



Full wwPDB EM Validation Report ⓘ

Oct 7, 2024 – 02:45 PM JST

PDB ID : 8I9W
EMDB ID : EMD-35286
Title : Cryo-EM structure of a Chaetomium thermophilum pre-60S ribosomal subunit
- Dbp10-3
Authors : Lau, B.; Huang, Z.; Beckmann, R.; Hurt, E.; Cheng, J.
Deposited on : 2023-02-07
Resolution : 3.10 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 : **FAILED**
Mogul : 1.8.5 (274361), 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 : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

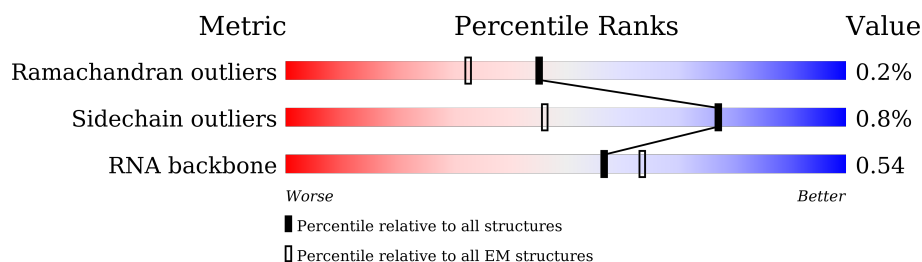
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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.








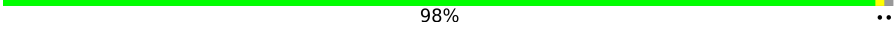
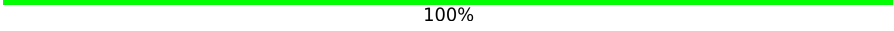




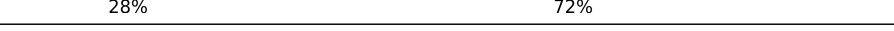


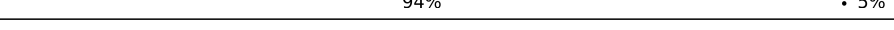




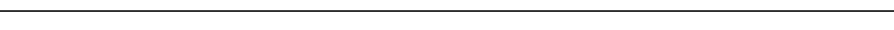

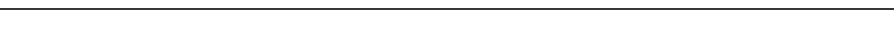
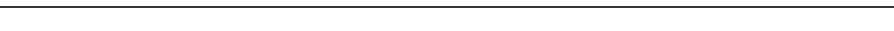


| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |
| RNA backbone | 6643 | 2191 |

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 $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | C1 | 3341 | |
| 2 | C2 | 319 | |
| 3 | CA | 316 | |
| 4 | CB | 391 | |
| 5 | CC | 801 | |
| 6 | CE | 598 | |
| 7 | CF | 270 | |
| 8 | CG | 184 | |
| 9 | CH | 661 | |


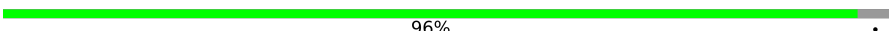

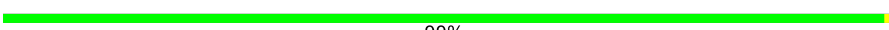






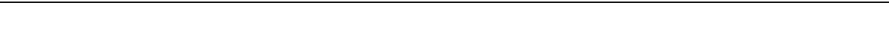

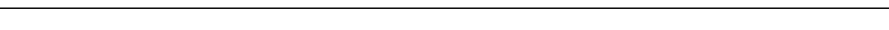
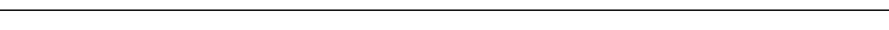
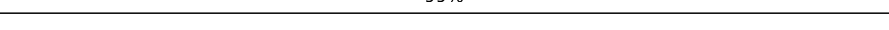



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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 10 | CI | 414 |  |
| 11 | CJ | 679 |  |
| 12 | CK | 261 |  |
| 13 | CL | 558 |  |
| 14 | CM | 249 |  |
| 14 | LF | 249 |  |
| 15 | CN | 246 |  |
| 16 | CO | 120 |  |
| 17 | CP | 751 |  |
| 18 | CQ | 225 |  |
| 19 | CR | 237 |  |
| 20 | CS | 834 |  |
| 21 | CT | 688 |  |
| 22 | CU | 451 |  |
| 23 | CV | 147 |  |
| 24 | CX | 203 |  |
| 25 | CY | 788 |  |
| 26 | Cb | 924 |  |
| 27 | Cz | 123 |  |
| 28 | LB | 392 |  |
| 29 | LC | 365 |  |
| 30 | LE | 200 |  |
| 31 | LG | 262 |  |
| 32 | LH | 192 |  |
| 33 | LK | 165 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 34 | LL | 213 |  54% 45% |
| 35 | LM | 142 |  96% . |
| 36 | LN | 203 |  87% . 10% |
| 37 | LO | 204 |  99% . |
| 38 | LP | 187 |  81% . 18% |
| 39 | LQ | 213 |  61% 39% |
| 40 | LS | 174 |  99% . |
| 41 | LT | 160 |  78% . 21% |
| 42 | LV | 139 |  96% . . |
| 43 | LX | 156 |  30% 70% |
| 44 | LY | 138 |  97% . |
| 45 | Ld | 120 |  90% . 9% |
| 46 | Le | 131 |  97% . |
| 47 | Lf | 109 |  99% . |
| 48 | Lh | 935 |  13% 87% |
| 49 | Li | 110 |  79% . 20% |
| 50 | Lj | 95 |  78% 22% |
| 51 | Lq | 217 |  93% . 5% |

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 136840 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called RNA (3341-MER).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 1 | C1 | 2163 | Total | C | N | O | P | 0 | 0 |
| | | | 46266 | 20653 | 8376 | 15074 | 2163 | | |

- Molecule 2 is a RNA chain called RNA (319-MER).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 2 | C2 | 256 | Total | C | N | O | P | 0 | 0 |
| | | | 5456 | 2435 | 974 | 1791 | 256 | | |

- Molecule 3 is a protein called Brix domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3 | CA | 251 | Total | C | N | O | S | 0 | 0 |
| | | | 2069 | 1324 | 381 | 357 | 7 | | |

- Molecule 4 is a protein called Ribosome biogenesis protein C8F11.04.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4 | CB | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 2063 | 1322 | 367 | 371 | 3 | | |

- Molecule 5 is a protein called Ribosome biogenesis protein ERB1.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---|---------|-------|
| 5 | CC | 291 | Total | C | N | O | P | S | 0 | 0 |
| | | | 2413 | 1530 | 403 | 471 | 2 | 7 | | |

- Molecule 6 is a protein called RNA helicase.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6 | CE | 463 | Total | C | N | O | S | 0 | 0 |
| | | | 3673 | 2352 | 643 | 667 | 11 | | |

There are 42 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| CE | 543 | LYS | - | insertion | UNP G0RYU9 |
| CE | 544 | SER | - | insertion | UNP G0RYU9 |
| CE | 545 | PHE | - | insertion | UNP G0RYU9 |
| CE | 546 | GLY | - | insertion | UNP G0RYU9 |
| CE | 547 | PHE | - | insertion | UNP G0RYU9 |
| CE | 548 | SER | - | insertion | UNP G0RYU9 |
| CE | 549 | THR | - | insertion | UNP G0RYU9 |
| CE | 550 | PRO | - | insertion | UNP G0RYU9 |
| CE | 551 | PRO | - | insertion | UNP G0RYU9 |
| CE | 552 | ARG | - | insertion | UNP G0RYU9 |
| CE | 553 | VAL | - | insertion | UNP G0RYU9 |
| CE | 554 | ASP | - | insertion | UNP G0RYU9 |
| CE | 555 | ILE | - | insertion | UNP G0RYU9 |
| CE | 556 | THR | - | insertion | UNP G0RYU9 |
| CE | 557 | LEU | - | insertion | UNP G0RYU9 |
| CE | 558 | SER | - | insertion | UNP G0RYU9 |
| CE | 559 | ALA | - | insertion | UNP G0RYU9 |
| CE | 560 | SER | - | insertion | UNP G0RYU9 |
| CE | 561 | LEU | - | insertion | UNP G0RYU9 |
| CE | 562 | SER | - | insertion | UNP G0RYU9 |
| CE | 563 | ARG | - | insertion | UNP G0RYU9 |
| CE | 564 | ASP | - | insertion | UNP G0RYU9 |
| CE | 565 | LYS | - | insertion | UNP G0RYU9 |
| CE | 566 | LYS | - | insertion | UNP G0RYU9 |
| CE | 567 | PRO | - | insertion | UNP G0RYU9 |
| CE | 568 | GLN | - | insertion | UNP G0RYU9 |
| CE | 569 | GLY | - | insertion | UNP G0RYU9 |
| CE | 570 | ARG | - | insertion | UNP G0RYU9 |
| CE | 571 | ARG | - | insertion | UNP G0RYU9 |
| CE | 572 | ALA | - | insertion | UNP G0RYU9 |
| CE | 573 | TYR | - | insertion | UNP G0RYU9 |
| CE | 574 | GLY | - | insertion | UNP G0RYU9 |
| CE | 575 | SER | - | insertion | UNP G0RYU9 |
| CE | 576 | GLN | - | insertion | UNP G0RYU9 |
| CE | 577 | PRO | - | insertion | UNP G0RYU9 |
| CE | 578 | ARG | - | insertion | UNP G0RYU9 |
| CE | 579 | GLN | - | insertion | UNP G0RYU9 |
| CE | 580 | GLY | - | insertion | UNP G0RYU9 |
| CE | 581 | GLY | - | insertion | UNP G0RYU9 |
| CE | 582 | ARG | - | insertion | UNP G0RYU9 |
| CE | 583 | TYR | - | insertion | UNP G0RYU9 |
| CE | 584 | LYS | - | insertion | UNP G0RYU9 |

- Molecule 7 is a protein called Ribosome assembly factor mrt4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7 | CF | 245 | Total | C | N | O | S | 0 | 0 |
| | | | 1945 | 1222 | 352 | 362 | 9 | | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| CF | 13 | ILE | THR | conflict | UNP G0S616 |
| CF | 139 | THR | PRO | conflict | UNP G0S616 |
| CF | 228 | ASN | SER | conflict | UNP G0S616 |
| CF | 259 | ILE | MET | conflict | UNP G0S616 |

- Molecule 8 is a protein called 60S ribosome subunit biogenesis protein NIP7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 8 | CG | 177 | Total | C | N | O | S | 0 | 0 |
| | | | 1396 | 884 | 247 | 253 | 12 | | |

- Molecule 9 is a protein called Nucleolar GTP-binding protein 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9 | CH | 503 | Total | C | N | O | S | 0 | 0 |
| | | | 4085 | 2594 | 712 | 763 | 16 | | |

- Molecule 10 is a protein called Putative RNA-binding protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10 | CI | 146 | Total | C | N | O | S | 0 | 0 |
| | | | 1196 | 763 | 224 | 204 | 5 | | |

