C | -6.07 | 94.60 | 111.00 |
| 45 | u | 1672 | U | N1-C1'-C2' | 6.04 | 121.85 | 114.00 |
| 53 | 3 | 71 | PRO | N-CA-CB | 6.02 | 110.52 | 103.30 |
| 45 | u | 1848 | C | C2'-C3'-O3' | 6.00 | 123.30 | 113.70 |
| 45 | u | 462 | G | O3'-P-O5' | 5.96 | 115.31 | 104.00 |
| 45 | u | 1390 | G | C2'-C3'-O3' | 5.93 | 123.19 | 113.70 |
| 29 | d | 78 | ARG | NE-CZ-NH1 | 5.92 | 123.26 | 120.30 |
| 34 | i | 85 | ARG | NE-CZ-NH1 | 5.91 | 123.26 | 120.30 |
| 55 | 5 | 513 | ARG | CA-C-N | 5.90 | 130.18 | 117.20 |
| 45 | u | 1696 | C | C2'-C3'-O3' | 5.89 | 123.13 | 113.70 |
| 45 | u | 1965 | G | P-O3'-C3' | 5.86 | 126.73 | 119.70 |
| 51 | 1 | 467 | PRO | N-CA-CB | 5.83 | 110.30 | 103.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 16 | Q | 104 | ARG | NE-CZ-NH1 | 5.81 | 123.21 | 120.30 |
| 5 | E | 72 | PRO | N-CA-CB | 5.80 | 110.26 | 103.30 |
| 45 | u | 978 | G | C2'-C3'-O3' | 5.80 | 122.97 | 113.70 |
| 49 | y | 56 | LEU | CA-CB-CG | 5.79 | 128.61 | 115.30 |
| 45 | u | 4951 | G | C2'-C3'-O3' | 5.78 | 122.95 | 113.70 |
| 45 | u | 4872 | G | C2'-C3'-O3' | 5.78 | 122.94 | 113.70 |
| 45 | u | 1329 | G | C2'-C3'-O3' | 5.76 | 122.92 | 113.70 |
| 45 | u | 4975 | G | C4'-C3'-O3' | -5.73 | 97.36 | 109.40 |
| 53 | 3 | 110 | PRO | N-CA-CB | 5.67 | 110.10 | 103.30 |
| 3 | C | 98 | GLY | N-CA-C | -5.64 | 99.01 | 113.10 |
| 18 | S | 83 | ARG | NE-CZ-NH1 | -5.62 | 117.49 | 120.30 |
| 53 | 3 | 56 | PRO | N-CA-CB | 5.55 | 109.96 | 103.30 |
| 6 | F | 91 | LEU | CA-CB-CG | 5.55 | 128.06 | 115.30 |
| 55 | 5 | 286 | LEU | C-N-CA | -5.52 | 107.89 | 121.70 |
| 2 | B | 36 | ASP | C-N-CD | 5.52 | 140.00 | 128.40 |
| 45 | u | 687 | U | N1-C1'-C2' | -5.48 | 105.97 | 112.00 |
| 45 | u | 4473 | A | N9-C1'-C2' | 5.46 | 121.10 | 114.00 |
| 45 | u | 2054 | U | N1-C1'-C2' | 5.46 | 121.10 | 114.00 |
| 53 | 3 | 113 | PRO | N-CA-CB | 5.46 | 109.85 | 103.30 |
| 45 | u | 979 | C | C2'-C3'-O3' | 5.45 | 122.43 | 113.70 |
| 45 | u | 210 | C | N1-C1'-C2' | 5.44 | 121.08 | 114.00 |
| 45 | u | 2028 | C | N1-C1'-C2' | -5.43 | 106.03 | 112.00 |
| 45 | u | 957 | G | P-O3'-C3' | 5.38 | 126.16 | 119.70 |
| 45 | u | 1365 | C | C4'-C3'-O3' | 5.38 | 123.77 | 113.00 |
| 55 | 5 | 292 | PRO | N-CA-CB | 5.37 | 109.74 | 103.30 |
| 45 | u | 215 | C | C4'-C3'-O3' | -5.36 | 98.14 | 109.40 |
| 24 | Y | 75 | ARG | NE-CZ-NH1 | 5.35 | 122.97 | 120.30 |
| 45 | u | 212 | A | N9-C1'-C2' | 5.35 | 120.95 | 114.00 |
| 55 | 5 | 4 | LEU | CA-CB-CG | 5.33 | 127.55 | 115.30 |
| 45 | u | 486 | C | C2'-C3'-O3' | 5.30 | 122.18 | 113.70 |
| 45 | u | 1266 | G | C2'-C3'-O3' | 5.29 | 122.17 | 113.70 |
| 33 | h | 22 | ASP | CB-CG-OD2 | 5.28 | 123.05 | 118.30 |
| 55 | 5 | 513 | ARG | C-N-CA | 5.26 | 134.85 | 121.70 |
| 3 | C | 262 | ASP | CB-CG-OD2 | 5.25 | 123.02 | 118.30 |
| 45 | u | 3715 | U | N1-C1'-C2' | -5.24 | 106.23 | 112.00 |
| 45 | u | 2586 | G | N9-C1'-C2' | 5.23 | 120.80 | 114.00 |
| 18 | S | 83 | ARG | CG-CD-NE | 5.22 | 122.76 | 111.80 |
| 45 | u | 223 | G | N9-C1'-C2' | -5.20 | 106.28 | 112.00 |
| 53 | 3 | 129 | LEU | CA-CB-CG | 5.17 | 127.19 | 115.30 |
| 7 | G | 231 | ASP | CB-CG-OD2 | 5.15 | 122.93 | 118.30 |
| 45 | u | 2661 | U | C2'-C3'-O3' | 5.13 | 121.91 | 113.70 |
| 32 | g | 66 | ARG | NE-CZ-NH1 | 5.12 | 122.86 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 42 | r | 17 | LEU | CA-CB-CG | 5.11 | 127.06 | 115.30 |
| 45 | u | 4731 | G | N9-C1'-C2' | 5.10 | 120.63 | 114.00 |
| 45 | u | 4481 | U | C5'-C4'-O4' | 5.09 | 115.21 | 109.10 |
| 55 | 5 | 100 | TYR | CA-CB-CG | 5.09 | 123.07 | 113.40 |
| 45 | u | 4965 | U | C2'-C3'-O3' | 5.07 | 121.81 | 113.70 |
| 39 | n | 21 | ARG | NE-CZ-NH2 | -5.06 | 117.77 | 120.30 |
| 45 | u | 1755 | C | C2'-C3'-O3' | 5.06 | 121.79 | 113.70 |
| 48 | x | 394 | LEU | CA-CB-CG | -5.05 | 103.68 | 115.30 |
| 45 | u | 680 | G | P-O3'-C3' | -5.04 | 113.65 | 119.70 |
| 3 | C | 67 | TRP | N-CA-C | -5.03 | 97.42 | 111.00 |
| 3 | C | 45 | ARG | NE-CZ-NH1 | 5.01 | 122.81 | 120.30 |
| 45 | u | 286 | U | N1-C1'-C2' | 5.00 | 120.50 | 114.00 |
| 45 | u | 2246 | C | C2'-C3'-O3' | 5.00 | 121.71 | 113.70 |

There are no chirality outliers.

All (41) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 52 | 2 | 15 | UNK | Peptide |
| 53 | 3 | 64 | ASP | Peptide |
| 53 | 3 | 67 | GLY | Peptide |
| 55 | 5 | 100 | TYR | Peptide |
| 55 | 5 | 263 | LEU | Peptide |
| 55 | 5 | 532 | ILE | Mainchain |
| 55 | 5 | 616 | ASP | Peptide |
| 55 | 5 | 655 | LYS | Peptide |
| 55 | 5 | 69 | HIS | Peptide |
| 56 | 6 | 20 | UNK | Peptide |
| 56 | 6 | 21 | UNK | Peptide |
| 56 | 6 | 80 | UNK | Peptide |
| 56 | 6 | 81 | UNK | Peptide |
| 56 | 6 | 89 | UNK | Peptide |
| 1 | A | 196 | TRP | Peptide |
| 2 | B | 17 | LEU | Peptide |
| 2 | B | 257 | TRP | Peptide |
| 2 | B | 258 | HIS | Peptide |
| 2 | B | 351 | LEU | Peptide |
| 3 | C | 245 | HIS | Peptide |
| 3 | C | 339 | THR | Peptide |
| 4 | D | 36 | LEU | Peptide |
| 5 | E | 123 | SER | Peptide |
| 7 | G | 238 | GLY | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 9 | I | 188 | LYS | Peptide |
| 9 | I | 202 | ASN | Peptide |
| 11 | L | 27 | ASN | Peptide |
| 11 | L | 46 | ILE | Peptide |
| 11 | L | 66 | TYR | Peptide |
| 17 | R | 19 | LYS | Peptide |
| 18 | S | 163 | HIS | Peptide |
| 18 | S | 164 | LYS | Peptide |
| 19 | T | 26 | PRO | Peptide |
| 20 | U | 27 | HIS | Peptide |
| 24 | Y | 7 | VAL | Peptide |
| 31 | f | 105 | LEU | Peptide |
| 42 | r | 106 | LEU | Peptide |
| 42 | r | 70 | GLN | Peptide |
| 45 | u | 2793 | G | Sidechain |
| 48 | x | 173 | TYR | Peptide |
| 48 | x | 42 | PHE | Peptide |

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|----------|-------------|----|
| 1 | A | 242/244 (99%) | 209 (86%) | 28 (12%) | 5 (2%) | 5 | 30 |
| 2 | B | 392/394 (100%) | 345 (88%) | 42 (11%) | 5 (1%) | 10 | 42 |
| 3 | C | 360/362 (99%) | 322 (89%) | 27 (8%) | 11 (3%) | 3 | 22 |
| 4 | D | 290/292 (99%) | 262 (90%) | 25 (9%) | 3 (1%) | 13 | 49 |
| 5 | E | 232/248 (94%) | 179 (77%) | 36 (16%) | 17 (7%) | 1 | 11 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 6 | F | 223/225 (99%) | 204 (92%) | 17 (8%) | 2 (1%) | 14 | 51 |
| 7 | G | 239/241 (99%) | 203 (85%) | 31 (13%) | 5 (2%) | 5 | 30 |
| 8 | H | 188/190 (99%) | 166 (88%) | 19 (10%) | 3 (2%) | 8 | 38 |
| 9 | I | 200/213 (94%) | 181 (90%) | 15 (8%) | 4 (2%) | 6 | 32 |
| 10 | J | 167/169 (99%) | 147 (88%) | 13 (8%) | 7 (4%) | 2 | 18 |
| 11 | L | 208/210 (99%) | 180 (86%) | 16 (8%) | 12 (6%) | 1 | 14 |
| 12 | M | 136/138 (99%) | 123 (90%) | 12 (9%) | 1 (1%) | 19 | 56 |
| 13 | N | 201/203 (99%) | 181 (90%) | 20 (10%) | 0 | 100 | 100 |
| 14 | O | 197/199 (99%) | 184 (93%) | 12 (6%) | 1 (0%) | 25 | 64 |
| 15 | P | 151/153 (99%) | 135 (89%) | 16 (11%) | 0 | 100 | 100 |
| 16 | Q | 185/187 (99%) | 169 (91%) | 14 (8%) | 2 (1%) | 12 | 46 |
| 17 | R | 178/180 (99%) | 166 (93%) | 9 (5%) | 3 (2%) | 7 | 36 |
| 18 | S | 173/175 (99%) | 157 (91%) | 12 (7%) | 4 (2%) | 5 | 28 |
| 19 | T | 157/159 (99%) | 139 (88%) | 15 (10%) | 3 (2%) | 6 | 32 |
| 20 | U | 97/99 (98%) | 82 (84%) | 11 (11%) | 4 (4%) | 2 | 18 |
| 21 | V | 129/131 (98%) | 115 (89%) | 13 (10%) | 1 (1%) | 16 | 54 |
| 22 | W | 61/63 (97%) | 56 (92%) | 4 (7%) | 1 (2%) | 8 | 38 |
| 23 | X | 117/119 (98%) | 109 (93%) | 6 (5%) | 2 (2%) | 7 | 36 |
| 24 | Y | 132/134 (98%) | 114 (86%) | 17 (13%) | 1 (1%) | 16 | 54 |
| 25 | Z | 133/135 (98%) | 113 (85%) | 13 (10%) | 7 (5%) | 1 | 15 |
| 26 | a | 145/147 (99%) | 122 (84%) | 19 (13%) | 4 (3%) | 4 | 24 |
| 27 | b | 73/75 (97%) | 67 (92%) | 5 (7%) | 1 (1%) | 9 | 40 |
| 28 | c | 92/94 (98%) | 89 (97%) | 3 (3%) | 0 | 100 | 100 |
| 29 | d | 105/107 (98%) | 91 (87%) | 13 (12%) | 1 (1%) | 13 | 49 |
| 30 | e | 126/128 (98%) | 115 (91%) | 6 (5%) | 5 (4%) | 2 | 18 |
| 31 | f | 107/109 (98%) | 94 (88%) | 8 (8%) | 5 (5%) | 2 | 17 |
| 32 | g | 112/114 (98%) | 103 (92%) | 8 (7%) | 1 (1%) | 14 | 51 |
| 33 | h | 120/122 (98%) | 106 (88%) | 10 (8%) | 4 (3%) | 3 | 21 |
| 34 | i | 100/102 (98%) | 92 (92%) | 6 (6%) | 2 (2%) | 6 | 32 |
| 35 | j | 84/86 (98%) | 71 (84%) | 8 (10%) | 5 (6%) | 1 | 14 |
| 36 | k | 67/69 (97%) | 56 (84%) | 7 (10%) | 4 (6%) | 1 | 14 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 37 | l | 48/50 (96%) | 40 (83%) | 7 (15%) | 1 (2%) | 5 | 30 |
| 38 | m | 50/52 (96%) | 44 (88%) | 6 (12%) | 0 | 100 | 100 |
| 39 | n | 21/23 (91%) | 21 (100%) | 0 | 0 | 100 | 100 |
| 40 | o | 102/104 (98%) | 92 (90%) | 7 (7%) | 3 (3%) | 3 | 23 |
| 41 | p | 89/91 (98%) | 80 (90%) | 8 (9%) | 1 (1%) | 12 | 46 |
| 42 | r | 132/136 (97%) | 113 (86%) | 12 (9%) | 7 (5%) | 1 | 15 |
| 43 | s | 196/198 (99%) | 164 (84%) | 22 (11%) | 10 (5%) | 1 | 16 |
| 44 | t | 161/163 (99%) | 102 (63%) | 33 (20%) | 26 (16%) | 0 | 3 |
| 48 | x | 420/426 (99%) | 373 (89%) | 46 (11%) | 1 (0%) | 44 | 78 |
| 49 | y | 60/62 (97%) | 52 (87%) | 8 (13%) | 0 | 100 | 100 |
| 50 | z | 27/29 (93%) | 25 (93%) | 1 (4%) | 1 (4%) | 2 | 20 |
| 51 | 1 | 134/162 (83%) | 129 (96%) | 5 (4%) | 0 | 100 | 100 |
| 53 | 3 | 118/120 (98%) | 99 (84%) | 18 (15%) | 1 (1%) | 16 | 54 |
| 54 | 4 | 32/34 (94%) | 31 (97%) | 1 (3%) | 0 | 100 | 100 |
| 55 | 5 | 632/696 (91%) | 538 (85%) | 88 (14%) | 6 (1%) | 14 | 51 |
| All | All | 8141/8362 (97%) | 7150 (88%) | 798 (10%) | 193 (2%) | 7 | 27 |

