



wwPDB EM Validation Summary Report ⓘ

Nov 22, 2022 – 01:37 AM EST

PDB ID : 7N2V
EMDB ID : EMD-24134
Title : Elongating 70S ribosome complex in a spectinomycin-stalled intermediate state of translocation bound to EF-G in an active, GTP conformation (INT1)
Authors : Rundlet, E.J.; Holm, M.; Schacherl, M.; Natchiar, K.S.; Altman, R.B.; Spahn, C.M.T.; Myasnikov, A.G.; Blanchard, S.C.
Deposited on : 2021-05-29
Resolution : 2.54 Å(reported)

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

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

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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

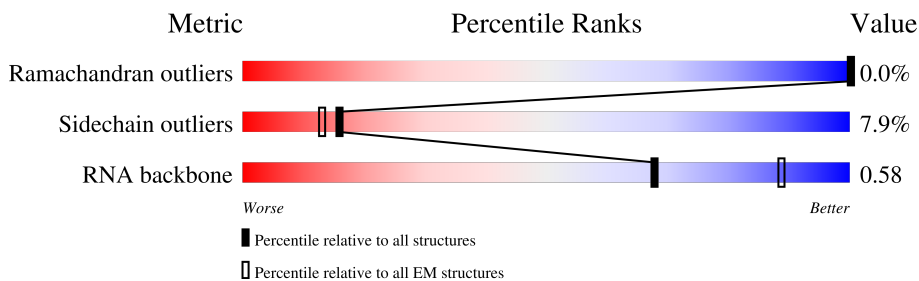
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.54 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |
| RNA backbone | 4643 | 859 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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 | 16 | 1534 | 84% 16% |
| 2 | SB | 241 | 88% 5% 7% |
| 3 | SC | 233 | 84% 7% 9% |
| 4 | SD | 206 | 93% 6% |
| 5 | SE | 167 | 90% 7% |
| 6 | SF | 135 | 70% 8% 21% |
| 7 | SG | 179 | 65% 19% 16% |
| 8 | SH | 130 | 95% 5% |
| 9 | SI | 130 | 87% 11% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 10 | SJ | 103 | 80% 17% |
| 11 | SK | 129 | 88% 8% |
| 12 | SL | 124 | 92% 7% |
| 13 | SM | 118 | 83% 11% |
| 14 | SN | 101 | 80% 16% |
| 15 | SO | 89 | 91% 8% |
| 16 | SP | 82 | 96% |
| 17 | SQ | 84 | 86% 10% 5% |
| 18 | SR | 75 | 79% 11% 11% |
| 19 | SS | 92 | 70% 21% 9% |
| 20 | ST | 87 | 93% 5% |
| 21 | SU | 71 | 92% 7% |
| 22 | mR | 60 | 17% 80% |
| 23 | 23 | 2904 | 81% 19% |
| 24 | 5 | 120 | 87% 13% |
| 25 | LB | 273 | 95% 5% |
| 26 | LC | 209 | 96% |
| 27 | LD | 201 | 97% |
| 28 | LE | 179 | 92% 7% |
| 29 | LF | 177 | 94% 6% |
| 30 | LI | 149 | 91% 8% |
| 31 | LJ | 165 | 70% 10% 21% |
| 32 | LK | 142 | 82% 12% 6% |
| 33 | LM | 142 | 95% 5% |
| 34 | LN | 123 | 96% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 35 | LO | 144 | 96% . |
| 36 | LP | 136 | 93% 7% |
| 37 | LQ | 127 | 89% 5% 6% |
| 38 | LR | 117 | 93% 6% . |
| 39 | LS | 115 | 96% . . |
| 40 | LT | 118 | 96% . . |
| 41 | LU | 103 | 94% 5% . |
| 42 | LV | 110 | 95% 5% |
| 43 | LW | 100 | 83% 10% 7% |
| 44 | LX | 104 | 93% . . . |
| 45 | LY | 94 | 93% 7% |
| 46 | La | 85 | 86% . 11% |
| 47 | Lb | 78 | 94% 5% . |
| 48 | Lc | 63 | 97% . . |
| 49 | Ld | 59 | 92% 7% . |
| 50 | Le | 70 | 80% 17% . |
| 51 | Lf | 57 | 95% . . . |
| 52 | Lg | 55 | 85% 9% 5% |
| 53 | Lh | 46 | 96% . |
| 54 | Li | 65 | 95% . . |
| 55 | Lj | 38 | 97% . |
| 56 | EF | 704 | 94% 6% |
| 57 | Pp | 3 | 33% 67% |
| 58 | Pt | 106 | 56% 14% . 28% |
| 59 | Dt | 106 | 52% 17% . 28% |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|------------|-------------|--------------|------------|------------------|-----------------|----------------|-------------------------|
| 64 | ATP | 23 | 3003 | X | - | - | - |

2 Entry composition [i](#)

There are 67 unique types of molecules in this entry. The entry contains 154120 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 16S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| | | | Total | C | N | O | P | | |
| 1 | 16 | 1534 | 32929 | 14693 | 6041 | 10661 | 1534 | 0 | 0 |

- Molecule 2 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 2 | SB | 224 | 1753 | 1109 | 315 | 321 | 8 | 0 | 0 |

- Molecule 3 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 3 | SC | 211 | 1653 | 1046 | 310 | 293 | 4 | 0 | 0 |

- Molecule 4 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 4 | SD | 205 | 1643 | 1026 | 315 | 298 | 4 | 0 | 0 |

- Molecule 5 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 5 | SE | 155 | 1144 | 711 | 216 | 211 | 6 | 0 | 0 |

- Molecule 6 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 6 | SF | 106 | 862 | 545 | 156 | 154 | 7 | 0 | 0 |

- Molecule 7 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 7 | SG | 151 | 1181 | 735 | 227 | 215 | 4 | 0 | 0 |

- Molecule 8 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 8 | SH | 129 | 979 | 616 | 173 | 184 | 6 | 0 | 0 |

- Molecule 9 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 9 | SI | 127 | 1022 | 634 | 206 | 179 | 3 | 0 | 0 |

- Molecule 10 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 10 | SJ | 99 | 795 | 498 | 152 | 144 | 1 | 0 | 0 |

- Molecule 11 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 11 | SK | 119 | 895 | 551 | 179 | 162 | 3 | 0 | 0 |

- Molecule 12 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 12 | SL | 123 | 957 | 591 | 196 | 165 | 5 | 0 | 0 |

- Molecule 13 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 13 | SM | 114 | 883 | 546 | 178 | 156 | 3 | 0 | 0 |

- Molecule 14 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14 | SN | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 805 | 499 | 164 | 139 | 3 | | |

- Molecule 15 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15 | SO | 88 | Total | C | N | O | S | 0 | 0 |
| | | | 714 | 439 | 144 | 130 | 1 | | |

- Molecule 16 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16 | SP | 82 | Total | C | N | O | S | 0 | 0 |
| | | | 649 | 406 | 128 | 114 | 1 | | |

- Molecule 17 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17 | SQ | 80 | Total | C | N | O | S | 0 | 0 |
| | | | 648 | 411 | 121 | 113 | 3 | | |

- Molecule 18 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 18 | SR | 67 | Total | C | N | O | S | 0 | 0 |
| | | | 555 | 351 | 106 | 97 | 1 | | |

- Molecule 19 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19 | SS | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 668 | 427 | 127 | 112 | 2 | | |

- Molecule 20 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20 | ST | 85 | Total | C | N | O | S | 0 | 0 |
| | | | 664 | 411 | 137 | 113 | 3 | | |

- Molecule 21 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 21 | SU | 70 | Total | C | N | O | S | 0 | 0 |
| | | | 589 | 366 | 125 | 97 | 1 | | |

- Molecule 22 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|-------|
| 22 | mR | 12 | Total | C | N | O | P | 0 | 0 |
| | | | 254 | 114 | 44 | 84 | 12 | | |

- Molecule 23 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 23 | 23 | 2904 | Total | C | N | O | P | 0 | 0 |
| | | | 62355 | 27824 | 11469 | 20158 | 2904 | | |

- Molecule 24 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 24 | 5 | 120 | Total | C | N | O | P | 0 | 0 |
| | | | 2570 | 1144 | 468 | 838 | 120 | | |

- Molecule 25 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 25 | LB | 271 | Total | C | N | O | S | 0 | 0 |
| | | | 2082 | 1288 | 423 | 364 | 7 | | |

- Molecule 26 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26 | LC | 209 | Total | C | N | O | S | 0 | 0 |
| | | | 1565 | 979 | 288 | 294 | 4 | | |

- Molecule 27 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27 | LD | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | |

- Molecule 28 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28 | LE | 177 | Total | C | N | O | S | 0 | 0 |
| | | | 1410 | 899 | 249 | 256 | 6 | | |

- Molecule 29 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29 | LF | 176 | Total | C | N | O | S | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | |

- Molecule 30 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30 | LI | 148 | Total | C | N | O | S | 0 | 0 |
| | | | 1101 | 694 | 196 | 210 | 1 | | |

- Molecule 31 is a protein called 50S ribosomal protein L10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31 | LJ | 131 | Total | C | N | O | S | 0 | 0 |
| | | | 992 | 629 | 175 | 184 | 4 | | |

- Molecule 32 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32 | LK | 134 | Total | C | N | O | S | 0 | 0 |
| | | | 979 | 619 | 169 | 185 | 6 | | |

- Molecule 33 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33 | LM | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | |

- Molecule 34 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34 | LN | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 938 | 587 | 180 | 165 | 6 | | |

- Molecule 35 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35 | LO | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1053 | 654 | 207 | 190 | 2 | | |

- Molecule 36 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36 | LP | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1075 | 686 | 205 | 178 | 6 | | |

- Molecule 37 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37 | LQ | 120 | Total | C | N | O | S | 0 | 0 |
| | | | 960 | 593 | 196 | 166 | 5 | | |

- Molecule 38 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 38 | LR | 116 | Total | C | N | O | 0 | 0 |
| | | | 892 | 552 | 178 | 162 | | |

- Molecule 39 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39 | LS | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 917 | 574 | 179 | 163 | 1 | | |

- Molecule 40 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 40 | LT | 117 | Total | C | N | O | 0 | 0 |
| | | | 947 | 604 | 192 | 151 | | |

- Molecule 41 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41 | LU | 103 | Total | C | N | O | S | 0 | 0 |
| | | | 816 | 516 | 153 | 145 | 2 | | |

- Molecule 42 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 42 | LV | 110 | 857 | 532 | 166 | 156 | 3 | 0 | 0 |

- Molecule 43 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 43 | LW | 93 | 738 | 466 | 139 | 131 | 2 | 0 | 0 |

- Molecule 44 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| | | | Total | C | N | O | | |
| 44 | LX | 102 | 779 | 492 | 146 | 141 | 0 | 0 |

- Molecule 45 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 45 | LY | 94 | 753 | 479 | 137 | 134 | 3 | 0 | 0 |

- Molecule 46 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 46 | La | 76 | 582 | 360 | 117 | 104 | 1 | 0 | 0 |

- Molecule 47 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 47 | Lb | 77 | 625 | 388 | 129 | 106 | 2 | 0 | 0 |

- Molecule 48 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 48 | Lc | 62 | 501 | 308 | 98 | 94 | 1 | 0 | 0 |

- Molecule 49 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 49 | Ld | 58 | Total | C | N | O | S | 0 | 0 |
| | | | 449 | 281 | 87 | 79 | 2 | | |

- Molecule 50 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 50 | Le | 68 | Total | C | N | O | S | 0 | 0 |
| | | | 533 | 330 | 101 | 96 | 6 | | |

- Molecule 51 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 51 | Lf | 56 | Total | C | N | O | S | 0 | 0 |
| | | | 444 | 269 | 94 | 80 | 1 | | |

- Molecule 52 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 52 | Lg | 52 | Total | C | N | O | 0 | 0 |
| | | | 427 | 275 | 78 | 74 | | |

- Molecule 53 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 53 | Lh | 46 | Total | C | N | O | S | 0 | 0 |
| | | | 377 | 228 | 90 | 57 | 2 | | |

- Molecule 54 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 54 | Li | 64 | Total | C | N | O | S | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | |

- Molecule 55 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 55 | Lj | 38 | Total | C | N | O | S | 0 | 0 |
| | | | 302 | 185 | 65 | 48 | 4 | | |

- Molecule 56 is a protein called Elongation factor G.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 56 | EF | 704 | 5388 | 3395 | 938 | 1033 | 22 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|----------------|
| EF | 1 | SER | - | expression tag | UNP A0A0H3PU63 |

- Molecule 57 is a protein called Nascent peptide.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|----|---|---|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 57 | Pp | 3 | 28 | 20 | 4 | 3 | 1 | 0 | 0 |

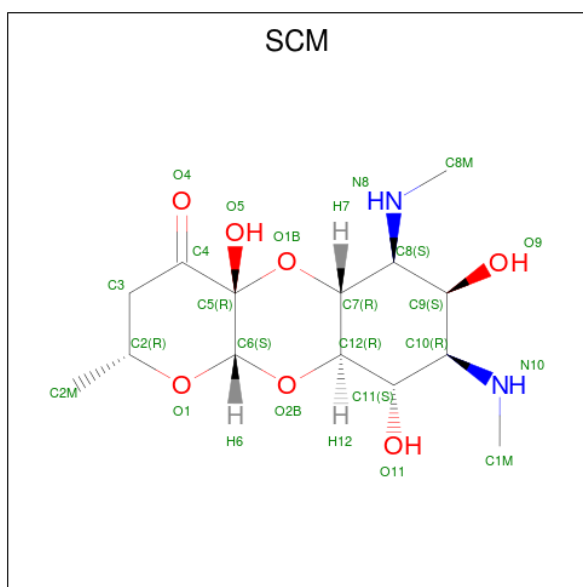
- Molecule 58 is a RNA chain called tRNA.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| | | | Total | C | N | O | P | S | | |
| 58 | Pt | 76 | 1636 | 733 | 284 | 542 | 76 | 1 | 0 | 0 |

- Molecule 59 is a RNA chain called tRNA.

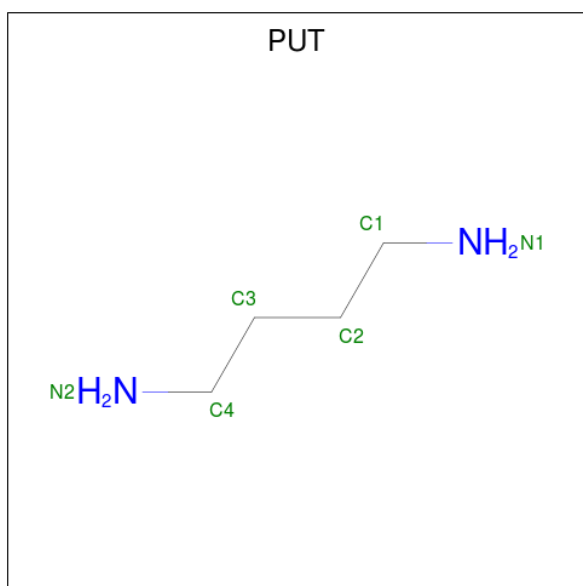
| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| | | | Total | C | N | O | P | S | | |
| 59 | Dt | 76 | 1641 | 735 | 294 | 534 | 76 | 2 | 0 | 0 |

- Molecule 60 is SPECTINOMYCIN (three-letter code: SCM) (formula: C₁₄H₂₄N₂O₇) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | AltConf | |
|-----|-------|----------|-------|----|---|---------|---|
| | | | Total | C | N | | O |
| 60 | 16 | 1 | 46 | 28 | 4 | 14 | 0 |
| 60 | 16 | 1 | 46 | 28 | 4 | 14 | 0 |
| 60 | 23 | 1 | 23 | 14 | 2 | 7 | 0 |

- Molecule 61 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 61 | 16 | 1 | Total | C | N | 0 |
| | | | 18 | 12 | 6 | |
| 61 | 16 | 1 | Total | C | N | 0 |
| | | | 18 | 12 | 6 | |
| 61 | 16 | 1 | Total | C | N | 0 |
| | | | 18 | 12 | 6 | |
| 61 | 23 | 1 | Total | C | N | 0 |
| | | | 78 | 52 | 26 | |
| 61 | 23 | 1 | Total | C | N | 0 |
| | | | 78 | 52 | 26 | |
| 61 | 23 | 1 | Total | C | N | 0 |
| | | | 78 | 52 | 26 | |
| 61 | 23 | 1 | Total | C | N | 0 |
| | | | 78 | 52 | 26 | |
| 61 | 23 | 1 | Total | C | N | 0 |
| | | | 78 | 52 | 26 | |
| 61 | 23 | 1 | Total | C | N | 0 |
| | | | 78 | 52 | 26 | |
| 61 | 23 | 1 | Total | C | N | 0 |
| | | | 78 | 52 | 26 | |
| 61 | 23 | 1 | Total | C | N | 0 |
| | | | 78 | 52 | 26 | |
| 61 | 23 | 1 | Total | C | N | 0 |
| | | | 78 | 52 | 26 | |
| 61 | 23 | 1 | Total | C | N | 0 |
| | | | 78 | 52 | 26 | |
| 61 | 23 | 1 | Total | C | N | 0 |
| | | | 78 | 52 | 26 | |
| 61 | 23 | 1 | Total | C | N | 0 |
| | | | 78 | 52 | 26 | |
| 61 | LC | 1 | Total | C | N | 0 |
| | | | 6 | 4 | 2 | |