- Molecule 11 is a protein called Pescadillo homolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 11 | CJ | 379 | Total | C | N | O | S | 0 | 0 |
| | | | 3092 | 1991 | 543 | 548 | 10 | | |

- Molecule 12 is a protein called Ribosome biogenesis protein NSA2 homolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 12 | CK | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1908 | 1199 | 375 | 330 | 4 | | |

- Molecule 13 is a protein called Putative GTP binding protein.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 13 | CL | 397 | Total | C | N | O | 0 | 0 |
| | | | 2239 | 1350 | 459 | 430 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| CL | 69 | ARG | ILE | conflict | UNP G0SEW3 |

- Molecule 14 is a protein called 60S ribosomal protein l7-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14 | CM | 223 | Total | C | N | O | S | 0 | 0 |
| | | | 1820 | 1169 | 340 | 308 | 3 | | |
| 14 | LF | 247 | Total | C | N | O | S | 0 | 0 |
| | | | 2017 | 1294 | 376 | 344 | 3 | | |

- Molecule 15 is a protein called Eukaryotic translation initiation factor 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 15 | CN | 246 | Total | C | N | O | S | 0 | 0 |
| | | | 1856 | 1158 | 322 | 369 | 7 | | |

- Molecule 16 is a protein called DUF2423 domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 16 | CO | 62 | Total | C | N | O | S | 0 | 0 |
| | | | 468 | 290 | 94 | 82 | 2 | | |

- Molecule 17 is a protein called RNA methyltransferase nop2-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 17 | CP | 356 | Total | C | N | O | S | 0 | 0 |
| | | | 2798 | 1777 | 495 | 510 | 16 | | |

- Molecule 18 is a protein called Ribosome biogenesis protein RLP24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 18 | CQ | 125 | Total | C | N | O | S | 0 | 0 |
| | | | 1056 | 664 | 219 | 163 | 10 | | |

- Molecule 19 is a protein called Nucleolar protein 16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19 | CR | 167 | Total | C | N | O | S | 0 | 0 |
| | | | 1354 | 827 | 278 | 247 | 2 | | |

- Molecule 20 is a protein called AdoMet-dependent rRNA methyltransferase SPB1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 20 | CS | 235 | Total | C | N | O | S | 0 | 0 |
| | | | 1891 | 1186 | 359 | 341 | 5 | | |

- Molecule 21 is a protein called Nucleolar complex-associated protein 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 21 | CT | 488 | Total | C | N | O | S | 0 | 0 |
| | | | 3911 | 2486 | 690 | 719 | 16 | | |

- Molecule 22 is a protein called rRNA-processing protein EBP2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22 | CU | 178 | Total | C | N | O | S | 0 | 0 |
| | | | 1415 | 876 | 265 | 271 | 3 | | |

- Molecule 23 is a protein called Putative 60S ribosomal protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23 | CV | 139 | Total | C | N | O | S | 0 | 0 |
| | | | 1073 | 672 | 213 | 188 | | | |

- Molecule 24 is a protein called 60S ribosomal subunit-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24 | CX | 88 | Total | C | N | O | S | 0 | 0 |
| | | | 701 | 435 | 128 | 135 | 3 | | |

- Molecule 25 is a protein called Putative NOC2 family protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 25 | CY | 361 | Total | C | N | O | S | 0 | 0 |
| | | | 2919 | 1874 | 525 | 509 | 11 | | |

- Molecule 26 is a protein called ATP-dependent RNA helicase DBP10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 26 | Cb | 634 | Total | C | N | O | S | 0 | 0 |
| | | | 5005 | 3183 | 907 | 902 | 13 | | |

- Molecule 27 is a protein called rRNA-processing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27 | Cz | 70 | Total | C | N | O | S | 0 | 0 |
| | | | 592 | 368 | 120 | 101 | 3 | | |

- Molecule 28 is a protein called 60S ribosomal protein L3-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 28 | LB | 339 | Total | C | N | O | S | 0 | 0 |
| | | | 2696 | 1713 | 491 | 480 | 12 | | |

- Molecule 29 is a protein called 60S ribosomal protein L4-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 29 | LC | 362 | Total | C | N | O | S | 0 | 0 |
| | | | 2752 | 1738 | 526 | 479 | 9 | | |

- Molecule 30 is a protein called 60S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30 | LE | 179 | Total | C | N | O | S | 0 | 0 |
| | | | 1403 | 898 | 255 | 247 | 3 | | |

- Molecule 31 is a protein called 60S ribosomal protein L8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 31 | LG | 204 | Total | C | N | O | S | 0 | 0 |
| | | | 1644 | 1060 | 297 | 282 | 5 | | |

- Molecule 32 is a protein called 60S ribosomal protein l9-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32 | LH | 190 | Total | C | N | O | S | 0 | 0 |
| | | | 1496 | 950 | 268 | 272 | 6 | | |

There are 37 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| LH | ? | - | GLY | deletion | UNP G0S0E5 |
| LH | ? | - | THR | deletion | UNP G0S0E5 |
| LH | ? | - | PHE | deletion | UNP G0S0E5 |
| LH | ? | - | ARG | deletion | UNP G0S0E5 |
| LH | ? | - | LYS | deletion | UNP G0S0E5 |
| LH | ? | - | PHE | deletion | UNP G0S0E5 |
| LH | ? | - | ARG | deletion | UNP G0S0E5 |
| LH | ? | - | ARG | deletion | UNP G0S0E5 |
| LH | ? | - | ASN | deletion | UNP G0S0E5 |
| LH | ? | - | ASP | deletion | UNP G0S0E5 |
| LH | ? | - | TYR | deletion | UNP G0S0E5 |
| LH | ? | - | THR | deletion | UNP G0S0E5 |
| LH | ? | - | PHE | deletion | UNP G0S0E5 |
| LH | ? | - | GLY | deletion | UNP G0S0E5 |
| LH | ? | - | ARG | deletion | UNP G0S0E5 |
| LH | ? | - | THR | deletion | UNP G0S0E5 |
| LH | ? | - | ARG | deletion | UNP G0S0E5 |
| LH | ? | - | GLY | deletion | UNP G0S0E5 |
| LH | ? | - | ARG | deletion | UNP G0S0E5 |
| LH | ? | - | GLU | deletion | UNP G0S0E5 |
| LH | ? | - | LYS | deletion | UNP G0S0E5 |
| LH | ? | - | LYS | deletion | UNP G0S0E5 |
| LH | ? | - | ARG | deletion | UNP G0S0E5 |
| LH | ? | - | GLY | deletion | UNP G0S0E5 |
| LH | ? | - | THR | deletion | UNP G0S0E5 |
| LH | ? | - | THR | deletion | UNP G0S0E5 |
| LH | ? | - | SER | deletion | UNP G0S0E5 |
| LH | ? | - | SER | deletion | UNP G0S0E5 |
| LH | ? | - | LYS | deletion | UNP G0S0E5 |
| LH | ? | - | ILE | deletion | UNP G0S0E5 |
| LH | ? | - | GLY | deletion | UNP G0S0E5 |
| LH | ? | - | GLU | deletion | UNP G0S0E5 |
| LH | ? | - | LEU | deletion | UNP G0S0E5 |
| LH | ? | - | ASP | deletion | UNP G0S0E5 |
| LH | ? | - | ILE | deletion | UNP G0S0E5 |
| LH | ? | - | ASN | deletion | UNP G0S0E5 |
| LH | ? | - | GLY | deletion | UNP G0S0E5 |

- Molecule 33 is a protein called 60S ribosomal protein L12-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33 | LK | 146 | Total | C | N | O | S | 0 | 0 |
| | | | 1112 | 701 | 203 | 206 | 2 | | |

- Molecule 34 is a protein called 60S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34 | LL | 117 | Total | C | N | O | S | 0 | 0 |
| | | | 964 | 608 | 206 | 148 | 2 | | |

- Molecule 35 is a protein called 60S ribosomal protein L14-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35 | LM | 137 | Total | C | N | O | S | 0 | 0 |
| | | | 1101 | 699 | 211 | 190 | 1 | | |

- Molecule 36 is a protein called Ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36 | LN | 183 | Total | C | N | O | S | 0 | 0 |
| | | | 1563 | 974 | 332 | 253 | 4 | | |

- Molecule 37 is a protein called 60S ribosomal protein L16-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 37 | LO | 204 | Total | C | N | O | S | 0 | 0 |
| | | | 1618 | 1039 | 306 | 267 | 6 | | |

- Molecule 38 is a protein called 60S ribosomal protein l17-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38 | LP | 153 | Total | C | N | O | S | 0 | 0 |
| | | | 1200 | 747 | 238 | 213 | 2 | | |

- Molecule 39 is a protein called Ribosomal protein L18-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39 | LQ | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1021 | 646 | 200 | 173 | 2 | | |

- Molecule 40 is a protein called 60S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40 | LS | 174 | Total | C | N | O | S | 0 | 0 |
| | | | 1433 | 922 | 267 | 239 | 5 | | |

- Molecule 41 is a protein called 60S ribosomal protein l21-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41 | LT | 126 | Total | C | N | O | S | 0 | 0 |
| | | | 1014 | 643 | 196 | 173 | 2 | | |

- Molecule 42 is a protein called 60S ribosomal protein l23-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42 | LV | 135 | Total | C | N | O | S | 0 | 0 |
| | | | 995 | 633 | 185 | 170 | 7 | | |

- Molecule 43 is a protein called 60S ribosomal protein L25-like protein.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 43 | LX | 47 | Total | C | N | O | 0 | 0 |
| | | | 354 | 224 | 72 | 58 | | |

- Molecule 44 is a protein called 60S ribosomal protein L26-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44 | LY | 134 | Total | C | N | O | S | 0 | 0 |
| | | | 1065 | 664 | 215 | 184 | 2 | | |

- Molecule 45 is a protein called Putative 60S ribosomal protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45 | Ld | 109 | Total | C | N | O | S | 0 | 0 |
| | | | 890 | 563 | 171 | 155 | 1 | | |

- Molecule 46 is a protein called 60S ribosomal protein L32-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46 | Le | 127 | Total | C | N | O | S | 0 | 0 |
| | | | 1025 | 645 | 209 | 164 | 7 | | |

- Molecule 47 is a protein called 60S ribosomal protein l33-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47 | Lf | 108 | Total | C | N | O | S | 0 | 0 |
| | | | 862 | 546 | 171 | 144 | 1 | | |

- Molecule 48 is a protein called dolichyl-diphosphooligosaccharide--protein glycotransferase.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 48 | Lh | 121 | Total | C | N | O | 0 | 0 |
| | | | 995 | 633 | 196 | 166 | | |

- Molecule 49 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49 | Li | 88 | Total | C | N | O | S | 0 | 0 |
| | | | 731 | 449 | 162 | 119 | 1 | | |