All (193) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 196 | TRP |
| 3 | C | 273 | LEU |
| 5 | E | 91 | PRO |
| 5 | E | 95 | ASP |
| 5 | E | 118 | PRO |
| 5 | E | 175 | LEU |
| 5 | E | 221 | PRO |
| 7 | G | 45 | ILE |
| 7 | G | 128 | VAL |
| 8 | H | 40 | HIS |
| 8 | H | 110 | SER |
| 9 | I | 47 | PRO |
| 11 | L | 64 | VAL |
| 11 | L | 67 | HIS |
| 17 | R | 36 | ASN |
| 18 | S | 165 | PRO |
| 20 | U | 47 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | Z | 84 | ARG |
| 26 | a | 90 | ALA |
| 29 | d | 94 | GLU |
| 30 | e | 92 | ASN |
| 31 | f | 80 | ASN |
| 33 | h | 7 | ARG |
| 36 | k | 61 | PRO |
| 40 | o | 32 | SER |
| 42 | r | 86 | ALA |
| 43 | s | 62 | ARG |
| 43 | s | 201 | PRO |
| 44 | t | 29 | ALA |
| 44 | t | 30 | PRO |
| 44 | t | 31 | LYS |
| 44 | t | 53 | TRP |
| 44 | t | 89 | PRO |
| 44 | t | 144 | ASP |
| 44 | t | 148 | PRO |
| 44 | t | 149 | HIS |
| 48 | x | 445 | THR |
| 55 | 5 | 84 | ILE |
| 55 | 5 | 89 | TYR |
| 1 | A | 217 | GLN |
| 2 | B | 38 | SER |
| 2 | B | 302 | ASN |
| 3 | C | 73 | VAL |
| 3 | C | 155 | GLU |
| 3 | C | 275 | SER |
| 4 | D | 187 | SER |
| 5 | E | 85 | LEU |
| 5 | E | 92 | VAL |
| 5 | E | 174 | PRO |
| 5 | E | 234 | GLU |
| 10 | J | 116 | GLY |
| 10 | J | 155 | HIS |
| 11 | L | 63 | THR |
| 11 | L | 143 | GLU |
| 11 | L | 172 | GLU |
| 17 | R | 130 | ASN |
| 18 | S | 88 | SER |
| 19 | T | 81 | LYS |
| 20 | U | 98 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | X | 131 | ASP |
| 25 | Z | 34 | SER |
| 26 | a | 76 | ASP |
| 30 | e | 44 | ARG |
| 34 | i | 11 | LEU |
| 35 | j | 36 | LYS |
| 35 | j | 39 | TYR |
| 42 | r | 67 | ARG |
| 42 | r | 71 | ARG |
| 43 | s | 70 | GLU |
| 43 | s | 106 | LYS |
| 43 | s | 109 | ALA |
| 44 | t | 5 | PHE |
| 44 | t | 26 | SER |
| 44 | t | 39 | PRO |
| 44 | t | 58 | ILE |
| 44 | t | 106 | PHE |
| 55 | 5 | 360 | TYR |
| 55 | 5 | 361 | TYR |
| 2 | B | 18 | PRO |
| 3 | C | 16 | GLU |
| 3 | C | 132 | ALA |
| 3 | C | 248 | ARG |
| 5 | E | 96 | LYS |
| 5 | E | 179 | ARG |
| 5 | E | 232 | GLU |
| 6 | F | 239 | GLU |
| 9 | I | 205 | PRO |
| 10 | J | 11 | PRO |
| 10 | J | 146 | ARG |
| 16 | Q | 14 | ARG |
| 17 | R | 19 | LYS |
| 21 | V | 14 | PHE |
| 25 | Z | 55 | ALA |
| 25 | Z | 124 | THR |
| 26 | a | 92 | LYS |
| 30 | e | 125 | PRO |
| 30 | e | 126 | ASN |
| 31 | f | 37 | ASP |
| 31 | f | 79 | GLY |
| 33 | h | 97 | LYS |
| 34 | i | 3 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36 | k | 32 | VAL |
| 37 | l | 47 | THR |
| 42 | r | 19 | LYS |
| 42 | r | 85 | ASN |
| 43 | s | 69 | LEU |
| 43 | s | 108 | PRO |
| 43 | s | 142 | GLY |
| 44 | t | 54 | LYS |
| 44 | t | 67 | ARG |
| 44 | t | 105 | THR |
| 44 | t | 137 | GLN |
| 53 | 3 | 64 | ASP |
| 55 | 5 | 661 | ASP |
| 1 | A | 180 | LEU |
| 2 | B | 54 | THR |
| 5 | E | 129 | PHE |
| 5 | E | 224 | GLN |
| 8 | H | 101 | ILE |
| 11 | L | 5 | ARG |
| 11 | L | 52 | SER |
| 19 | T | 29 | THR |
| 24 | Y | 83 | GLU |
| 25 | Z | 31 | ASP |
| 26 | a | 98 | ALA |
| 30 | e | 89 | LEU |
| 32 | g | 65 | MET |
| 33 | h | 89 | ARG |
| 36 | k | 29 | LYS |
| 41 | p | 41 | PHE |
| 44 | t | 2 | PRO |
| 44 | t | 18 | THR |
| 1 | A | 130 | SER |
| 2 | B | 309 | LEU |
| 4 | D | 20 | PHE |
| 5 | E | 218 | LEU |
| 5 | E | 229 | PHE |
| 7 | G | 123 | ALA |
| 7 | G | 125 | LYS |
| 10 | J | 153 | ALA |
| 11 | L | 6 | ASN |
| 11 | L | 103 | ARG |
| 16 | Q | 148 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | U | 27 | HIS |
| 25 | Z | 91 | LEU |
| 31 | f | 107 | PRO |
| 33 | h | 40 | ALA |
| 35 | j | 34 | CYS |
| 35 | j | 61 | THR |
| 36 | k | 21 | LYS |
| 40 | o | 77 | CYS |
| 42 | r | 11 | ARG |
| 43 | s | 34 | ASN |
| 44 | t | 7 | PRO |
| 55 | 5 | 616 | ASP |
| 1 | A | 67 | TYR |
| 3 | C | 222 | ARG |
| 3 | C | 309 | ILE |
| 10 | J | 124 | GLY |
| 11 | L | 100 | PRO |
| 11 | L | 169 | ILE |
| 14 | O | 49 | ARG |
| 18 | S | 5 | GLY |
| 20 | U | 67 | LYS |
| 22 | W | 15 | PRO |
| 31 | f | 106 | TYR |
| 35 | j | 60 | GLY |
| 40 | o | 33 | LEU |
| 44 | t | 10 | ILE |
| 44 | t | 19 | GLY |
| 44 | t | 22 | VAL |
| 3 | C | 133 | LEU |
| 9 | I | 99 | ILE |
| 27 | b | 21 | ILE |
| 43 | s | 73 | PRO |
| 4 | D | 125 | VAL |
| 11 | L | 134 | PRO |
| 25 | Z | 90 | PRO |
| 3 | C | 265 | GLY |
| 5 | E | 103 | VAL |
| 6 | F | 230 | VAL |
| 7 | G | 238 | GLY |
| 9 | I | 201 | PRO |
| 19 | T | 44 | GLY |
| 10 | J | 174 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | M | 7 | VAL |
| 18 | S | 155 | PRO |
| 44 | t | 3 | PRO |
| 44 | t | 98 | ILE |
| 23 | X | 119 | ILE |
| 42 | r | 69 | GLY |
| 44 | t | 23 | GLY |
| 50 | z | 71 | VAL |

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 | 187/187 (100%) | 161 (86%) | 26 (14%) | 3 | 14 |
| 2 | B | 336/342 (98%) | 291 (87%) | 45 (13%) | 3 | 14 |
| 3 | C | 302/302 (100%) | 260 (86%) | 42 (14%) | 3 | 14 |
| 4 | D | 247/247 (100%) | 218 (88%) | 29 (12%) | 4 | 17 |
| 5 | E | 208/221 (94%) | 185 (89%) | 23 (11%) | 5 | 18 |
| 6 | F | 194/195 (100%) | 165 (85%) | 29 (15%) | 2 | 12 |
| 7 | G | 206/206 (100%) | 182 (88%) | 24 (12%) | 4 | 17 |
| 8 | H | 169/169 (100%) | 148 (88%) | 21 (12%) | 4 | 16 |
| 9 | I | 174/180 (97%) | 153 (88%) | 21 (12%) | 4 | 16 |
| 10 | J | 142/142 (100%) | 126 (89%) | 16 (11%) | 4 | 18 |
| 11 | L | 176/176 (100%) | 145 (82%) | 31 (18%) | 1 | 9 |
| 12 | M | 117/117 (100%) | 102 (87%) | 15 (13%) | 3 | 15 |
| 13 | N | 171/171 (100%) | 152 (89%) | 19 (11%) | 5 | 18 |
| 14 | O | 171/171 (100%) | 144 (84%) | 27 (16%) | 2 | 11 |
| 15 | P | 134/134 (100%) | 120 (90%) | 14 (10%) | 5 | 20 |
| 16 | Q | 163/163 (100%) | 145 (89%) | 18 (11%) | 5 | 19 |
| 17 | R | 159/159 (100%) | 140 (88%) | 19 (12%) | 4 | 17 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 18 | S | 156/156 (100%) | 132 (85%) | 24 (15%) | 2 | 12 |
| 19 | T | 139/139 (100%) | 122 (88%) | 17 (12%) | 4 | 16 |
| 20 | U | 89/89 (100%) | 82 (92%) | 7 (8%) | 10 | 29 |
| 21 | V | 101/101 (100%) | 84 (83%) | 17 (17%) | 1 | 10 |
| 22 | W | 55/55 (100%) | 50 (91%) | 5 (9%) | 7 | 25 |
| 23 | X | 107/107 (100%) | 97 (91%) | 10 (9%) | 7 | 24 |
| 24 | Y | 124/124 (100%) | 107 (86%) | 17 (14%) | 3 | 14 |
| 25 | Z | 117/117 (100%) | 109 (93%) | 8 (7%) | 13 | 34 |
| 26 | a | 119/119 (100%) | 107 (90%) | 12 (10%) | 6 | 21 |
| 27 | b | 62/62 (100%) | 57 (92%) | 5 (8%) | 9 | 29 |
| 28 | c | 79/79 (100%) | 66 (84%) | 13 (16%) | 2 | 10 |
| 29 | d | 98/98 (100%) | 82 (84%) | 16 (16%) | 2 | 11 |
| 30 | e | 114/114 (100%) | 99 (87%) | 15 (13%) | 3 | 15 |
| 31 | f | 88/88 (100%) | 76 (86%) | 12 (14%) | 3 | 14 |
| 32 | g | 98/98 (100%) | 83 (85%) | 15 (15%) | 2 | 12 |
| 33 | h | 109/109 (100%) | 97 (89%) | 12 (11%) | 5 | 19 |
| 34 | i | 86/86 (100%) | 81 (94%) | 5 (6%) | 17 | 38 |
| 35 | j | 73/73 (100%) | 62 (85%) | 11 (15%) | 2 | 12 |
| 36 | k | 64/64 (100%) | 56 (88%) | 8 (12%) | 3 | 16 |
| 37 | l | 47/47 (100%) | 40 (85%) | 7 (15%) | 2 | 12 |
| 38 | m | 48/48 (100%) | 39 (81%) | 9 (19%) | 1 | 8 |
| 39 | n | 22/22 (100%) | 18 (82%) | 4 (18%) | 1 | 8 |
| 40 | o | 92/92 (100%) | 79 (86%) | 13 (14%) | 3 | 14 |
| 41 | p | 74/74 (100%) | 68 (92%) | 6 (8%) | 9 | 29 |
| 42 | r | 120/120 (100%) | 96 (80%) | 24 (20%) | 1 | 7 |
| 43 | s | 166/166 (100%) | 156 (94%) | 10 (6%) | 16 | 38 |
| 44 | t | 136/136 (100%) | 128 (94%) | 8 (6%) | 16 | 38 |
| 48 | x | 360/362 (99%) | 346 (96%) | 14 (4%) | 27 | 49 |
| 49 | y | 53/53 (100%) | 49 (92%) | 4 (8%) | 11 | 31 |
| 50 | z | 26/26 (100%) | 22 (85%) | 4 (15%) | 2 | 12 |
| 51 | 1 | 20/122 (16%) | 20 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 53 | 3 | 61/101 (60%) | 58 (95%) | 3 (5%) | 21 | 43 |
| 54 | 4 | 30/30 (100%) | 27 (90%) | 3 (10%) | 6 | 21 |
| 55 | 5 | 528/607 (87%) | 512 (97%) | 16 (3%) | 36 | 56 |
| All | All | 6917/7166 (96%) | 6144 (89%) | 773 (11%) | 7 | 18 |