- Molecule 62 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 62 | 16 | 63 | Total | Mg | 0 |
| | | | 63 | 63 | |
| 62 | SK | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|--------------|-----------|---------|
| 62 | SN | 1 | Total 1 | Mg 1 | 0 |
| 62 | SR | 1 | Total 1 | Mg 1 | 0 |
| 62 | 23 | 264 | Total 264 | Mg 264 | 0 |
| 62 | 5 | 6 | Total 6 | Mg 6 | 0 |
| 62 | LB | 1 | Total 1 | Mg 1 | 0 |
| 62 | LC | 1 | Total 1 | Mg 1 | 0 |
| 62 | LD | 1 | Total 1 | Mg 1 | 0 |
| 62 | LO | 1 | Total 1 | Mg 1 | 0 |
| 62 | LQ | 1 | Total 1 | Mg 1 | 0 |
| 62 | Lf | 1 | Total 1 | Mg 1 | 0 |
| 62 | EF | 1 | Total 1 | Mg 1 | 0 |
| 62 | Pt | 1 | Total 1 | Mg 1 | 0 |

- Molecule 63 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

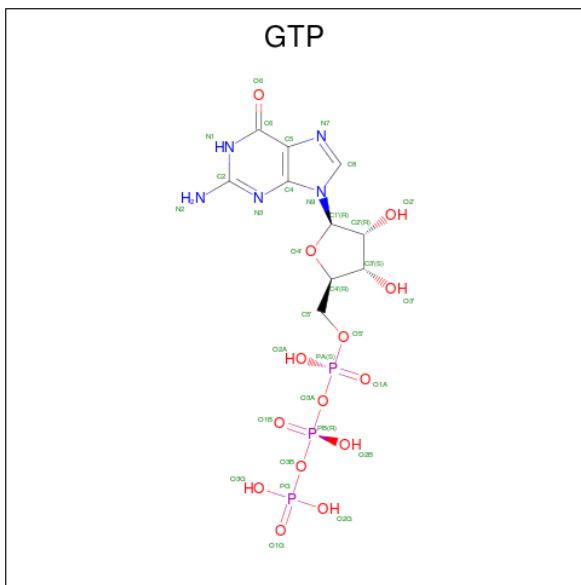
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|---------|---------|
| 63 | SB | 1 | Total 1 | Zn 1 | 0 |
| 63 | Le | 1 | Total 1 | Zn 1 | 0 |
| 63 | Lj | 1 | Total 1 | Zn 1 | 0 |

- Molecule 64 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| | | | Total | C | N | |
| 65 | 23 | 1 | 20 | 14 | 6 | 0 |

- Molecule 66 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| | | | Total | C | N | O | P | |
| 66 | EF | 1 | 32 | 10 | 5 | 14 | 3 | 0 |

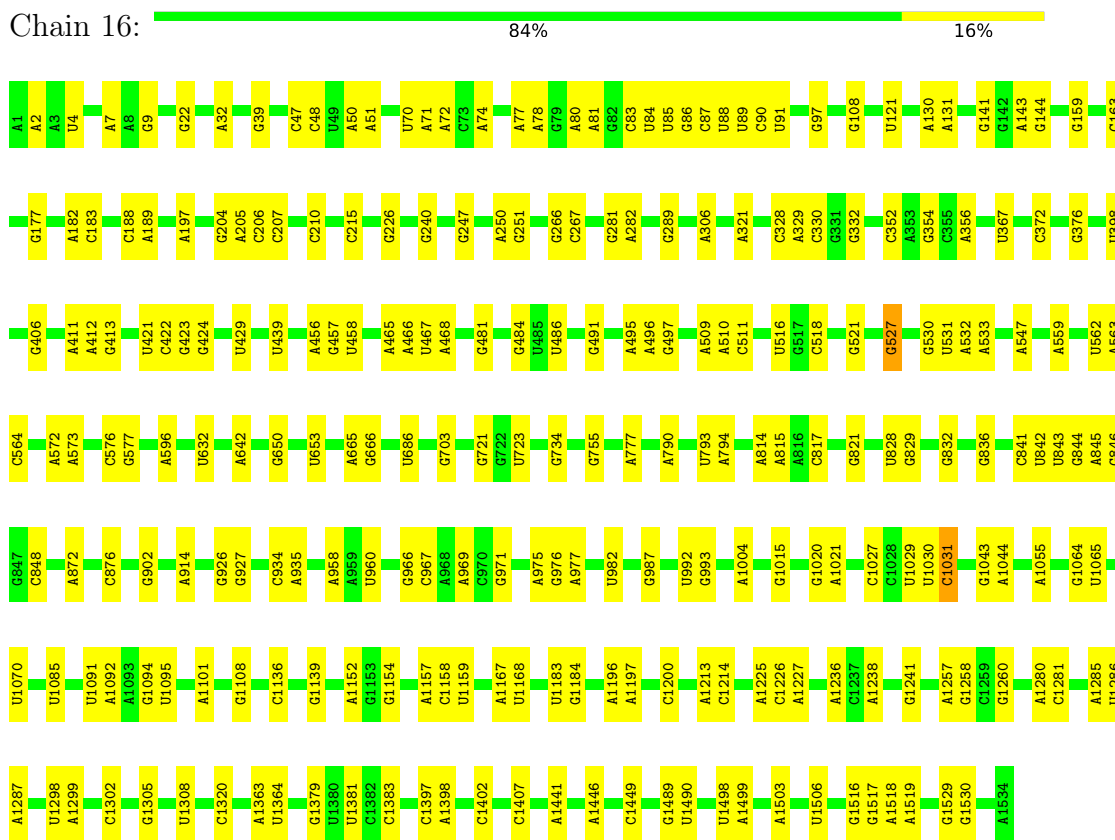
- Molecule 67 is water.

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| | | | Total | O | |
| 67 | 16 | 1 | 1 | 1 | 0 |
| 67 | SB | 1 | 1 | 1 | 0 |
| 67 | 23 | 22 | 22 | 22 | 0 |
| 67 | LB | 1 | 1 | 1 | 0 |
| 67 | EF | 1 | 1 | 1 | 0 |

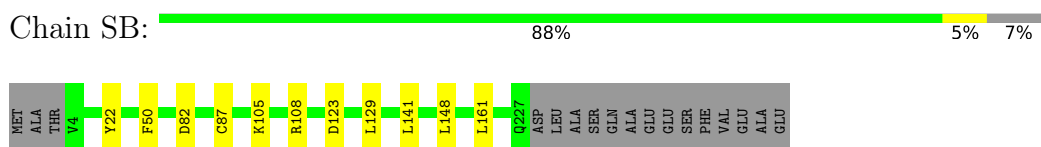
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

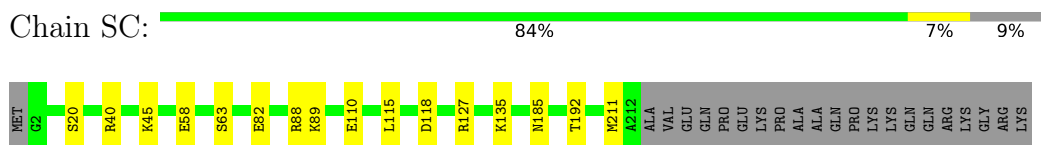
- Molecule 1: 16S rRNA



- Molecule 2: 30S ribosomal protein S2

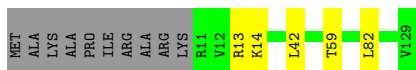
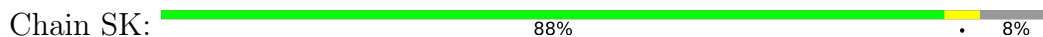


- Molecule 3: 30S ribosomal protein S3





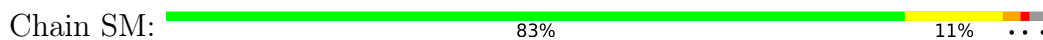
- Molecule 11: 30S ribosomal protein S11



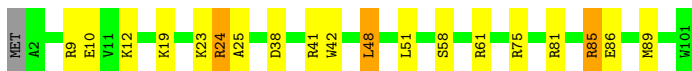
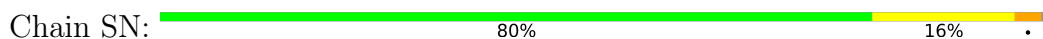
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14



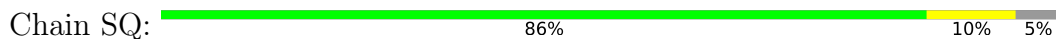
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

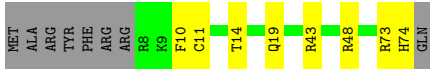
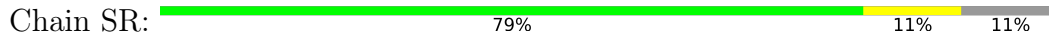


- Molecule 17: 30S ribosomal protein S17

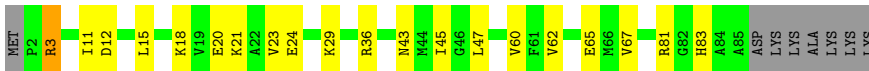
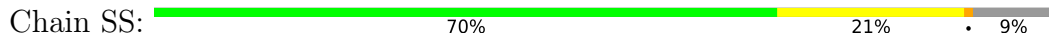




- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



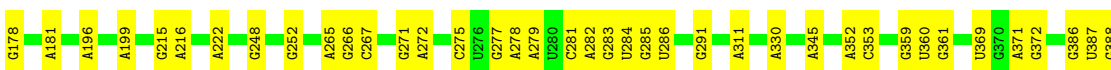
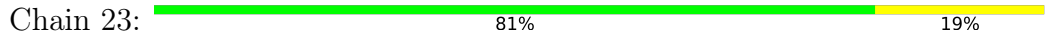
- Molecule 21: 30S ribosomal protein S21

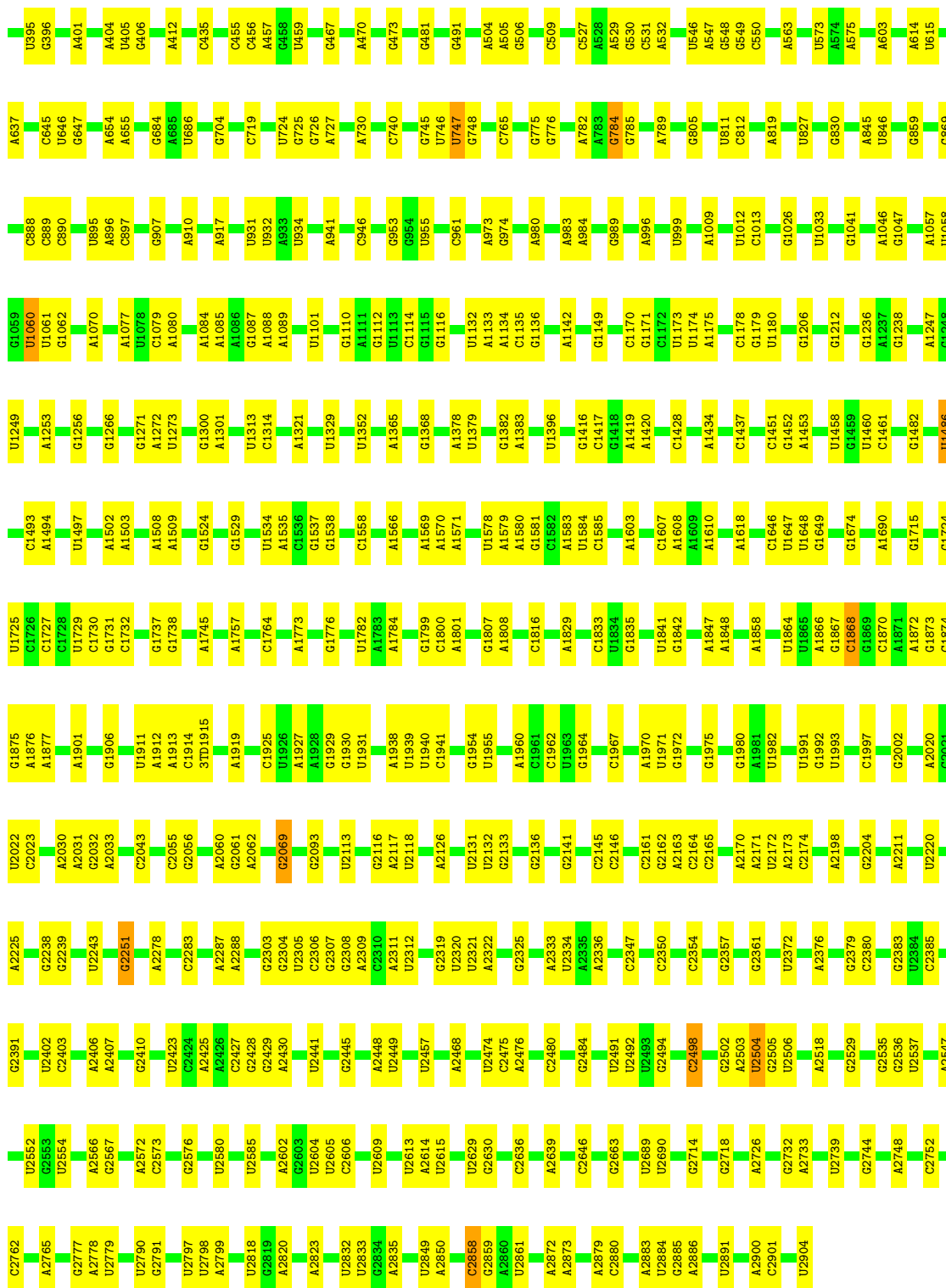


- Molecule 22: mRNA

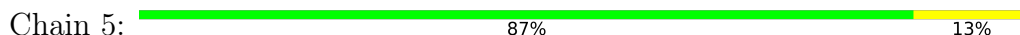


- Molecule 23: 23S rRNA






• Molecule 24: 5S rRNA



ARG
ASP
ALA
LYS
GLU
ALA
ALA

- Molecule 32: 50S ribosomal protein L11

Chain LK:  82% 12% 6%

MET
ALA
LYS
LYS
VAL
GLN
ALA
ALA
Y8
L28
I59
L79
L80
K81
K87
S90
K95
D96
K97
K100
I101
S102
K113
D121
T132
S135
M136
V139
V140
E141
ASP

- Molecule 33: 50S ribosomal protein L13

Chain LM:  95% 5%

M1
K7
R37
G38
K39
D60
R95
R96
D141
I142

- Molecule 34: 50S ribosomal protein L14

Chain LN:  96% ..

M1
R31
R70
E110
K114
V122
LEU

- Molecule 35: 50S ribosomal protein L15

Chain LO:  96% .


M1
S42
T87
K70
I73
V89
T121
E144

- Molecule 36: 50S ribosomal protein L16

Chain LP:  93% 7%

M1
L2
Q3
R6
R18
K68
R59
4P481
L102
K123
M136

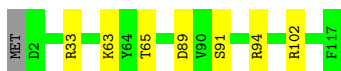
- Molecule 37: 50S ribosomal protein L17

Chain LQ:  89% 5% 6%

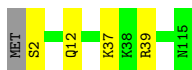
M3
R2
S14
S15
S27
T57
S89
R118
S119
E120
LYS
ALA
GLU
ALA
ALA
ALA
ALA
GLU

- Molecule 38: 50S ribosomal protein L18

Chain LR:  93% 6% .