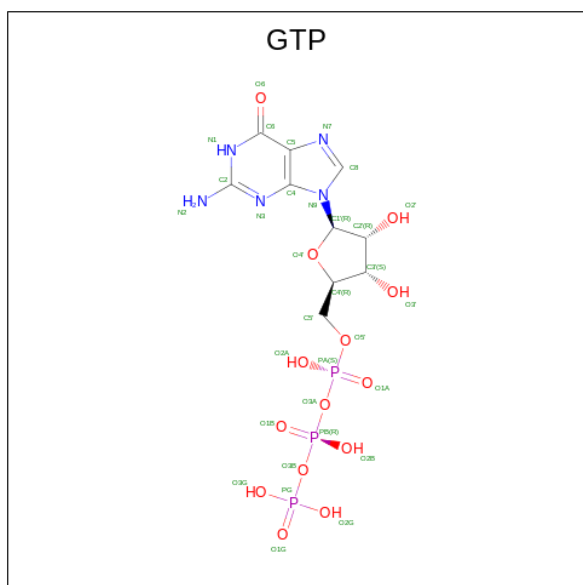
- Molecule 50 is a protein called Ribosomal protein L37.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 50 | Lj | 74 | Total | C | N | O | S | 0 | 0 |
| | | | 595 | 365 | 132 | 93 | 5 | | |

- Molecule 51 is a protein called Ribosomal protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 51 | Lq | 207 | Total | C | N | O | S | 0 | 0 |
| | | | 1600 | 1016 | 285 | 291 | 8 | | |

- Molecule 52 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

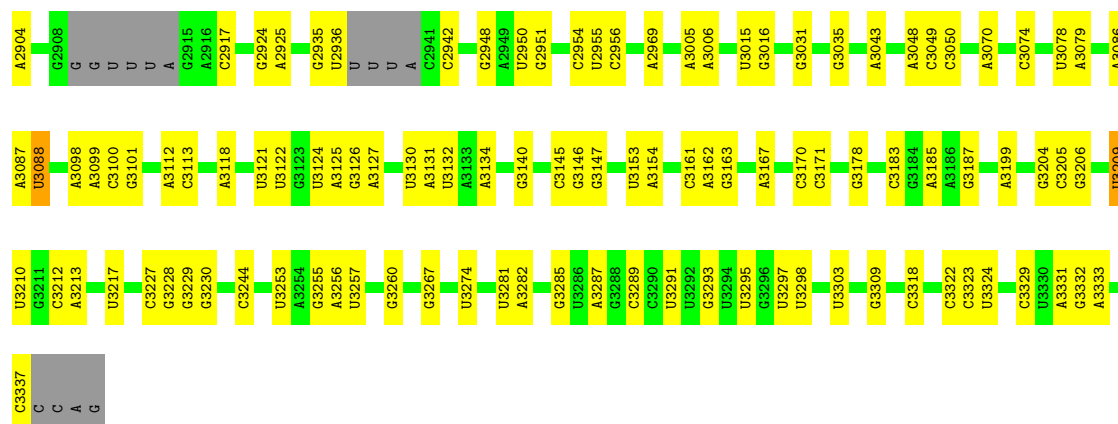


| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 52 | CH | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |

- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|---------|---------|
| 53 | CQ | 1 | Total 1 | Zn 1 | 0 |
| 53 | Lj | 1 | Total 1 | Zn 1 | 0 |

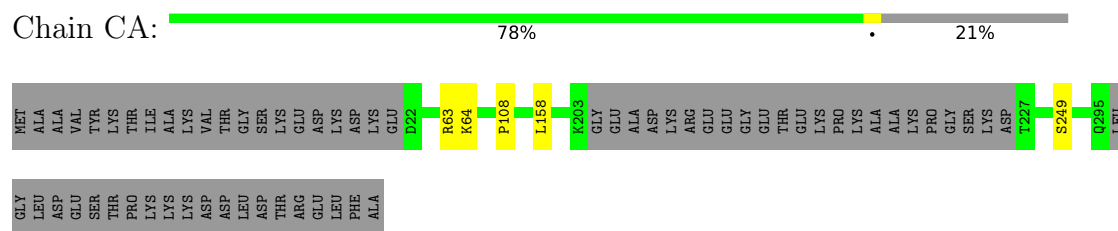




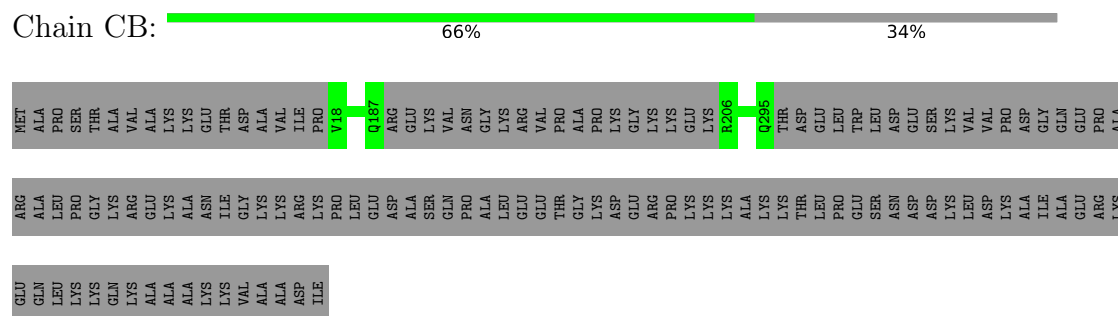
- Molecule 2: RNA (319-MER)



- Molecule 3: Brix domain-containing protein



- Molecule 4: Ribosome biogenesis protein C8F11.04



- Molecule 5: Ribosome biogenesis protein ERB1



67% 31%



| Category | Percentage |
|--------------|------------|
| Satisfied | 57% |
| Dissatisfied | 43% |



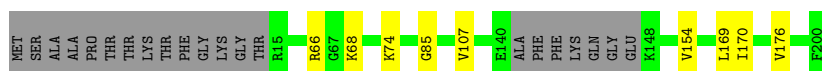
85% • 14%



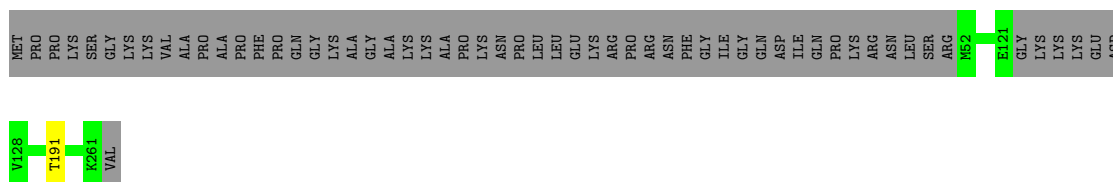
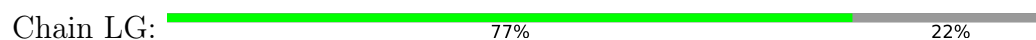
99%



| Response | Percentage |
|----------|------------|
| Yes | 85% |
| No | 10% |



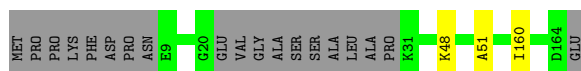
- Molecule 31: 60S ribosomal protein L8



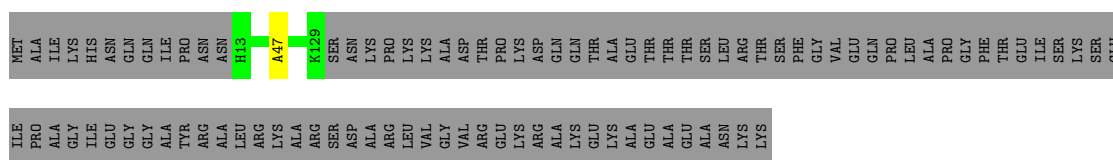
- Molecule 32: 60S ribosomal protein L9-like protein



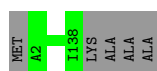
- Molecule 33: 60S ribosomal protein L12-like protein



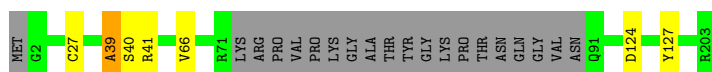
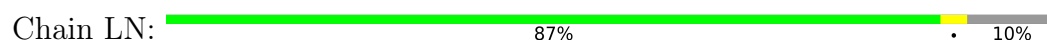
- Molecule 34: 60S ribosomal protein L13



- Molecule 35: 60S ribosomal protein L14-like protein



- Molecule 36: Ribosomal protein L15


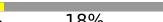


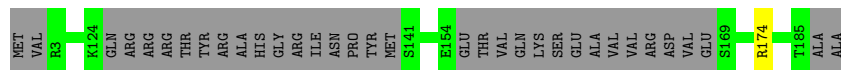
- Molecule 37: 60S ribosomal protein L16-like protein

Chain LO:  99%



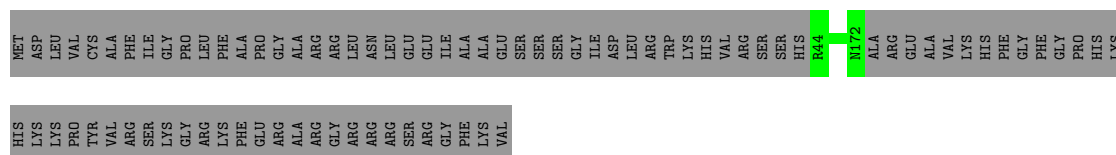
- Molecule 38: 60S ribosomal protein l17-like protein

Chain LP:  81%  18%



- Molecule 39: Ribosomal protein L18-like protein

Chain LQ:  61%  39%


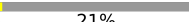


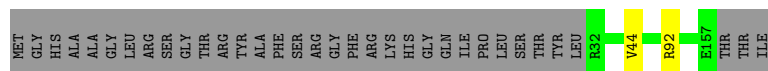
- Molecule 40: 60S ribosomal protein L20

Chain LS:  99%



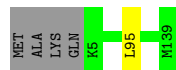
- Molecule 41: 60S ribosomal protein l21-like protein

Chain LT:  78%  21%



- Molecule 42: 60S ribosomal protein l23-like protein

Chain LV:  96%

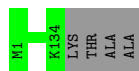


- Molecule 43: 60S ribosomal protein L25-like protein

Chain LX:  30%  70%

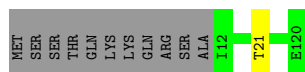
- Molecule 44: 60S ribosomal protein L26-like protein

Chain LY: 97%



- Molecule 45: Putative 60S ribosomal protein

Chain Ld:  90% 9%



- Molecule 46: 60S ribosomal protein L32-like protein

Chain Le: 97%



- Molecule 47: 60S ribosomal protein l33-like protein

Chain Lf:  99%



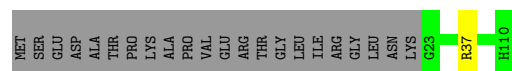
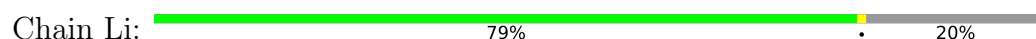
- Molecule 48: dolichyl-diphosphooligosaccharide--protein glycotransferase

Chain Lh:  13% 87%

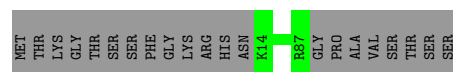
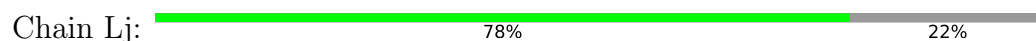