All (773) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 5 | ILE |
| 1 | A | 44 | ILE |
| 1 | A | 49 | ILE |
| 1 | A | 64 | ARG |
| 1 | A | 82 | ILE |
| 1 | A | 96 | LEU |
| 1 | A | 97 | ASN |
| 1 | A | 102 | LEU |
| 1 | A | 125 | LYS |
| 1 | A | 128 | ARG |
| 1 | A | 142 | GLU |
| 1 | A | 158 | ILE |
| 1 | A | 163 | ARG |
| 1 | A | 175 | ILE |
| 1 | A | 180 | LEU |
| 1 | A | 193 | ARG |
| 1 | A | 194 | ASN |
| 1 | A | 200 | ARG |
| 1 | A | 207 | VAL |
| 1 | A | 218 | HIS |
| 1 | A | 221 | LYS |
| 1 | A | 226 | ARG |
| 1 | A | 227 | ARG |
| 1 | A | 233 | ARG |
| 1 | A | 235 | VAL |
| 1 | A | 242 | ARG |
| 2 | B | 4 | ARG |
| 2 | B | 10 | ARG |
| 2 | B | 17 | LEU |
| 2 | B | 19 | ARG |
| 2 | B | 21 | ARG |
| 2 | B | 31 | SER |
| 2 | B | 43 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 56 | ILE |
| 2 | B | 61 | ASP |
| 2 | B | 62 | ARG |
| 2 | B | 66 | LYS |
| 2 | B | 67 | VAL |
| 2 | B | 90 | VAL |
| 2 | B | 97 | ARG |
| 2 | B | 99 | LEU |
| 2 | B | 101 | THR |
| 2 | B | 103 | LYS |
| 2 | B | 115 | LYS |
| 2 | B | 116 | ARG |
| 2 | B | 135 | LYS |
| 2 | B | 138 | GLN |
| 2 | B | 146 | LEU |
| 2 | B | 162 | VAL |
| 2 | B | 167 | GLN |
| 2 | B | 173 | LEU |
| 2 | B | 203 | GLN |
| 2 | B | 213 | GLN |
| 2 | B | 214 | ASP |
| 2 | B | 228 | TYR |
| 2 | B | 244 | THR |
| 2 | B | 248 | LEU |
| 2 | B | 258 | HIS |
| 2 | B | 261 | ARG |
| 2 | B | 262 | VAL |
| 2 | B | 309 | LEU |
| 2 | B | 314 | ILE |
| 2 | B | 329 | ASP |
| 2 | B | 333 | LEU |
| 2 | B | 340 | THR |
| 2 | B | 352 | LEU |
| 2 | B | 356 | LYS |
| 2 | B | 357 | ARG |
| 2 | B | 366 | LYS |
| 2 | B | 381 | THR |
| 2 | B | 383 | GLU |
| 3 | C | 14 | LYS |
| 3 | C | 20 | LYS |
| 3 | C | 44 | LEU |
| 3 | C | 54 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 55 | SER |
| 3 | C | 57 | LEU |
| 3 | C | 66 | SER |
| 3 | C | 71 | ARG |
| 3 | C | 80 | ARG |
| 3 | C | 95 | MET |
| 3 | C | 101 | MET |
| 3 | C | 113 | ARG |
| 3 | C | 114 | ARG |
| 3 | C | 122 | TYR |
| 3 | C | 124 | ILE |
| 3 | C | 144 | ILE |
| 3 | C | 147 | VAL |
| 3 | C | 150 | LEU |
| 3 | C | 155 | GLU |
| 3 | C | 159 | GLU |
| 3 | C | 165 | LYS |
| 3 | C | 175 | LYS |
| 3 | C | 179 | ASP |
| 3 | C | 188 | ARG |
| 3 | C | 193 | LYS |
| 3 | C | 204 | ARG |
| 3 | C | 208 | CYS |
| 3 | C | 222 | ARG |
| 3 | C | 232 | VAL |
| 3 | C | 237 | ILE |
| 3 | C | 246 | VAL |
| 3 | C | 267 | TRP |
| 3 | C | 281 | MET |
| 3 | C | 284 | MET |
| 3 | C | 287 | THR |
| 3 | C | 294 | LYS |
| 3 | C | 307 | LYS |
| 3 | C | 312 | ARG |
| 3 | C | 333 | LYS |
| 3 | C | 342 | ARG |
| 3 | C | 345 | ARG |
| 3 | C | 348 | LYS |
| 4 | D | 4 | VAL |
| 4 | D | 22 | ARG |
| 4 | D | 33 | ARG |
| 4 | D | 37 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 50 | ARG |
| 4 | D | 66 | TYR |
| 4 | D | 89 | LYS |
| 4 | D | 94 | ASN |
| 4 | D | 104 | LEU |
| 4 | D | 110 | LEU |
| 4 | D | 111 | ASN |
| 4 | D | 124 | GLU |
| 4 | D | 128 | ASP |
| 4 | D | 152 | ARG |
| 4 | D | 179 | ARG |
| 4 | D | 189 | GLU |
| 4 | D | 196 | ARG |
| 4 | D | 202 | GLN |
| 4 | D | 206 | ASP |
| 4 | D | 208 | MET |
| 4 | D | 225 | GLN |
| 4 | D | 234 | ASP |
| 4 | D | 248 | ARG |
| 4 | D | 249 | GLU |
| 4 | D | 256 | LYS |
| 4 | D | 264 | LYS |
| 4 | D | 268 | ARG |
| 4 | D | 279 | ARG |
| 4 | D | 293 | ARG |
| 5 | E | 43 | ASN |
| 5 | E | 46 | LEU |
| 5 | E | 52 | ARG |
| 5 | E | 55 | ARG |
| 5 | E | 58 | MET |
| 5 | E | 101 | ARG |
| 5 | E | 105 | LEU |
| 5 | E | 126 | ARG |
| 5 | E | 134 | ARG |
| 5 | E | 136 | LEU |
| 5 | E | 137 | ARG |
| 5 | E | 148 | ILE |
| 5 | E | 162 | LYS |
| 5 | E | 190 | VAL |
| 5 | E | 197 | ILE |
| 5 | E | 206 | LYS |
| 5 | E | 212 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | E | 230 | ASP |
| 5 | E | 233 | LYS |
| 5 | E | 250 | ASP |
| 5 | E | 254 | LEU |
| 5 | E | 282 | LEU |
| 5 | E | 284 | PHE |
| 6 | F | 33 | LYS |
| 6 | F | 41 | GLN |
| 6 | F | 44 | LEU |
| 6 | F | 49 | ARG |
| 6 | F | 68 | ARG |
| 6 | F | 70 | GLU |
| 6 | F | 72 | ARG |
| 6 | F | 76 | MET |
| 6 | F | 82 | ASN |
| 6 | F | 90 | LYS |
| 6 | F | 91 | LEU |
| 6 | F | 100 | ILE |
| 6 | F | 101 | ASN |
| 6 | F | 127 | LEU |
| 6 | F | 137 | ILE |
| 6 | F | 154 | GLU |
| 6 | F | 179 | ARG |
| 6 | F | 181 | LEU |
| 6 | F | 189 | MET |
| 6 | F | 190 | GLU |
| 6 | F | 192 | LEU |
| 6 | F | 201 | LYS |
| 6 | F | 202 | ARG |
| 6 | F | 214 | LYS |
| 6 | F | 216 | SER |
| 6 | F | 234 | ASP |
| 6 | F | 239 | GLU |
| 6 | F | 248 | ARG |
| 6 | F | 249 | MET |
| 7 | G | 28 | VAL |
| 7 | G | 73 | ARG |
| 7 | G | 75 | LYS |
| 7 | G | 81 | ASN |
| 7 | G | 90 | GLN |
| 7 | G | 95 | LEU |
| 7 | G | 106 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | G | 110 | LYS |
| 7 | G | 112 | GLN |
| 7 | G | 131 | LYS |
| 7 | G | 148 | GLU |
| 7 | G | 150 | LYS |
| 7 | G | 151 | LYS |
| 7 | G | 154 | LEU |
| 7 | G | 170 | LEU |
| 7 | G | 173 | LEU |
| 7 | G | 175 | ARG |
| 7 | G | 177 | MET |
| 7 | G | 189 | ARG |
| 7 | G | 202 | VAL |
| 7 | G | 210 | GLU |
| 7 | G | 217 | LYS |
| 7 | G | 220 | GLU |
| 7 | G | 240 | ASN |
| 8 | H | 1 | MET |
| 8 | H | 20 | LEU |
| 8 | H | 26 | ILE |
| 8 | H | 28 | LYS |
| 8 | H | 41 | ILE |
| 8 | H | 52 | LYS |
| 8 | H | 54 | ARG |
| 8 | H | 57 | VAL |
| 8 | H | 59 | LYS |
| 8 | H | 66 | GLU |
| 8 | H | 74 | CYS |
| 8 | H | 78 | GLN |
| 8 | H | 98 | HIS |
| 8 | H | 111 | LEU |
| 8 | H | 125 | ARG |
| 8 | H | 128 | MET |
| 8 | H | 129 | ARG |
| 8 | H | 162 | GLN |
| 8 | H | 173 | ARG |
| 8 | H | 177 | ASP |
| 8 | H | 183 | GLU |
| 9 | I | 13 | LYS |
| 9 | I | 35 | ASP |
| 9 | I | 36 | LEU |
| 9 | I | 39 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | I | 43 | VAL |
| 9 | I | 48 | LEU |
| 9 | I | 76 | MET |
| 9 | I | 88 | ARG |
| 9 | I | 116 | ARG |
| 9 | I | 136 | MET |
| 9 | I | 139 | ARG |
| 9 | I | 144 | ASN |
| 9 | I | 153 | ARG |
| 9 | I | 163 | GLN |
| 9 | I | 164 | LYS |
| 9 | I | 180 | GLU |
| 9 | I | 195 | CYS |
| 9 | I | 198 | LYS |
| 9 | I | 202 | ASN |
| 9 | I | 208 | LYS |
| 9 | I | 212 | LEU |
| 10 | J | 15 | LEU |
| 10 | J | 16 | ARG |
| 10 | J | 33 | LEU |
| 10 | J | 34 | THR |
| 10 | J | 49 | VAL |
| 10 | J | 55 | TYR |
| 10 | J | 72 | CYS |
| 10 | J | 90 | ARG |
| 10 | J | 91 | GLU |
| 10 | J | 110 | GLN |
| 10 | J | 111 | GLU |
| 10 | J | 113 | ILE |
| 10 | J | 146 | ARG |
| 10 | J | 151 | ILE |
| 10 | J | 167 | GLN |
| 10 | J | 168 | GLN |
| 11 | L | 10 | LEU |
| 11 | L | 28 | GLN |
| 11 | L | 35 | ARG |
| 11 | L | 49 | ARG |
| 11 | L | 59 | VAL |
| 11 | L | 61 | CYS |
| 11 | L | 64 | VAL |
| 11 | L | 67 | HIS |
| 11 | L | 74 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | L | 77 | SER |
| 11 | L | 92 | ARG |
| 11 | L | 94 | ILE |
| 11 | L | 99 | ASP |
| 11 | L | 107 | THR |
| 11 | L | 111 | GLN |
| 11 | L | 113 | ASN |
| 11 | L | 115 | GLN |
| 11 | L | 121 | ARG |
| 11 | L | 123 | LYS |
| 11 | L | 129 | ARG |
| 11 | L | 130 | LYS |
| 11 | L | 143 | GLU |
| 11 | L | 145 | LYS |
| 11 | L | 158 | ARG |
| 11 | L | 162 | LYS |
| 11 | L | 165 | LYS |
| 11 | L | 186 | ARG |
| 11 | L | 190 | ARG |
| 11 | L | 195 | ARG |
| 11 | L | 198 | ARG |
| 11 | L | 201 | GLU |
| 12 | M | 5 | ARG |
| 12 | M | 8 | GLU |
| 12 | M | 25 | VAL |
| 12 | M | 33 | GLN |
| 12 | M | 38 | VAL |
| 12 | M | 48 | GLN |
| 12 | M | 53 | LYS |
| 12 | M | 57 | LEU |
| 12 | M | 61 | ILE |
| 12 | M | 70 | GLN |
| 12 | M | 96 | GLU |
| 12 | M | 105 | THR |
| 12 | M | 118 | MET |
| 12 | M | 119 | ARG |
| 12 | M | 130 | LEU |
| 13 | N | 9 | GLU |
| 13 | N | 17 | ASP |
| 13 | N | 26 | ARG |
| 13 | N | 32 | GLN |
| 13 | N | 61 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | N | 64 | ILE |
| 13 | N | 72 | LYS |
| 13 | N | 77 | LYS |
| 13 | N | 80 | THR |
| 13 | N | 87 | HIS |
| 13 | N | 89 | VAL |
| 13 | N | 104 | GLU |
| 13 | N | 108 | ARG |
| 13 | N | 136 | ASP |
| 13 | N | 147 | ASP |
| 13 | N | 174 | LEU |
| 13 | N | 197 | THR |
| 13 | N | 199 | GLN |
| 13 | N | 202 | ARG |
| 14 | O | 5 | GLN |
| 14 | O | 18 | ARG |
| 14 | O | 31 | ARG |
| 14 | O | 36 | VAL |
| 14 | O | 37 | ARG |
| 14 | O | 38 | CYS |
| 14 | O | 42 | ASN |
| 14 | O | 49 | ARG |
| 14 | O | 60 | LYS |
| 14 | O | 61 | ARG |
| 14 | O | 62 | MET |
| 14 | O | 67 | SER |
| 14 | O | 74 | ARG |
| 14 | O | 82 | ARG |
| 14 | O | 85 | ARG |
| 14 | O | 103 | LYS |
| 14 | O | 117 | ARG |
| 14 | O | 128 | ARG |
| 14 | O | 130 | LYS |
| 14 | O | 145 | VAL |
| 14 | O | 165 | LYS |
| 14 | O | 175 | MET |
| 14 | O | 179 | LYS |
| 14 | O | 187 | LYS |
| 14 | O | 195 | VAL |
| 14 | O | 201 | PHE |
| 14 | O | 202 | LEU |
| 15 | P | 5 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | P | 7 | ASP |
| 15 | P | 25 | HIS |
| 15 | P | 57 | CYS |
| 15 | P | 69 | ARG |
| 15 | P | 86 | LYS |
| 15 | P | 91 | LEU |
| 15 | P | 92 | LEU |
| 15 | P | 99 | GLU |
| 15 | P | 100 | SER |
| 15 | P | 105 | LYS |
| 15 | P | 127 | ARG |
| 15 | P | 128 | ARG |
| 15 | P | 147 | GLU |
| 16 | Q | 13 | VAL |
| 16 | Q | 31 | LEU |
| 16 | Q | 37 | ARG |
| 16 | Q | 54 | SER |
| 16 | Q | 63 | LEU |
| 16 | Q | 75 | ARG |
| 16 | Q | 78 | LYS |
| 16 | Q | 85 | THR |
| 16 | Q | 89 | ASP |
| 16 | Q | 91 | ARG |
| 16 | Q | 93 | GLN |
| 16 | Q | 95 | VAL |
| 16 | Q | 97 | LYS |
| 16 | Q | 108 | ARG |
| 16 | Q | 112 | ARG |
| 16 | Q | 140 | SER |
| 16 | Q | 143 | ARG |
| 16 | Q | 187 | LYS |
| 17 | R | 10 | LEU |
| 17 | R | 15 | LEU |
| 17 | R | 39 | GLN |
| 17 | R | 40 | GLN |
| 17 | R | 43 | LYS |
| 17 | R | 50 | ILE |
| 17 | R | 52 | ARG |
| 17 | R | 75 | HIS |
| 17 | R | 89 | MET |
| 17 | R | 98 | ARG |
| 17 | R | 99 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17 | R | 106 | LEU |
| 17 | R | 107 | ARG |
| 17 | R | 113 | LYS |
| 17 | R | 117 | ARG |
| 17 | R | 123 | LEU |
| 17 | R | 133 | LYS |
| 17 | R | 138 | LEU |
| 17 | R | 178 | GLN |
| 18 | S | 2 | LYS |
| 18 | S | 8 | ARG |
| 18 | S | 9 | GLU |
| 18 | S | 17 | LEU |
| 18 | S | 39 | VAL |
| 18 | S | 43 | ARG |
| 18 | S | 67 | VAL |
| 18 | S | 70 | LYS |
| 18 | S | 82 | LEU |
| 18 | S | 83 | ARG |
| 18 | S | 84 | TYR |
| 18 | S | 86 | SER |
| 18 | S | 91 | HIS |
| 18 | S | 95 | ARG |
| 18 | S | 98 | ARG |
| 18 | S | 100 | LEU |
| 18 | S | 102 | THR |
| 18 | S | 125 | GLN |
| 18 | S | 127 | MET |
| 18 | S | 132 | ILE |
| 18 | S | 147 | ASP |
| 18 | S | 149 | LYS |
| 18 | S | 156 | HIS |
| 18 | S | 159 | LEU |
| 19 | T | 5 | LYS |
| 19 | T | 9 | ARG |
| 19 | T | 17 | ARG |
| 19 | T | 33 | ILE |
| 19 | T | 41 | ASP |
| 19 | T | 52 | MET |
| 19 | T | 60 | LYS |
| 19 | T | 81 | LYS |
| 19 | T | 96 | ILE |
| 19 | T | 99 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | T | 117 | LYS |
| 19 | T | 118 | GLU |
| 19 | T | 131 | GLN |
| 19 | T | 142 | ARG |
| 19 | T | 144 | ASN |
| 19 | T | 157 | GLU |
| 19 | T | 159 | MET |
| 20 | U | 33 | ILE |
| 20 | U | 46 | ARG |
| 20 | U | 65 | ARG |
| 20 | U | 67 | LYS |
| 20 | U | 80 | LYS |
| 20 | U | 97 | ARG |
| 20 | U | 99 | TRP |
| 21 | V | 15 | ARG |
| 21 | V | 18 | LEU |
| 21 | V | 31 | ASN |
| 21 | V | 35 | LYS |
| 21 | V | 46 | LYS |
| 21 | V | 51 | ARG |
| 21 | V | 57 | VAL |
| 21 | V | 60 | MET |
| 21 | V | 61 | VAL |
| 21 | V | 82 | ILE |
| 21 | V | 91 | LYS |
| 21 | V | 97 | TYR |
| 21 | V | 99 | GLU |
| 21 | V | 106 | VAL |
| 21 | V | 109 | LYS |
| 21 | V | 113 | LYS |
| 21 | V | 123 | LYS |
| 22 | W | 4 | GLU |
| 22 | W | 27 | LYS |
| 22 | W | 41 | LEU |
| 22 | W | 43 | LYS |
| 22 | W | 57 | ARG |
| 23 | X | 39 | LYS |
| 23 | X | 41 | ARG |
| 23 | X | 50 | LYS |
| 23 | X | 52 | LEU |
| 23 | X | 59 | LYS |
| 23 | X | 94 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | X | 111 | GLN |
| 23 | X | 129 | ARG |
| 23 | X | 145 | ASP |
| 23 | X | 152 | LYS |
| 24 | Y | 2 | LYS |
| 24 | Y | 7 | VAL |
| 24 | Y | 8 | THR |
| 24 | Y | 28 | LYS |
| 24 | Y | 34 | LEU |
| 24 | Y | 50 | ARG |
| 24 | Y | 52 | ASP |
| 24 | Y | 55 | VAL |
| 24 | Y | 59 | ARG |
| 24 | Y | 65 | GLN |
| 24 | Y | 72 | GLN |
| 24 | Y | 74 | TYR |
| 24 | Y | 79 | VAL |
| 24 | Y | 87 | ARG |
| 24 | Y | 104 | VAL |
| 24 | Y | 115 | ARG |
| 24 | Y | 126 | ARG |
| 25 | Z | 11 | VAL |
| 25 | Z | 17 | ARG |
| 25 | Z | 57 | MET |
| 25 | Z | 59 | LYS |
| 25 | Z | 67 | LYS |
| 25 | Z | 93 | LYS |
| 25 | Z | 108 | ARG |
| 25 | Z | 112 | ARG |
| 26 | a | 10 | LYS |
| 26 | a | 12 | ARG |
| 26 | a | 39 | HIS |
| 26 | a | 40 | HIS |
| 26 | a | 46 | ASP |
| 26 | a | 47 | LYS |
| 26 | a | 52 | TYR |
| 26 | a | 59 | ARG |
| 26 | a | 63 | LEU |
| 26 | a | 84 | GLU |
| 26 | a | 122 | VAL |
| 26 | a | 132 | ARG |
| 27 | b | 22 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27 | b | 28 | ARG |
| 27 | b | 39 | PHE |
| 27 | b | 43 | MET |
| 27 | b | 51 | LYS |
| 28 | c | 28 | VAL |
| 28 | c | 37 | MET |
| 28 | c | 40 | GLN |
| 28 | c | 50 | ASN |
| 28 | c | 59 | GLU |
| 28 | c | 61 | GLU |
| 28 | c | 77 | ASN |
| 28 | c | 78 | ASN |
| 28 | c | 81 | LEU |
| 28 | c | 87 | LYS |
| 28 | c | 91 | VAL |
| 28 | c | 94 | LEU |
| 28 | c | 98 | ASP |
| 29 | d | 19 | GLU |
| 29 | d | 23 | ARG |
| 29 | d | 26 | THR |
| 29 | d | 31 | LYS |
| 29 | d | 36 | VAL |
| 29 | d | 44 | ARG |
| 29 | d | 48 | GLU |
| 29 | d | 75 | LYS |
| 29 | d | 78 | ARG |
| 29 | d | 79 | ASN |
| 29 | d | 85 | ARG |
| 29 | d | 90 | ARG |
| 29 | d | 94 | GLU |
| 29 | d | 102 | LEU |
| 29 | d | 107 | THR |
| 29 | d | 116 | ASN |
| 30 | e | 11 | LYS |
| 30 | e | 21 | ILE |
| 30 | e | 22 | ARG |
| 30 | e | 24 | GLN |
| 30 | e | 30 | LYS |
| 30 | e | 32 | LYS |
| 30 | e | 46 | ARG |
| 30 | e | 48 | ARG |
| 30 | e | 64 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | e | 78 | LEU |
| 30 | e | 91 | CYS |
| 30 | e | 104 | SER |
| 30 | e | 106 | LYS |
| 30 | e | 107 | ASN |
| 30 | e | 113 | GLU |
| 31 | f | 16 | ARG |
| 31 | f | 33 | VAL |
| 31 | f | 36 | ARG |
| 31 | f | 38 | GLU |
| 31 | f | 40 | GLU |
| 31 | f | 46 | ARG |
| 31 | f | 52 | LYS |
| 31 | f | 56 | ASN |
| 31 | f | 69 | VAL |
| 31 | f | 84 | VAL |
| 31 | f | 100 | ARG |
| 31 | f | 101 | ILE |
| 32 | g | 5 | LEU |
| 32 | g | 6 | THR |
| 32 | g | 11 | LEU |
| 32 | g | 14 | ASN |
| 32 | g | 15 | THR |
| 32 | g | 21 | ARG |
| 32 | g | 32 | TYR |
| 32 | g | 54 | ARG |
| 32 | g | 60 | ARG |
| 32 | g | 64 | LEU |
| 32 | g | 66 | ARG |
| 32 | g | 73 | HIS |
| 32 | g | 90 | ARG |
| 32 | g | 100 | GLN |
| 32 | g | 115 | LYS |
| 33 | h | 10 | ARG |
| 33 | h | 28 | LEU |
| 33 | h | 46 | LYS |
| 33 | h | 65 | GLN |
| 33 | h | 67 | GLU |
| 33 | h | 88 | THR |
| 33 | h | 89 | ARG |
| 33 | h | 97 | LYS |
| 33 | h | 104 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33 | h | 117 | ARG |
| 33 | h | 121 | VAL |
| 33 | h | 122 | LYS |
| 34 | i | 33 | LEU |
| 34 | i | 86 | LYS |
| 34 | i | 87 | ARG |
| 34 | i | 89 | GLU |
| 34 | i | 103 | LYS |
| 35 | j | 2 | THR |
| 35 | j | 3 | LYS |
| 35 | j | 15 | THR |
| 35 | j | 20 | ARG |
| 35 | j | 25 | LYS |
| 35 | j | 29 | LEU |
| 35 | j | 33 | THR |
| 35 | j | 61 | THR |
| 35 | j | 63 | ARG |
| 35 | j | 68 | LYS |
| 35 | j | 79 | ARG |
| 36 | k | 18 | LYS |
| 36 | k | 29 | LYS |
| 36 | k | 31 | ASN |
| 36 | k | 37 | ARG |
| 36 | k | 39 | SER |
| 36 | k | 57 | LYS |
| 36 | k | 69 | LEU |
| 36 | k | 70 | LYS |
| 37 | l | 8 | ARG |
| 37 | l | 16 | LYS |
| 37 | l | 17 | GLN |
| 37 | l | 21 | ARG |
| 37 | l | 36 | ARG |
| 37 | l | 46 | ARG |
| 37 | l | 49 | LEU |
| 38 | m | 79 | GLU |
| 38 | m | 82 | LEU |
| 38 | m | 85 | LEU |
| 38 | m | 88 | LYS |
| 38 | m | 97 | ARG |
| 38 | m | 98 | LYS |
| 38 | m | 106 | ARG |
| 38 | m | 111 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38 | m | 119 | ASN |
| 39 | n | 2 | ARG |
| 39 | n | 9 | ARG |
| 39 | n | 13 | LEU |
| 39 | n | 21 | ARG |
| 40 | o | 17 | LYS |
| 40 | o | 24 | THR |
| 40 | o | 26 | TYR |
| 40 | o | 31 | ASP |
| 40 | o | 33 | LEU |
| 40 | o | 36 | GLN |
| 40 | o | 55 | ILE |
| 40 | o | 61 | LYS |
| 40 | o | 69 | ARG |
| 40 | o | 82 | MET |
| 40 | o | 89 | LYS |
| 40 | o | 96 | ASP |
| 40 | o | 102 | GLN |
| 41 | p | 16 | THR |
| 41 | p | 24 | LYS |
| 41 | p | 49 | ARG |
| 41 | p | 54 | ILE |
| 41 | p | 60 | CYS |
| 41 | p | 84 | ARG |
| 42 | r | 17 | LEU |
| 42 | r | 18 | ILE |
| 42 | r | 20 | ARG |
| 42 | r | 21 | ASN |
| 42 | r | 24 | THR |
| 42 | r | 26 | SER |
| 42 | r | 28 | GLU |
| 42 | r | 31 | ASN |
| 42 | r | 32 | LEU |
| 42 | r | 37 | SER |
| 42 | r | 39 | ARG |
| 42 | r | 41 | ASN |
| 42 | r | 60 | VAL |
| 42 | r | 67 | ARG |
| 42 | r | 70 | GLN |
| 42 | r | 71 | ARG |
| 42 | r | 80 | THR |
| 42 | r | 103 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42 | r | 107 | ARG |
| 42 | r | 108 | MET |
| 42 | r | 118 | LEU |
| 42 | r | 122 | LYS |
| 42 | r | 125 | MET |
| 42 | r | 135 | LYS |
| 43 | s | 38 | LYS |
| 43 | s | 44 | ARG |
| 43 | s | 62 | ARG |
| 43 | s | 68 | HIS |
| 43 | s | 94 | ASP |
| 43 | s | 146 | LYS |
| 43 | s | 149 | ARG |
| 43 | s | 174 | LEU |
| 43 | s | 185 | PHE |
| 43 | s | 191 | GLN |
| 44 | t | 1 | MET |
| 44 | t | 14 | TYR |
| 44 | t | 40 | LYS |
| 44 | t | 95 | GLN |
| 44 | t | 104 | ILE |
| 44 | t | 106 | PHE |
| 44 | t | 114 | ARG |
| 44 | t | 123 | ARG |
| 48 | x | 45 | CYS |
| 48 | x | 64 | TRP |
| 48 | x | 65 | MET |
| 48 | x | 202 | ASN |
| 48 | x | 207 | MET |
| 48 | x | 241 | ASN |
| 48 | x | 244 | ASN |
| 48 | x | 355 | LEU |
| 48 | x | 406 | GLU |
| 48 | x | 414 | ASN |
| 48 | x | 436 | ASP |
| 48 | x | 441 | ILE |
| 48 | x | 458 | PHE |
| 48 | x | 461 | PHE |
| 49 | y | 40 | THR |
| 49 | y | 59 | ILE |
| 49 | y | 62 | ASN |
| 49 | y | 63 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50 | z | 73 | VAL |
| 50 | z | 76 | MET |
| 50 | z | 81 | ILE |
| 50 | z | 87 | LEU |
| 53 | 3 | 88 | LEU |
| 53 | 3 | 90 | SER |
| 53 | 3 | 93 | LEU |
| 54 | 4 | 21 | LEU |
| 54 | 4 | 31 | ASN |
| 54 | 4 | 34 | LYS |
| 55 | 5 | 9 | LEU |
| 55 | 5 | 31 | PHE |
| 55 | 5 | 82 | ARG |
| 55 | 5 | 123 | PHE |
| 55 | 5 | 173 | ILE |
| 55 | 5 | 175 | CYS |
| 55 | 5 | 178 | LEU |
| 55 | 5 | 285 | TYR |
| 55 | 5 | 286 | LEU |
| 55 | 5 | 367 | LEU |
| 55 | 5 | 524 | SER |
| 55 | 5 | 554 | ARG |
| 55 | 5 | 562 | THR |
| 55 | 5 | 597 | LEU |
| 55 | 5 | 601 | ARG |
| 55 | 5 | 602 | ILE |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 50 | HIS |
| 2 | B | 68 | ASN |
| 5 | E | 217 | GLN |
| 7 | G | 29 | ASN |
| 14 | O | 96 | GLN |
| 42 | r | 121 | GLN |
| 48 | x | 202 | ASN |
| 48 | x | 241 | ASN |
| 48 | x | 244 | ASN |
| 48 | x | 300 | ASN |
| 48 | x | 414 | ASN |
| 48 | x | 465 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49 | y | 63 | ASN |
| 54 | 4 | 12 | ASN |
| 55 | 5 | 46 | HIS |
| 55 | 5 | 168 | ASN |
| 55 | 5 | 217 | ASN |
| 55 | 5 | 222 | HIS |
| 55 | 5 | 352 | HIS |
| 55 | 5 | 531 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 45 | u | 3643/3662 (99%) | 1188 (32%) | 0 |
| 46 | v | 119/120 (99%) | 19 (15%) | 0 |
| 47 | w | 155/156 (99%) | 52 (33%) | 0 |
| All | All | 3917/3938 (99%) | 1259 (32%) | 0 |