- Molecule 39: 50S ribosomal protein L19



- Molecule 40: 50S ribosomal protein L20



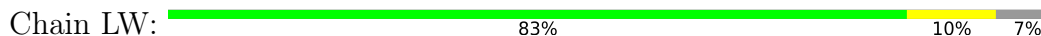
- Molecule 41: 50S ribosomal protein L21



- Molecule 42: 50S ribosomal protein L22



- Molecule 43: 50S ribosomal protein L23



- Molecule 44: 50S ribosomal protein L24

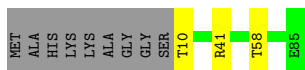
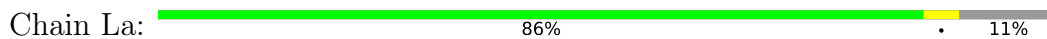


- Molecule 45: 50S ribosomal protein L25





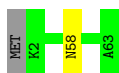
- Molecule 46: 50S ribosomal protein L27



- Molecule 47: 50S ribosomal protein L28



- Molecule 48: 50S ribosomal protein L29



- Molecule 49: 50S ribosomal protein L30



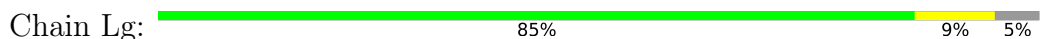
- Molecule 50: 50S ribosomal protein L31



- Molecule 51: 50S ribosomal protein L32



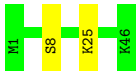
- Molecule 52: 50S ribosomal protein L33





- Molecule 53: 50S ribosomal protein L34

Chain Lh: 96%



- Molecule 54: 50S ribosomal protein L35

Chain Li: 95%



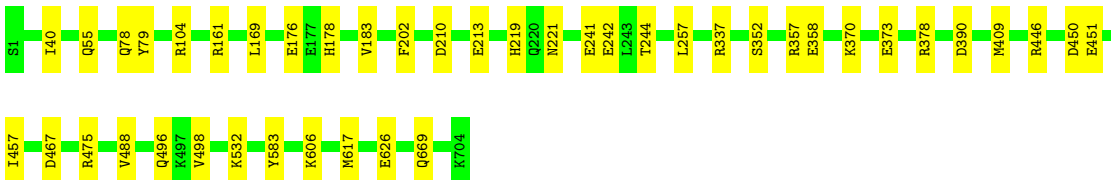
- Molecule 55: 50S ribosomal protein L36

Chain Lj: 97%



- Molecule 56: Elongation factor G

Chain EF: 94% 6%



- Molecule 57: Nascent peptide

Chain Pp: 33% 67%

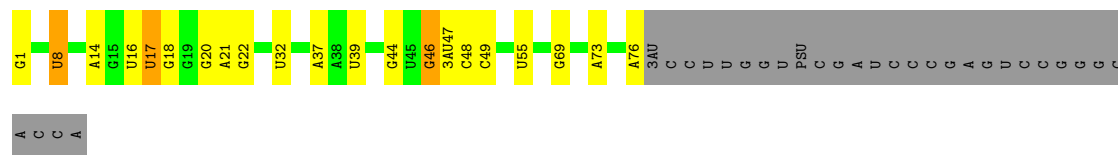


- Molecule 58: tRNA

Chain Pt: 56% 14% 28%



- Molecule 59: tRNA



A
C
C
A

4 Experimental information

| Property | Value | Source |
|--------------------------------------|---------------------|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 33688 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING ONLY | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 87 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: OMU, 3AU, ZN, 4SU, MA6, SCM, MIA, D2T, 6MZ, ATP, 2MG, 7MG, 5MU, T6A, PUT, OMG, MG, 1MG, 2MA, 4D4, U8U, 5MC, 3TD, 4OC, GTP, SPD, OMC, UR3, H2U, PSU

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 | 16 | 0.65 | 1/36619 (0.0%) | 0.78 | 8/57122 (0.0%) |
| 2 | SB | 0.40 | 0/1784 | 0.63 | 1/2403 (0.0%) |
| 3 | SC | 0.39 | 0/1680 | 0.65 | 0/2263 |
| 4 | SD | 0.36 | 0/1665 | 0.60 | 0/2227 |
| 5 | SE | 0.42 | 0/1157 | 0.63 | 0/1557 |
| 6 | SF | 0.40 | 0/881 | 0.67 | 1/1189 (0.1%) |
| 7 | SG | 0.46 | 0/1195 | 0.83 | 5/1602 (0.3%) |
| 8 | SH | 0.39 | 0/989 | 0.57 | 0/1326 |
| 9 | SI | 0.53 | 1/1034 (0.1%) | 0.71 | 0/1375 |
| 10 | SJ | 0.40 | 0/805 | 0.78 | 0/1089 |
| 11 | SK | 0.42 | 0/911 | 0.70 | 0/1229 |
| 12 | SL | 0.38 | 0/960 | 0.64 | 0/1286 |
| 13 | SM | 0.46 | 0/892 | 0.89 | 3/1193 (0.3%) |
| 14 | SN | 0.44 | 0/817 | 0.91 | 3/1088 (0.3%) |
| 15 | SO | 0.37 | 0/722 | 0.59 | 0/964 |
| 16 | SP | 0.39 | 0/659 | 0.61 | 0/884 |
| 17 | SQ | 0.40 | 0/657 | 0.64 | 0/881 |
| 18 | SR | 0.38 | 0/564 | 0.60 | 0/756 |
| 19 | SS | 0.47 | 0/685 | 0.77 | 1/922 (0.1%) |
| 20 | ST | 0.32 | 0/670 | 0.55 | 0/888 |
| 21 | SU | 0.50 | 0/597 | 0.67 | 0/792 |
| 22 | mR | 0.55 | 0/283 | 0.73 | 0/438 |
| 23 | 23 | 0.79 | 1/69284 (0.0%) | 0.78 | 15/108082 (0.0%) |
| 24 | 5 | 0.72 | 1/2873 (0.0%) | 0.76 | 0/4478 |
| 25 | LB | 0.43 | 0/2121 | 0.62 | 0/2852 |
| 26 | LC | 0.42 | 0/1586 | 0.59 | 0/2134 |
| 27 | LD | 0.39 | 0/1571 | 0.58 | 0/2113 |
| 28 | LE | 0.48 | 1/1434 (0.1%) | 0.72 | 1/1926 (0.1%) |
| 29 | LF | 0.37 | 0/1343 | 0.62 | 0/1816 |
| 30 | LI | 0.37 | 0/1112 | 0.81 | 5/1503 (0.3%) |
| 31 | LJ | 0.42 | 0/1006 | 0.67 | 1/1358 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 32 | LK | 0.51 | 0/993 | 0.66 | 0/1341 |
| 33 | LM | 0.43 | 0/1152 | 0.57 | 0/1551 |
| 34 | LN | 0.41 | 0/947 | 0.66 | 0/1268 |
| 35 | LO | 0.41 | 0/1062 | 0.63 | 0/1413 |
| 36 | LP | 0.42 | 0/1081 | 0.65 | 0/1443 |
| 37 | LQ | 0.39 | 0/973 | 0.60 | 0/1301 |
| 38 | LR | 0.41 | 0/902 | 0.63 | 0/1209 |
| 39 | LS | 0.41 | 0/929 | 0.61 | 0/1242 |
| 40 | LT | 0.43 | 0/960 | 0.56 | 0/1278 |
| 41 | LU | 0.43 | 0/829 | 0.62 | 0/1107 |
| 42 | LV | 0.39 | 0/864 | 0.59 | 0/1156 |
| 43 | LW | 0.38 | 0/744 | 0.58 | 0/994 |
| 44 | LX | 0.41 | 0/787 | 0.60 | 0/1051 |
| 45 | LY | 0.40 | 0/766 | 0.56 | 0/1025 |
| 46 | La | 0.41 | 0/589 | 0.60 | 0/779 |
| 47 | Lb | 0.44 | 0/635 | 0.69 | 1/848 (0.1%) |
| 48 | Lc | 0.43 | 0/502 | 0.65 | 0/667 |
| 49 | Ld | 0.41 | 0/453 | 0.65 | 0/605 |
| 50 | Le | 0.45 | 0/543 | 0.72 | 0/726 |
| 51 | Lf | 0.42 | 0/450 | 0.62 | 0/599 |
| 52 | Lg | 0.42 | 0/434 | 0.65 | 0/576 |
| 53 | Lh | 0.40 | 0/380 | 0.67 | 0/498 |
| 54 | Li | 0.38 | 0/513 | 0.64 | 1/676 (0.1%) |
| 55 | Lj | 0.39 | 0/303 | 0.62 | 0/397 |
| 56 | EF | 0.40 | 0/5490 | 0.61 | 1/7437 (0.0%) |
| 57 | Pp | 0.45 | 0/28 | 1.11 | 0/34 |
| 58 | Pt | 0.53 | 2/1684 (0.1%) | 0.78 | 0/2615 |
| 59 | Dt | 0.60 | 1/1654 (0.1%) | 0.80 | 1/2572 (0.0%) |
| All | All | 0.65 | 8/165203 (0.0%) | 0.75 | 48/246144 (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 |
|-----|-------|---------------------|---------------------|
| 3 | SC | 0 | 2 |
| 4 | SD | 0 | 3 |
| 5 | SE | 0 | 1 |
| 9 | SI | 0 | 3 |
| 10 | SJ | 0 | 2 |
| 12 | SL | 0 | 1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 13 | SM | 0 | 4 |
| 14 | SN | 0 | 2 |
| 17 | SQ | 0 | 3 |
| 19 | SS | 0 | 1 |
| 21 | SU | 0 | 1 |
| 25 | LB | 0 | 3 |
| 27 | LD | 0 | 1 |
| 28 | LE | 0 | 3 |
| 30 | LI | 0 | 2 |
| 34 | LN | 0 | 2 |
| 36 | LP | 0 | 2 |
| 37 | LQ | 0 | 2 |
| 38 | LR | 0 | 1 |
| 41 | LU | 0 | 1 |
| 44 | LX | 0 | 1 |
| 45 | LY | 0 | 1 |
| 46 | La | 0 | 1 |
| 49 | Ld | 0 | 1 |
| 51 | Lf | 0 | 2 |
| 55 | Lj | 0 | 1 |
| 56 | EF | 0 | 3 |
| All | All | 0 | 50 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 59 | Dt | 1 | G | OP3-P | -10.87 | 1.48 | 1.61 |
| 23 | 23 | 1 | G | OP3-P | -10.70 | 1.48 | 1.61 |
| 24 | 5 | 1 | U | OP3-P | -10.20 | 1.49 | 1.61 |
| 58 | Pt | 1 | G | OP3-P | -10.15 | 1.49 | 1.61 |
| 28 | LE | 93 | GLY | C-N | -8.57 | 1.14 | 1.34 |

The worst 5 of 48 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1 | 16 | 1490 | U | O5'-P-OP1 | -29.78 | 74.96 | 110.70 |
| 1 | 16 | 1490 | U | OP1-P-OP2 | -26.97 | 79.15 | 119.60 |
| 1 | 16 | 1490 | U | O5'-P-OP2 | 17.20 | 131.33 | 110.70 |
| 14 | SN | 25 | ALA | N-CA-CB | -15.22 | 88.78 | 110.10 |
| 1 | 16 | 1489 | G | OP1-P-O3' | 13.97 | 135.93 | 105.20 |

There are no chirality outliers.

5 of 50 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 3 | SC | 40 | ARG | Sidechain |
| 3 | SC | 88 | ARG | Sidechain |
| 4 | SD | 26 | ARG | Sidechain |
| 4 | SD | 44 | ARG | Sidechain |
| 4 | SD | 56 | ARG | Sidechain |

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 | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 2 | SB | 222/241 (92%) | 210 (95%) | 12 (5%) | 0 | 100 | 100 |
| 3 | SC | 209/233 (90%) | 200 (96%) | 9 (4%) | 0 | 100 | 100 |
| 4 | SD | 203/206 (98%) | 201 (99%) | 2 (1%) | 0 | 100 | 100 |
| 5 | SE | 153/167 (92%) | 150 (98%) | 3 (2%) | 0 | 100 | 100 |
| 6 | SF | 104/135 (77%) | 101 (97%) | 3 (3%) | 0 | 100 | 100 |
| 7 | SG | 149/179 (83%) | 141 (95%) | 8 (5%) | 0 | 100 | 100 |
| 8 | SH | 127/130 (98%) | 126 (99%) | 1 (1%) | 0 | 100 | 100 |
| 9 | SI | 125/130 (96%) | 118 (94%) | 7 (6%) | 0 | 100 | 100 |
| 10 | SJ | 97/103 (94%) | 91 (94%) | 6 (6%) | 0 | 100 | 100 |
| 11 | SK | 117/129 (91%) | 111 (95%) | 6 (5%) | 0 | 100 | 100 |
| 12 | SL | 120/124 (97%) | 114 (95%) | 6 (5%) | 0 | 100 | 100 |
| 13 | SM | 112/118 (95%) | 108 (96%) | 4 (4%) | 0 | 100 | 100 |
| 14 | SN | 98/101 (97%) | 94 (96%) | 4 (4%) | 0 | 100 | 100 |
| 15 | SO | 86/89 (97%) | 83 (96%) | 3 (4%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|----------|-------------|-----|
| 16 | SP | 80/82 (98%) | 76 (95%) | 4 (5%) | 0 | 100 | 100 |
| 17 | SQ | 78/84 (93%) | 77 (99%) | 1 (1%) | 0 | 100 | 100 |
| 18 | SR | 65/75 (87%) | 60 (92%) | 5 (8%) | 0 | 100 | 100 |
| 19 | SS | 82/92 (89%) | 75 (92%) | 7 (8%) | 0 | 100 | 100 |
| 20 | ST | 83/87 (95%) | 83 (100%) | 0 | 0 | 100 | 100 |
| 21 | SU | 68/71 (96%) | 67 (98%) | 1 (2%) | 0 | 100 | 100 |
| 25 | LB | 269/273 (98%) | 262 (97%) | 7 (3%) | 0 | 100 | 100 |
| 26 | LC | 207/209 (99%) | 198 (96%) | 8 (4%) | 1 (0%) | 29 | 40 |
| 27 | LD | 199/201 (99%) | 193 (97%) | 6 (3%) | 0 | 100 | 100 |
| 28 | LE | 175/179 (98%) | 168 (96%) | 7 (4%) | 0 | 100 | 100 |
| 29 | LF | 174/177 (98%) | 169 (97%) | 5 (3%) | 0 | 100 | 100 |
| 30 | LI | 146/149 (98%) | 129 (88%) | 17 (12%) | 0 | 100 | 100 |
| 31 | LJ | 129/165 (78%) | 121 (94%) | 8 (6%) | 0 | 100 | 100 |
| 32 | LK | 132/142 (93%) | 121 (92%) | 11 (8%) | 0 | 100 | 100 |
| 33 | LM | 140/142 (99%) | 138 (99%) | 2 (1%) | 0 | 100 | 100 |
| 34 | LN | 120/123 (98%) | 117 (98%) | 3 (2%) | 0 | 100 | 100 |
| 35 | LO | 142/144 (99%) | 137 (96%) | 5 (4%) | 0 | 100 | 100 |
| 36 | LP | 133/136 (98%) | 133 (100%) | 0 | 0 | 100 | 100 |
| 37 | LQ | 118/127 (93%) | 113 (96%) | 5 (4%) | 0 | 100 | 100 |
| 38 | LR | 114/117 (97%) | 107 (94%) | 7 (6%) | 0 | 100 | 100 |
| 39 | LS | 112/115 (97%) | 109 (97%) | 3 (3%) | 0 | 100 | 100 |
| 40 | LT | 115/118 (98%) | 115 (100%) | 0 | 0 | 100 | 100 |
| 41 | LU | 101/103 (98%) | 95 (94%) | 6 (6%) | 0 | 100 | 100 |
| 42 | LV | 108/110 (98%) | 101 (94%) | 7 (6%) | 0 | 100 | 100 |
| 43 | LW | 91/100 (91%) | 87 (96%) | 4 (4%) | 0 | 100 | 100 |
| 44 | LX | 100/104 (96%) | 94 (94%) | 6 (6%) | 0 | 100 | 100 |
| 45 | LY | 92/94 (98%) | 92 (100%) | 0 | 0 | 100 | 100 |
| 46 | La | 74/85 (87%) | 73 (99%) | 1 (1%) | 0 | 100 | 100 |
| 47 | Lb | 75/78 (96%) | 72 (96%) | 3 (4%) | 0 | 100 | 100 |
| 48 | Lc | 60/63 (95%) | 58 (97%) | 2 (3%) | 0 | 100 | 100 |
| 49 | Ld | 56/59 (95%) | 55 (98%) | 1 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 50 | Le | 66/70 (94%) | 58 (88%) | 8 (12%) | 0 | 100 | 100 |
| 51 | Lf | 54/57 (95%) | 54 (100%) | 0 | 0 | 100 | 100 |
| 52 | Lg | 50/55 (91%) | 49 (98%) | 1 (2%) | 0 | 100 | 100 |
| 53 | Lh | 44/46 (96%) | 43 (98%) | 1 (2%) | 0 | 100 | 100 |
| 54 | Li | 62/65 (95%) | 57 (92%) | 5 (8%) | 0 | 100 | 100 |
| 55 | Lj | 36/38 (95%) | 35 (97%) | 1 (3%) | 0 | 100 | 100 |
| 56 | EF | 702/704 (100%) | 664 (95%) | 38 (5%) | 0 | 100 | 100 |
| 57 | Pp | 1/3 (33%) | 1 (100%) | 0 | 0 | 100 | 100 |
| All | All | 6575/6927 (95%) | 6304 (96%) | 270 (4%) | 1 (0%) | 100 | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | LC | 149 | ASN |