[illegible]

- Molecule 49: 60S ribosomal protein L36



- Molecule 50: Ribosomal protein L37



- Molecule 51: Ribosomal protein



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 30333 | 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 ($e^-/\text{\AA}^2$) | 44 | Depositor |
| Minimum defocus (nm) | 800 | Depositor |
| Maximum defocus (nm) | 2500 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------|-------------|-----------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | C1 | 0.31 | 0/51760 | 0.82 | 35/80668 (0.0%) |
| 2 | C2 | 0.31 | 0/6097 | 0.77 | 0/9499 |
| 3 | CA | 0.33 | 0/2115 | 0.58 | 1/2840 (0.0%) |
| 4 | CB | 0.30 | 0/2109 | 0.58 | 0/2866 |
| 5 | CC | 0.28 | 0/2461 | 0.54 | 0/3348 |
| 6 | CE | 0.28 | 0/3743 | 0.53 | 0/5045 |
| 7 | CF | 0.27 | 0/1982 | 0.60 | 0/2671 |
| 8 | CG | 0.33 | 0/1422 | 0.59 | 0/1920 |
| 9 | CH | 0.32 | 0/4162 | 0.56 | 0/5618 |
| 10 | CI | 0.30 | 0/1225 | 0.66 | 1/1645 (0.1%) |
| 11 | CJ | 0.27 | 0/3171 | 0.56 | 1/4286 (0.0%) |
| 12 | CK | 0.28 | 0/1940 | 0.57 | 0/2601 |
| 13 | CL | 0.25 | 0/2247 | 0.49 | 0/3076 |
| 14 | CM | 0.29 | 0/1851 | 0.58 | 0/2481 |
| 14 | LF | 0.31 | 0/2055 | 0.56 | 1/2758 (0.0%) |
| 15 | CN | 0.27 | 0/1881 | 0.56 | 0/2560 |
| 16 | CO | 0.26 | 0/470 | 0.54 | 0/619 |
| 17 | CP | 0.36 | 0/2859 | 0.62 | 1/3870 (0.0%) |
| 18 | CQ | 0.31 | 0/1077 | 0.67 | 0/1427 |
| 19 | CR | 0.26 | 0/1369 | 0.56 | 0/1828 |
| 20 | CS | 0.25 | 0/1912 | 0.51 | 0/2534 |
| 21 | CT | 0.27 | 0/3974 | 0.54 | 0/5357 |
| 22 | CU | 0.30 | 0/1428 | 0.57 | 0/1910 |
| 23 | CV | 0.27 | 0/1091 | 0.54 | 0/1468 |
| 24 | CX | 0.29 | 0/705 | 0.54 | 0/938 |
| 25 | CY | 0.28 | 0/2971 | 0.60 | 0/4006 |
| 26 | Cb | 0.29 | 0/5097 | 0.56 | 0/6868 |
| 27 | Cz | 0.26 | 0/598 | 0.55 | 0/785 |
| 28 | LB | 0.33 | 0/2748 | 0.59 | 0/3684 |
| 29 | LC | 0.29 | 0/2809 | 0.54 | 0/3787 |
| 30 | LE | 0.44 | 0/1428 | 0.67 | 0/1921 |
| 31 | LG | 0.34 | 0/1667 | 0.60 | 0/2230 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 32 | LH | 0.34 | 0/1516 | 0.59 | 0/2038 |
| 33 | LK | 0.27 | 0/1124 | 0.56 | 0/1507 |
| 34 | LL | 0.31 | 0/983 | 0.63 | 0/1318 |
| 35 | LM | 0.30 | 0/1120 | 0.57 | 0/1507 |
| 36 | LN | 0.34 | 0/1595 | 0.65 | 2/2132 (0.1%) |
| 37 | LO | 0.32 | 0/1652 | 0.56 | 0/2215 |
| 38 | LP | 0.24 | 0/1217 | 0.54 | 0/1636 |
| 39 | LQ | 0.28 | 0/1033 | 0.59 | 0/1391 |
| 40 | LS | 0.28 | 0/1468 | 0.56 | 0/1975 |
| 41 | LT | 0.24 | 0/1033 | 0.51 | 0/1389 |
| 42 | LV | 0.29 | 0/1013 | 0.52 | 0/1361 |
| 43 | LX | 0.25 | 0/361 | 0.50 | 0/482 |
| 44 | LY | 0.26 | 0/1079 | 0.57 | 0/1443 |
| 45 | Ld | 0.34 | 0/904 | 0.55 | 0/1209 |
| 46 | Le | 0.27 | 0/1043 | 0.55 | 0/1389 |
| 47 | Lf | 0.29 | 0/883 | 0.59 | 0/1187 |
| 48 | Lh | 0.31 | 0/1006 | 0.64 | 1/1338 (0.1%) |
| 49 | Li | 0.28 | 0/738 | 0.61 | 0/971 |
| 50 | Lj | 0.29 | 0/606 | 0.63 | 0/803 |
| 51 | Lq | 0.28 | 0/1621 | 0.59 | 0/2180 |
| All | All | 0.30 | 0/144419 | 0.69 | 43/206585 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 28 | LB | 0 | 1 |
| 36 | LN | 0 | 1 |
| 51 | Lq | 0 | 1 |
| All | All | 0 | 3 |

There are no bond length outliers.

All (43) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | C1 | 1050 | C | N3-C2-O2 | -12.14 | 113.41 | 121.90 |
| 1 | C1 | 1050 | C | N1-C2-O2 | 10.77 | 125.36 | 118.90 |
| 1 | C1 | 136 | C | N3-C2-O2 | -8.71 | 115.80 | 121.90 |
| 1 | C1 | 2723 | C | N3-C2-O2 | -7.43 | 116.70 | 121.90 |
| 1 | C1 | 2452 | C | N3-C2-O2 | -7.21 | 116.85 | 121.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | C1 | 3209 | U | P-O3'-C3' | 7.18 | 128.31 | 119.70 |
| 1 | C1 | 1051 | C | N3-C2-O2 | -6.91 | 117.06 | 121.90 |
| 1 | C1 | 3267 | G | C4'-C3'-C2' | -6.61 | 96.00 | 102.60 |
| 1 | C1 | 1051 | C | C6-N1-C2 | -6.57 | 117.67 | 120.30 |
| 1 | C1 | 83 | C | C2-N3-C4 | -6.50 | 116.65 | 119.90 |
| 1 | C1 | 127 | G | N3-C4-N9 | 6.49 | 129.89 | 126.00 |
| 1 | C1 | 249 | C | N3-C2-O2 | -6.35 | 117.46 | 121.90 |
| 1 | C1 | 72 | C | C2-N3-C4 | -6.30 | 116.75 | 119.90 |
| 1 | C1 | 3015 | U | C2-N1-C1' | 6.29 | 125.25 | 117.70 |
| 1 | C1 | 136 | C | N1-C2-O2 | 6.23 | 122.64 | 118.90 |
| 1 | C1 | 799 | C | N3-C2-O2 | -6.16 | 117.59 | 121.90 |
| 10 | CI | 313 | ARG | CB-CG-CD | 6.12 | 127.52 | 111.60 |
| 48 | Lh | 27 | LEU | CA-CB-CG | 5.87 | 128.79 | 115.30 |
| 1 | C1 | 1050 | C | C6-N1-C2 | -5.76 | 118.00 | 120.30 |
| 14 | LF | 13 | LEU | CA-CB-CG | 5.74 | 128.51 | 115.30 |
| 1 | C1 | 249 | C | N1-C2-O2 | 5.69 | 122.31 | 118.90 |
| 36 | LN | 39 | ALA | C-N-CA | 5.67 | 135.88 | 121.70 |
| 1 | C1 | 1157 | C | C6-N1-C2 | 5.63 | 122.55 | 120.30 |
| 1 | C1 | 2752 | G | C5-C6-O6 | 5.54 | 131.92 | 128.60 |
| 1 | C1 | 83 | C | N1-C2-N3 | 5.51 | 123.06 | 119.20 |
| 1 | C1 | 127 | G | C8-N9-C1' | -5.48 | 119.88 | 127.00 |
| 1 | C1 | 127 | G | C4-N9-C1' | 5.42 | 133.55 | 126.50 |
| 1 | C1 | 1134 | G | O4'-C1'-N9 | 5.36 | 112.49 | 108.20 |
| 17 | CP | 576 | PHE | CB-CA-C | -5.32 | 99.75 | 110.40 |
| 1 | C1 | 2752 | G | N1-C6-O6 | -5.32 | 116.71 | 119.90 |
| 1 | C1 | 442 | C | C2-N1-C1' | 5.27 | 124.60 | 118.80 |
| 1 | C1 | 3015 | U | N1-C2-O2 | 5.27 | 126.49 | 122.80 |
| 36 | LN | 127 | TYR | CB-CA-C | -5.26 | 99.87 | 110.40 |
| 1 | C1 | 799 | C | N1-C2-O2 | 5.26 | 122.06 | 118.90 |
| 3 | CA | 108 | PRO | CB-CA-C | -5.26 | 98.84 | 112.00 |
| 11 | CJ | 119 | PRO | CA-N-CD | -5.23 | 104.17 | 111.50 |
| 1 | C1 | 1204 | G | O4'-C1'-N9 | 5.14 | 112.31 | 108.20 |
| 1 | C1 | 398 | G | O4'-C1'-N9 | 5.13 | 112.30 | 108.20 |
| 1 | C1 | 136 | C | C6-N1-C2 | -5.09 | 118.26 | 120.30 |
| 1 | C1 | 1072 | G | N1-C2-N2 | -5.08 | 111.63 | 116.20 |
| 1 | C1 | 3289 | C | N1-C2-O2 | 5.08 | 121.95 | 118.90 |
| 1 | C1 | 3088 | U | C2-N1-C1' | 5.07 | 123.79 | 117.70 |
| 1 | C1 | 1073 | G | N1-C2-N2 | -5.05 | 111.65 | 116.20 |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 28 | LB | 17 | LEU | Peptide |
| 36 | LN | 39 | ALA | Peptide |
| 51 | Lq | 60 | ARG | 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 | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 3 | CA | 247/316 (78%) | 232 (94%) | 15 (6%) | 0 | 100 | 100 |
| 4 | CB | 256/391 (66%) | 239 (93%) | 17 (7%) | 0 | 100 | 100 |
| 5 | CC | 283/801 (35%) | 268 (95%) | 14 (5%) | 1 (0%) | 30 | 63 |
| 6 | CE | 459/598 (77%) | 444 (97%) | 15 (3%) | 0 | 100 | 100 |
| 7 | CF | 243/270 (90%) | 230 (95%) | 11 (4%) | 2 (1%) | 16 | 48 |
| 8 | CG | 175/184 (95%) | 167 (95%) | 8 (5%) | 0 | 100 | 100 |
| 9 | CH | 499/661 (76%) | 470 (94%) | 28 (6%) | 1 (0%) | 44 | 74 |
| 10 | CI | 144/414 (35%) | 134 (93%) | 10 (7%) | 0 | 100 | 100 |
| 11 | CJ | 373/679 (55%) | 355 (95%) | 18 (5%) | 0 | 100 | 100 |
| 12 | CK | 234/261 (90%) | 221 (94%) | 13 (6%) | 0 | 100 | 100 |
| 13 | CL | 393/558 (70%) | 361 (92%) | 29 (7%) | 3 (1%) | 16 | 48 |
| 14 | CM | 219/249 (88%) | 209 (95%) | 10 (5%) | 0 | 100 | 100 |
| 14 | LF | 245/249 (98%) | 237 (97%) | 7 (3%) | 1 (0%) | 30 | 63 |
| 15 | CN | 244/246 (99%) | 228 (93%) | 16 (7%) | 0 | 100 | 100 |
| 16 | CO | 56/120 (47%) | 55 (98%) | 1 (2%) | 0 | 100 | 100 |
| 17 | CP | 354/751 (47%) | 332 (94%) | 21 (6%) | 1 (0%) | 37 | 68 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 18 | CQ | 123/225 (55%) | 119 (97%) | 4 (3%) | 0 | 100 | 100 |
| 19 | CR | 159/237 (67%) | 156 (98%) | 3 (2%) | 0 | 100 | 100 |
| 20 | CS | 221/834 (26%) | 213 (96%) | 8 (4%) | 0 | 100 | 100 |
| 21 | CT | 478/688 (70%) | 456 (95%) | 21 (4%) | 1 (0%) | 44 | 74 |
| 22 | CU | 174/451 (39%) | 169 (97%) | 4 (2%) | 1 (1%) | 22 | 53 |
| 23 | CV | 137/147 (93%) | 134 (98%) | 2 (2%) | 1 (1%) | 19 | 51 |
| 24 | CX | 86/203 (42%) | 84 (98%) | 2 (2%) | 0 | 100 | 100 |
| 25 | CY | 351/788 (44%) | 323 (92%) | 27 (8%) | 1 (0%) | 37 | 68 |
| 26 | Cb | 622/924 (67%) | 575 (92%) | 45 (7%) | 2 (0%) | 37 | 68 |
| 27 | Cz | 68/123 (55%) | 66 (97%) | 2 (3%) | 0 | 100 | 100 |
| 28 | LB | 335/392 (86%) | 315 (94%) | 18 (5%) | 2 (1%) | 22 | 53 |
| 29 | LC | 360/365 (99%) | 344 (96%) | 16 (4%) | 0 | 100 | 100 |
| 30 | LE | 175/200 (88%) | 167 (95%) | 7 (4%) | 1 (1%) | 22 | 53 |
| 31 | LG | 200/262 (76%) | 192 (96%) | 8 (4%) | 0 | 100 | 100 |
| 32 | LH | 188/192 (98%) | 181 (96%) | 7 (4%) | 0 | 100 | 100 |
| 33 | LK | 142/165 (86%) | 134 (94%) | 6 (4%) | 2 (1%) | 9 | 34 |
| 34 | LL | 115/213 (54%) | 106 (92%) | 8 (7%) | 1 (1%) | 14 | 45 |
| 35 | LM | 135/142 (95%) | 128 (95%) | 7 (5%) | 0 | 100 | 100 |
| 36 | LN | 179/203 (88%) | 168 (94%) | 9 (5%) | 2 (1%) | 12 | 39 |
| 37 | LO | 202/204 (99%) | 190 (94%) | 10 (5%) | 2 (1%) | 13 | 42 |
| 38 | LP | 147/187 (79%) | 144 (98%) | 3 (2%) | 0 | 100 | 100 |
| 39 | LQ | 127/213 (60%) | 122 (96%) | 5 (4%) | 0 | 100 | 100 |
| 40 | LS | 172/174 (99%) | 166 (96%) | 6 (4%) | 0 | 100 | 100 |
| 41 | LT | 124/160 (78%) | 119 (96%) | 4 (3%) | 1 (1%) | 16 | 48 |
| 42 | LV | 133/139 (96%) | 131 (98%) | 2 (2%) | 0 | 100 | 100 |
| 43 | LX | 43/156 (28%) | 43 (100%) | 0 | 0 | 100 | 100 |
| 44 | LY | 132/138 (96%) | 128 (97%) | 4 (3%) | 0 | 100 | 100 |
| 45 | Ld | 107/120 (89%) | 102 (95%) | 5 (5%) | 0 | 100 | 100 |
| 46 | Le | 125/131 (95%) | 120 (96%) | 5 (4%) | 0 | 100 | 100 |
| 47 | Lf | 106/109 (97%) | 103 (97%) | 3 (3%) | 0 | 100 | 100 |
| 48 | Lh | 119/935 (13%) | 111 (93%) | 8 (7%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 49 | Li | 86/110 (78%) | 85 (99%) | 1 (1%) | 0 | 100 | 100 |
| 50 | Lj | 72/95 (76%) | 69 (96%) | 3 (4%) | 0 | 100 | 100 |
| 51 | Lq | 205/217 (94%) | 180 (88%) | 25 (12%) | 0 | 100 | 100 |
| All | All | 10572/16590 (64%) | 10025 (95%) | 521 (5%) | 26 (0%) | 45 | 74 |