All (1259) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | u | 2 | G |
| 45 | u | 8 | U |
| 45 | u | 9 | C |
| 45 | u | 10 | A |
| 45 | u | 12 | A |
| 45 | u | 13 | U |
| 45 | u | 21 | G |
| 45 | u | 25 | A |
| 45 | u | 30 | C |
| 45 | u | 39 | A |
| 45 | u | 42 | A |
| 45 | u | 43 | U |
| 45 | u | 44 | A |
| 45 | u | 48 | G |
| 45 | u | 49 | U |
| 45 | u | 56 | A |
| 45 | u | 58 | G |
| 45 | u | 59 | A |
| 45 | u | 64 | A |
| 45 | u | 65 | A |
| 45 | u | 69 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | u | 71 | C |
| 45 | u | 72 | C |
| 45 | u | 73 | A |
| 45 | u | 74 | G |
| 45 | u | 91 | G |
| 45 | u | 93 | G |
| 45 | u | 94 | A |
| 45 | u | 95 | G |
| 45 | u | 108 | A |
| 45 | u | 109 | G |
| 45 | u | 110 | C |
| 45 | u | 116 | G |
| 45 | u | 118 | C |
| 45 | u | 119 | G |
| 45 | u | 120 | A |
| 45 | u | 121 | A |
| 45 | u | 126 | C |
| 45 | u | 128 | C |
| 45 | u | 129 | C |
| 45 | u | 134 | G |
| 45 | u | 135 | G |
| 45 | u | 136 | C |
| 45 | u | 143 | C |
| 45 | u | 144 | G |
| 45 | u | 146 | G |
| 45 | u | 157 | U |
| 45 | u | 159 | C |
| 45 | u | 160 | G |
| 45 | u | 161 | G |
| 45 | u | 164 | G |
| 45 | u | 166 | C |
| 45 | u | 167 | C |
| 45 | u | 170 | C |
| 45 | u | 171 | U |
| 45 | u | 172 | C |
| 45 | u | 173 | C |
| 45 | u | 174 | C |
| 45 | u | 175 | C |
| 45 | u | 177 | G |
| 45 | u | 183 | C |
| 45 | u | 184 | U |
| 45 | u | 185 | C |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | u | 186 | G |
| 45 | u | 187 | U |
| 45 | u | 188 | G |
| 45 | u | 189 | G |
| 45 | u | 197 | A |
| 45 | u | 200 | U |
| 45 | u | 201 | C |
| 45 | u | 202 | C |
| 45 | u | 203 | U |
| 45 | u | 205 | C |
| 45 | u | 206 | U |
| 45 | u | 210 | C |
| 45 | u | 211 | G |
| 45 | u | 216 | C |
| 45 | u | 217 | C |
| 45 | u | 218 | A |
| 45 | u | 219 | G |
| 45 | u | 220 | C |
| 45 | u | 221 | C |
| 45 | u | 224 | U |
| 45 | u | 226 | G |
| 45 | u | 227 | A |
| 45 | u | 233 | U |
| 45 | u | 234 | G |
| 45 | u | 246 | G |
| 45 | u | 253 | G |
| 45 | u | 255 | C |
| 45 | u | 257 | C |
| 45 | u | 265 | C |
| 45 | u | 266 | C |
| 45 | u | 267 | G |
| 45 | u | 272 | U |
| 45 | u | 276 | C |
| 45 | u | 277 | G |
| 45 | u | 278 | G |
| 45 | u | 280 | G |
| 45 | u | 286 | U |
| 45 | u | 296 | A |
| 45 | u | 297 | U |
| 45 | u | 300 | A |
| 45 | u | 306 | A |
| 45 | u | 309 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | u | 315 | G |
| 45 | u | 316 | U |
| 45 | u | 319 | A |
| 45 | u | 321 | U |
| 45 | u | 322 | C |
| 45 | u | 326 | C |
| 45 | u | 328 | A |
| 45 | u | 334 | A |
| 45 | u | 337 | U |
| 45 | u | 340 | C |
| 45 | u | 347 | A |
| 45 | u | 349 | A |
| 45 | u | 350 | C |
| 45 | u | 353 | A |
| 45 | u | 357 | U |
| 45 | u | 361 | C |
| 45 | u | 362 | A |
| 45 | u | 363 | A |
| 45 | u | 385 | A |
| 45 | u | 386 | A |
| 45 | u | 387 | G |
| 45 | u | 399 | G |
| 45 | u | 405 | U |
| 45 | u | 406 | C |
| 45 | u | 407 | A |
| 45 | u | 409 | G |
| 45 | u | 410 | A |
| 45 | u | 412 | G |
| 45 | u | 413 | G |
| 45 | u | 424 | U |
| 45 | u | 429 | A |
| 45 | u | 431 | G |
| 45 | u | 432 | U |
| 45 | u | 434 | A |
| 45 | u | 446 | C |
| 45 | u | 448 | G |
| 45 | u | 449 | C |
| 45 | u | 451 | C |
| 45 | u | 452 | A |
| 45 | u | 453 | G |
| 45 | u | 454 | U |
| 45 | u | 455 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | u | 458 | C |
| 45 | u | 466 | A |
| 45 | u | 467 | U |
| 45 | u | 468 | U |
| 45 | u | 469 | C |
| 45 | u | 470 | A |
| 45 | u | 471 | A |
| 45 | u | 473 | C |
| 45 | u | 485 | C |
| 45 | u | 486 | C |
| 45 | u | 487 | G |
| 45 | u | 498 | C |
| 45 | u | 499 | G |
| 45 | u | 500 | G |
| 45 | u | 501 | C |
| 45 | u | 502 | C |
| 45 | u | 503 | C |
| 45 | u | 504 | G |
| 45 | u | 506 | C |
| 45 | u | 509 | A |
| 45 | u | 510 | U |
| 45 | u | 513 | U |
| 45 | u | 514 | U |
| 45 | u | 515 | C |
| 45 | u | 519 | C |
| 45 | u | 649 | A |
| 45 | u | 654 | C |
| 45 | u | 655 | C |
| 45 | u | 663 | G |
| 45 | u | 664 | G |
| 45 | u | 665 | C |
| 45 | u | 666 | G |
| 45 | u | 667 | A |
| 45 | u | 668 | C |
| 45 | u | 681 | G |
| 45 | u | 682 | G |
| 45 | u | 683 | C |
| 45 | u | 684 | G |
| 45 | u | 685 | C |
| 45 | u | 686 | A |
| 45 | u | 687 | U |
| 45 | u | 689 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | u | 690 | C |
| 45 | u | 692 | A |
| 45 | u | 694 | C |
| 45 | u | 695 | G |
| 45 | u | 696 | C |
| 45 | u | 697 | G |
| 45 | u | 701 | G |
| 45 | u | 703 | G |
| 45 | u | 707 | C |
| 45 | u | 718 | C |
| 45 | u | 721 | G |
| 45 | u | 722 | G |
| 45 | u | 724 | C |
| 45 | u | 728 | U |
| 45 | u | 729 | G |
| 45 | u | 730 | G |
| 45 | u | 737 | C |
| 45 | u | 742 | G |
| 45 | u | 745 | G |
| 45 | u | 746 | A |
| 45 | u | 747 | A |
| 45 | u | 748 | G |
| 45 | u | 749 | G |
| 45 | u | 756 | G |
| 45 | u | 911 | U |
| 45 | u | 914 | U |
| 45 | u | 915 | A |
| 45 | u | 917 | A |
| 45 | u | 918 | G |
| 45 | u | 919 | C |
| 45 | u | 920 | C |
| 45 | u | 925 | C |
| 45 | u | 927 | G |
| 45 | u | 928 | C |
| 45 | u | 929 | A |
| 45 | u | 930 | G |
| 45 | u | 931 | C |
| 45 | u | 932 | A |
| 45 | u | 933 | G |
| 45 | u | 934 | C |
| 45 | u | 935 | A |
| 45 | u | 936 | C |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | u | 937 | U |
| 45 | u | 938 | C |
| 45 | u | 939 | G |
| 45 | u | 940 | C |
| 45 | u | 942 | G |
| 45 | u | 943 | A |
| 45 | u | 944 | A |
| 45 | u | 945 | U |
| 45 | u | 946 | C |
| 45 | u | 947 | C |
| 45 | u | 957 | G |
| 45 | u | 958 | G |
| 45 | u | 960 | A |
| 45 | u | 961 | G |
| 45 | u | 962 | C |
| 45 | u | 963 | G |
| 45 | u | 964 | A |
| 45 | u | 965 | G |
| 45 | u | 966 | A |
| 45 | u | 967 | C |
| 45 | u | 968 | C |
| 45 | u | 969 | C |
| 45 | u | 970 | G |
| 45 | u | 971 | U |
| 45 | u | 972 | C |
| 45 | u | 973 | G |
| 45 | u | 976 | G |
| 45 | u | 977 | C |
| 45 | u | 978 | G |
| 45 | u | 979 | C |
| 45 | u | 982 | U |
| 45 | u | 983 | C |
| 45 | u | 984 | C |
| 45 | u | 989 | U |
| 45 | u | 990 | C |
| 45 | u | 992 | C |
| 45 | u | 1051 | G |
| 45 | u | 1070 | G |
| 45 | u | 1072 | C |
| 45 | u | 1073 | G |
| 45 | u | 1075 | G |
| 45 | u | 1076 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | u | 1083 | U |
| 45 | u | 1097 | C |
| 45 | u | 1175 | A |
| 45 | u | 1176 | C |
| 45 | u | 1177 | U |
| 45 | u | 1181 | C |
| 45 | u | 1182 | C |
| 45 | u | 1183 | C |
| 45 | u | 1193 | C |
| 45 | u | 1204 | C |
| 45 | u | 1209 | U |
| 45 | u | 1211 | G |
| 45 | u | 1212 | G |
| 45 | u | 1214 | C |
| 45 | u | 1215 | C |
| 45 | u | 1219 | G |
| 45 | u | 1221 | G |
| 45 | u | 1222 | A |
| 45 | u | 1233 | G |
| 45 | u | 1234 | G |
| 45 | u | 1235 | G |
| 45 | u | 1236 | C |
| 45 | u | 1237 | C |
| 45 | u | 1238 | A |
| 45 | u | 1239 | C |
| 45 | u | 1240 | G |
| 45 | u | 1241 | C |
| 45 | u | 1242 | G |
| 45 | u | 1243 | C |
| 45 | u | 1244 | G |
| 45 | u | 1245 | C |
| 45 | u | 1255 | A |
| 45 | u | 1256 | G |
| 45 | u | 1259 | G |
| 45 | u | 1266 | G |
| 45 | u | 1267 | C |
| 45 | u | 1268 | G |
| 45 | u | 1269 | G |
| 45 | u | 1270 | A |
| 45 | u | 1272 | C |
| 45 | u | 1273 | G |
| 45 | u | 1274 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | u | 1275 | G |
| 45 | u | 1279 | A |
| 45 | u | 1280 | C |
| 45 | u | 1281 | G |
| 45 | u | 1285 | U |
| 45 | u | 1286 | C |
| 45 | u | 1287 | G |
| 45 | u | 1288 | G |
| 45 | u | 1289 | C |
| 45 | u | 1293 | G |
| 45 | u | 1294 | A |
| 45 | u | 1295 | C |
| 45 | u | 1296 | G |
| 45 | u | 1297 | U |
| 45 | u | 1301 | C |
| 45 | u | 1303 | A |
| 45 | u | 1304 | C |
| 45 | u | 1313 | C |
| 45 | u | 1326 | A |
| 45 | u | 1330 | A |
| 45 | u | 1337 | A |
| 45 | u | 1344 | C |
| 45 | u | 1354 | A |
| 45 | u | 1358 | G |
| 45 | u | 1364 | U |
| 45 | u | 1365 | C |
| 45 | u | 1366 | G |
| 45 | u | 1367 | C |
| 45 | u | 1368 | A |
| 45 | u | 1369 | C |
| 45 | u | 1370 | G |
| 45 | u | 1371 | A |
| 45 | u | 1372 | A |
| 45 | u | 1376 | C |
| 45 | u | 1377 | G |
| 45 | u | 1378 | C |
| 45 | u | 1379 | C |
| 45 | u | 1380 | G |
| 45 | u | 1381 | U |
| 45 | u | 1387 | A |
| 45 | u | 1390 | G |
| 45 | u | 1394 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | u | 1397 | A |
| 45 | u | 1398 | A |
| 45 | u | 1399 | G |
| 45 | u | 1407 | C |
| 45 | u | 1408 | G |
| 45 | u | 1409 | C |
| 45 | u | 1410 | U |
| 45 | u | 1411 | C |
| 45 | u | 1413 | C |
| 45 | u | 1414 | C |
| 45 | u | 1416 | G |
| 45 | u | 1418 | C |
| 45 | u | 1420 | A |
| 45 | u | 1421 | G |
| 45 | u | 1429 | C |
| 45 | u | 1432 | G |
| 45 | u | 1435 | G |
| 45 | u | 1436 | C |
| 45 | u | 1439 | C |
| 45 | u | 1440 | U |
| 45 | u | 1441 | C |
| 45 | u | 1442 | C |
| 45 | u | 1445 | U |
| 45 | u | 1446 | C |
| 45 | u | 1448 | G |
| 45 | u | 1449 | C |
| 45 | u | 1455 | G |
| 45 | u | 1456 | C |
| 45 | u | 1457 | G |
| 45 | u | 1475 | G |
| 45 | u | 1477 | C |
| 45 | u | 1478 | C |
| 45 | u | 1481 | C |
| 45 | u | 1482 | G |
| 45 | u | 1483 | C |
| 45 | u | 1484 | G |
| 45 | u | 1485 | C |
| 45 | u | 1486 | C |
| 45 | u | 1489 | G |
| 45 | u | 1497 | A |
| 45 | u | 1498 | G |
| 45 | u | 1501 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | u | 1502 | G |
| 45 | u | 1504 | G |
| 45 | u | 1514 | U |
| 45 | u | 1516 | G |
| 45 | u | 1518 | A |
| 45 | u | 1523 | A |
| 45 | u | 1524 | A |
| 45 | u | 1533 | A |
| 45 | u | 1534 | A |
| 45 | u | 1547 | A |
| 45 | u | 1563 | A |
| 45 | u | 1564 | A |
| 45 | u | 1566 | C |
| 45 | u | 1568 | C |
| 45 | u | 1578 | U |
| 45 | u | 1582 | U |
| 45 | u | 1586 | G |
| 45 | u | 1591 | U |
| 45 | u | 1592 | G |
| 45 | u | 1596 | U |
| 45 | u | 1602 | U |
| 45 | u | 1612 | G |
| 45 | u | 1613 | A |
| 45 | u | 1614 | C |
| 45 | u | 1624 | G |
| 45 | u | 1625 | G |
| 45 | u | 1631 | A |
| 45 | u | 1633 | G |
| 45 | u | 1634 | A |
| 45 | u | 1636 | U |
| 45 | u | 1638 | A |
| 45 | u | 1641 | G |
| 45 | u | 1654 | G |
| 45 | u | 1655 | C |
| 45 | u | 1656 | U |
| 45 | u | 1661 | C |
| 45 | u | 1670 | G |
| 45 | u | 1676 | C |
| 45 | u | 1677 | U |
| 45 | u | 1691 | G |
| 45 | u | 1692 | C |
| 45 | u | 1696 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | u | 1697 | G |
| 45 | u | 1698 | C |
| 45 | u | 1699 | A |
| 45 | u | 1719 | A |
| 45 | u | 1720 | C |
| 45 | u | 1721 | G |
| 45 | u | 1722 | C |
| 45 | u | 1724 | G |
| 45 | u | 1725 | U |
| 45 | u | 1733 | G |
| 45 | u | 1734 | G |
| 45 | u | 1735 | U |
| 45 | u | 1742 | A |
| 45 | u | 1746 | A |
| 45 | u | 1750 | G |
| 45 | u | 1753 | G |
| 45 | u | 1754 | U |
| 45 | u | 1755 | C |
| 45 | u | 1756 | U |
| 45 | u | 1757 | U |
| 45 | u | 1758 | G |
| 45 | u | 1760 | G |
| 45 | u | 1761 | G |
| 45 | u | 1764 | G |
| 45 | u | 1767 | A |
| 45 | u | 1768 | C |
| 45 | u | 1772 | C |
| 45 | u | 1776 | A |
| 45 | u | 1777 | C |
| 45 | u | 1781 | U |
| 45 | u | 1787 | A |
| 45 | u | 1799 | G |
| 45 | u | 1800 | U |
| 45 | u | 1803 | G |
| 45 | u | 1804 | A |
| 45 | u | 1805 | A |
| 45 | u | 1812 | C |
| 45 | u | 1815 | G |
| 45 | u | 1818 | G |
| 45 | u | 1819 | G |
| 45 | u | 1820 | C |
| 45 | u | 1821 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | u | 1822 | U |
| 45 | u | 1828 | C |
| 45 | u | 1830 | G |
| 45 | u | 1832 | C |
| 45 | u | 1833 | G |
| 45 | u | 1834 | U |
| 45 | u | 1835 | G |
| 45 | u | 1836 | G |
| 45 | u | 1847 | C |
| 45 | u | 1848 | C |
| 45 | u | 1855 | G |
| 45 | u | 1867 | A |
| 45 | u | 1869 | G |
| 45 | u | 1882 | U |
| 45 | u | 1885 | G |
| 45 | u | 1886 | G |
| 45 | u | 1889 | U |
| 45 | u | 1892 | A |
| 45 | u | 1897 | A |
| 45 | u | 1899 | G |
| 45 | u | 1900 | C |
| 45 | u | 1910 | G |
| 45 | u | 1918 | U |
| 45 | u | 1919 | G |
| 45 | u | 1920 | C |
| 45 | u | 1921 | C |
| 45 | u | 1922 | G |
| 45 | u | 1923 | A |
| 45 | u | 1931 | C |
| 45 | u | 1947 | U |
| 45 | u | 1952 | G |
| 45 | u | 1955 | G |
| 45 | u | 1956 | A |
| 45 | u | 1957 | U |
| 45 | u | 1958 | A |
| 45 | u | 1959 | U |
| 45 | u | 1960 | A |
| 45 | u | 1961 | G |
| 45 | u | 1964 | A |
| 45 | u | 1968 | G |
| 45 | u | 1969 | G |
| 45 | u | 1975 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | u | 1976 | G |
| 45 | u | 1977 | C |
| 45 | u | 1979 | A |
| 45 | u | 1980 | U |
| 45 | u | 1981 | G |
| 45 | u | 1983 | A |
| 45 | u | 1984 | A |
| 45 | u | 1985 | G |
| 45 | u | 1986 | U |
| 45 | u | 1987 | C |
| 45 | u | 1988 | G |
| 45 | u | 1990 | A |
| 45 | u | 1991 | A |
| 45 | u | 1992 | U |
| 45 | u | 1993 | C |
| 45 | u | 1997 | U |
| 45 | u | 1998 | A |
| 45 | u | 2001 | G |
| 45 | u | 2002 | A |
| 45 | u | 2003 | G |
| 45 | u | 2004 | U |
| 45 | u | 2005 | G |
| 45 | u | 2008 | U |
| 45 | u | 2010 | A |
| 45 | u | 2011 | C |
| 45 | u | 2019 | C |
| 45 | u | 2020 | U |
| 45 | u | 2021 | G |
| 45 | u | 2024 | G |
| 45 | u | 2025 | A |
| 45 | u | 2026 | A |
| 45 | u | 2027 | U |
| 45 | u | 2028 | C |
| 45 | u | 2044 | U |
| 45 | u | 2046 | G |
| 45 | u | 2047 | A |
| 45 | u | 2048 | U |
| 45 | u | 2052 | G |
| 45 | u | 2055 | G |
| 45 | u | 2056 | G |
| 45 | u | 2062 | C |
| 45 | u | 2064 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | u | 2068 | C |
| 45 | u | 2069 | A |
| 45 | u | 2070 | U |
| 45 | u | 2071 | A |
| 45 | u | 2079 | G |
| 45 | u | 2084 | C |
| 45 | u | 2085 | G |
| 45 | u | 2089 | G |
| 45 | u | 2090 | U |
| 45 | u | 2091 | C |
| 45 | u | 2092 | G |
| 45 | u | 2093 | A |
| 45 | u | 2094 | G |
| 45 | u | 2095 | A |
| 45 | u | 2097 | U |
| 45 | u | 2100 | A |
| 45 | u | 2101 | C |
| 45 | u | 2103 | G |
| 45 | u | 2107 | C |
| 45 | u | 2108 | G |
| 45 | u | 2109 | G |
| 45 | u | 2110 | C |
| 45 | u | 2111 | G |
| 45 | u | 2112 | G |
| 45 | u | 2113 | G |
| 45 | u | 2114 | G |
| 45 | u | 2115 | G |
| 45 | u | 2116 | C |
| 45 | u | 2117 | G |
| 45 | u | 2118 | G |
| 45 | u | 2119 | C |
| 45 | u | 2120 | G |
| 45 | u | 2122 | G |
| 45 | u | 2123 | C |
| 45 | u | 2124 | G |
| 45 | u | 2125 | C |
| 45 | u | 2126 | G |
| 45 | u | 2127 | C |
| 45 | u | 2129 | C |
| 45 | u | 2130 | G |
| 45 | u | 2131 | C |
| 45 | u | 2247 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | u | 2248 | C |
| 45 | u | 2250 | C |
| 45 | u | 2251 | G |
| 45 | u | 2252 | G |
| 45 | u | 2253 | A |
| 45 | u | 2254 | G |
| 45 | u | 2255 | C |
| 45 | u | 2256 | C |
| 45 | u | 2257 | C |
| 45 | u | 2258 | C |
| 45 | u | 2259 | G |
| 45 | u | 2260 | C |
| 45 | u | 2261 | G |
| 45 | u | 2263 | A |
| 45 | u | 2264 | C |
| 45 | u | 2265 | G |
| 45 | u | 2266 | C |
| 45 | u | 2267 | U |
| 45 | u | 2268 | A |
| 45 | u | 2269 | C |
| 45 | u | 2270 | G |
| 45 | u | 2274 | C |
| 45 | u | 2275 | G |