5.3.2 Protein sidechains [i](#)

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 | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 2 | SB | 186/199 (94%) | 176 (95%) | 10 (5%) | 22 | 29 |
| 3 | SC | 172/190 (90%) | 158 (92%) | 14 (8%) | 11 | 14 |
| 4 | SD | 172/173 (99%) | 162 (94%) | 10 (6%) | 20 | 26 |
| 5 | SE | 118/126 (94%) | 115 (98%) | 3 (2%) | 47 | 62 |
| 6 | SF | 92/116 (79%) | 82 (89%) | 10 (11%) | 6 | 6 |
| 7 | SG | 124/147 (84%) | 94 (76%) | 30 (24%) | 0 | 0 |
| 8 | SH | 104/105 (99%) | 98 (94%) | 6 (6%) | 20 | 26 |
| 9 | SI | 105/107 (98%) | 95 (90%) | 10 (10%) | 8 | 10 |
| 10 | SJ | 87/90 (97%) | 72 (83%) | 15 (17%) | 2 | 2 |
| 11 | SK | 92/99 (93%) | 87 (95%) | 5 (5%) | 22 | 29 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 12 | SL | 102/103 (99%) | 95 (93%) | 7 (7%) | 15 | 20 |
| 13 | SM | 92/96 (96%) | 79 (86%) | 13 (14%) | 3 | 3 |
| 14 | SN | 83/84 (99%) | 66 (80%) | 17 (20%) | 1 | 1 |
| 15 | SO | 76/77 (99%) | 69 (91%) | 7 (9%) | 9 | 11 |
| 16 | SP | 65/65 (100%) | 62 (95%) | 3 (5%) | 27 | 36 |
| 17 | SQ | 74/78 (95%) | 69 (93%) | 5 (7%) | 16 | 20 |
| 18 | SR | 58/65 (89%) | 50 (86%) | 8 (14%) | 3 | 3 |
| 19 | SS | 72/79 (91%) | 53 (74%) | 19 (26%) | 0 | 0 |
| 20 | ST | 65/66 (98%) | 61 (94%) | 4 (6%) | 18 | 24 |
| 21 | SU | 60/61 (98%) | 56 (93%) | 4 (7%) | 16 | 21 |
| 25 | LB | 216/218 (99%) | 206 (95%) | 10 (5%) | 27 | 36 |
| 26 | LC | 164/164 (100%) | 156 (95%) | 8 (5%) | 25 | 34 |
| 27 | LD | 165/165 (100%) | 158 (96%) | 7 (4%) | 30 | 40 |
| 28 | LE | 148/150 (99%) | 138 (93%) | 10 (7%) | 16 | 20 |
| 29 | LF | 137/138 (99%) | 127 (93%) | 10 (7%) | 14 | 18 |
| 30 | LI | 113/114 (99%) | 107 (95%) | 6 (5%) | 22 | 30 |
| 31 | LJ | 100/123 (81%) | 85 (85%) | 15 (15%) | 3 | 2 |
| 32 | LK | 104/110 (94%) | 87 (84%) | 17 (16%) | 2 | 2 |
| 33 | LM | 116/116 (100%) | 109 (94%) | 7 (6%) | 19 | 25 |
| 34 | LN | 103/104 (99%) | 101 (98%) | 2 (2%) | 57 | 72 |
| 35 | LO | 103/103 (100%) | 97 (94%) | 6 (6%) | 20 | 26 |
| 36 | LP | 108/108 (100%) | 102 (94%) | 6 (6%) | 21 | 28 |
| 37 | LQ | 100/103 (97%) | 94 (94%) | 6 (6%) | 19 | 25 |
| 38 | LR | 86/87 (99%) | 80 (93%) | 6 (7%) | 15 | 19 |
| 39 | LS | 99/100 (99%) | 95 (96%) | 4 (4%) | 31 | 43 |
| 40 | LT | 89/90 (99%) | 85 (96%) | 4 (4%) | 27 | 37 |
| 41 | LU | 84/84 (100%) | 78 (93%) | 6 (7%) | 14 | 19 |
| 42 | LV | 93/93 (100%) | 87 (94%) | 6 (6%) | 17 | 23 |
| 43 | LW | 80/84 (95%) | 70 (88%) | 10 (12%) | 4 | 4 |
| 44 | LX | 83/85 (98%) | 78 (94%) | 5 (6%) | 19 | 25 |
| 45 | LY | 78/78 (100%) | 72 (92%) | 6 (8%) | 13 | 16 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 46 | La | 58/63 (92%) | 56 (97%) | 2 (3%) | 37 | 50 |
| 47 | Lb | 67/68 (98%) | 64 (96%) | 3 (4%) | 27 | 37 |
| 48 | Lc | 54/55 (98%) | 53 (98%) | 1 (2%) | 57 | 72 |
| 49 | Ld | 48/49 (98%) | 45 (94%) | 3 (6%) | 18 | 23 |
| 50 | Le | 60/62 (97%) | 48 (80%) | 12 (20%) | 1 | 1 |
| 51 | Lf | 47/48 (98%) | 46 (98%) | 1 (2%) | 53 | 68 |
| 52 | Lg | 47/49 (96%) | 42 (89%) | 5 (11%) | 6 | 7 |
| 53 | Lh | 38/38 (100%) | 36 (95%) | 2 (5%) | 22 | 30 |
| 54 | Li | 51/52 (98%) | 50 (98%) | 1 (2%) | 55 | 70 |
| 55 | Lj | 34/34 (100%) | 34 (100%) | 0 | 100 | 100 |
| 56 | EF | 561/578 (97%) | 522 (93%) | 39 (7%) | 15 | 19 |
| 57 | Pp | 3/3 (100%) | 1 (33%) | 2 (67%) | 0 | 0 |
| All | All | 5436/5642 (96%) | 5008 (92%) | 428 (8%) | 16 | 15 |

5 of 428 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | LE | 134 | GLU |
| 33 | LM | 60 | ASP |
| 56 | EF | 219 | HIS |
| 29 | LF | 50 | LEU |
| 31 | LJ | 101 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | LK | 31 | GLN |
| 56 | EF | 558 | GLN |
| 37 | LQ | 62 | ASN |
| 56 | EF | 645 | GLN |
| 56 | EF | 55 | GLN |

5.3.3 RNA [i](#)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | 16 | 1530/1534 (99%) | 234 (15%) | 10 (0%) |

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| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 22 | mR | 11/60 (18%) | 2 (18%) | 0 |
| 23 | 23 | 2899/2904 (99%) | 517 (17%) | 28 (0%) |
| 24 | 5 | 119/120 (99%) | 15 (12%) | 1 (0%) |
| 58 | Pt | 73/106 (68%) | 12 (16%) | 0 |
| 59 | Dt | 73/106 (68%) | 15 (20%) | 0 |
| All | All | 4705/4830 (97%) | 795 (16%) | 39 (0%) |

5 of 795 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 16 | 2 | A |
| 1 | 16 | 4 | U |
| 1 | 16 | 7 | A |
| 1 | 16 | 9 | G |
| 1 | 16 | 22 | G |

5 of 39 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | 23 | 1508 | A |
| 23 | 23 | 2536 | G |
| 23 | 23 | 1570 | A |
| 23 | 23 | 2145 | C |
| 23 | 23 | 2858 | C |

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

47 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 |
| 23 | PSU | 23 | 2457 | 23 | 18,21,22 | 4.02 | 8 (44%) | 22,30,33 | 2.15 | 5 (22%) |
| 23 | 6MZ | 23 | 2030 | 23 | 18,25,26 | 1.90 | 4 (22%) | 16,36,39 | 3.27 | 3 (18%) |
| 59 | 7MG | Dt | 46 | 59 | 22,26,27 | 3.66 | 10 (45%) | 29,39,42 | 2.00 | 9 (31%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 23 | OMU | 23 | 2552 | 23 | 19,22,23 | 2.83 | 8 (42%) | 26,31,34 | 1.89 | 5 (19%) |
| 1 | MA6 | 16 | 1519 | 1 | 19,26,27 | 1.12 | 2 (10%) | 18,38,41 | 1.95 | 6 (33%) |
| 1 | MA6 | 16 | 1518 | 1 | 19,26,27 | 1.10 | 2 (10%) | 18,38,41 | 3.48 | 2 (11%) |
| 23 | PSU | 23 | 2580 | 23 | 18,21,22 | 4.04 | 8 (44%) | 22,30,33 | 1.95 | 6 (27%) |
| 59 | PSU | Dt | 39 | 59 | 18,21,22 | 4.11 | 7 (38%) | 22,30,33 | 1.91 | 5 (22%) |
| 12 | D2T | SL | 89 | 12 | 7,9,10 | 1.05 | 0 | 6,11,13 | 2.27 | 2 (33%) |
| 23 | 1MG | 23 | 745 | 23 | 18,26,27 | 2.85 | 5 (27%) | 19,39,42 | 1.47 | 4 (21%) |
| 23 | 3TD | 23 | 1915 | 23 | 18,22,23 | 4.24 | 6 (33%) | 22,32,35 | 1.62 | 2 (9%) |
| 1 | 7MG | 16 | 527 | 1 | 22,26,27 | 1.38 | 3 (13%) | 29,39,42 | 2.54 | 8 (27%) |
| 58 | T6A | Pt | 37 | 58 | 27,34,35 | 2.05 | 7 (25%) | 29,49,52 | 2.15 | 7 (24%) |
| 23 | PSU | 23 | 2504 | 23 | 18,21,22 | 4.02 | 7 (38%) | 22,30,33 | 1.84 | 5 (22%) |
| 23 | 7MG | 23 | 2069 | 23 | 22,26,27 | 1.39 | 3 (13%) | 29,39,42 | 2.56 | 7 (24%) |
| 1 | PSU | 16 | 516 | 1 | 18,21,22 | 4.08 | 7 (38%) | 22,30,33 | 1.77 | 4 (18%) |
| 59 | PSU | Dt | 55 | 59 | 18,21,22 | 4.26 | 7 (38%) | 22,30,33 | 1.94 | 5 (22%) |
| 23 | PSU | 23 | 955 | 23 | 18,21,22 | 4.02 | 7 (38%) | 22,30,33 | 2.02 | 5 (22%) |
| 36 | 4D4 | LP | 81 | 36 | 9,11,12 | 2.45 | 3 (33%) | 8,13,15 | 0.97 | 0 |
| 23 | PSU | 23 | 1911 | 23 | 18,21,22 | 4.06 | 8 (44%) | 22,30,33 | 1.75 | 4 (18%) |
| 59 | 4SU | Dt | 8 | 59 | 18,21,22 | 4.13 | 8 (44%) | 26,30,33 | 2.32 | 5 (19%) |
| 23 | 6MZ | 23 | 1618 | 23 | 18,25,26 | 1.82 | 3 (16%) | 16,36,39 | 2.94 | 4 (25%) |
| 58 | 3AU | Pt | 47 | 58 | 24,28,29 | 1.00 | 1 (4%) | 33,40,43 | 1.43 | 3 (9%) |
| 59 | MIA | Dt | 37 | 59 | 24,31,32 | 2.30 | 3 (12%) | 26,44,47 | 2.55 | 9 (34%) |
| 23 | PSU | 23 | 2604 | 23 | 18,21,22 | 3.99 | 7 (38%) | 22,30,33 | 1.94 | 5 (22%) |
| 23 | 5MU | 23 | 747 | 23 | 19,22,23 | 4.73 | 7 (36%) | 28,32,35 | 3.73 | 10 (35%) |
| 23 | OMC | 23 | 2498 | 62,23 | 19,22,23 | 2.83 | 8 (42%) | 26,31,34 | 0.77 | 0 |
| 23 | 2MG | 23 | 1835 | 23 | 18,26,27 | 2.33 | 7 (38%) | 16,38,41 | 1.55 | 4 (25%) |
| 1 | 2MG | 16 | 1516 | 1 | 18,26,27 | 2.42 | 7 (38%) | 16,38,41 | 1.42 | 4 (25%) |
| 58 | 7MG | Pt | 46 | 58 | 22,26,27 | 3.78 | 10 (45%) | 29,39,42 | 2.10 | 9 (31%) |
| 1 | 4OC | 16 | 1402 | 1,62 | 20,23,24 | 2.99 | 8 (40%) | 26,32,35 | 0.91 | 1 (3%) |
| 1 | 5MC | 16 | 1407 | 1 | 18,22,23 | 3.43 | 7 (38%) | 26,32,35 | 1.03 | 2 (7%) |
| 23 | PSU | 23 | 2605 | 23 | 18,21,22 | 4.06 | 8 (44%) | 22,30,33 | 1.91 | 5 (22%) |
| 58 | PSU | Pt | 39 | 58 | 18,21,22 | 4.16 | 7 (38%) | 22,30,33 | 1.93 | 5 (22%) |
| 23 | 2MG | 23 | 2445 | 23 | 18,26,27 | 2.33 | 7 (38%) | 16,38,41 | 1.54 | 4 (25%) |
| 23 | 5MU | 23 | 1939 | 23 | 19,22,23 | 4.73 | 7 (36%) | 28,32,35 | 3.82 | 9 (32%) |
| 23 | 5MC | 23 | 1962 | 23 | 18,22,23 | 3.38 | 7 (38%) | 26,32,35 | 0.99 | 1 (3%) |
| 1 | 2MG | 16 | 966 | 1 | 18,26,27 | 2.38 | 7 (38%) | 16,38,41 | 1.46 | 4 (25%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 23 | 2MA | 23 | 2503 | 62,23 | 17,25,26 | 2.39 | 5 (29%) | 17,37,40 | 1.43 | 3 (17%) |
| 58 | U8U | Pt | 34 | 58,22 | 19,24,25 | 1.70 | 3 (15%) | 23,34,37 | 1.19 | 4 (17%) |
| 1 | UR3 | 16 | 1498 | 1 | 19,22,23 | 2.72 | 6 (31%) | 26,32,35 | 1.28 | 1 (3%) |
| 59 | PSU | Dt | 32 | 59 | 18,21,22 | 4.13 | 7 (38%) | 22,30,33 | 1.91 | 5 (22%) |
| 1 | 5MC | 16 | 967 | 1 | 18,22,23 | 3.42 | 7 (38%) | 26,32,35 | 1.03 | 1 (3%) |
| 23 | OMG | 23 | 2251 | 58,23 | 18,26,27 | 2.37 | 8 (44%) | 19,38,41 | 1.54 | 4 (21%) |
| 23 | H2U | 23 | 2449 | 23 | 18,21,22 | 2.86 | 5 (27%) | 21,30,33 | 2.15 | 5 (23%) |
| 23 | PSU | 23 | 746 | 62,23 | 18,21,22 | 4.06 | 7 (38%) | 22,30,33 | 1.70 | 5 (22%) |
| 59 | 3AU | Dt | 47 | 59 | 24,28,29 | 1.05 | 1 (4%) | 33,40,43 | 1.49 | 4 (12%) |