All (26) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | CF | 239 | ALA |
| 21 | CT | 502 | ARG |
| 36 | LN | 40 | SER |
| 37 | LO | 191 | VAL |
| 17 | CP | 442 | GLU |
| 22 | CU | 359 | ASP |
| 25 | CY | 523 | PRO |
| 26 | Cb | 294 | ARG |
| 28 | LB | 18 | PRO |
| 33 | LK | 51 | ALA |
| 7 | CF | 188 | ALA |
| 13 | CL | 224 | ASP |
| 13 | CL | 439 | ASP |
| 26 | Cb | 576 | PHE |
| 28 | LB | 368 | HIS |
| 9 | CH | 197 | ALA |
| 23 | CV | 85 | SER |
| 30 | LE | 85 | GLY |
| 14 | LF | 118 | ASN |
| 36 | LN | 124 | ASP |
| 13 | CL | 446 | ASP |
| 33 | LK | 160 | ILE |
| 37 | LO | 192 | ASP |
| 41 | LT | 44 | VAL |
| 34 | LL | 47 | ALA |
| 5 | CC | 251 | 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 | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 3 | CA | 223/276 (81%) | 219 (98%) | 4 (2%) | 54 | 76 |
| 4 | CB | 222/329 (68%) | 222 (100%) | 0 | 100 | 100 |
| 5 | CC | 266/708 (38%) | 262 (98%) | 4 (2%) | 60 | 80 |
| 6 | CE | 398/517 (77%) | 397 (100%) | 1 (0%) | 91 | 95 |
| 7 | CF | 214/236 (91%) | 213 (100%) | 1 (0%) | 86 | 92 |
| 8 | CG | 150/155 (97%) | 149 (99%) | 1 (1%) | 81 | 90 |
| 9 | CH | 448/575 (78%) | 440 (98%) | 8 (2%) | 54 | 76 |
| 10 | CI | 121/336 (36%) | 120 (99%) | 1 (1%) | 79 | 89 |
| 11 | CJ | 330/579 (57%) | 330 (100%) | 0 | 100 | 100 |
| 12 | CK | 204/225 (91%) | 203 (100%) | 1 (0%) | 86 | 92 |
| 13 | CL | 72/458 (16%) | 72 (100%) | 0 | 100 | 100 |
| 14 | CM | 191/215 (89%) | 191 (100%) | 0 | 100 | 100 |
| 14 | LF | 213/215 (99%) | 212 (100%) | 1 (0%) | 86 | 92 |
| 15 | CN | 206/206 (100%) | 205 (100%) | 1 (0%) | 86 | 92 |
| 16 | CO | 48/99 (48%) | 48 (100%) | 0 | 100 | 100 |
| 17 | CP | 302/632 (48%) | 297 (98%) | 5 (2%) | 56 | 78 |
| 18 | CQ | 107/192 (56%) | 107 (100%) | 0 | 100 | 100 |
| 19 | CR | 144/206 (70%) | 144 (100%) | 0 | 100 | 100 |
| 20 | CS | 188/716 (26%) | 187 (100%) | 1 (0%) | 86 | 92 |
| 21 | CT | 427/600 (71%) | 425 (100%) | 2 (0%) | 86 | 92 |
| 22 | CU | 149/376 (40%) | 149 (100%) | 0 | 100 | 100 |
| 23 | CV | 109/112 (97%) | 109 (100%) | 0 | 100 | 100 |
| 24 | CX | 76/172 (44%) | 76 (100%) | 0 | 100 | 100 |
| 25 | CY | 313/686 (46%) | 311 (99%) | 2 (1%) | 84 | 91 |
| 26 | Cb | 535/779 (69%) | 526 (98%) | 9 (2%) | 56 | 78 |
| 27 | Cz | 60/107 (56%) | 60 (100%) | 0 | 100 | 100 |
| 28 | LB | 289/331 (87%) | 287 (99%) | 2 (1%) | 81 | 90 |
| 29 | LC | 283/285 (99%) | 283 (100%) | 0 | 100 | 100 |
| 30 | LE | 151/166 (91%) | 143 (95%) | 8 (5%) | 19 | 48 |
| 31 | LG | 175/222 (79%) | 174 (99%) | 1 (1%) | 84 | 91 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|-------------|-----|
| 32 | LH | 167/169 (99%) | 165 (99%) | 2 (1%) | 67 | 83 |
| 33 | LK | 121/136 (89%) | 120 (99%) | 1 (1%) | 79 | 89 |
| 34 | LL | 99/176 (56%) | 99 (100%) | 0 | 100 | 100 |
| 35 | LM | 115/117 (98%) | 115 (100%) | 0 | 100 | 100 |
| 36 | LN | 164/180 (91%) | 161 (98%) | 3 (2%) | 54 | 76 |
| 37 | LO | 163/163 (100%) | 163 (100%) | 0 | 100 | 100 |
| 38 | LP | 123/152 (81%) | 122 (99%) | 1 (1%) | 79 | 89 |
| 39 | LQ | 110/178 (62%) | 110 (100%) | 0 | 100 | 100 |
| 40 | LS | 154/154 (100%) | 153 (99%) | 1 (1%) | 84 | 91 |
| 41 | LT | 109/135 (81%) | 108 (99%) | 1 (1%) | 75 | 88 |
| 42 | LV | 99/102 (97%) | 98 (99%) | 1 (1%) | 73 | 86 |
| 43 | LX | 36/129 (28%) | 36 (100%) | 0 | 100 | 100 |
| 44 | LY | 117/119 (98%) | 117 (100%) | 0 | 100 | 100 |
| 45 | Ld | 95/105 (90%) | 94 (99%) | 1 (1%) | 70 | 84 |
| 46 | Le | 110/114 (96%) | 110 (100%) | 0 | 100 | 100 |
| 47 | Lf | 89/90 (99%) | 89 (100%) | 0 | 100 | 100 |
| 48 | Lh | 108/781 (14%) | 107 (99%) | 1 (1%) | 75 | 88 |
| 49 | Li | 75/93 (81%) | 74 (99%) | 1 (1%) | 65 | 82 |
| 50 | Lj | 61/78 (78%) | 61 (100%) | 0 | 100 | 100 |
| 51 | Lq | 179/189 (95%) | 174 (97%) | 5 (3%) | 38 | 66 |
| All | All | 8908/14071 (63%) | 8837 (99%) | 71 (1%) | 77 | 89 |