| 45 | u | 2279 | A |
| 45 | u | 2288 | G |
| 45 | u | 2289 | C |
| 45 | u | 2299 | G |
| 45 | u | 2300 | A |
| 45 | u | 2301 | G |
| 45 | u | 2312 | U |
| 45 | u | 2313 | A |
| 45 | u | 2314 | G |
| 45 | u | 2324 | C |
| 45 | u | 2331 | G |
| 45 | u | 2332 | A |
| 45 | u | 2333 | G |
| 45 | u | 2335 | C |
| 45 | u | 2337 | C |
| 45 | u | 2348 | G |
| 45 | u | 2351 | C |
| 45 | u | 2360 | A |
| 45 | u | 2364 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | u | 2370 | A |
| 45 | u | 2382 | A |
| 45 | u | 2383 | C |
| 45 | u | 2395 | A |
| 45 | u | 2396 | A |
| 45 | u | 2399 | G |
| 45 | u | 2417 | A |
| 45 | u | 2422 | C |
| 45 | u | 2424 | G |
| 45 | u | 2425 | U |
| 45 | u | 2428 | A |
| 45 | u | 2429 | A |
| 45 | u | 2433 | G |
| 45 | u | 2434 | G |
| 45 | u | 2440 | U |
| 45 | u | 2441 | C |
| 45 | u | 2447 | U |
| 45 | u | 2450 | G |
| 45 | u | 2458 | C |
| 45 | u | 2469 | C |
| 45 | u | 2471 | G |
| 45 | u | 2473 | A |
| 45 | u | 2474 | G |
| 45 | u | 2475 | G |
| 45 | u | 2485 | U |
| 45 | u | 2488 | C |
| 45 | u | 2489 | C |
| 45 | u | 2490 | U |
| 45 | u | 2491 | C |
| 45 | u | 2493 | G |
| 45 | u | 2495 | U |
| 45 | u | 2499 | C |
| 45 | u | 2503 | G |
| 45 | u | 2504 | C |
| 45 | u | 2505 | C |
| 45 | u | 2506 | G |
| 45 | u | 2507 | A |
| 45 | u | 2512 | A |
| 45 | u | 2513 | A |
| 45 | u | 2514 | G |
| 45 | u | 2519 | U |
| 45 | u | 2521 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | u | 2527 | A |
| 45 | u | 2530 | U |
| 45 | u | 2536 | A |
| 45 | u | 2537 | A |
| 45 | u | 2544 | G |
| 45 | u | 2546 | G |
| 45 | u | 2547 | G |
| 45 | u | 2553 | A |
| 45 | u | 2554 | U |
| 45 | u | 2555 | G |
| 45 | u | 2564 | G |
| 45 | u | 2566 | G |
| 45 | u | 2568 | C |
| 45 | u | 2571 | C |
| 45 | u | 2575 | U |
| 45 | u | 2577 | C |
| 45 | u | 2583 | C |
| 45 | u | 2587 | A |
| 45 | u | 2588 | C |
| 45 | u | 2589 | C |
| 45 | u | 2591 | A |
| 45 | u | 2601 | A |
| 45 | u | 2602 | G |
| 45 | u | 2611 | A |
| 45 | u | 2620 | G |
| 45 | u | 2623 | A |
| 45 | u | 2627 | C |
| 45 | u | 2638 | G |
| 45 | u | 2640 | G |
| 45 | u | 2647 | A |
| 45 | u | 2653 | C |
| 45 | u | 2661 | U |
| 45 | u | 2662 | G |
| 45 | u | 2663 | G |
| 45 | u | 2669 | C |
| 45 | u | 2673 | G |
| 45 | u | 2676 | A |
| 45 | u | 2679 | G |
| 45 | u | 2681 | G |
| 45 | u | 2686 | G |
| 45 | u | 2687 | U |
| 45 | u | 2688 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | u | 2695 | A |
| 45 | u | 2696 | A |
| 45 | u | 2704 | C |
| 45 | u | 2708 | U |
| 45 | u | 2710 | C |
| 45 | u | 2711 | G |
| 45 | u | 2712 | G |
| 45 | u | 2714 | G |
| 45 | u | 2716 | C |
| 45 | u | 2721 | G |
| 45 | u | 2724 | G |
| 45 | u | 2725 | A |
| 45 | u | 2726 | G |
| 45 | u | 2733 | C |
| 45 | u | 2740 | U |
| 45 | u | 2743 | A |
| 45 | u | 2754 | G |
| 45 | u | 2755 | A |
| 45 | u | 2756 | G |
| 45 | u | 2760 | G |
| 45 | u | 2761 | U |
| 45 | u | 2762 | G |
| 45 | u | 2767 | U |
| 45 | u | 2768 | C |
| 45 | u | 2769 | U |
| 45 | u | 2770 | C |
| 45 | u | 2772 | C |
| 45 | u | 2787 | A |
| 45 | u | 2788 | U |
| 45 | u | 2789 | A |
| 45 | u | 2790 | U |
| 45 | u | 2794 | C |
| 45 | u | 2795 | A |
| 45 | u | 2796 | G |
| 45 | u | 2798 | A |
| 45 | u | 2806 | A |
| 45 | u | 2807 | A |
| 45 | u | 2814 | C |
| 45 | u | 2824 | C |
| 45 | u | 2825 | A |
| 45 | u | 2826 | U |
| 45 | u | 2827 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | u | 2828 | U |
| 45 | u | 2829 | U |
| 45 | u | 2835 | A |
| 45 | u | 2838 | G |
| 45 | u | 2839 | U |
| 45 | u | 2842 | G |
| 45 | u | 2855 | G |
| 45 | u | 2859 | G |
| 45 | u | 2862 | G |
| 45 | u | 2869 | U |
| 45 | u | 2896 | G |
| 45 | u | 2897 | G |
| 45 | u | 2898 | G |
| 45 | u | 2904 | U |
| 45 | u | 2905 | C |
| 45 | u | 2910 | G |
| 45 | u | 3594 | C |
| 45 | u | 3595 | U |
| 45 | u | 3596 | A |
| 45 | u | 3597 | G |
| 45 | u | 3598 | C |
| 45 | u | 3605 | C |
| 45 | u | 3606 | U |
| 45 | u | 3615 | G |
| 45 | u | 3617 | G |
| 45 | u | 3625 | G |
| 45 | u | 3626 | G |
| 45 | u | 3630 | A |
| 45 | u | 3635 | A |
| 45 | u | 3644 | U |
| 45 | u | 3653 | A |
| 45 | u | 3662 | A |
| 45 | u | 3668 | C |
| 45 | u | 3670 | C |
| 45 | u | 3671 | G |
| 45 | u | 3673 | C |
| 45 | u | 3674 | G |
| 45 | u | 3680 | U |
| 45 | u | 3682 | A |
| 45 | u | 3689 | G |
| 45 | u | 3692 | A |
| 45 | u | 3696 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | u | 3698 | G |
| 45 | u | 3702 | A |
| 45 | u | 3709 | U |
| 45 | u | 3710 | G |
| 45 | u | 3711 | A |
| 45 | u | 3712 | A |
| 45 | u | 3717 | A |
| 45 | u | 3718 | A |
| 45 | u | 3722 | G |
| 45 | u | 3728 | A |
| 45 | u | 3729 | U |
| 45 | u | 3737 | A |
| 45 | u | 3740 | G |
| 45 | u | 3748 | A |
| 45 | u | 3750 | G |
| 45 | u | 3752 | C |
| 45 | u | 3753 | G |
| 45 | u | 3755 | G |
| 45 | u | 3756 | A |
| 45 | u | 3759 | A |
| 45 | u | 3760 | A |
| 45 | u | 3764 | U |
| 45 | u | 3773 | U |
| 45 | u | 3774 | A |
| 45 | u | 3775 | A |
| 45 | u | 3776 | G |
| 45 | u | 3777 | G |
| 45 | u | 3778 | U |
| 45 | u | 3780 | G |
| 45 | u | 3783 | A |
| 45 | u | 3784 | A |
| 45 | u | 3786 | U |
| 45 | u | 3788 | C |
| 45 | u | 3798 | U |
| 45 | u | 3799 | A |
| 45 | u | 3802 | U |
| 45 | u | 3810 | C |
| 45 | u | 3811 | G |
| 45 | u | 3812 | C |
| 45 | u | 3813 | A |
| 45 | u | 3814 | U |
| 45 | u | 3817 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | u | 3819 | G |
| 45 | u | 3822 | U |
| 45 | u | 3831 | U |
| 45 | u | 3836 | A |
| 45 | u | 3838 | U |
| 45 | u | 3839 | G |
| 45 | u | 3840 | U |
| 45 | u | 3859 | G |
| 45 | u | 3867 | A |
| 45 | u | 3877 | A |
| 45 | u | 3878 | C |
| 45 | u | 3879 | G |
| 45 | u | 3889 | G |
| 45 | u | 3897 | G |
| 45 | u | 3900 | G |
| 45 | u | 3901 | A |
| 45 | u | 3905 | A |
| 45 | u | 3906 | A |
| 45 | u | 3907 | G |
| 45 | u | 3912 | U |
| 45 | u | 3915 | U |
| 45 | u | 3916 | G |
| 45 | u | 3917 | A |
| 45 | u | 3924 | C |
| 45 | u | 3925 | U |
| 45 | u | 3926 | C |
| 45 | u | 3927 | U |
| 45 | u | 3938 | G |
| 45 | u | 3939 | G |
| 45 | u | 3943 | A |
| 45 | u | 3946 | G |
| 45 | u | 4069 | U |
| 45 | u | 4070 | U |
| 45 | u | 4076 | G |
| 45 | u | 4084 | G |
| 45 | u | 4085 | A |
| 45 | u | 4086 | G |
| 45 | u | 4087 | G |
| 45 | u | 4088 | C |
| 45 | u | 4091 | G |
| 45 | u | 4092 | G |
| 45 | u | 4093 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | u | 4094 | G |
| 45 | u | 4097 | G |
| 45 | u | 4104 | G |
| 45 | u | 4105 | A |
| 45 | u | 4107 | G |
| 45 | u | 4112 | C |
| 45 | u | 4114 | C |
| 45 | u | 4115 | G |
| 45 | u | 4116 | C |
| 45 | u | 4117 | U |
| 45 | u | 4118 | U |
| 45 | u | 4119 | C |
| 45 | u | 4120 | U |
| 45 | u | 4121 | G |
| 45 | u | 4122 | G |
| 45 | u | 4125 | C |
| 45 | u | 4127 | A |
| 45 | u | 4134 | C |
| 45 | u | 4143 | G |
| 45 | u | 4144 | C |
| 45 | u | 4145 | C |
| 45 | u | 4155 | C |
| 45 | u | 4161 | G |
| 45 | u | 4162 | C |
| 45 | u | 4163 | U |
| 45 | u | 4165 | C |
| 45 | u | 4166 | G |
| 45 | u | 4168 | G |
| 45 | u | 4170 | A |
| 45 | u | 4171 | C |
| 45 | u | 4182 | G |
| 45 | u | 4183 | G |
| 45 | u | 4184 | G |
| 45 | u | 4191 | G |
| 45 | u | 4203 | A |
| 45 | u | 4208 | U |
| 45 | u | 4212 | A |
| 45 | u | 4213 | A |
| 45 | u | 4216 | G |
| 45 | u | 4217 | G |
| 45 | u | 4218 | U |
| 45 | u | 4219 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | u | 4225 | G |
| 45 | u | 4226 | G |
| 45 | u | 4229 | U |
| 45 | u | 4232 | U |
| 45 | u | 4233 | A |
| 45 | u | 4238 | G |
| 45 | u | 4241 | C |
| 45 | u | 4251 | A |
| 45 | u | 4254 | G |
| 45 | u | 4258 | C |
| 45 | u | 4265 | U |
| 45 | u | 4266 | G |
| 45 | u | 4267 | G |
| 45 | u | 4268 | A |
| 45 | u | 4271 | A |
| 45 | u | 4273 | A |
| 45 | u | 4282 | A |
| 45 | u | 4291 | G |
| 45 | u | 4297 | G |
| 45 | u | 4302 | U |
| 45 | u | 4303 | C |
| 45 | u | 4304 | A |
| 45 | u | 4305 | G |
| 45 | u | 4306 | U |
| 45 | u | 4307 | A |
| 45 | u | 4311 | A |
| 45 | u | 4312 | U |
| 45 | u | 4313 | A |
| 45 | u | 4314 | C |
| 45 | u | 4317 | A |
| 45 | u | 4318 | C |
| 45 | u | 4319 | C |
| 45 | u | 4329 | G |
| 45 | u | 4330 | G |
| 45 | u | 4331 | G |
| 45 | u | 4332 | C |
| 45 | u | 4335 | C |
| 45 | u | 4336 | A |
| 45 | u | 4349 | C |
| 45 | u | 4350 | C |
| 45 | u | 4354 | U |
| 45 | u | 4355 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | u | 4360 | U |
| 45 | u | 4367 | G |
| 45 | u | 4368 | G |
| 45 | u | 4372 | U |
| 45 | u | 4373 | G |
| 45 | u | 4377 | G |
| 45 | u | 4378 | A |
| 45 | u | 4379 | A |
| 45 | u | 4380 | A |
| 45 | u | 4387 | C |
| 45 | u | 4391 | G |
| 45 | u | 4394 | A |
| 45 | u | 4395 | U |
| 45 | u | 4396 | A |
| 45 | u | 4398 | C |
| 45 | u | 4405 | G |
| 45 | u | 4419 | U |
| 45 | u | 4420 | U |
| 45 | u | 4421 | C |
| 45 | u | 4422 | A |
| 45 | u | 4424 | A |
| 45 | u | 4426 | C |
| 45 | u | 4430 | G |
| 45 | u | 4432 | C |
| 45 | u | 4433 | G |
| 45 | u | 4438 | U |
| 45 | u | 4439 | U |
| 45 | u | 4441 | A |
| 45 | u | 4444 | C |
| 45 | u | 4448 | G |
| 45 | u | 4449 | A |
| 45 | u | 4450 | U |
| 45 | u | 4453 | C |
| 45 | u | 4454 | G |
| 45 | u | 4464 | A |
| 45 | u | 4471 | U |
| 45 | u | 4472 | G |
| 45 | u | 4473 | A |
| 45 | u | 4475 | G |
| 45 | u | 4476 | C |
| 45 | u | 4481 | U |
| 45 | u | 4482 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | u | 4484 | A |
| 45 | u | 4488 | A |
| 45 | u | 4491 | G |
| 45 | u | 4495 | G |
| 45 | u | 4500 | U |
| 45 | u | 4510 | A |
| 45 | u | 4511 | A |
| 45 | u | 4512 | U |
| 45 | u | 4513 | A |
| 45 | u | 4515 | G |
| 45 | u | 4519 | C |
| 45 | u | 4520 | G |
| 45 | u | 4522 | G |
| 45 | u | 4524 | G |
| 45 | u | 4527 | G |
| 45 | u | 4528 | G |
| 45 | u | 4529 | G |
| 45 | u | 4535 | A |
| 45 | u | 4548 | A |
| 45 | u | 4549 | G |
| 45 | u | 4550 | G |
| 45 | u | 4557 | U |
| 45 | u | 4567 | G |
| 45 | u | 4570 | G |
| 45 | u | 4573 | G |
| 45 | u | 4575 | G |
| 45 | u | 4577 | U |
| 45 | u | 4583 | C |
| 45 | u | 4584 | A |
| 45 | u | 4585 | U |
| 45 | u | 4586 | G |
| 45 | u | 4590 | A |
| 45 | u | 4591 | U |
| 45 | u | 4606 | G |
| 45 | u | 4618 | G |
| 45 | u | 4636 | U |
| 45 | u | 4637 | G |
| 45 | u | 4641 | U |
| 45 | u | 4647 | G |
| 45 | u | 4648 | A |
| 45 | u | 4656 | A |
| 45 | u | 4657 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | u | 4661 | G |
| 45 | u | 4670 | C |
| 45 | u | 4672 | A |
| 45 | u | 4677 | U |
| 45 | u | 4687 | A |
| 45 | u | 4694 | G |
| 45 | u | 4695 | C |
| 45 | u | 4700 | A |
| 45 | u | 4701 | A |
| 45 | u | 4702 | G |
| 45 | u | 4709 | U |
| 45 | u | 4719 | G |
| 45 | u | 4720 | C |
| 45 | u | 4721 | G |
| 45 | u | 4730 | C |
| 45 | u | 4731 | G |
| 45 | u | 4732 | G |
| 45 | u | 4733 | C |
| 45 | u | 4734 | A |
| 45 | u | 4737 | G |
| 45 | u | 4741 | C |
| 45 | u | 4745 | G |
| 45 | u | 4746 | C |
| 45 | u | 4749 | C |
| 45 | u | 4750 | G |
| 45 | u | 4753 | U |
| 45 | u | 4754 | G |
| 45 | u | 4756 | C |
| 45 | u | 4758 | U |
| 45 | u | 4760 | G |
| 45 | u | 4764 | A |
| 45 | u | 4768 | G |
| 45 | u | 4770 | U |
| 45 | u | 4771 | C |
| 45 | u | 4774 | C |
| 45 | u | 4869 | U |
| 45 | u | 4871 | C |
| 45 | u | 4872 | G |
| 45 | u | 4873 | G |
| 45 | u | 4874 | A |
| 45 | u | 4875 | G |
| 45 | u | 4876 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | u | 4877 | G |
| 45 | u | 4878 | C |
| 45 | u | 4883 | C |
| 45 | u | 4884 | G |
| 45 | u | 4885 | U |
| 45 | u | 4886 | C |
| 45 | u | 4889 | G |
| 45 | u | 4890 | G |
| 45 | u | 4893 | A |
| 45 | u | 4895 | C |
| 45 | u | 4896 | G |
| 45 | u | 4898 | G |
| 45 | u | 4900 | C |
| 45 | u | 4901 | G |
| 45 | u | 4904 | G |
| 45 | u | 4906 | C |
| 45 | u | 4910 | G |
| 45 | u | 4911 | A |
| 45 | u | 4912 | G |
| 45 | u | 4913 | G |
| 45 | u | 4924 | C |
| 45 | u | 4926 | C |
| 45 | u | 4927 | G |
| 45 | u | 4930 | C |
| 45 | u | 4931 | G |
| 45 | u | 4932 | U |
| 45 | u | 4934 | A |
| 45 | u | 4935 | C |
| 45 | u | 4936 | G |
| 45 | u | 4939 | C |
| 45 | u | 4942 | C |
| 45 | u | 4945 | G |
| 45 | u | 4948 | C |
| 45 | u | 4949 | G |
| 45 | u | 4950 | U |
| 45 | u | 4951 | G |
| 45 | u | 4952 | G |
| 45 | u | 4959 | U |
| 45 | u | 4964 | C |
| 45 | u | 4965 | U |
| 45 | u | 4966 | A |
| 45 | u | 4967 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | u | 4975 | G |
| 45 | u | 4976 | U |
| 45 | u | 4985 | U |
| 45 | u | 4988 | U |
| 45 | u | 4989 | U |
| 45 | u | 4990 | C |
| 45 | u | 4991 | U |
| 45 | u | 5007 | A |
| 45 | u | 5013 | C |
| 45 | u | 5014 | A |
| 45 | u | 5017 | G |
| 45 | u | 5018 | C |
| 45 | u | 5022 | U |
| 45 | u | 5023 | C |
| 45 | u | 5024 | C |
| 45 | u | 5025 | C |
| 45 | u | 5026 | U |
| 45 | u | 5027 | C |
| 45 | u | 5028 | G |
| 45 | u | 5031 | G |
| 45 | u | 5033 | G |
| 45 | u | 5041 | G |
| 45 | u | 5047 | C |
| 45 | u | 5050 | C |
| 45 | u | 5052 | C |
| 45 | u | 5053 | U |
| 45 | u | 5054 | C |
| 45 | u | 5056 | A |
| 45 | u | 5058 | A |
| 45 | u | 5060 | A |
| 45 | u | 5061 | A |
| 45 | u | 5062 | G |
| 45 | u | 5066 | U |
| 46 | v | 7 | G |
| 46 | v | 11 | A |
| 46 | v | 21 | G |
| 46 | v | 25 | G |
| 46 | v | 33 | U |
| 46 | v | 40 | U |
| 46 | v | 51 | G |
| 46 | v | 53 | U |
| 46 | v | 54 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46 | v | 64 | G |
| 46 | v | 74 | A |
| 46 | v | 76 | U |
| 46 | v | 97 | G |
| 46 | v | 99 | G |
| 46 | v | 100 | A |
| 46 | v | 106 | G |
| 46 | v | 110 | G |
| 46 | v | 111 | C |
| 46 | v | 120 | U |
| 47 | w | 2 | G |
| 47 | w | 3 | A |
| 47 | w | 34 | U |
| 47 | w | 35 | C |
| 47 | w | 38 | U |
| 47 | w | 39 | G |
| 47 | w | 49 | G |
| 47 | w | 51 | U |
| 47 | w | 52 | A |
| 47 | w | 55 | U |
| 47 | w | 57 | C |
| 47 | w | 59 | A |
| 47 | w | 62 | A |
| 47 | w | 63 | U |
| 47 | w | 74 | U |
| 47 | w | 75 | G |
| 47 | w | 79 | G |
| 47 | w | 80 | A |
| 47 | w | 81 | C |
| 47 | w | 82 | A |
| 47 | w | 83 | C |
| 47 | w | 84 | A |
| 47 | w | 85 | U |
| 47 | w | 86 | U |
| 47 | w | 87 | G |
| 47 | w | 94 | G |
| 47 | w | 95 | A |
| 47 | w | 99 | U |
| 47 | w | 101 | C |
| 47 | w | 103 | A |
| 47 | w | 104 | A |
| 47 | w | 105 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47 | w | 107 | C |
| 47 | w | 109 | C |
| 47 | w | 110 | U |
| 47 | w | 111 | U |
| 47 | w | 112 | G |
| 47 | w | 113 | C |
| 47 | w | 114 | G |
| 47 | w | 115 | G |
| 47 | w | 117 | C |
| 47 | w | 121 | G |
| 47 | w | 122 | G |
| 47 | w | 123 | U |
| 47 | w | 124 | U |
| 47 | w | 125 | C |
| 47 | w | 126 | C |
| 47 | w | 127 | U |
| 47 | w | 137 | A |
| 47 | w | 143 | G |
| 47 | w | 150 | C |
| 47 | w | 156 | U |