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 |
|-----|------|-------|------|------|---------|-------------|---------|
| 23 | PSU | 23 | 2457 | 23 | - | 0/7/25/26 | 0/2/2/2 |
| 23 | 6MZ | 23 | 2030 | 23 | - | 2/5/27/28 | 0/3/3/3 |
| 59 | 7MG | Dt | 46 | 59 | - | 2/7/37/38 | 0/3/3/3 |
| 23 | OMU | 23 | 2552 | 23 | - | 0/9/27/28 | 0/2/2/2 |
| 1 | MA6 | 16 | 1519 | 1 | - | 6/7/29/30 | 0/3/3/3 |
| 1 | MA6 | 16 | 1518 | 1 | - | 0/7/29/30 | 0/3/3/3 |
| 23 | PSU | 23 | 2580 | 23 | - | 1/7/25/26 | 0/2/2/2 |
| 59 | PSU | Dt | 39 | 59 | - | 0/7/25/26 | 0/2/2/2 |
| 12 | D2T | SL | 89 | 12 | - | 1/7/12/14 | - |
| 23 | 1MG | 23 | 745 | 23 | - | 0/3/25/26 | 0/3/3/3 |
| 23 | 3TD | 23 | 1915 | 23 | - | 3/7/25/26 | 0/2/2/2 |
| 1 | 7MG | 16 | 527 | 1 | - | 3/7/37/38 | 0/3/3/3 |
| 58 | T6A | Pt | 37 | 58 | - | 10/19/41/42 | 0/3/3/3 |
| 23 | PSU | 23 | 2504 | 23 | - | 0/7/25/26 | 0/2/2/2 |
| 23 | 7MG | 23 | 2069 | 23 | - | 1/7/37/38 | 0/3/3/3 |
| 1 | PSU | 16 | 516 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 59 | PSU | Dt | 55 | 59 | - | 0/7/25/26 | 0/2/2/2 |
| 23 | PSU | 23 | 955 | 23 | - | 0/7/25/26 | 0/2/2/2 |
| 36 | 4D4 | LP | 81 | 36 | - | 1/11/12/14 | - |
| 23 | PSU | 23 | 1911 | 23 | - | 3/7/25/26 | 0/2/2/2 |
| 59 | 4SU | Dt | 8 | 59 | - | 0/7/25/26 | 0/2/2/2 |
| 23 | 6MZ | 23 | 1618 | 23 | - | 4/5/27/28 | 0/3/3/3 |
| 58 | 3AU | Pt | 47 | 58 | - | 9/16/34/35 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|-------|---------|-------------|---------|
| 59 | MIA | Dt | 37 | 59 | - | 6/11/33/34 | 0/3/3/3 |
| 23 | PSU | 23 | 2604 | 23 | - | 0/7/25/26 | 0/2/2/2 |
| 23 | 5MU | 23 | 747 | 23 | - | 1/7/25/26 | 0/2/2/2 |
| 23 | OMC | 23 | 2498 | 62,23 | - | 2/9/27/28 | 0/2/2/2 |
| 23 | 2MG | 23 | 1835 | 23 | - | 2/5/27/28 | 0/3/3/3 |
| 1 | 2MG | 16 | 1516 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 58 | 7MG | Pt | 46 | 58 | - | 4/7/37/38 | 0/3/3/3 |
| 1 | 4OC | 16 | 1402 | 1,62 | - | 1/9/29/30 | 0/2/2/2 |
| 1 | 5MC | 16 | 1407 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 23 | PSU | 23 | 2605 | 23 | - | 0/7/25/26 | 0/2/2/2 |
| 58 | PSU | Pt | 39 | 58 | - | 0/7/25/26 | 0/2/2/2 |
| 23 | 2MG | 23 | 2445 | 23 | - | 0/5/27/28 | 0/3/3/3 |
| 23 | 5MU | 23 | 1939 | 23 | - | 0/7/25/26 | 0/2/2/2 |
| 23 | 5MC | 23 | 1962 | 23 | - | 2/7/25/26 | 0/2/2/2 |
| 1 | 2MG | 16 | 966 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 23 | 2MA | 23 | 2503 | 62,23 | - | 2/3/25/26 | 0/3/3/3 |
| 58 | U8U | Pt | 34 | 58,22 | - | 2/9/28/29 | 0/2/2/2 |
| 1 | UR3 | 16 | 1498 | 1 | - | 2/7/25/26 | 0/2/2/2 |
| 59 | PSU | Dt | 32 | 59 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MC | 16 | 967 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 23 | OMG | 23 | 2251 | 58,23 | - | 3/5/27/28 | 0/3/3/3 |
| 23 | H2U | 23 | 2449 | 23 | - | 1/7/38/39 | 0/2/2/2 |
| 23 | PSU | 23 | 746 | 62,23 | - | 1/7/25/26 | 0/2/2/2 |
| 59 | 3AU | Dt | 47 | 59 | - | 10/16/34/35 | 0/2/2/2 |

The worst 5 of 280 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 23 | 23 | 1915 | 3TD | C6-C5 | 12.52 | 1.49 | 1.35 |
| 59 | Dt | 55 | PSU | C6-C5 | 11.00 | 1.48 | 1.35 |
| 58 | Pt | 39 | PSU | C6-C5 | 10.81 | 1.47 | 1.35 |
| 59 | Dt | 39 | PSU | C6-C5 | 10.66 | 1.47 | 1.35 |
| 59 | Dt | 32 | PSU | C6-C5 | 10.66 | 1.47 | 1.35 |

The worst 5 of 210 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16 | 1518 | MA6 | N1-C6-N6 | -13.49 | 102.86 | 117.06 |
| 23 | 23 | 1939 | 5MU | C5-C4-N3 | 12.84 | 126.27 | 115.31 |
| 23 | 23 | 747 | 5MU | C5-C4-N3 | 12.28 | 125.80 | 115.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 23 | 23 | 2030 | 6MZ | C1'-N9-C4 | -11.73 | 106.03 | 126.64 |
| 23 | 23 | 1939 | 5MU | C5-C6-N1 | -10.86 | 112.17 | 123.34 |

There are no chirality outliers.

5 of 85 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 1 | 16 | 527 | 7MG | C3'-C4'-C5'-O5' |
| 1 | 16 | 1519 | MA6 | O4'-C4'-C5'-O5' |
| 1 | 16 | 1519 | MA6 | C3'-C4'-C5'-O5' |
| 1 | 16 | 1519 | MA6 | C5-C6-N6-C9 |
| 1 | 16 | 1519 | MA6 | C5-C6-N6-C10 |

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 372 ligands modelled in this entry, 347 are monoatomic - leaving 25 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 |
| 61 | PUT | 23 | 3004 | - | 5,5,5 | 0.19 | 0 | 4,4,4 | 0.56 | 0 |
| 61 | PUT | 23 | 3006 | - | 5,5,5 | 0.22 | 0 | 4,4,4 | 0.50 | 0 |
| 64 | ATP | 23 | 3002 | - | 26,33,33 | 0.66 | 0 | 31,52,52 | 0.78 | 1 (3%) |
| 64 | ATP | 23 | 3003 | - | 26,33,33 | 0.66 | 0 | 31,52,52 | 0.72 | 1 (3%) |
| 60 | SCM | 23 | 3001 | - | 23,25,25 | 1.36 | 3 (13%) | 26,39,39 | 1.56 | 5 (19%) |
| 61 | PUT | 23 | 3016 | - | 5,5,5 | 0.23 | 0 | 4,4,4 | 0.49 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 60 | SCM | 16 | 1602 | - | 23,25,25 | 1.35 | 2 (8%) | 26,39,39 | 1.31 | 3 (11%) |
| 61 | PUT | LC | 301 | 26 | 5,5,5 | 0.23 | 0 | 4,4,4 | 0.77 | 0 |
| 61 | PUT | 23 | 3012 | - | 5,5,5 | 0.23 | 0 | 4,4,4 | 0.49 | 0 |
| 65 | SPD | 23 | 3018 | - | 9,9,9 | 0.31 | 0 | 8,8,8 | 0.96 | 0 |
| 61 | PUT | 23 | 3007 | - | 5,5,5 | 0.16 | 0 | 4,4,4 | 0.20 | 0 |
| 61 | PUT | 23 | 3011 | - | 5,5,5 | 0.24 | 0 | 4,4,4 | 0.46 | 0 |
| 61 | PUT | 23 | 3009 | - | 5,5,5 | 0.23 | 0 | 4,4,4 | 0.51 | 0 |
| 61 | PUT | 23 | 3010 | - | 5,5,5 | 0.21 | 0 | 4,4,4 | 0.56 | 0 |
| 65 | SPD | 23 | 3017 | - | 9,9,9 | 0.31 | 0 | 8,8,8 | 0.91 | 0 |
| 61 | PUT | 23 | 3005 | - | 5,5,5 | 0.24 | 0 | 4,4,4 | 0.44 | 0 |
| 61 | PUT | 16 | 1605 | - | 5,5,5 | 0.17 | 0 | 4,4,4 | 0.21 | 0 |
| 60 | SCM | 16 | 1601 | - | 23,25,25 | 1.33 | 1 (4%) | 26,39,39 | 1.37 | 3 (11%) |
| 61 | PUT | 16 | 1604 | - | 5,5,5 | 0.17 | 0 | 4,4,4 | 0.21 | 0 |
| 61 | PUT | 23 | 3013 | - | 5,5,5 | 0.16 | 0 | 4,4,4 | 0.62 | 0 |
| 61 | PUT | 16 | 1603 | - | 5,5,5 | 0.24 | 0 | 4,4,4 | 0.50 | 0 |
| 66 | GTP | EF | 901 | 62 | 26,34,34 | 5.13 | 14 (53%) | 32,54,54 | 1.88 | 7 (21%) |
| 61 | PUT | 23 | 3014 | - | 5,5,5 | 0.21 | 0 | 4,4,4 | 0.44 | 0 |
| 61 | PUT | 23 | 3015 | - | 5,5,5 | 0.24 | 0 | 4,4,4 | 0.42 | 0 |
| 61 | PUT | 23 | 3008 | - | 5,5,5 | 0.24 | 0 | 4,4,4 | 0.51 | 0 |

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 |
|-----|------|-------|------|------|---------|------------|---------|
| 61 | PUT | 23 | 3004 | - | - | 2/3/3/3 | - |
| 61 | PUT | 23 | 3006 | - | - | 1/3/3/3 | - |
| 64 | ATP | 23 | 3003 | - | 1/1/7/7 | 6/18/38/38 | 0/3/3/3 |
| 64 | ATP | 23 | 3002 | - | - | 3/18/38/38 | 0/3/3/3 |
| 60 | SCM | 23 | 3001 | - | - | 0/4/57/57 | 0/3/3/3 |
| 61 | PUT | 23 | 3016 | - | - | 1/3/3/3 | - |
| 60 | SCM | 16 | 1602 | - | - | 0/4/57/57 | 0/3/3/3 |
| 61 | PUT | LC | 301 | 26 | - | 1/3/3/3 | - |
| 61 | PUT | 23 | 3012 | - | - | 2/3/3/3 | - |
| 65 | SPD | 23 | 3018 | - | - | 0/7/7/7 | - |
| 61 | PUT | 23 | 3007 | - | - | 3/3/3/3 | - |
| 61 | PUT | 23 | 3011 | - | - | 1/3/3/3 | - |
| 61 | PUT | 23 | 3009 | - | - | 1/3/3/3 | - |
| 61 | PUT | 23 | 3010 | - | - | 1/3/3/3 | - |
| 65 | SPD | 23 | 3017 | - | - | 4/7/7/7 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 61 | PUT | 23 | 3005 | - | - | 0/3/3/3 | - |
| 61 | PUT | 16 | 1605 | - | - | 3/3/3/3 | - |
| 60 | SCM | 16 | 1601 | - | - | 2/4/57/57 | 0/3/3/3 |
| 61 | PUT | 16 | 1604 | - | - | 0/3/3/3 | - |
| 61 | PUT | 23 | 3013 | - | - | 2/3/3/3 | - |
| 61 | PUT | 16 | 1603 | - | - | 0/3/3/3 | - |
| 66 | GTP | EF | 901 | 62 | - | 2/18/38/38 | 0/3/3/3 |
| 61 | PUT | 23 | 3014 | - | - | 2/3/3/3 | - |
| 61 | PUT | 23 | 3015 | - | - | 2/3/3/3 | - |
| 61 | PUT | 23 | 3008 | - | - | 0/3/3/3 | - |

The worst 5 of 20 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 66 | EF | 901 | GTP | C2'-C1' | -16.82 | 1.28 | 1.53 |
| 66 | EF | 901 | GTP | O4'-C1' | 14.42 | 1.61 | 1.41 |
| 66 | EF | 901 | GTP | O4'-C4' | -6.48 | 1.30 | 1.45 |
| 66 | EF | 901 | GTP | C2-N3 | 6.17 | 1.48 | 1.33 |
| 66 | EF | 901 | GTP | C4-N3 | 4.70 | 1.48 | 1.37 |

The worst 5 of 20 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 66 | EF | 901 | GTP | PA-O3A-PB | -6.50 | 110.52 | 132.83 |
| 60 | 16 | 1601 | SCM | C8M-N8-C8 | -4.31 | 108.11 | 114.38 |
| 66 | EF | 901 | GTP | C5-C6-N1 | 3.89 | 120.83 | 113.95 |
| 60 | 23 | 3001 | SCM | C1M-N10-C10 | -3.46 | 109.34 | 114.38 |
| 66 | EF | 901 | GTP | C2-N1-C6 | -3.43 | 118.79 | 125.10 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 64 | 23 | 3003 | ATP | C4' |

5 of 39 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 60 | 16 | 1601 | SCM | C9-C10-N10-C1M |
| 60 | 16 | 1601 | SCM | C11-C10-N10-C1M |
| 64 | 23 | 3002 | ATP | PB-O3B-PG-O3G |