All (71) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | CA | 63 | ARG |
| 3 | CA | 64 | LYS |
| 3 | CA | 158 | LEU |
| 3 | CA | 249 | SER |
| 5 | CC | 157 | VAL |
| 5 | CC | 161 | ASP |
| 5 | CC | 164 | ASP |
| 5 | CC | 406 | ARG |
| 6 | CE | 488 | ASN |
| 7 | CF | 91 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | CG | 58 | CYS |
| 9 | CH | 128 | LYS |
| 9 | CH | 174 | PHE |
| 9 | CH | 179 | LYS |
| 9 | CH | 201 | LYS |
| 9 | CH | 286 | LEU |
| 9 | CH | 289 | MET |
| 9 | CH | 290 | ASP |
| 9 | CH | 291 | ILE |
| 10 | CI | 313 | ARG |
| 12 | CK | 149 | ARG |
| 15 | CN | 123 | ARG |
| 17 | CP | 286 | ASN |
| 17 | CP | 397 | HIS |
| 17 | CP | 517 | VAL |
| 17 | CP | 562 | LEU |
| 17 | CP | 563 | THR |
| 20 | CS | 834 | ARG |
| 21 | CT | 277 | ARG |
| 21 | CT | 413 | LYS |
| 25 | CY | 701 | ARG |
| 25 | CY | 747 | ARG |
| 26 | Cb | 162 | ARG |
| 26 | Cb | 291 | VAL |
| 26 | Cb | 509 | LEU |
| 26 | Cb | 512 | VAL |
| 26 | Cb | 584 | GLU |
| 26 | Cb | 587 | ARG |
| 26 | Cb | 589 | ASN |
| 26 | Cb | 821 | ARG |
| 26 | Cb | 871 | LYS |
| 28 | LB | 18 | PRO |
| 28 | LB | 378 | LYS |
| 30 | LE | 66 | ARG |
| 30 | LE | 68 | LYS |
| 30 | LE | 74 | LYS |
| 30 | LE | 107 | VAL |
| 30 | LE | 154 | VAL |
| 30 | LE | 169 | LEU |
| 30 | LE | 170 | ILE |
| 30 | LE | 176 | VAL |
| 14 | LF | 94 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31 | LG | 191 | THR |
| 32 | LH | 92 | LEU |
| 32 | LH | 105 | LEU |
| 33 | LK | 48 | LYS |
| 36 | LN | 27 | CYS |
| 36 | LN | 41 | ARG |
| 36 | LN | 66 | VAL |
| 38 | LP | 174 | ARG |
| 40 | LS | 119 | ARG |
| 41 | LT | 92 | ARG |
| 42 | LV | 95 | LEU |
| 45 | Ld | 21 | THR |
| 48 | Lh | 17 | LYS |
| 49 | Li | 37 | ARG |
| 51 | Lq | 16 | LEU |
| 51 | Lq | 17 | LEU |
| 51 | Lq | 24 | LYS |
| 51 | Lq | 39 | LYS |
| 51 | Lq | 92 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | CA | 193 | ASN |
| 4 | CB | 234 | HIS |
| 4 | CB | 277 | ASN |
| 7 | CF | 38 | GLN |
| 9 | CH | 73 | GLN |
| 9 | CH | 258 | GLN |
| 10 | CI | 269 | HIS |
| 11 | CJ | 259 | GLN |
| 11 | CJ | 381 | GLN |
| 12 | CK | 4 | ASN |
| 15 | CN | 162 | HIS |
| 16 | CO | 42 | GLN |
| 17 | CP | 343 | GLN |
| 17 | CP | 437 | ASN |
| 17 | CP | 474 | ASN |
| 19 | CR | 148 | GLN |
| 20 | CS | 744 | GLN |
| 21 | CT | 436 | GLN |
| 21 | CT | 602 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | CU | 217 | HIS |
| 22 | CU | 305 | GLN |
| 23 | CV | 17 | ASN |
| 23 | CV | 23 | GLN |
| 24 | CX | 102 | ASN |
| 25 | CY | 443 | ASN |
| 25 | CY | 481 | ASN |
| 25 | CY | 509 | HIS |
| 26 | Cb | 210 | ASN |
| 26 | Cb | 437 | ASN |
| 26 | Cb | 517 | ASN |
| 29 | LC | 280 | ASN |
| 14 | LF | 99 | ASN |
| 14 | LF | 116 | GLN |
| 14 | LF | 119 | ASN |
| 14 | LF | 178 | ASN |
| 33 | LK | 70 | GLN |
| 35 | LM | 106 | GLN |
| 40 | LS | 8 | GLN |
| 40 | LS | 62 | ASN |
| 51 | Lq | 200 | ASN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | C1 | 2145/3341 (64%) | 455 (21%) | 27 (1%) |
| 2 | C2 | 254/319 (79%) | 60 (23%) | 6 (2%) |
| All | All | 2399/3660 (65%) | 515 (21%) | 33 (1%) |