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

8 monosaccharides are modelled in this entry.

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 | $\# Z > 2$ |
| 59 | NAG | K | 1 | 59,55 | 14,14,15 | 0.49 | 0 | 17,19,21 | 0.63 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 59 | NAG | K | 2 | 59 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.53 | 0 |
| 59 | BMA | K | 3 | 59 | 11,11,12 | 0.67 | 0 | 15,15,17 | 0.88 | 1 (6%) |
| 59 | MAN | K | 4 | 59 | 11,11,12 | 0.82 | 0 | 15,15,17 | 1.66 | 2 (13%) |
| 59 | MAN | K | 5 | 59 | 11,11,12 | 0.71 | 0 | 15,15,17 | 1.25 | 2 (13%) |
| 59 | MAN | K | 6 | 59 | 11,11,12 | 0.92 | 1 (9%) | 15,15,17 | 0.99 | 2 (13%) |
| 59 | MAN | K | 7 | 59 | 11,11,12 | 1.26 | 1 (9%) | 15,15,17 | 1.29 | 2 (13%) |
| 59 | MAN | K | 8 | 59 | 11,11,12 | 0.68 | 0 | 15,15,17 | 1.04 | 2 (13%) |

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|-------|---------|-----------|---------|
| 59 | NAG | K | 1 | 59,55 | - | 2/6/23/26 | 0/1/1/1 |
| 59 | NAG | K | 2 | 59 | - | 1/6/23/26 | 0/1/1/1 |
| 59 | BMA | K | 3 | 59 | - | 2/2/19/22 | 0/1/1/1 |
| 59 | MAN | K | 4 | 59 | - | 0/2/19/22 | 0/1/1/1 |
| 59 | MAN | K | 5 | 59 | - | 1/2/19/22 | 0/1/1/1 |
| 59 | MAN | K | 6 | 59 | - | 0/2/19/22 | 0/1/1/1 |
| 59 | MAN | K | 7 | 59 | - | 0/2/19/22 | 0/1/1/1 |
| 59 | MAN | K | 8 | 59 | - | 2/2/19/22 | 0/1/1/1 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 59 | K | 7 | MAN | C2-C3 | 2.51 | 1.56 | 1.52 |
| 59 | K | 6 | MAN | O5-C1 | -2.12 | 1.40 | 1.43 |

All (11) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 59 | K | 4 | MAN | C1-O5-C5 | 4.40 | 118.15 | 112.19 |
| 59 | K | 4 | MAN | O2-C2-C3 | -3.75 | 102.62 | 110.14 |
| 59 | K | 7 | MAN | C1-O5-C5 | 3.21 | 116.55 | 112.19 |
| 59 | K | 5 | MAN | O2-C2-C3 | -3.06 | 104.02 | 110.14 |
| 59 | K | 5 | MAN | C1-O5-C5 | 3.01 | 116.27 | 112.19 |
| 59 | K | 8 | MAN | C1-O5-C5 | 2.80 | 115.98 | 112.19 |
| 59 | K | 7 | MAN | O3-C3-C2 | 2.54 | 114.86 | 109.99 |
| 59 | K | 6 | MAN | O2-C2-C3 | -2.48 | 105.16 | 110.14 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 59 | K | 8 | MAN | O2-C2-C3 | -2.19 | 105.76 | 110.14 |
| 59 | K | 3 | BMA | C1-O5-C5 | 2.12 | 115.07 | 112.19 |
| 59 | K | 6 | MAN | C1-O5-C5 | 2.04 | 114.96 | 112.19 |

There are no chirality outliers.

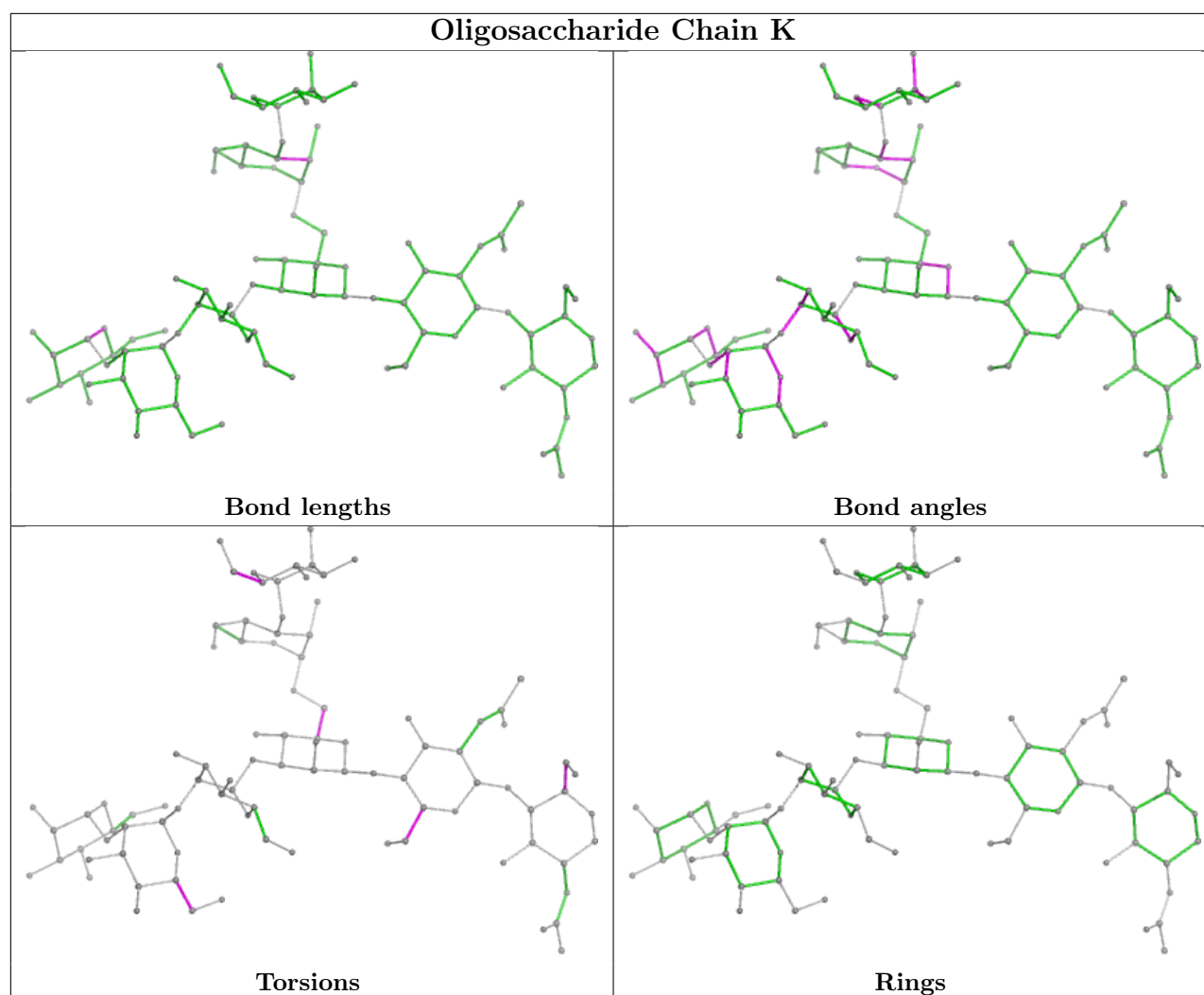
All (8) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 59 | K | 3 | BMA | C4-C5-C6-O6 |
| 59 | K | 3 | BMA | O5-C5-C6-O6 |
| 59 | K | 8 | MAN | O5-C5-C6-O6 |
| 59 | K | 8 | MAN | C4-C5-C6-O6 |
| 59 | K | 1 | NAG | C4-C5-C6-O6 |
| 59 | K | 1 | NAG | O5-C5-C6-O6 |
| 59 | K | 5 | MAN | O5-C5-C6-O6 |
| 59 | K | 2 | NAG | C4-C5-C6-O6 |

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

Of 165 ligands modelled in this entry, 164 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | # $ Z > 2$ | Counts | RMSZ | # $ Z > 2$ |
| 62 | 9UB | 5 | 809 | - | 41,43,43 | 2.31 | 9 (21%) | 47,59,59 | 1.65 | 13 (27%) |

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 |
|-----|------|-------|-----|------|---------|------------|---------|
| 62 | 9UB | 5 | 809 | - | - | 4/39/62/62 | 0/1/1/1 |

All (9) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 62 | 5 | 809 | 9UB | P26-O25 | 8.10 | 1.67 | 1.58 |
| 62 | 5 | 809 | 9UB | P26-C29 | 7.18 | 1.91 | 1.80 |
| 62 | 5 | 809 | 9UB | C37-C39 | -3.65 | 1.46 | 1.53 |
| 62 | 5 | 809 | 9UB | C41-N40 | 3.35 | 1.45 | 1.34 |
| 62 | 5 | 809 | 9UB | C06-C07 | 2.98 | 1.57 | 1.51 |
| 62 | 5 | 809 | 9UB | C11-C12 | 2.68 | 1.56 | 1.51 |
| 62 | 5 | 809 | 9UB | C16-C17 | 2.37 | 1.56 | 1.51 |
| 62 | 5 | 809 | 9UB | C18-C17 | 2.32 | 1.56 | 1.50 |
| 62 | 5 | 809 | 9UB | C20-C19 | 2.05 | 1.55 | 1.49 |

All (13) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 62 | 5 | 809 | 9UB | C18-C17-C16 | 4.23 | 122.39 | 115.27 |
| 62 | 5 | 809 | 9UB | C20-C19-C17 | -3.49 | 120.01 | 126.04 |
| 62 | 5 | 809 | 9UB | C01-C02-C03 | 2.72 | 120.61 | 114.60 |
| 62 | 5 | 809 | 9UB | C32-O31-C30 | 2.61 | 117.72 | 113.16 |
| 62 | 5 | 809 | 9UB | C39-N40-C41 | -2.61 | 116.83 | 123.18 |
| 62 | 5 | 809 | 9UB | O31-C32-C35 | 2.44 | 114.12 | 109.69 |
| 62 | 5 | 809 | 9UB | O27-P26-C29 | 2.41 | 111.04 | 105.72 |
| 62 | 5 | 809 | 9UB | C08-C07-C06 | 2.37 | 119.26 | 115.27 |
| 62 | 5 | 809 | 9UB | C15-C14-C12 | -2.29 | 122.14 | 127.66 |
| 62 | 5 | 809 | 9UB | C10-C09-C07 | -2.28 | 122.18 | 127.66 |
| 62 | 5 | 809 | 9UB | C18-C17-C19 | -2.23 | 117.95 | 123.68 |
| 62 | 5 | 809 | 9UB | C13-C12-C11 | 2.21 | 118.99 | 115.27 |
| 62 | 5 | 809 | 9UB | C33-C32-C35 | -2.16 | 107.95 | 113.00 |