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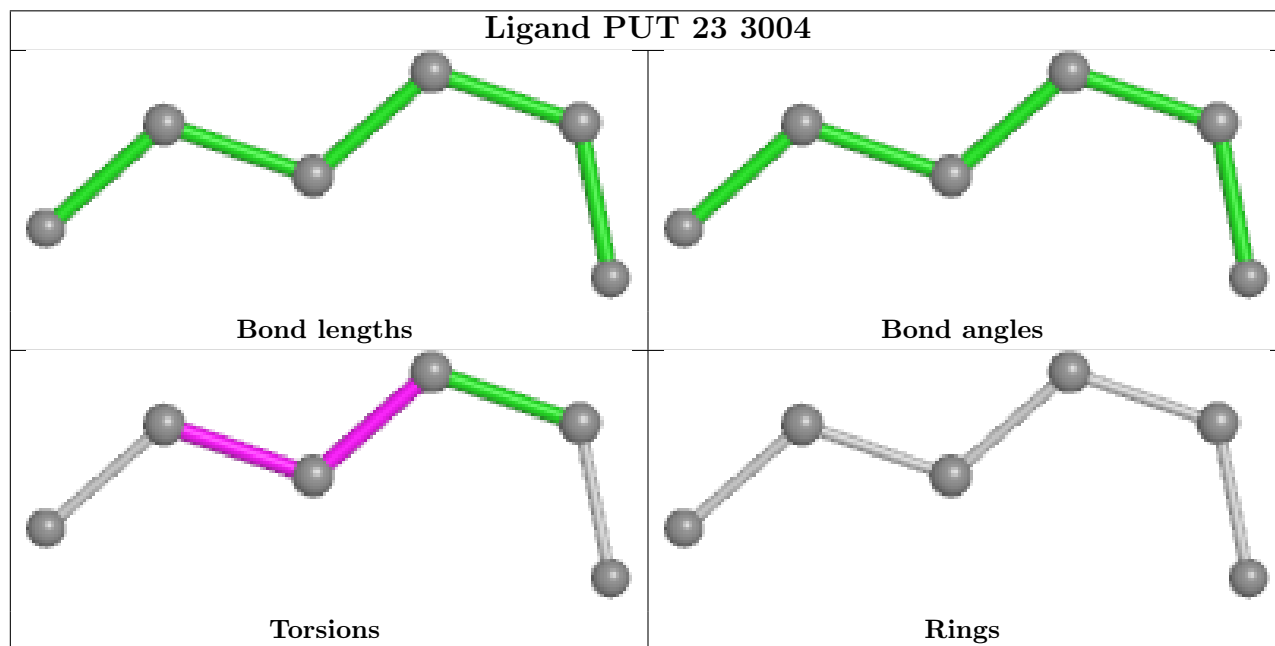
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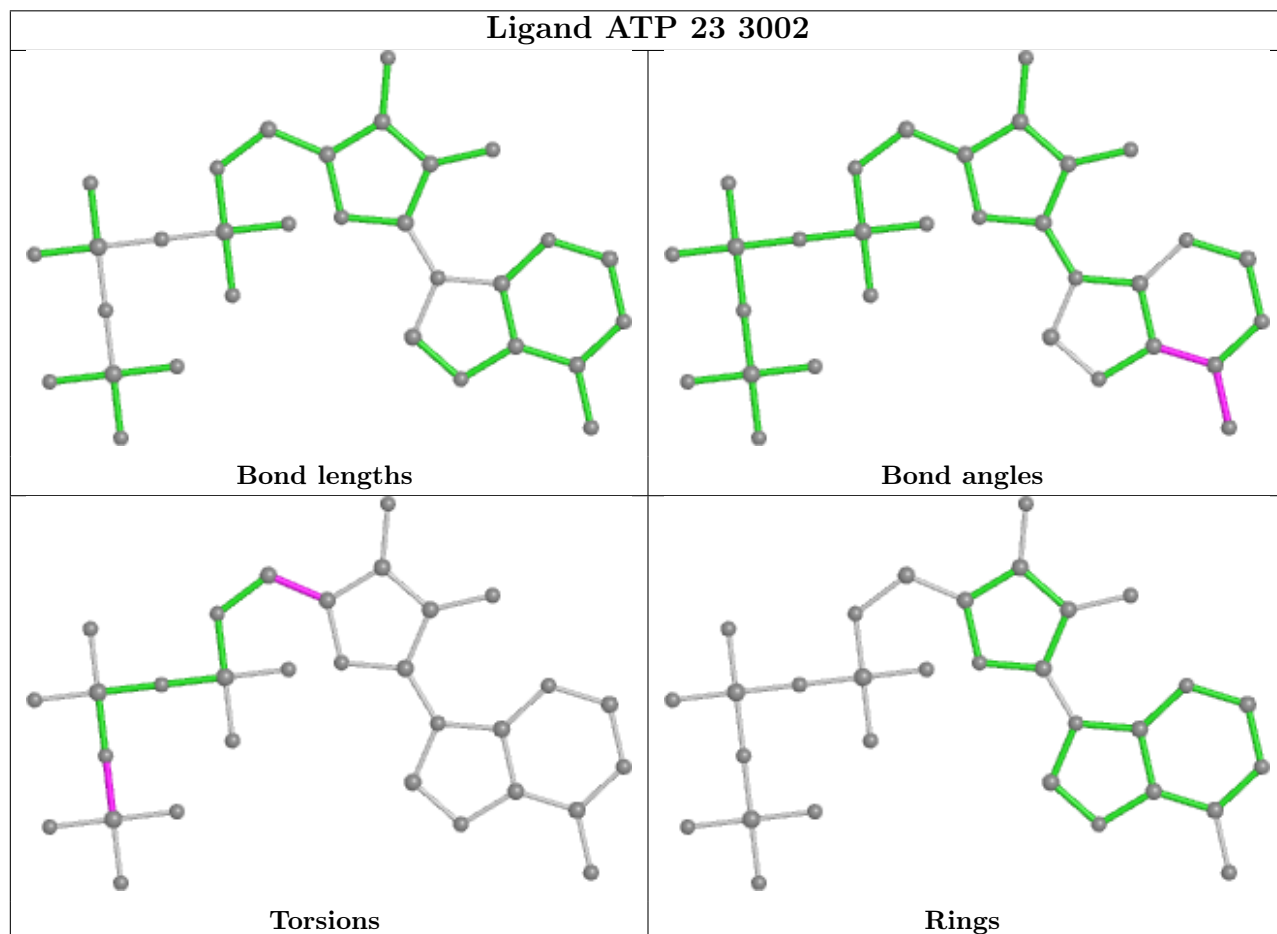
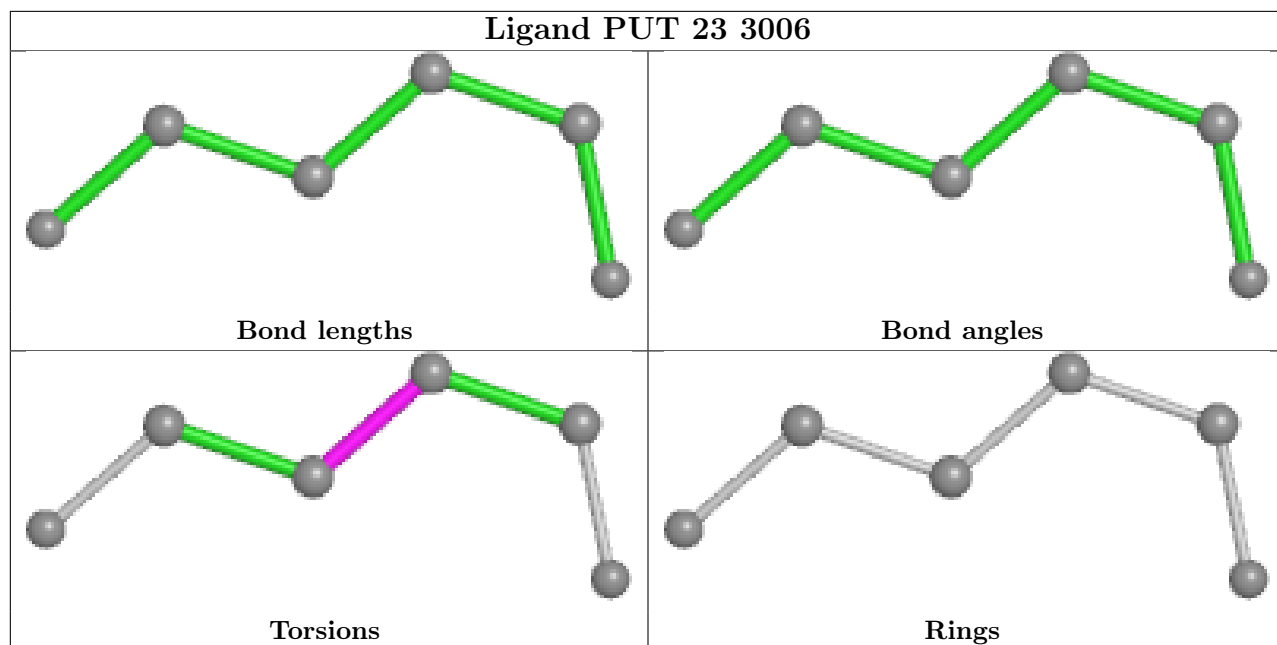
| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 64 | 23 | 3002 | ATP | O4'-C4'-C5'-O5' |
| 64 | 23 | 3003 | ATP | C5'-O5'-PA-O1A |

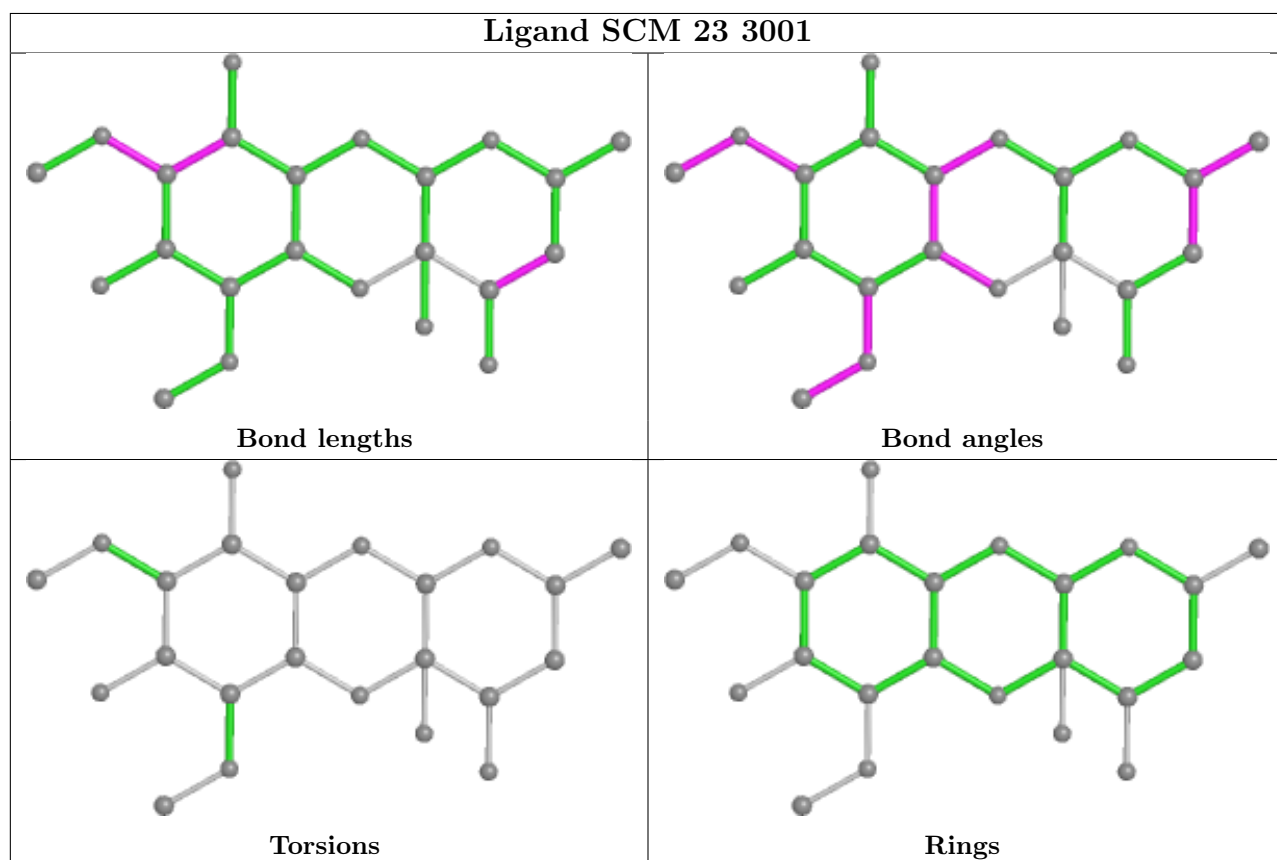
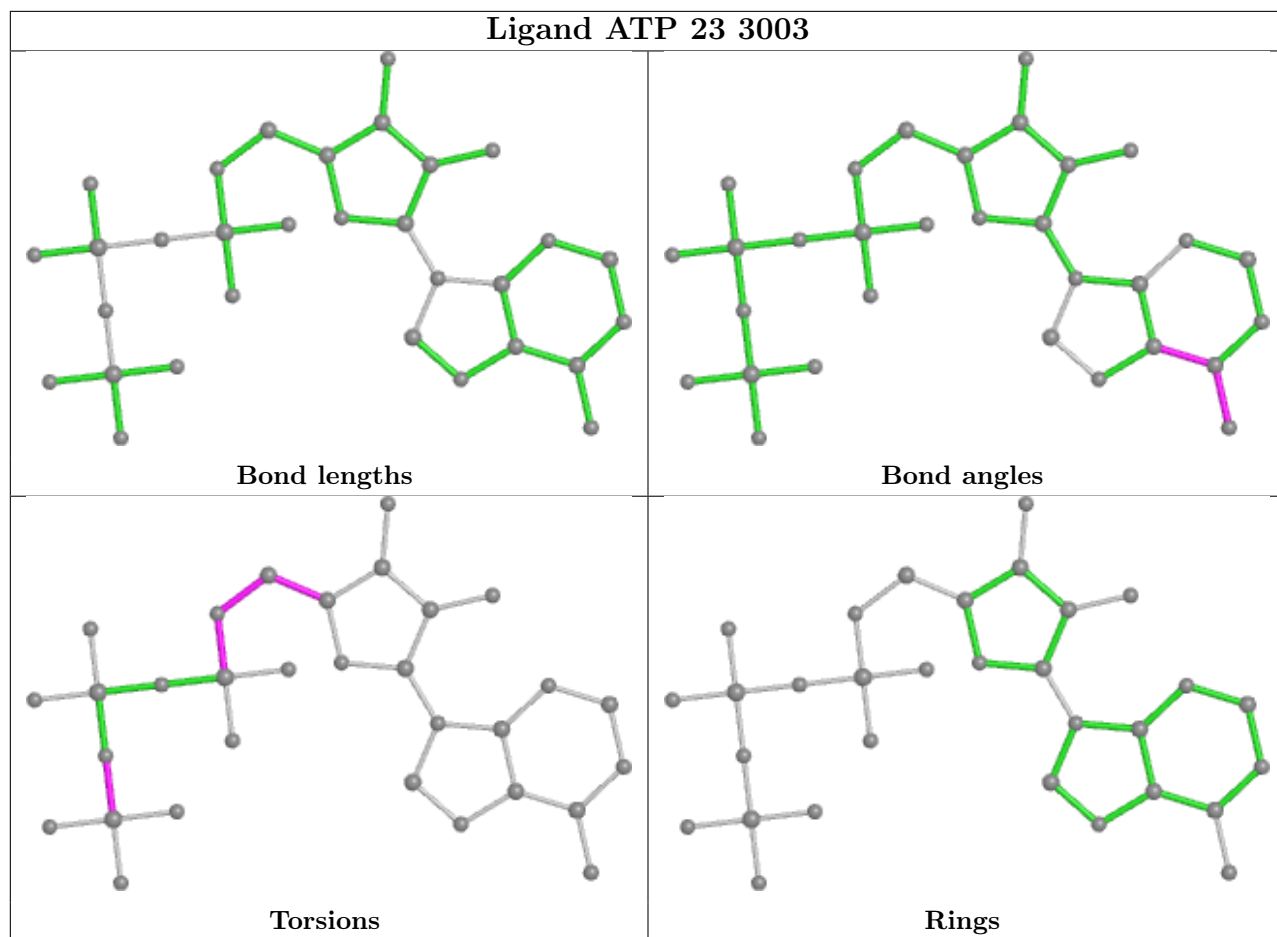
There are no ring outliers.

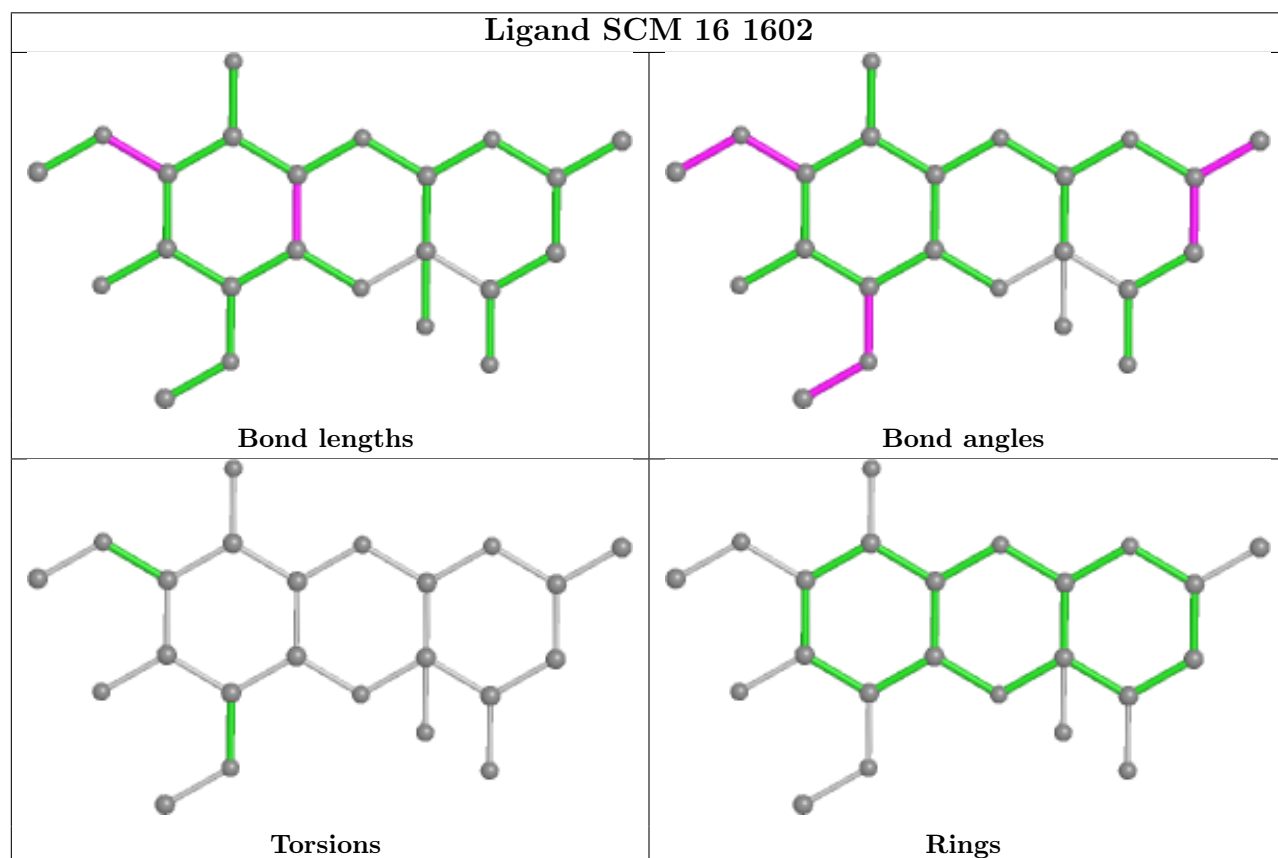
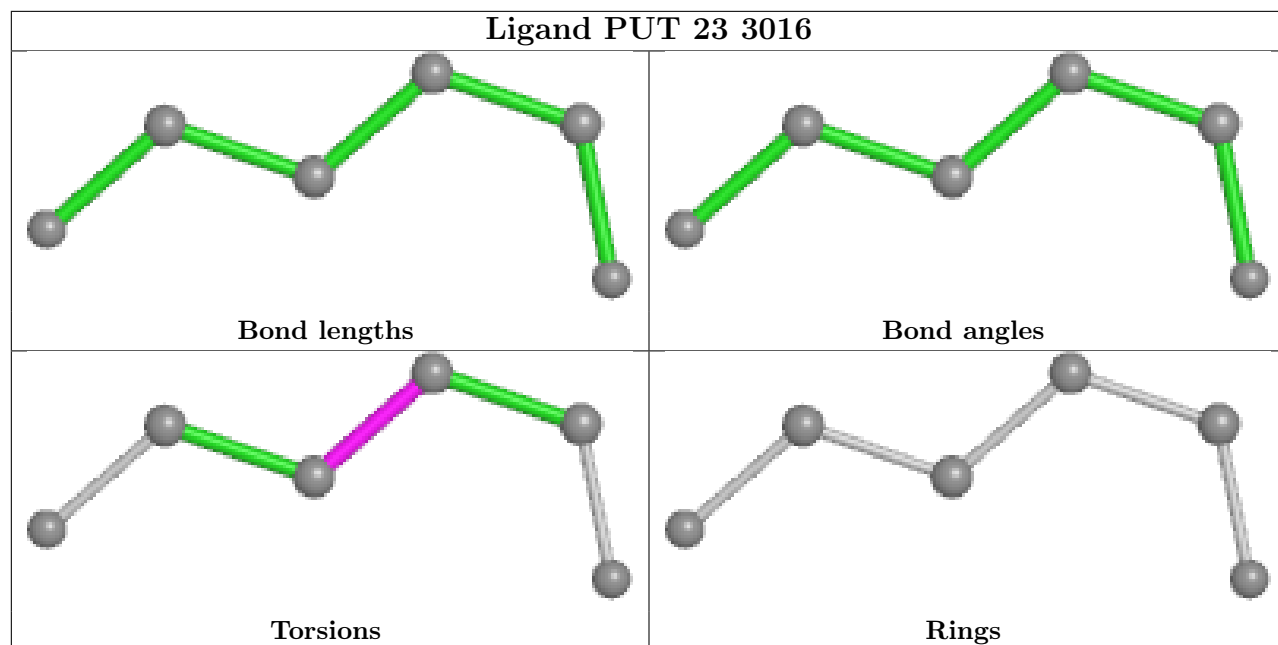
No monomer is involved in short contacts.