All (515) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C1 | 14 | U |
| 1 | C1 | 26 | A |
| 1 | C1 | 41 | G |
| 1 | C1 | 49 | A |
| 1 | C1 | 59 | G |
| 1 | C1 | 60 | A |
| 1 | C1 | 65 | A |
| 1 | C1 | 66 | A |
| 1 | C1 | 74 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C1 | 92 | G |
| 1 | C1 | 93 | C |
| 1 | C1 | 94 | G |
| 1 | C1 | 96 | G |
| 1 | C1 | 105 | C |
| 1 | C1 | 110 | G |
| 1 | C1 | 111 | C |
| 1 | C1 | 116 | A |
| 1 | C1 | 122 | A |
| 1 | C1 | 128 | G |
| 1 | C1 | 129 | C |
| 1 | C1 | 131 | U |
| 1 | C1 | 132 | C |
| 1 | C1 | 133 | G |
| 1 | C1 | 134 | G |
| 1 | C1 | 135 | C |
| 1 | C1 | 136 | C |
| 1 | C1 | 138 | G |
| 1 | C1 | 143 | G |
| 1 | C1 | 150 | G |
| 1 | C1 | 151 | G |
| 1 | C1 | 152 | A |
| 1 | C1 | 156 | G |
| 1 | C1 | 163 | U |
| 1 | C1 | 176 | U |
| 1 | C1 | 177 | U |
| 1 | C1 | 180 | G |
| 1 | C1 | 183 | U |
| 1 | C1 | 193 | C |
| 1 | C1 | 203 | C |
| 1 | C1 | 206 | A |
| 1 | C1 | 211 | G |
| 1 | C1 | 212 | A |
| 1 | C1 | 225 | G |
| 1 | C1 | 232 | G |
| 1 | C1 | 240 | U |
| 1 | C1 | 244 | U |
| 1 | C1 | 253 | U |
| 1 | C1 | 257 | A |
| 1 | C1 | 258 | C |
| 1 | C1 | 261 | G |
| 1 | C1 | 262 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C1 | 275 | G |
| 1 | C1 | 276 | A |
| 1 | C1 | 277 | A |
| 1 | C1 | 287 | A |
| 1 | C1 | 299 | A |
| 1 | C1 | 300 | A |
| 1 | C1 | 302 | U |
| 1 | C1 | 309 | A |
| 1 | C1 | 310 | A |
| 1 | C1 | 315 | A |
| 1 | C1 | 321 | C |
| 1 | C1 | 325 | C |
| 1 | C1 | 330 | A |
| 1 | C1 | 331 | C |
| 1 | C1 | 342 | C |
| 1 | C1 | 343 | A |
| 1 | C1 | 344 | A |
| 1 | C1 | 368 | G |
| 1 | C1 | 390 | U |
| 1 | C1 | 391 | A |
| 1 | C1 | 393 | C |
| 1 | C1 | 394 | A |
| 1 | C1 | 395 | C |
| 1 | C1 | 413 | G |
| 1 | C1 | 414 | A |
| 1 | C1 | 433 | U |
| 1 | C1 | 434 | G |
| 1 | C1 | 439 | C |
| 1 | C1 | 444 | G |
| 1 | C1 | 446 | U |
| 1 | C1 | 447 | C |
| 1 | C1 | 457 | U |
| 1 | C1 | 458 | C |
| 1 | C1 | 459 | U |
| 1 | C1 | 469 | A |
| 1 | C1 | 470 | C |
| 1 | C1 | 472 | C |
| 1 | C1 | 474 | G |
| 1 | C1 | 477 | G |
| 1 | C1 | 488 | A |
| 1 | C1 | 493 | C |
| 1 | C1 | 508 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C1 | 509 | A |
| 1 | C1 | 510 | U |
| 1 | C1 | 511 | A |
| 1 | C1 | 513 | A |
| 1 | C1 | 517 | C |
| 1 | C1 | 521 | G |
| 1 | C1 | 526 | G |
| 1 | C1 | 534 | U |
| 1 | C1 | 535 | C |
| 1 | C1 | 544 | U |
| 1 | C1 | 546 | A |
| 1 | C1 | 547 | U |
| 1 | C1 | 548 | A |
| 1 | C1 | 559 | U |
| 1 | C1 | 579 | A |
| 1 | C1 | 582 | A |
| 1 | C1 | 587 | G |
| 1 | C1 | 589 | U |
| 1 | C1 | 590 | C |
| 1 | C1 | 591 | U |
| 1 | C1 | 592 | G |
| 1 | C1 | 594 | A |
| 1 | C1 | 596 | G |
| 1 | C1 | 598 | A |
| 1 | C1 | 607 | U |
| 1 | C1 | 608 | A |
| 1 | C1 | 609 | A |
| 1 | C1 | 614 | C |
| 1 | C1 | 623 | C |
| 1 | C1 | 633 | A |
| 1 | C1 | 647 | A |
| 1 | C1 | 663 | G |
| 1 | C1 | 664 | A |
| 1 | C1 | 668 | U |
| 1 | C1 | 674 | U |
| 1 | C1 | 678 | A |
| 1 | C1 | 712 | A |
| 1 | C1 | 716 | C |
| 1 | C1 | 718 | U |
| 1 | C1 | 719 | C |
| 1 | C1 | 731 | G |
| 1 | C1 | 739 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | C1 | 742 | A |
| 1 | C1 | 744 | G |
| 1 | C1 | 748 | U |
| 1 | C1 | 749 | C |
| 1 | C1 | 751 | G |
| 1 | C1 | 752 | A |
| 1 | C1 | 755 | G |
| 1 | C1 | 757 | U |
| 1 | C1 | 758 | U |
| 1 | C1 | 761 | A |
| 1 | C1 | 762 | G |
| 1 | C1 | 766 | G |
| 1 | C1 | 767 | A |
| 1 | C1 | 787 | A |
| 1 | C1 | 798 | A |
| 1 | C1 | 799 | C |
| 1 | C1 | 800 | U |
| 1 | C1 | 801 | A |
| 1 | C1 | 887 | G |
| 1 | C1 | 889 | G |
| 1 | C1 | 896 | A |
| 1 | C1 | 898 | A |
| 1 | C1 | 925 | A |
| 1 | C1 | 932 | A |
| 1 | C1 | 933 | A |
| 1 | C1 | 934 | G |
| 1 | C1 | 941 | U |
| 1 | C1 | 942 | C |
| 1 | C1 | 943 | A |
| 1 | C1 | 944 | G |
| 1 | C1 | 959 | C |
| 1 | C1 | 960 | C |
| 1 | C1 | 965 | G |
| 1 | C1 | 974 | G |
| 1 | C1 | 975 | G |
| 1 | C1 | 976 | U |
| 1 | C1 | 982 | G |
| 1 | C1 | 983 | A |
| 1 | C1 | 1031 | C |
| 1 | C1 | 1033 | U |
| 1 | C1 | 1039 | A |
| 1 | C1 | 1046 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | C1 | 1047 | A |
| 1 | C1 | 1048 | G |
| 1 | C1 | 1049 | C |
| 1 | C1 | 1050 | C |
| 1 | C1 | 1054 | G |
| 1 | C1 | 1057 | A |
| 1 | C1 | 1058 | C |
| 1 | C1 | 1063 | C |
| 1 | C1 | 1064 | U |
| 1 | C1 | 1065 | G |
| 1 | C1 | 1073 | G |
| 1 | C1 | 1074 | C |
| 1 | C1 | 1076 | U |
| 1 | C1 | 1079 | G |
| 1 | C1 | 1080 | A |
| 1 | C1 | 1085 | A |
| 1 | C1 | 1086 | U |
| 1 | C1 | 1095 | G |
| 1 | C1 | 1097 | G |
| 1 | C1 | 1098 | G |
| 1 | C1 | 1114 | C |
| 1 | C1 | 1122 | G |
| 1 | C1 | 1124 | G |
| 1 | C1 | 1125 | A |
| 1 | C1 | 1126 | U |
| 1 | C1 | 1135 | A |
| 1 | C1 | 1141 | A |
| 1 | C1 | 1157 | C |
| 1 | C1 | 1158 | C |
| 1 | C1 | 1159 | G |
| 1 | C1 | 1163 | U |
| 1 | C1 | 1164 | G |
| 1 | C1 | 1172 | A |
| 1 | C1 | 1174 | C |
| 1 | C1 | 1175 | A |
| 1 | C1 | 1178 | C |
| 1 | C1 | 1179 | A |
| 1 | C1 | 1180 | C |
| 1 | C1 | 1184 | A |
| 1 | C1 | 1189 | G |
| 1 | C1 | 1190 | C |
| 1 | C1 | 1191 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | C1 | 1204 | G |
| 1 | C1 | 1218 | G |
| 1 | C1 | 1227 | A |
| 1 | C1 | 1228 | G |
| 1 | C1 | 1240 | U |
| 1 | C1 | 1245 | A |
| 1 | C1 | 1247 | U |
| 1 | C1 | 1254 | C |
| 1 | C1 | 1268 | A |
| 1 | C1 | 1269 | A |
| 1 | C1 | 1271 | G |
| 1 | C1 | 1272 | U |
| 1 | C1 | 1286 | A |
| 1 | C1 | 1287 | U |
| 1 | C1 | 1288 | G |
| 1 | C1 | 1289 | G |
| 1 | C1 | 1291 | U |
| 1 | C1 | 1294 | C |
| 1 | C1 | 1295 | G |
| 1 | C1 | 1298 | C |
| 1 | C1 | 1312 | A |
| 1 | C1 | 1314 | A |
| 1 | C1 | 1330 | A |
| 1 | C1 | 1331 | G |
| 1 | C1 | 1332 | A |
| 1 | C1 | 1333 | A |
| 1 | C1 | 1334 | A |
| 1 | C1 | 1335 | C |
| 1 | C1 | 1336 | G |
| 1 | C1 | 1337 | A |
| 1 | C1 | 1347 | G |
| 1 | C1 | 1368 | A |
| 1 | C1 | 1374 | G |
| 1 | C1 | 1381 | A |
| 1 | C1 | 1399 | G |
| 1 | C1 | 1401 | A |
| 1 | C1 | 1416 | G |
| 1 | C1 | 1419 | C |
| 1 | C1 | 1434 | A |
| 1 | C1 | 1861 | G |
| 1 | C1 | 1864 | C |
| 1 | C1 | 1865 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | C1 | 1866 | A |
| 1 | C1 | 1867 | U |
| 1 | C1 | 1874 | A |
| 1 | C1 | 1875 | A |
| 1 | C1 | 1883 | C |
| 1 | C1 | 1886 | C |
| 1 | C1 | 1897 | C |
| 1 | C1 | 1900 | A |
| 1 | C1 | 1901 | A |
| 1 | C1 | 2075 | A |
| 1 | C1 | 2088 | A |
| 1 | C1 | 2287 | G |
| 1 | C1 | 2288 | A |
| 1 | C1 | 2294 | A |
| 1 | C1 | 2295 | C |
| 1 | C1 | 2297 | G |
| 1 | C1 | 2298 | U |
| 1 | C1 | 2302 | U |
| 1 | C1 | 2310 | A |
| 1 | C1 | 2325 | A |
| 1 | C1 | 2327 | C |
| 1 | C1 | 2332 | G |
| 1 | C1 | 2335 | A |
| 1 | C1 | 2338 | G |
| 1 | C1 | 2339 | G |
| 1 | C1 | 2342 | U |
| 1 | C1 | 2343 | G |
| 1 | C1 | 2345 | C |
| 1 | C1 | 2347 | A |
| 1 | C1 | 2350 | U |
| 1 | C1 | 2355 | G |
| 1 | C1 | 2356 | G |
| 1 | C1 | 2359 | A |
| 1 | C1 | 2361 | A |
| 1 | C1 | 2362 | G |
| 1 | C1 | 2363 | A |
| 1 | C1 | 2364 | A |
| 1 | C1 | 2396 | U |
| 1 | C1 | 2397 | G |
| 1 | C1 | 2399 | G |
| 1 | C1 | 2407 | A |
| 1 | C1 | 2410 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | C1 | 2414 | G |
| 1 | C1 | 2415 | U |
| 1 | C1 | 2424 | G |
| 1 | C1 | 2425 | G |
| 1 | C1 | 2428 | G |
| 1 | C1 | 2430 | A |
| 1 | C1 | 2433 | U |
| 1 | C1 | 2434 | U |
| 1 | C1 | 2435 | C |
| 1 | C1 | 2436 | G |
| 1 | C1 | 2437 | G |
| 1 | C1 | 2438 | C |
| 1 | C1 | 2439 | G |
| 1 | C1 | 2444 | U |
| 1 | C1 | 2449 | U |
| 1 | C1 | 2453 | A |
| 1 | C1 | 2455 | U |
| 1 | C1 | 2456 | A |
| 1 | C1 | 2464 | U |
| 1 | C1 | 2465 | G |
| 1 | C1 | 2467 | U |
| 1 | C1 | 2484 | G |
| 1 | C1 | 2551 | A |
| 1 | C1 | 2560 | G |
| 1 | C1 | 2564 | G |
| 1 | C1 | 2730 | C |
| 1 | C1 | 2740 | U |
| 1 | C1 | 2749 | G |
| 1 | C1 | 2759 | A |
| 1 | C1 | 2760 | A |
| 1 | C1 | 2761 | A |
| 1 | C1 | 2775 | A |
| 1 | C1 | 2777 | A |
| 1 | C1 | 2778 | A |
| 1 | C1 | 2782 | G |
| 1 | C1 | 2783 | C |
| 1 | C1 | 2784 | U |
| 1 | C1 | 2785 | U |
| 1 | C1 | 2806 | G |
| 1 | C1 | 2818 | U |
| 1 | C1 | 2819 | U |
| 1 | C1 | 2820 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | C1 | 2845 | A |
| 1 | C1 | 2847 | C |
| 1 | C1 | 2856 | G |
| 1 | C1 | 2857 | C |
| 1 | C1 | 2862 | U |
| 1 | C1 | 2869 | A |
| 1 | C1 | 2889 | C |
| 1 | C1 | 2893 | U |
| 1 | C1 | 2894 | A |
| 1 | C1 | 2899 | A |
| 1 | C1 | 2902 | U |
| 1 | C1 | 2904 | A |
| 1 | C1 | 2917 | C |
| 1 | C1 | 2924 | G |
| 1 | C1 | 2925 | A |
| 1 | C1 | 2935 | G |
| 1 | C1 | 2936 | U |
| 1 | C1 | 2942 | C |
| 1 | C1 | 2948 | G |
| 1 | C1 | 2950 | U |
| 1 | C1 | 2951 | G |
| 1 | C1 | 2954 | C |
| 1 | C1 | 2955 | U |
| 1 | C1 | 2956 | C |
| 1 | C1 | 2969 | A |
| 1 | C1 | 3005 | A |
| 1 | C1 | 3006 | A |
| 1 | C1 | 3016 | G |
| 1 | C1 | 3031 | G |
| 1 | C1 | 3035 | G |
| 1 | C1 | 3043 | A |
| 1 | C1 | 3048 | A |
| 1 | C1 | 3049 | C |
| 1 | C1 | 3050 | C |
| 1 | C1 | 3070 | A |
| 1 | C1 | 3074 | C |
| 1 | C1 | 3079 | A |
| 1 | C1 | 3086 | A |
| 1 | C1 | 3087 | A |
| 1 | C1 | 3088 | U |
| 1 | C1 | 3098 | A |
| 1 | C1 | 3099 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | C1 | 3100 | C |
| 1 | C1 | 3101 | G |
| 1 | C1 | 3112 | A |
| 1 | C1 | 3113 | C |
| 1 | C1 | 3118 | A |
| 1 | C1 | 3121 | U |
| 1 | C1 | 3122 | U |
| 1 | C1 | 3124 | U |
| 1 | C1 | 3125 | A |
| 1 | C1 | 3126 | G |
| 1 | C1 | 3127 | A |
| 1 | C1 | 3130 | U |
| 1 | C1 | 3131 | A |
| 1 | C1 | 3132 | U |
| 1 | C1 | 3134 | A |
| 1 | C1 | 3140 | G |
| 1 | C1 | 3145 | C |
| 1 | C1 | 3146 | G |
| 1 | C1 | 3147 | G |
| 1 | C1 | 3153 | U |
| 1 | C1 | 3154 | A |
| 1 | C1 | 3161 | C |
| 1 | C1 | 3162 | A |
| 1 | C1 | 3163 | G |
| 1 | C1 | 3167 | A |
| 1 | C1 | 3170 | C |
| 1 | C1 | 3171 | C |
| 1 | C1 | 3178 | G |
| 1 | C1 | 3183 | C |
| 1 | C1 | 3185 | A |
| 1 | C1 | 3187 | G |
| 1 | C1 | 3199 | A |
| 1 | C1 | 3205 | C |
| 1 | C1 | 3206 | G |
| 1 | C1 | 3210 | U |
| 1 | C1 | 3212 | C |
| 1 | C1 | 3213 | A |
| 1 | C1 | 3217 | U |
| 1 | C1 | 3227 | C |
| 1 | C1 | 3228 | G |
| 1 | C1 | 3229 | G |
| 1 | C1 | 3230 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | C1 | 3244 | C |
| 1 | C1 | 3253 | U |
| 1 | C1 | 3255 | G |
| 1 | C1 | 3256 | A |
| 1 | C1 | 3257 | U |
| 1 | C1 | 3260 | G |
| 1 | C1 | 3274 | U |
| 1 | C1 | 3281 | U |
| 1 | C1 | 3282 | A |
| 1 | C1 | 3285 | G |
| 1 | C1 | 3287 | A |
| 1 | C1 | 3291 | U |
| 1 | C1 | 3293 | G |
| 1 | C1 | 3295 | U |
| 1 | C1 | 3298 | U |
| 1 | C1 | 3303 | U |
| 1 | C1 | 3309 | G |
| 1 | C1 | 3318 | C |
| 1 | C1 | 3322 | C |
| 1 | C1 | 3323 | C |
| 1 | C1 | 3324 | U |
| 1 | C1 | 3329 | C |
| 1 | C1 | 3331 | A |
| 1 | C1 | 3332 | G |
| 1 | C1 | 3333 | A |
| 1 | C1 | 3337 | C |
| 2 | C2 | 23 | U |
| 2 | C2 | 34 | U |
| 2 | C2 | 35 | C |
| 2 | C2 | 39 | G |
| 2 | C2 | 59 | A |
| 2 | C2 | 62 | A |
| 2 | C2 | 63 | G |
| 2 | C2 | 81 | U |
| 2 | C2 | 82 | U |
| 2 | C2 | 84 | C |
| 2 | C2 | 86 | U |
| 2 | C2 | 87 | G |
| 2 | C2 | 88 | A |
| 2 | C2 | 90 | U |
| 2 | C2 | 95 | G |
| 2 | C2 | 97 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C2 | 100 | U |
| 2 | C2 | 103 | G |
| 2 | C2 | 104 | A |
| 2 | C2 | 105 | A |
| 2 | C2 | 106 | C |
| 2 | C2 | 110 | C |
| 2 | C2 | 111 | A |
| 2 | C2 | 112 | U |
| 2 | C2 | 113 | U |
| 2 | C2 | 125 | U |
| 2 | C2 | 151 | C |
| 2 | C2 | 158 | U |
| 2 | C2 | 159 | C |
| 2 | C2 | 160 | A |
| 2 | C2 | 163 | C |
| 2 | C2 | 164 | A |
| 2 | C2 | 165 | U |
| 2 | C2 | 166 | C |
| 2 | C2 | 170 | C |
| 2 | C2 | 173 | U |
| 2 | C2 | 174 | G |
| 2 | C2 | 180 | G |
| 2 | C2 | 181 | U |
| 2 | C2 | 182 | G |
| 2 | C2 | 183 | U |
| 2 | C2 | 189 | A |
| 2 | C2 | 192 | C |
| 2 | C2 | 195 | G |
| 2 | C2 | 196 | G |
| 2 | C2 | 212 | G |
| 2 | C2 | 213 | A |
| 2 | C2 | 214 | A |
| 2 | C2 | 215 | A |
| 2 | C2 | 216 | A |
| 2 | C2 | 219 | A |
| 2 | C2 | 221 | U |
| 2 | C2 | 222 | G |
| 2 | C2 | 289 | G |
| 2 | C2 | 291 | G |
| 2 | C2 | 292 | C |
| 2 | C2 | 295 | G |
| 2 | C2 | 300 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C2 | 301 | A |
| 2 | C2 | 305 | C |