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 62 | 5 | 809 | 9UB | C20-O21-P22-O25 |
| 62 | 5 | 809 | 9UB | C20-O21-P22-O23 |
| 62 | 5 | 809 | 9UB | C20-O21-P22-O24 |

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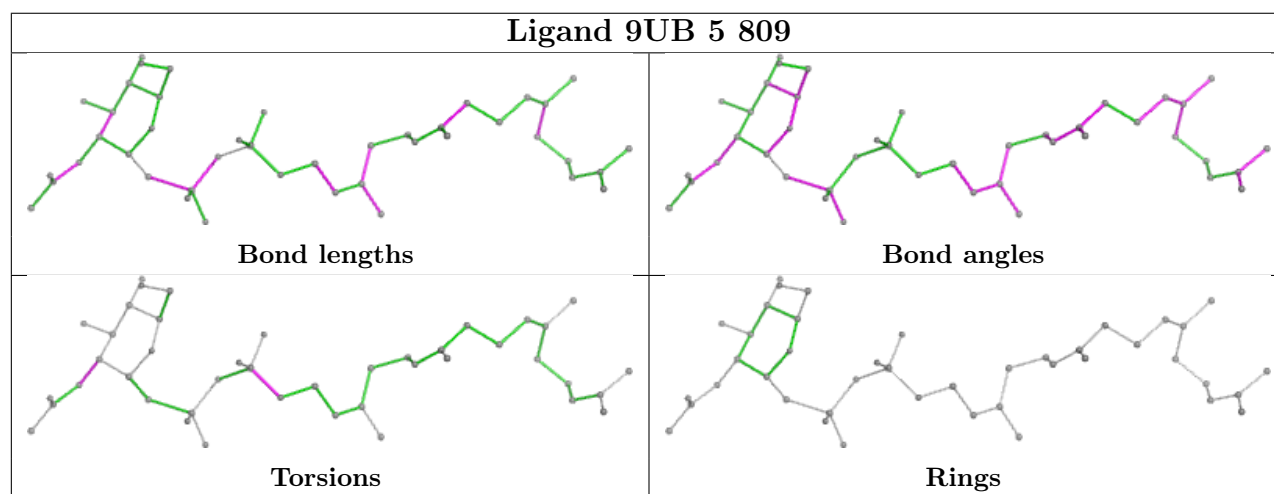
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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 62 | 5 | 809 | 9UB | C30-C39-N40-C41 |

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 45 | u | 21 |

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| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 55 | 5 | 4 |
| 58 | 8 | 2 |
| 56 | 6 | 2 |
| 48 | x | 2 |
| 51 | 1 | 1 |
| 52 | 2 | 1 |
| 42 | r | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | u | 4776:G | O3' | 4859:C | P | 17.95 |
| 1 | u | 757:G | O3' | 906:C | P | 17.49 |
| 1 | u | 519:C | O3' | 642:G | P | 16.73 |
| 1 | u | 2910:G | O3' | 3583:U | P | 16.46 |
| 1 | 8 | 566:UNK | C | 577:UNK | N | 15.56 |
| 1 | 1 | 573:VAL | C | 582:UNK | N | 15.25 |
| 1 | u | 2131:C | O3' | 2243:C | P | 14.50 |
| 1 | u | 3950:U | O3' | 4065:G | P | 14.39 |
| 1 | u | 997:C | O3' | 1047:C | P | 13.95 |
| 1 | 6 | 46:UNK | C | 53:UNK | N | 13.30 |
| 1 | 2 | 42:UNK | C | 50:UNK | N | 12.33 |
| 1 | 8 | 598:UNK | C | 600:UNK | N | 11.54 |
| 1 | 6 | 82:UNK | C | 88:UNK | N | 10.20 |
| 1 | x | 312:PHE | C | 337:PRO | N | 9.61 |
| 1 | u | 1051:G | O3' | 1064:G | P | 8.98 |
| 1 | x | 133:MET | C | 145:SER | N | 8.39 |
| 1 | u | 1222:A | O3' | 1232:G | P | 5.15 |
| 1 | u | 2016:C | O3' | 2017:A | P | 4.53 |
| 1 | u | 1100:U | O3' | 1167:C | P | 4.42 |
| 1 | u | 1699:A | O3' | 1718:C | P | 4.00 |
| 1 | r | 121:GLN | C | 122:LYS | N | 2.97 |
| 1 | u | 1840:G | O3' | 1842:G | P | 2.91 |
| 1 | u | 4939:C | O3' | 4941:G | P | 2.80 |
| 1 | 5 | 502:PHE | C | 503:ASP | N | 2.78 |
| 1 | u | 4942:C | O3' | 4944:C | P | 2.73 |
| 1 | u | 1823:G | O3' | 1825:A | P | 2.56 |
| 1 | 5 | 590:SER | C | 591:ASP | N | 2.33 |
| 1 | u | 692:A | O3' | 693:C | P | 2.00 |
| 1 | u | 197:A | O3' | 198:A | P | 1.77 |
| 1 | u | 472:C | O3' | 473:C | P | 1.37 |
| 1 | u | 1965:G | O3' | 1966:C | P | 1.33 |
| 1 | u | 680:G | O3' | 681:G | P | 1.20 |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | 5 | 550:THR | C | 551:HIS | N | 0.96 |
| 1 | 5 | 545:ASN | C | 546:THR | N | 0.91 |

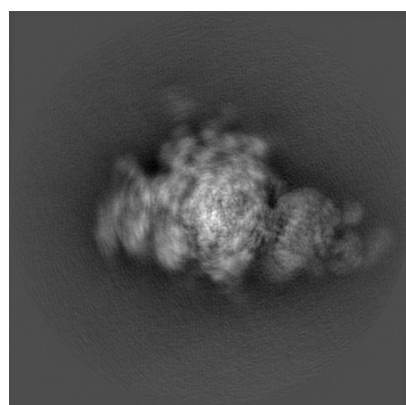
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4317. These allow visual inspection of the internal detail of the map and identification of artifacts.

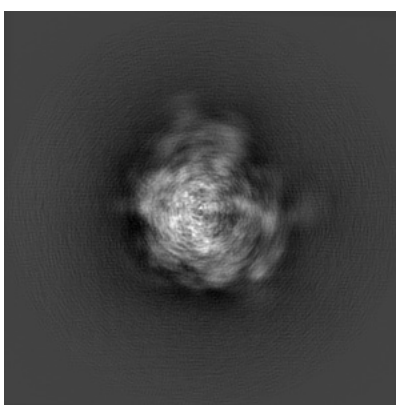
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

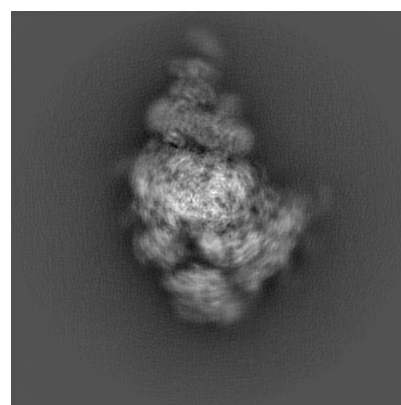
6.1.1 Primary map



X



Y

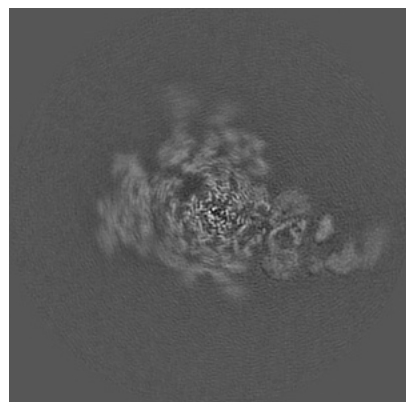


Z

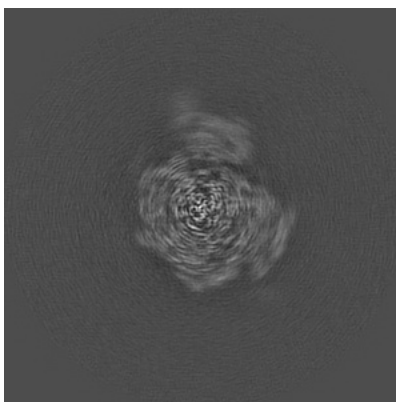
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

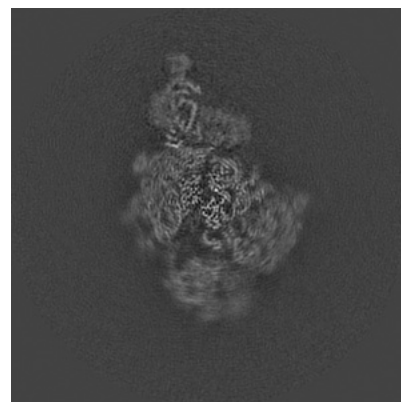
6.2.1 Primary map



X Index: 250



Y Index: 250

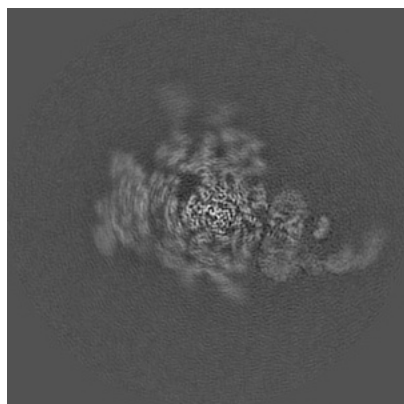


Z Index: 250

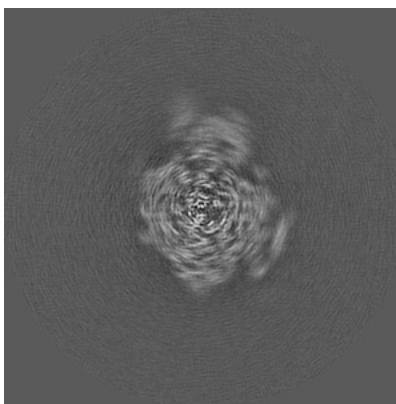
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

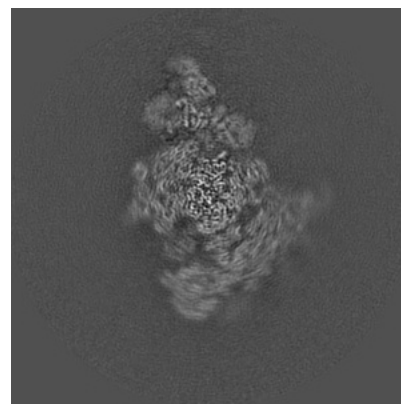
6.3.1 Primary map



X Index: 253



Y Index: 245

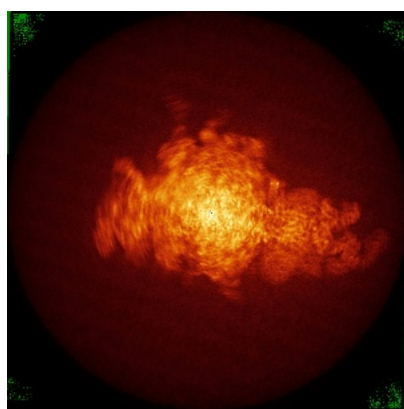


Z Index: 235

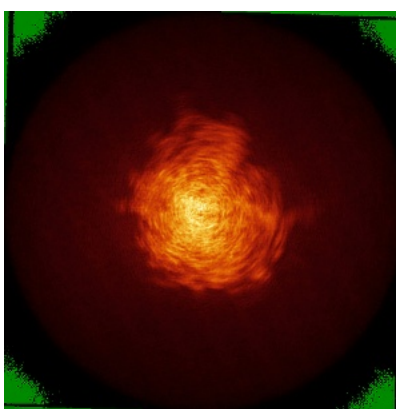
The images above show the largest variance slices of the map in three orthogonal directions.

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

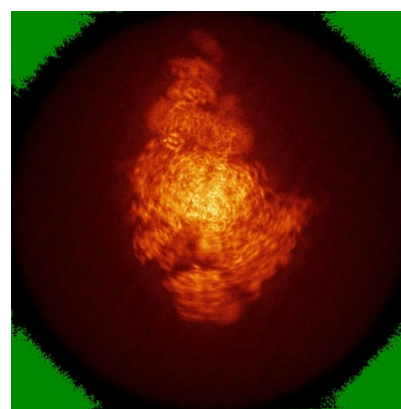
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

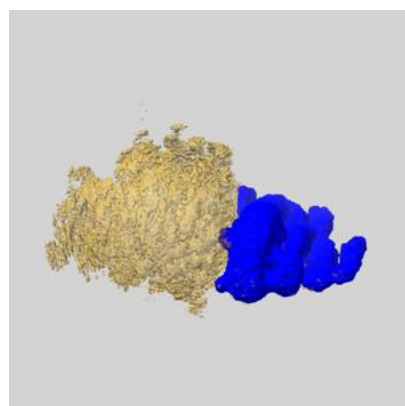
6.6 Mask visualisation [i](#)

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

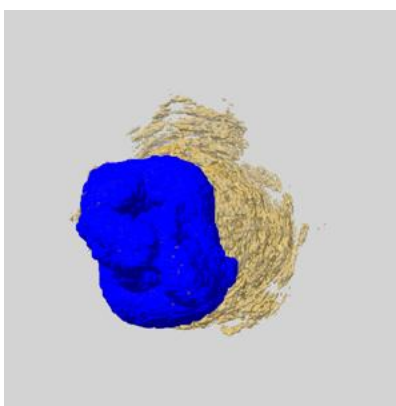
A mask typically either:

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

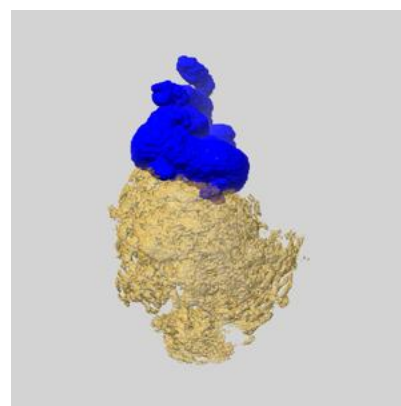
6.6.1 emd_4317_msk_1.map [i](#)