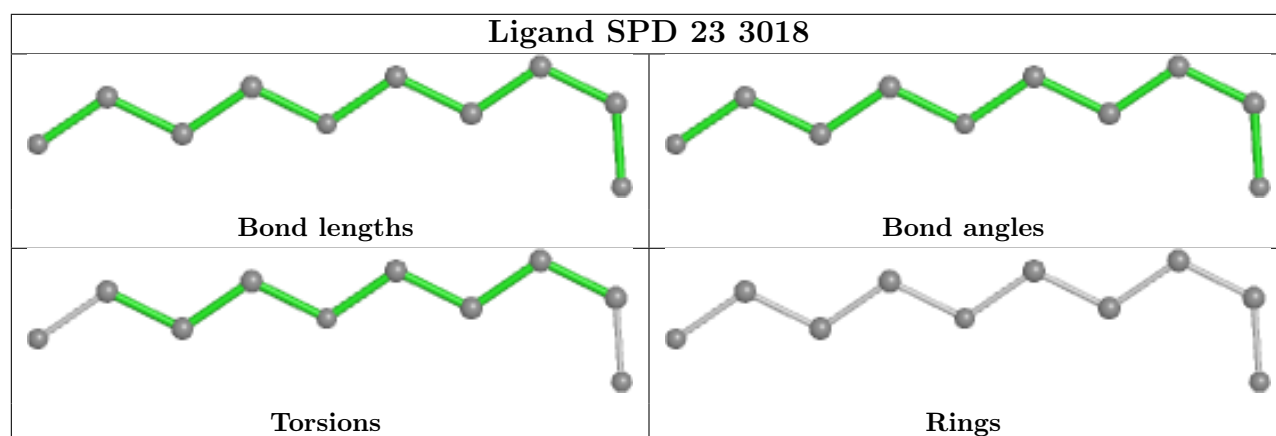
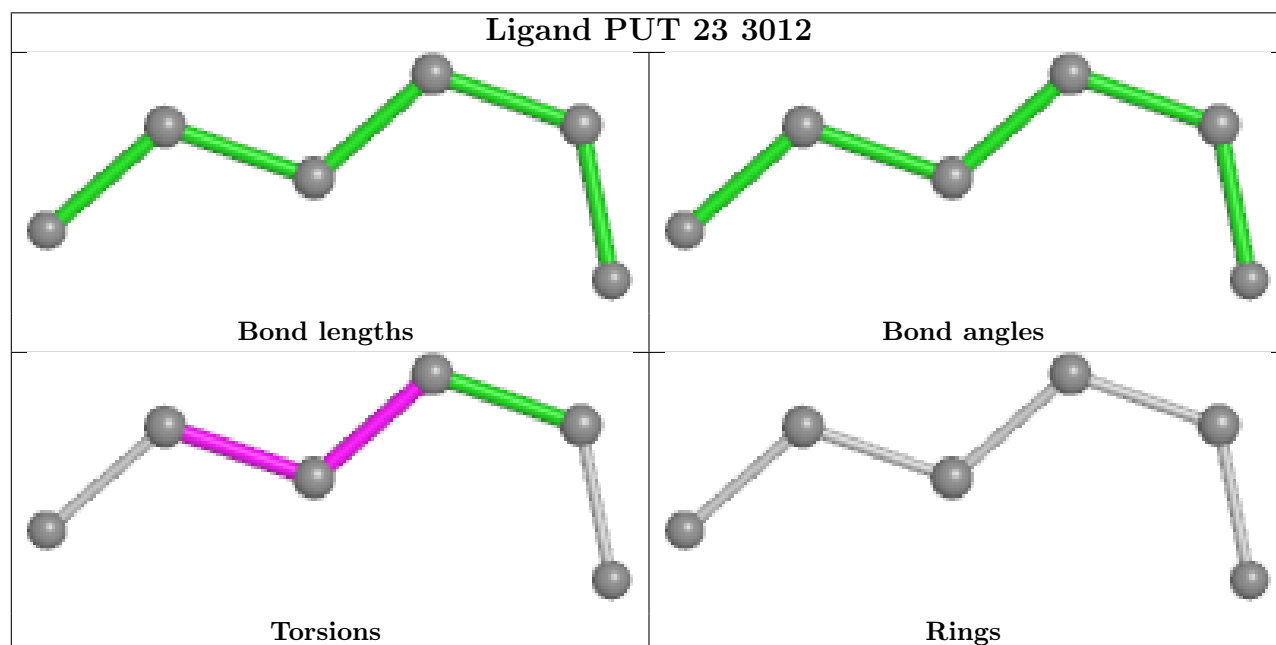
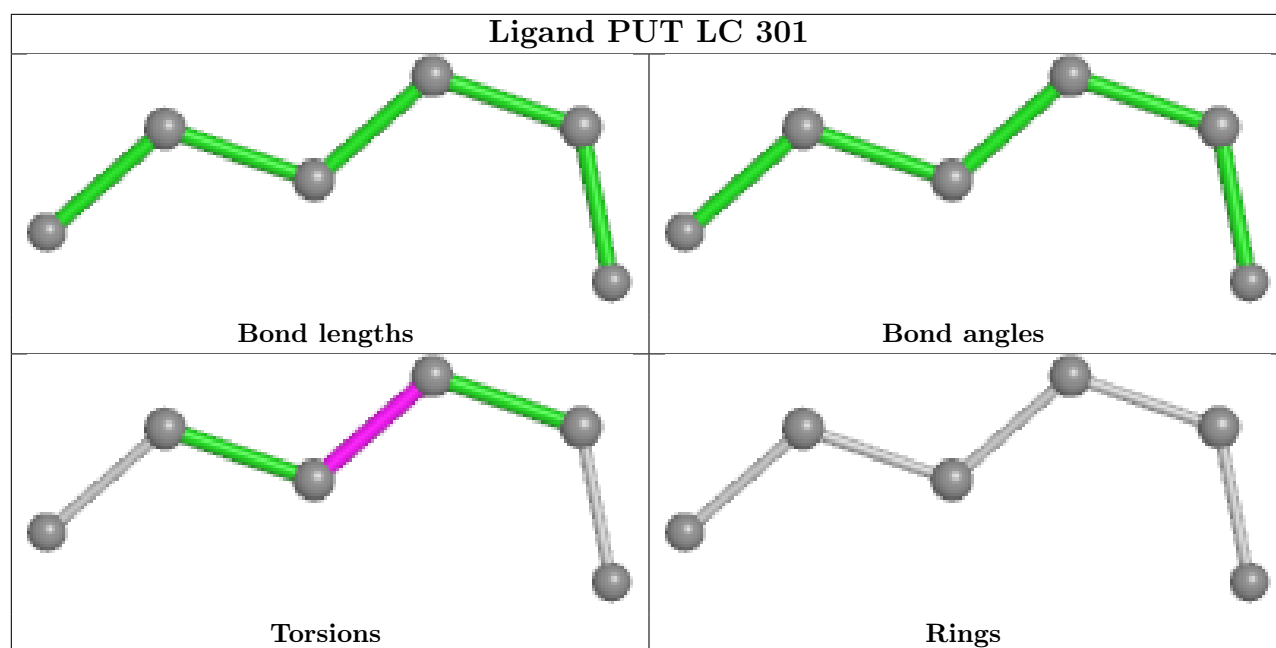
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

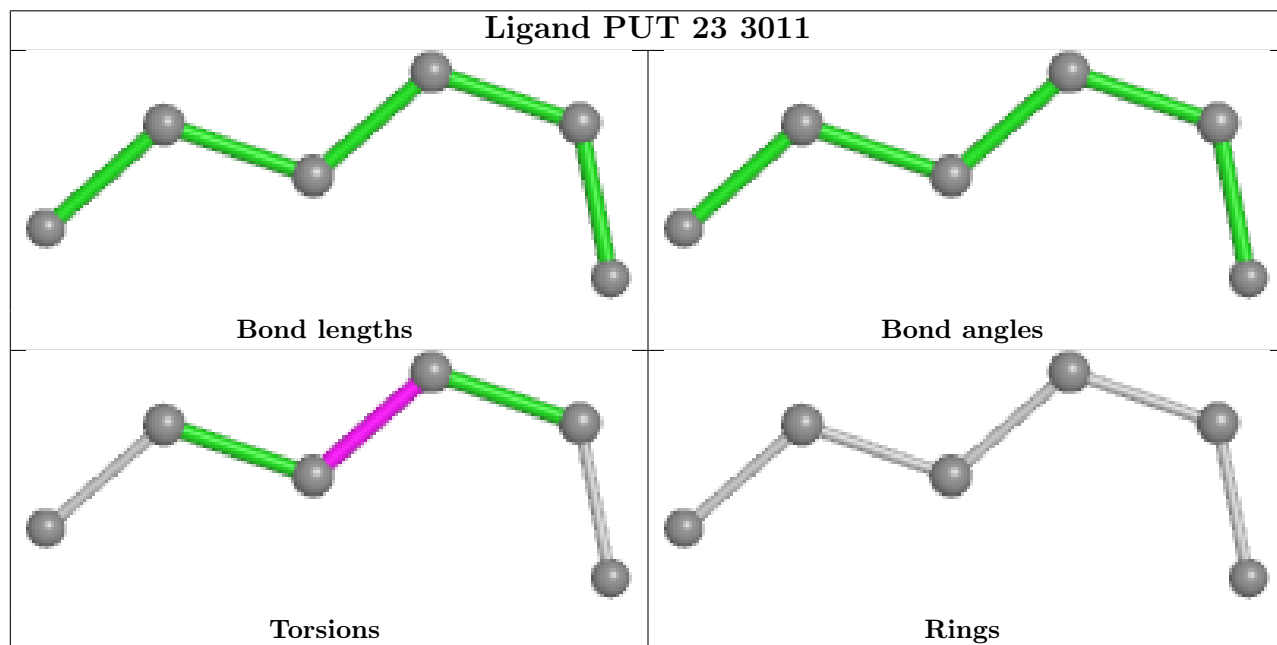
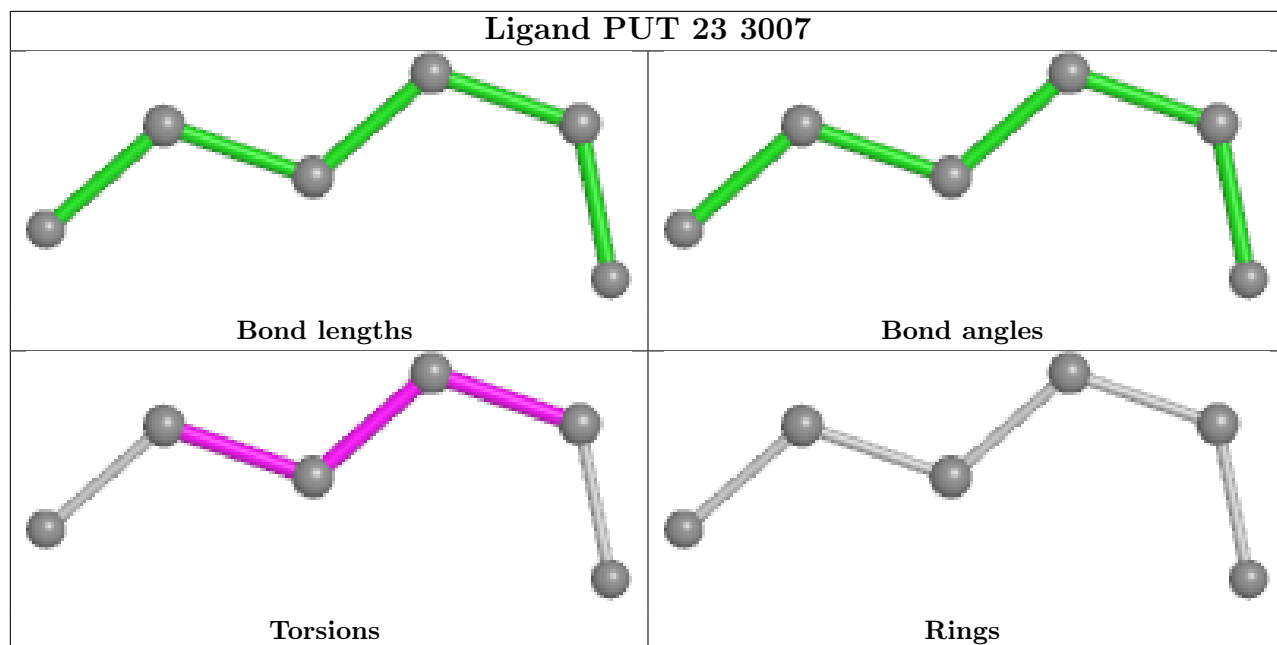