All (33) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | C1 | 150 | G |
| 1 | C1 | 445 | A |
| 1 | C1 | 446 | U |
| 1 | C1 | 508 | G |
| 1 | C1 | 510 | U |
| 1 | C1 | 886 | U |
| 1 | C1 | 897 | G |
| 1 | C1 | 959 | C |
| 1 | C1 | 1063 | C |
| 1 | C1 | 1134 | G |
| 1 | C1 | 2301 | C |
| 1 | C1 | 2360 | A |
| 1 | C1 | 2777 | A |
| 1 | C1 | 2817 | U |
| 1 | C1 | 2898 | A |
| 1 | C1 | 3005 | A |
| 1 | C1 | 3078 | U |
| 1 | C1 | 3112 | A |
| 1 | C1 | 3131 | A |
| 1 | C1 | 3162 | A |
| 1 | C1 | 3204 | G |
| 1 | C1 | 3209 | U |
| 1 | C1 | 3212 | C |
| 1 | C1 | 3229 | G |
| 1 | C1 | 3255 | G |
| 1 | C1 | 3257 | U |
| 1 | C1 | 3297 | U |
| 2 | C2 | 87 | G |
| 2 | C2 | 102 | U |
| 2 | C2 | 163 | C |
| 2 | C2 | 164 | A |
| 2 | C2 | 180 | G |
| 2 | C2 | 181 | U |

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

2 non-standard protein/DNA/RNA residues 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 |
| 5 | SEP | CC | 160 | 5 | 8,9,10 | 0.62 | 0 | 8,12,14 | 0.76 | 0 |
| 5 | TPO | CC | 163 | 5 | 8,10,11 | 0.66 | 0 | 10,14,16 | 1.01 | 1 (10%) |

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 |
|-----|------|-------|-----|------|---------|-----------|-------|
| 5 | SEP | CC | 160 | 5 | - | 4/5/8/10 | - |
| 5 | TPO | CC | 163 | 5 | - | 1/9/11/13 | - |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 5 | CC | 163 | TPO | O-C-CA | -2.42 | 118.43 | 124.78 |

There are no chirality outliers.

All (5) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 5 | CC | 160 | SEP | CB-OG-P-O1P |
| 5 | CC | 160 | SEP | CB-OG-P-O2P |
| 5 | CC | 160 | SEP | CB-OG-P-O3P |
| 5 | CC | 160 | SEP | N-CA-CB-OG |
| 5 | CC | 163 | TPO | O-C-CA-CB |

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 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 | $\# Z > 2$ |
| 52 | GTP | CH | 1001 | - | 26,34,34 | 0.97 | 2 (7%) | 32,54,54 | 0.78 | 1 (3%) |

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 |
|-----|------|-------|------|------|---------|------------|---------|
| 52 | GTP | CH | 1001 | - | - | 7/18/38/38 | 0/3/3/3 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 52 | CH | 1001 | GTP | C5-C6 | -2.63 | 1.42 | 1.47 |
| 52 | CH | 1001 | GTP | C8-N7 | -2.07 | 1.31 | 1.35 |

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 52 | CH | 1001 | GTP | O6-C6-C5 | 2.08 | 128.44 | 124.37 |

There are no chirality outliers.

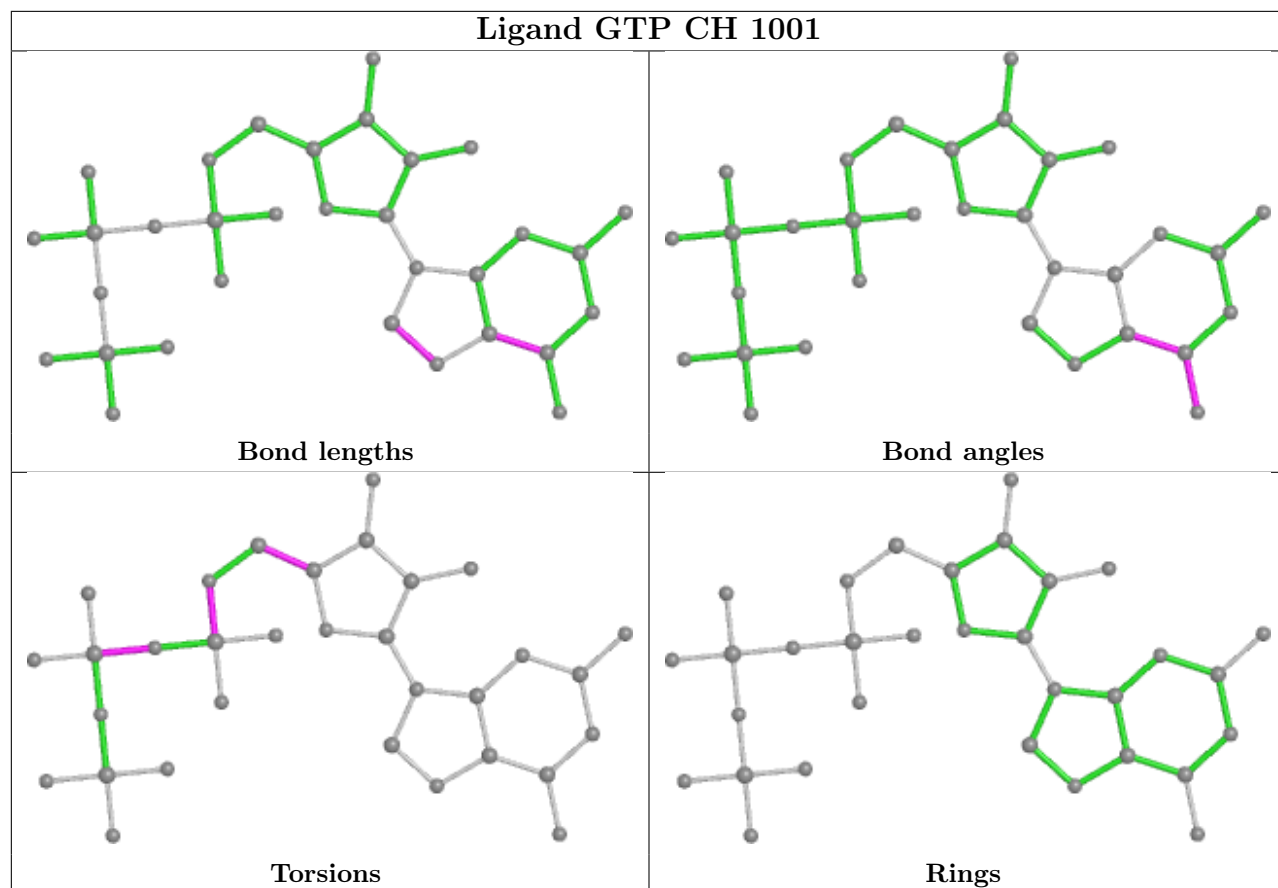
All (7) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 52 | CH | 1001 | GTP | C5'-O5'-PA-O1A |
| 52 | CH | 1001 | GTP | C5'-O5'-PA-O2A |
| 52 | CH | 1001 | GTP | O4'-C4'-C5'-O5' |
| 52 | CH | 1001 | GTP | C3'-C4'-C5'-O5' |
| 52 | CH | 1001 | GTP | C5'-O5'-PA-O3A |
| 52 | CH | 1001 | GTP | PA-O3A-PB-O2B |
| 52 | CH | 1001 | GTP | PA-O3A-PB-O1B |

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.