X



Y

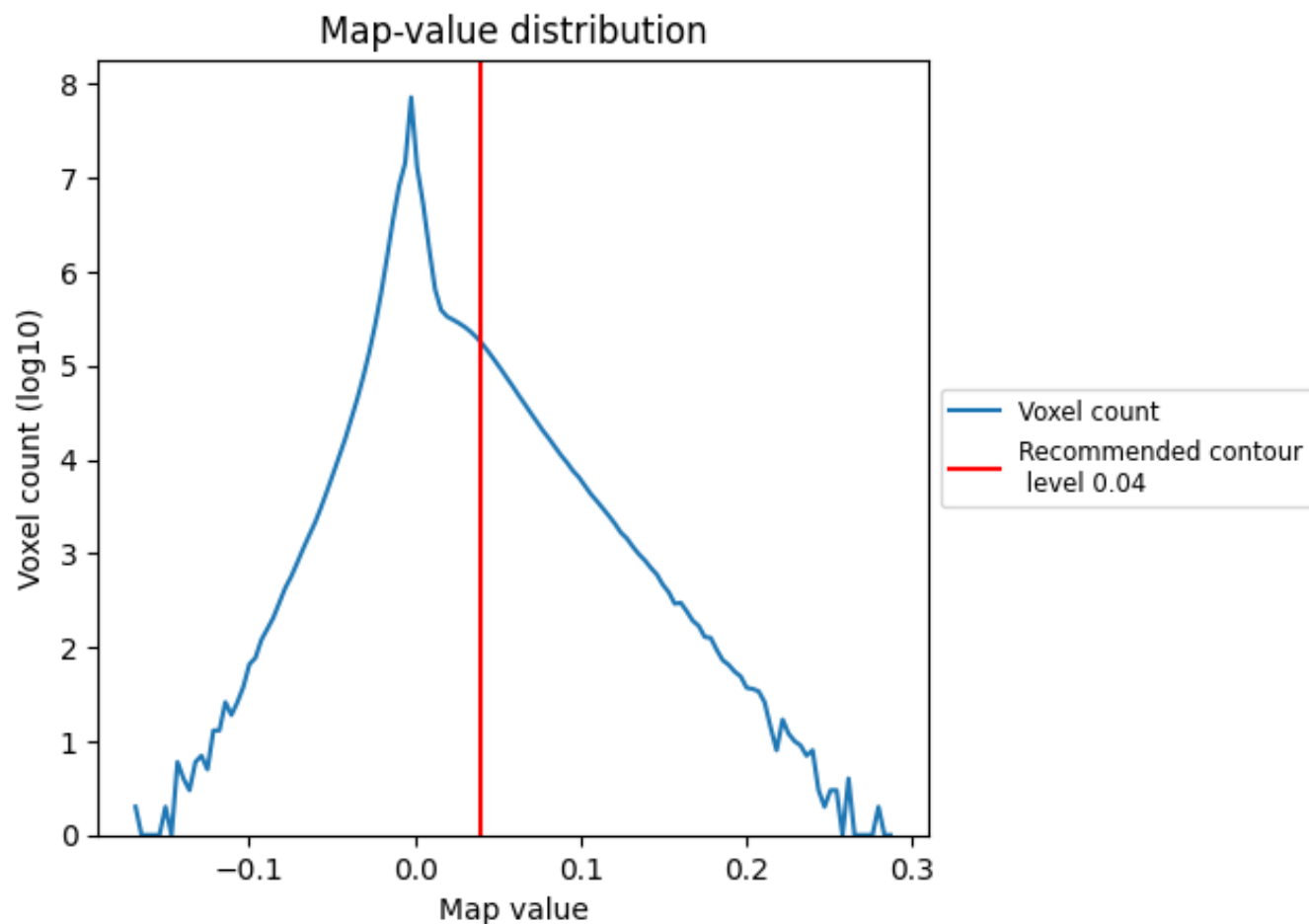


Z

7 Map analysis [i](#)

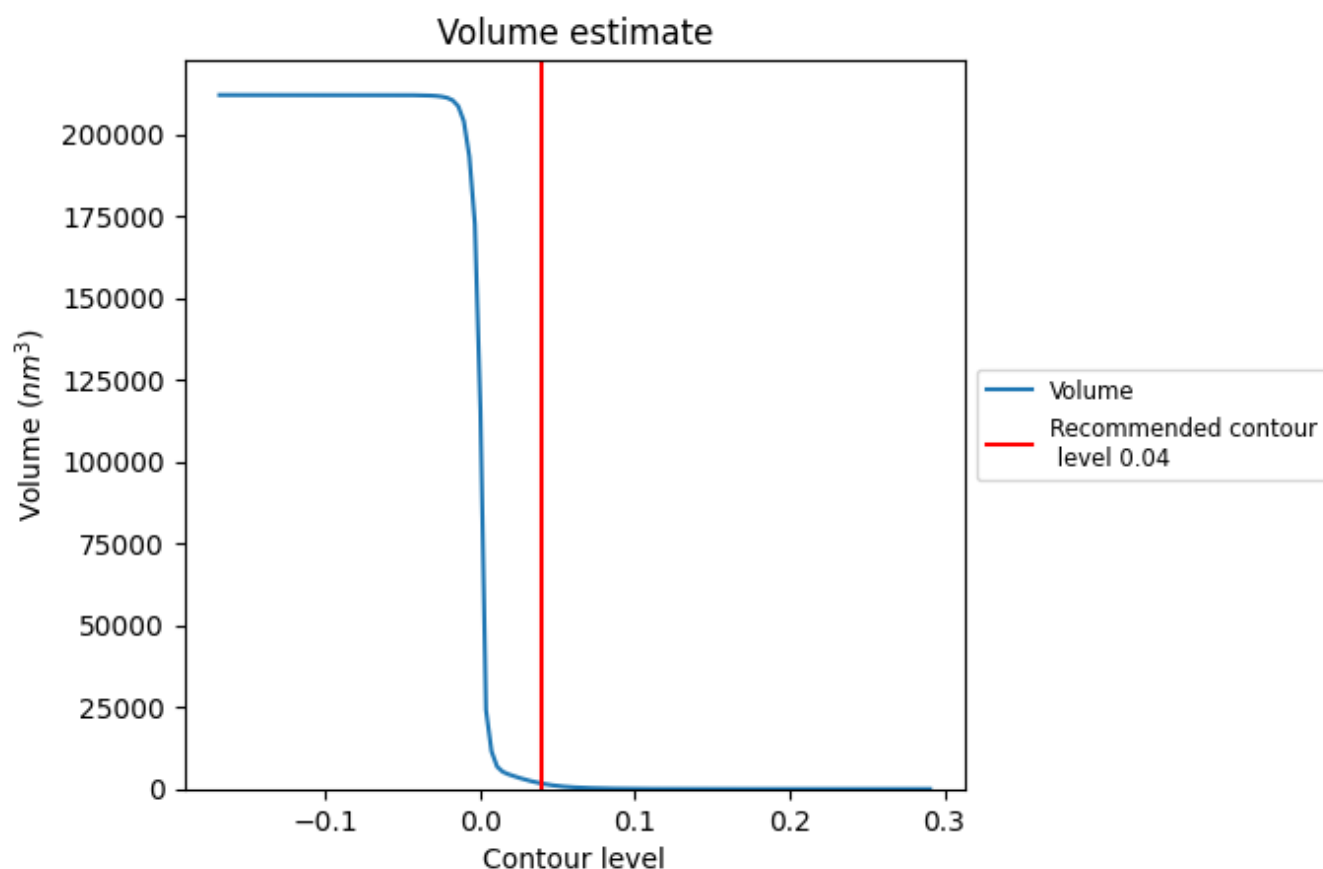
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

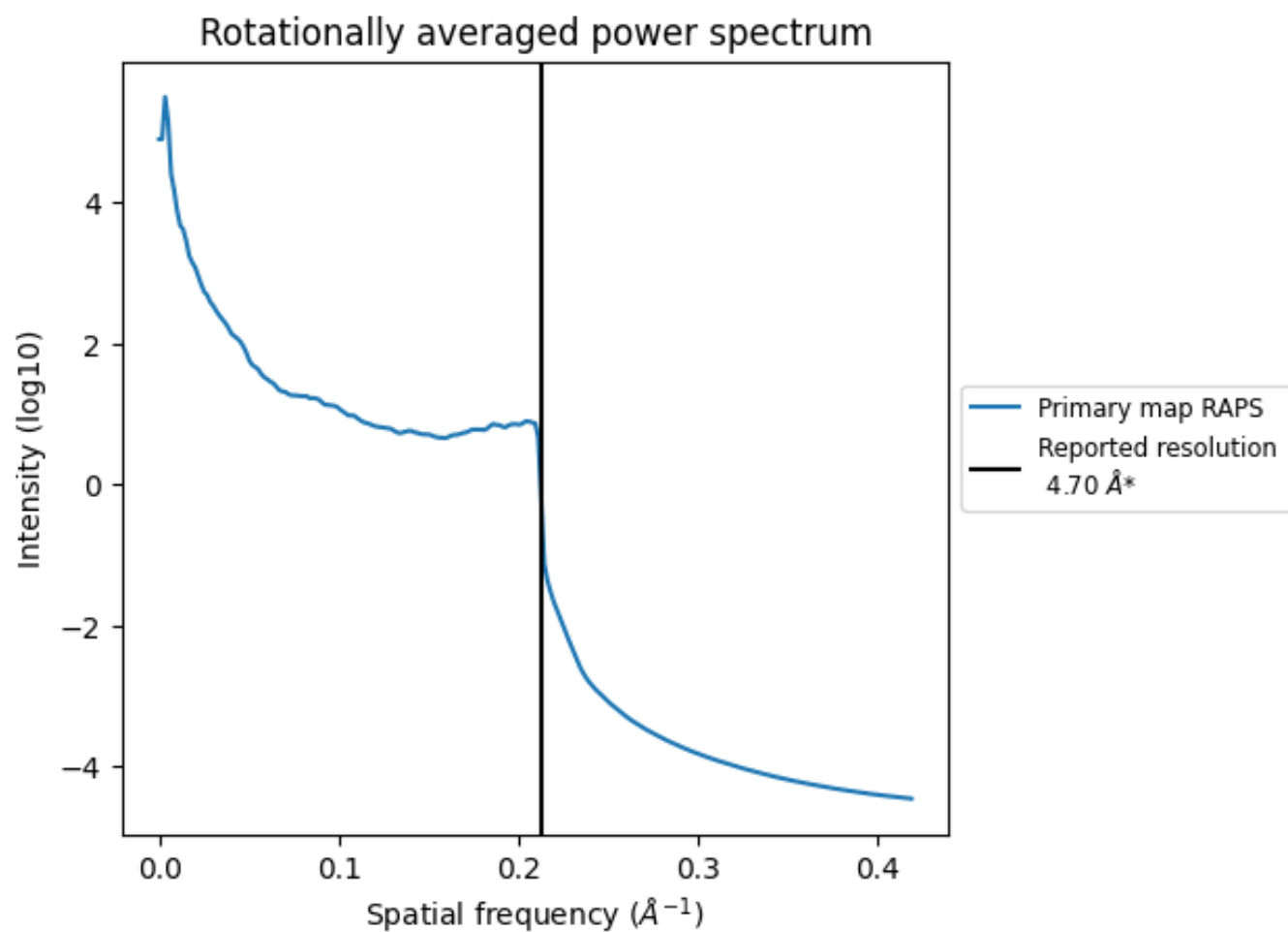
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1641 nm^3 ; this corresponds to an approximate mass of 1482 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 0.213 Å⁻¹

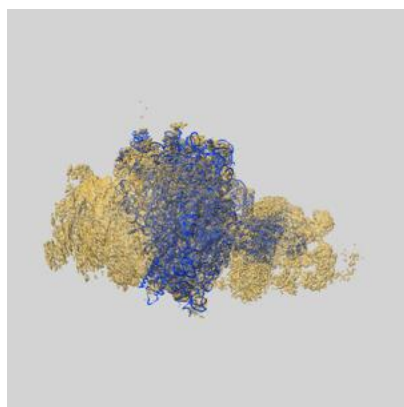
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

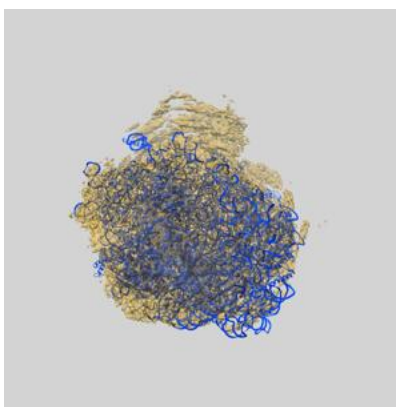
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4317 and PDB model 6FTJ. Per-residue inclusion information can be found in section [3](#) on page [18](#).

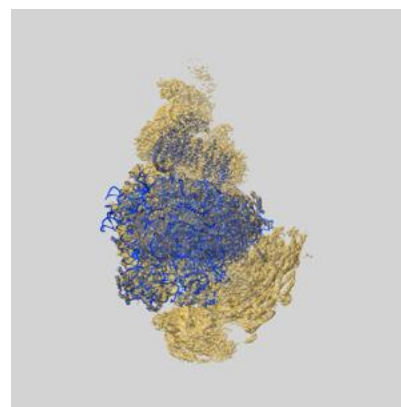
9.1 Map-model overlay [i](#)



X



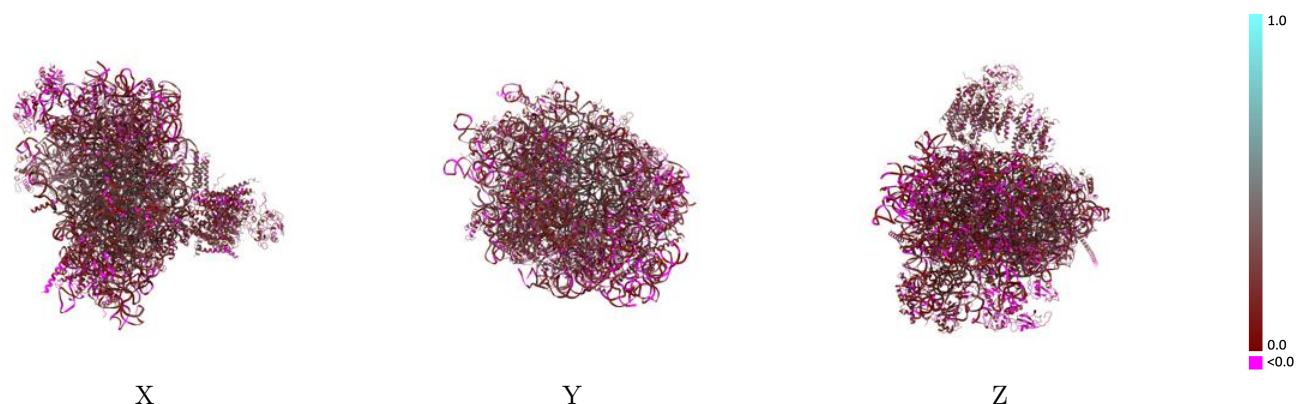
Y



Z

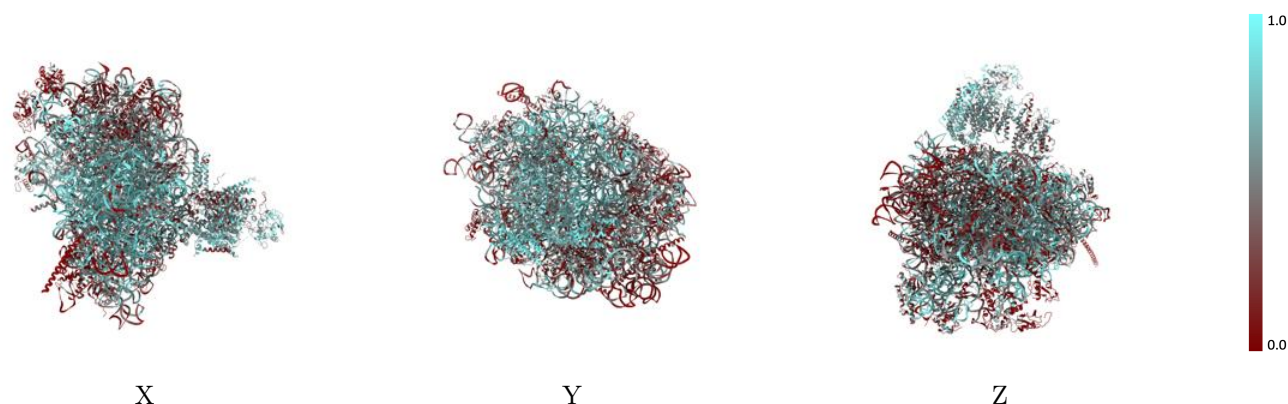
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



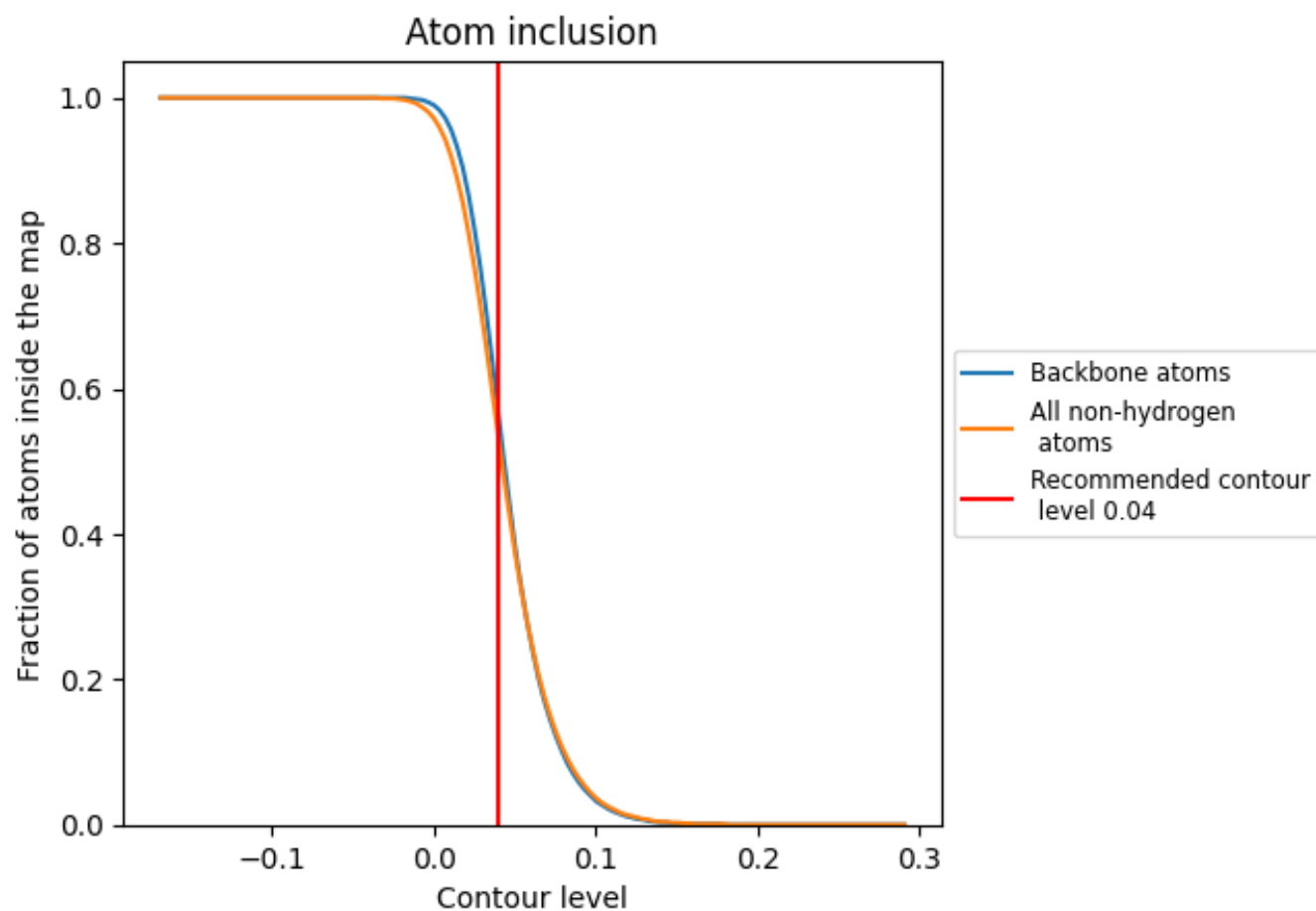
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 57% of all backbone atoms, 53% 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 (0.04) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.5340 |  0.1740 |
| 1 |  0.6550 |  0.1980 |
| 2 |  0.7600 |  0.2210 |
| 3 |  0.5740 |  0.1750 |
| 4 |  0.6090 |  0.2080 |
| 5 |  0.5850 |  0.1790 |
| 6 |  0.8470 |  0.2550 |
| 7 |  0.8160 |  0.2140 |
| 8 |  0.7770 |  0.2330 |
| A |  0.3640 |  0.1920 |
| B |  0.3700 |  0.1570 |
| C |  0.3320 |  0.1680 |
| D |  0.3630 |  0.1080 |
| E |  0.2450 |  0.0940 |
| F |  0.2580 |  0.1230 |
| G |  0.2180 |  0.1030 |
| H |  0.2080 |  0.0760 |
| I |  0.3290 |  0.1670 |
| J |  0.3870 |  0.1220 |
| K |  0.5210 |  0.1490 |
| L |  0.3220 |  0.1430 |
| M |  0.2970 |  0.1060 |
| N |  0.3930 |  0.1800 |
| O |  0.2380 |  0.1060 |
| P |  0.5140 |  0.2280 |
| Q |  0.3310 |  0.1600 |
| R |  0.3910 |  0.1490 |
| S |  0.2490 |  0.1080 |
| T |  0.2310 |  0.1230 |
| U |  0.4110 |  0.1380 |
| V |  0.3350 |  0.1830 |
| W |  0.3930 |  0.1850 |
| X |  0.4090 |  0.1880 |
| Y |  0.4170 |  0.1650 |
| Z |  0.3620 |  0.1310 |



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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| a |  0.3010 |  0.1530 |
| b |  0.3340 |  0.1360 |
| c |  0.3160 |  0.1520 |
| d |  0.4640 |  0.2090 |
| e |  0.2440 |  0.1380 |
| f |  0.1830 |  0.0770 |
| g |  0.3030 |  0.1600 |
| h |  0.4390 |  0.1690 |
| i |  0.3370 |  0.1660 |
| j |  0.5720 |  0.2520 |
| k |  0.3000 |  0.1370 |
| l |  0.5580 |  0.2660 |
| m |  0.2520 |  0.0870 |
| n |  0.4530 |  0.1880 |
| o |  0.4210 |  0.1890 |
| p |  0.3220 |  0.1620 |
| r |  0.3350 |  0.1260 |
| s |  0.1440 |  0.0380 |
| t |  0.1180 |  0.0100 |
| u |  0.6530 |  0.1930 |
| v |  0.7110 |  0.1640 |
| w |  0.7430 |  0.2300 |
| x |  0.5500 |  0.1930 |
| y |  0.5620 |  0.1960 |
| z |  0.2620 |  0.0520 |