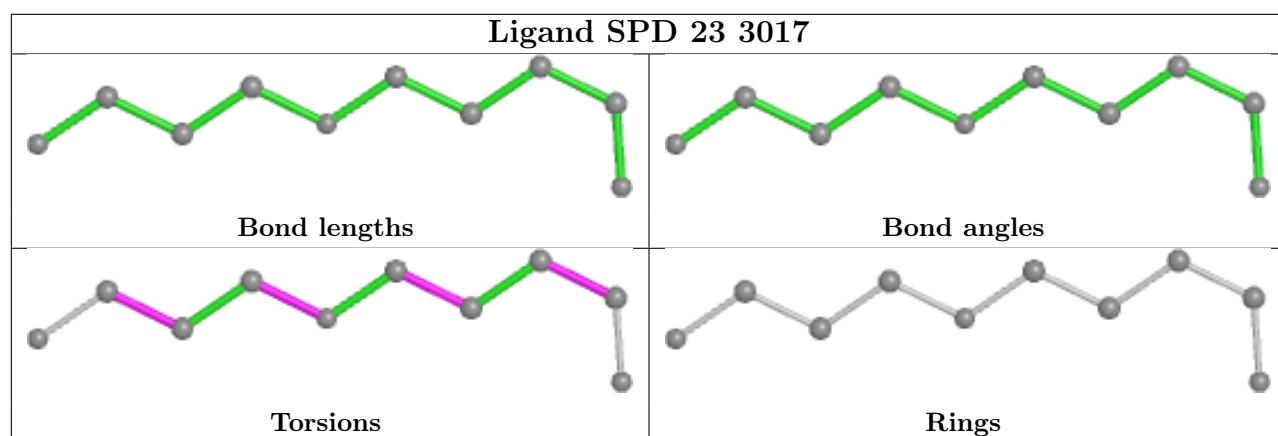
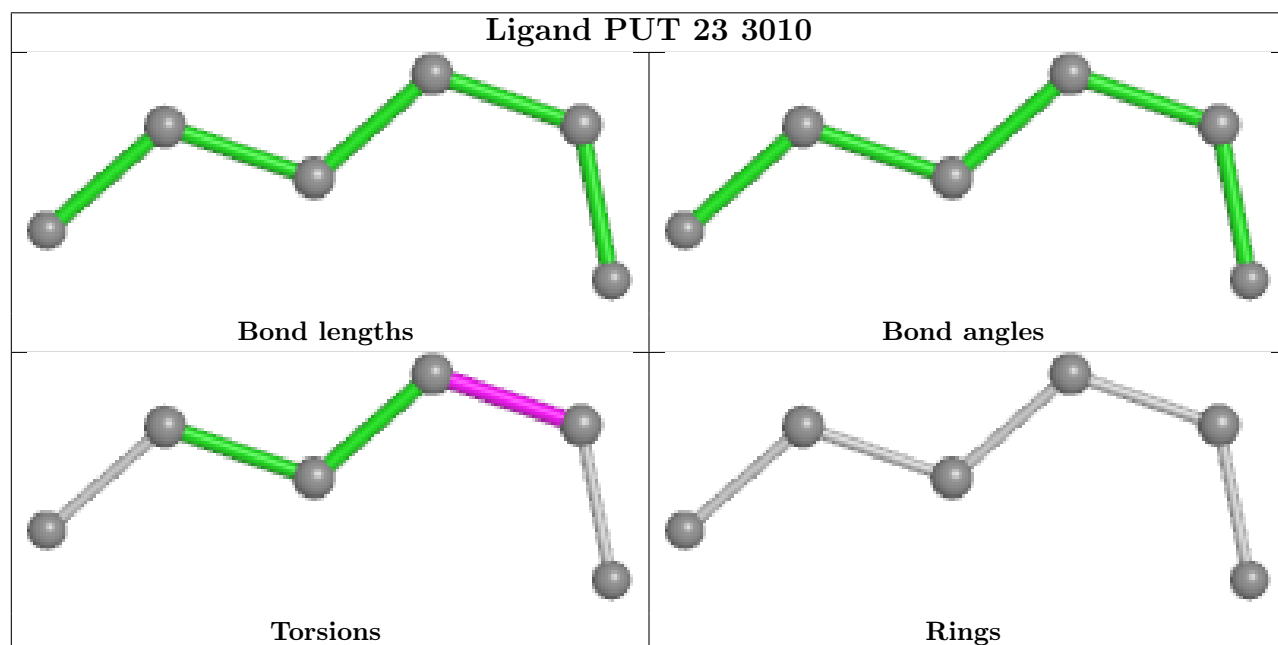
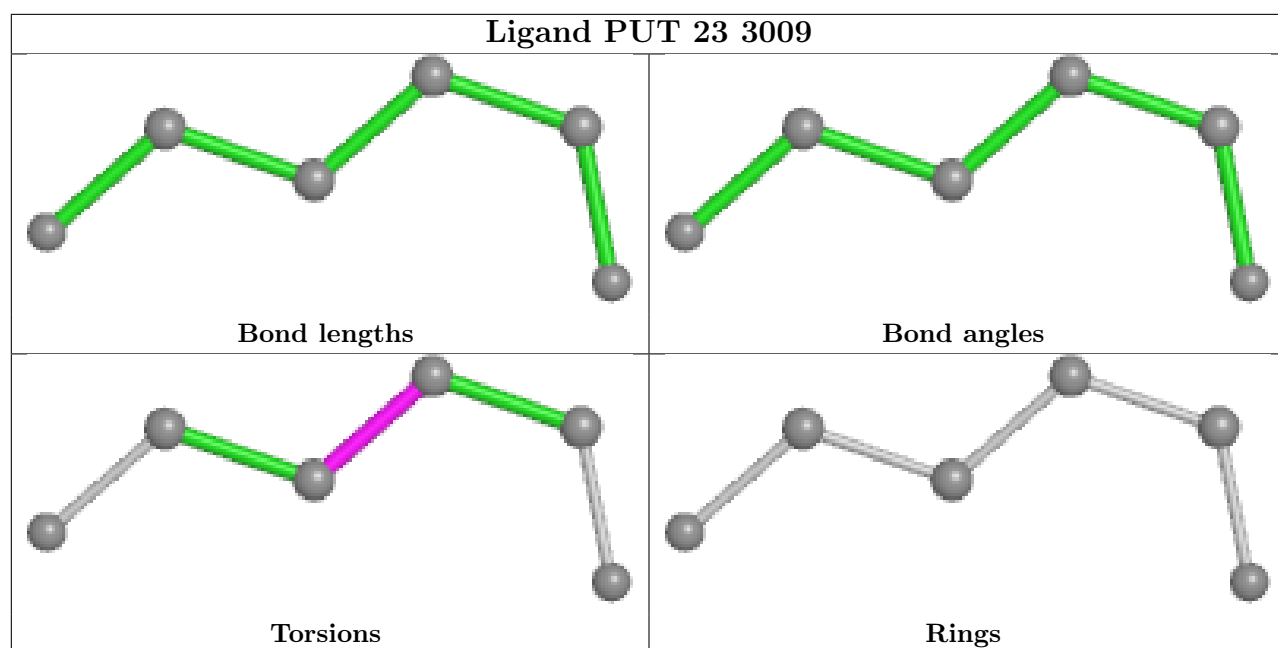


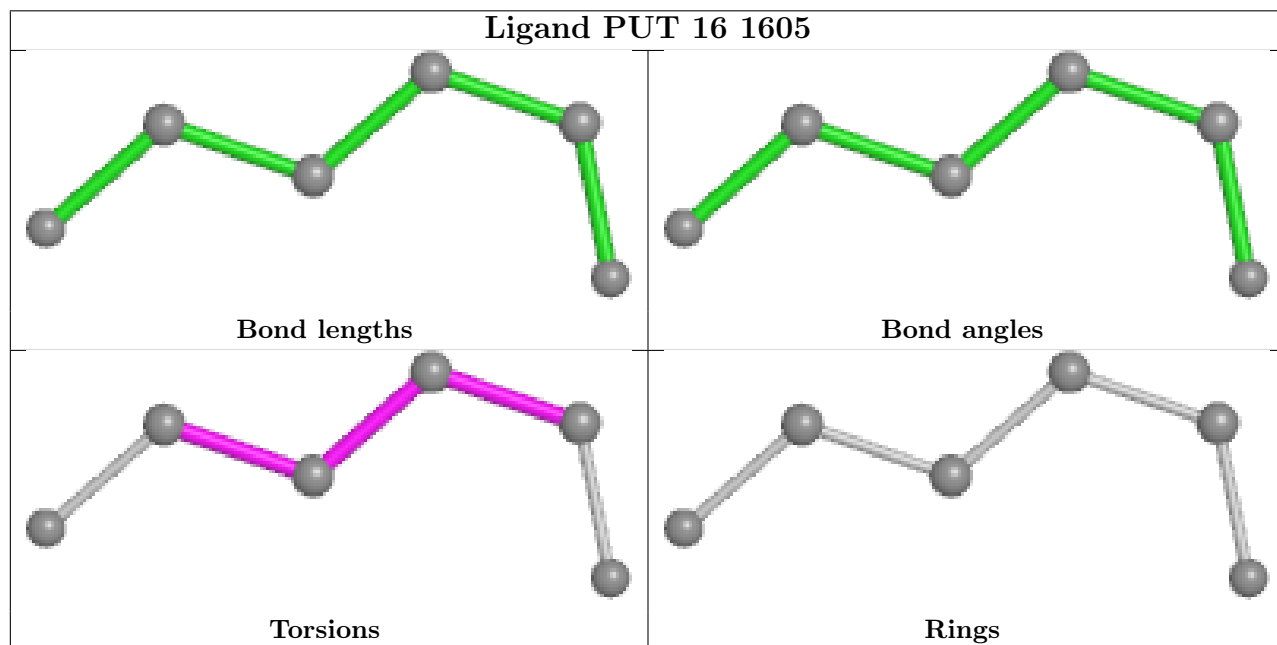
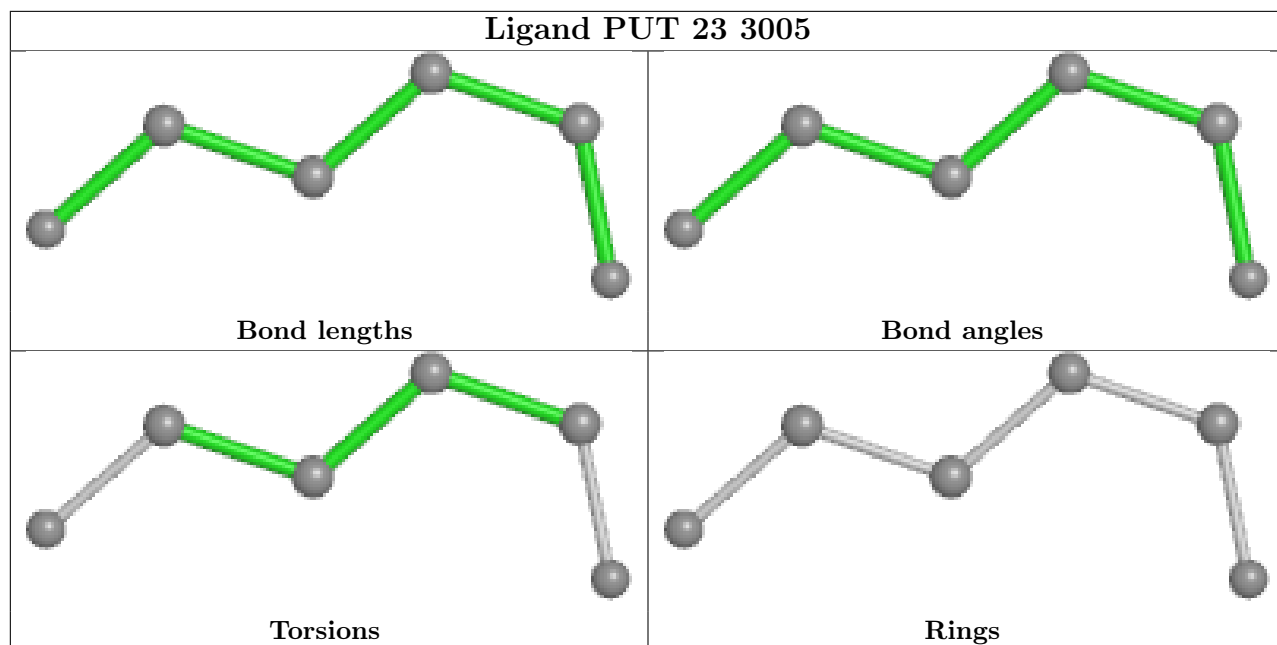


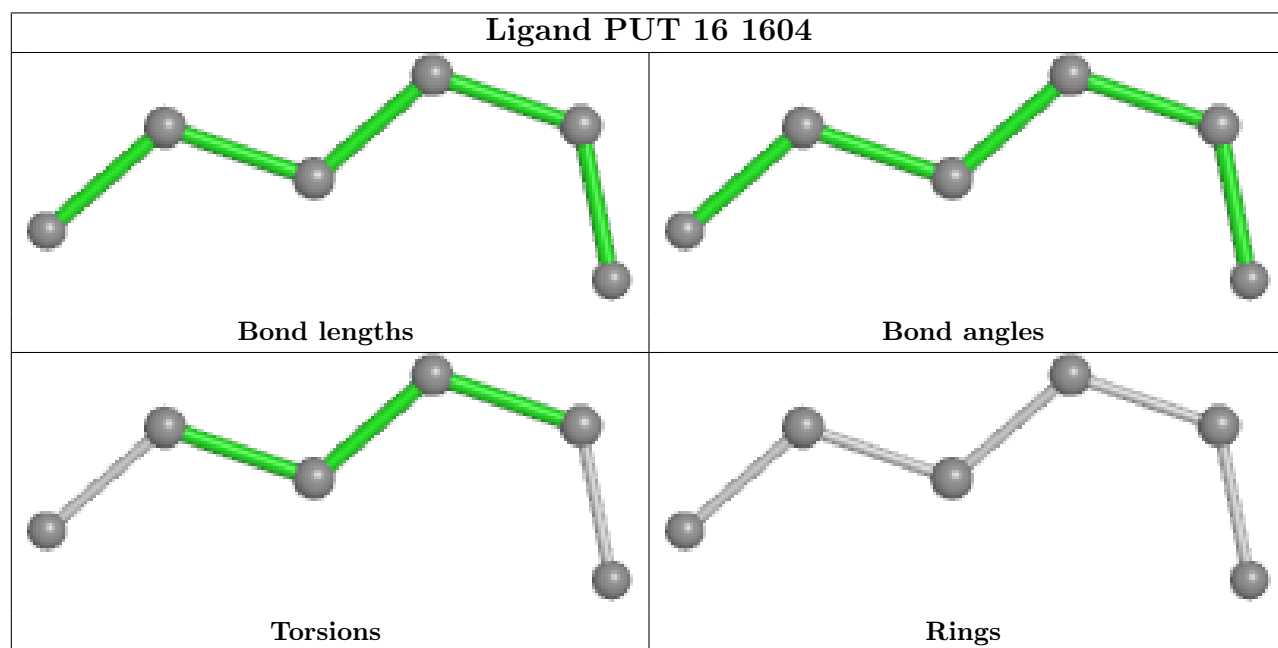
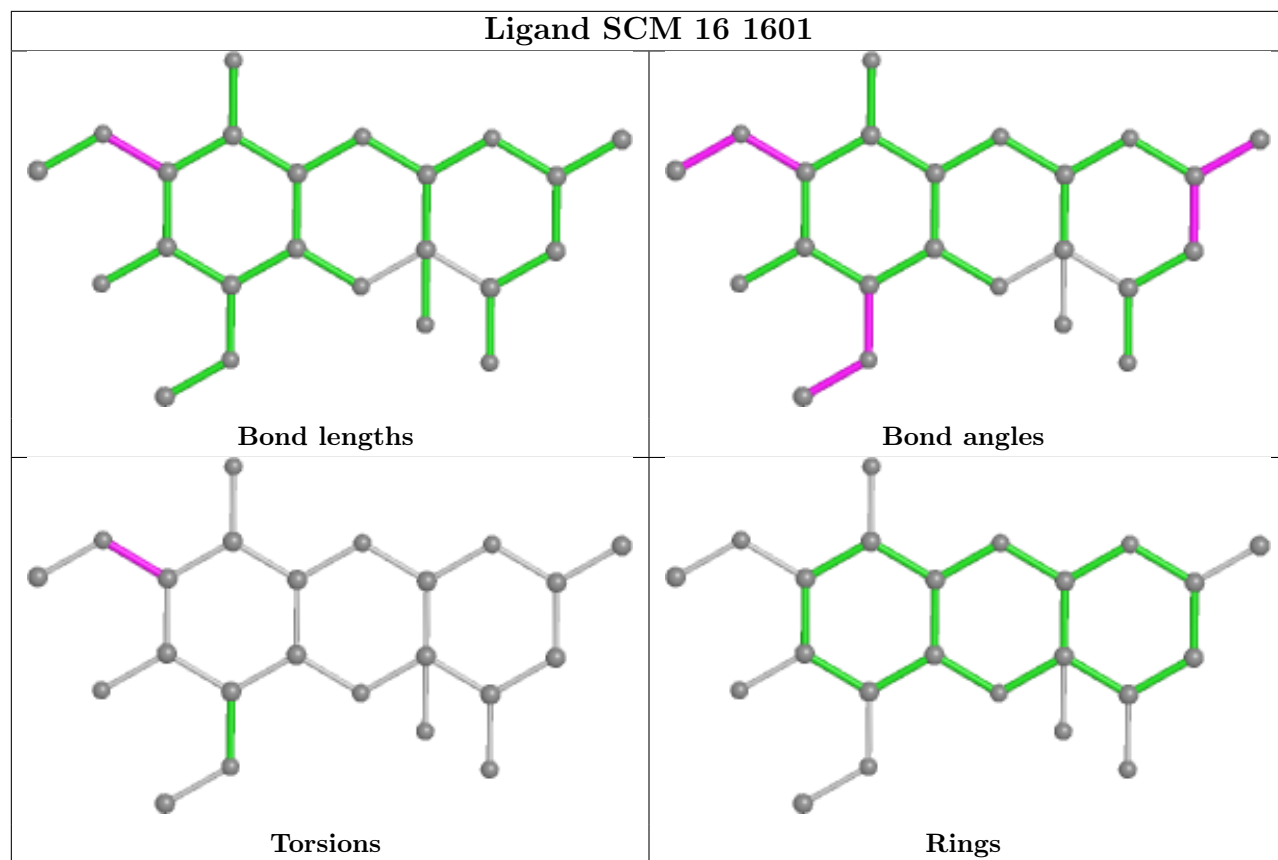


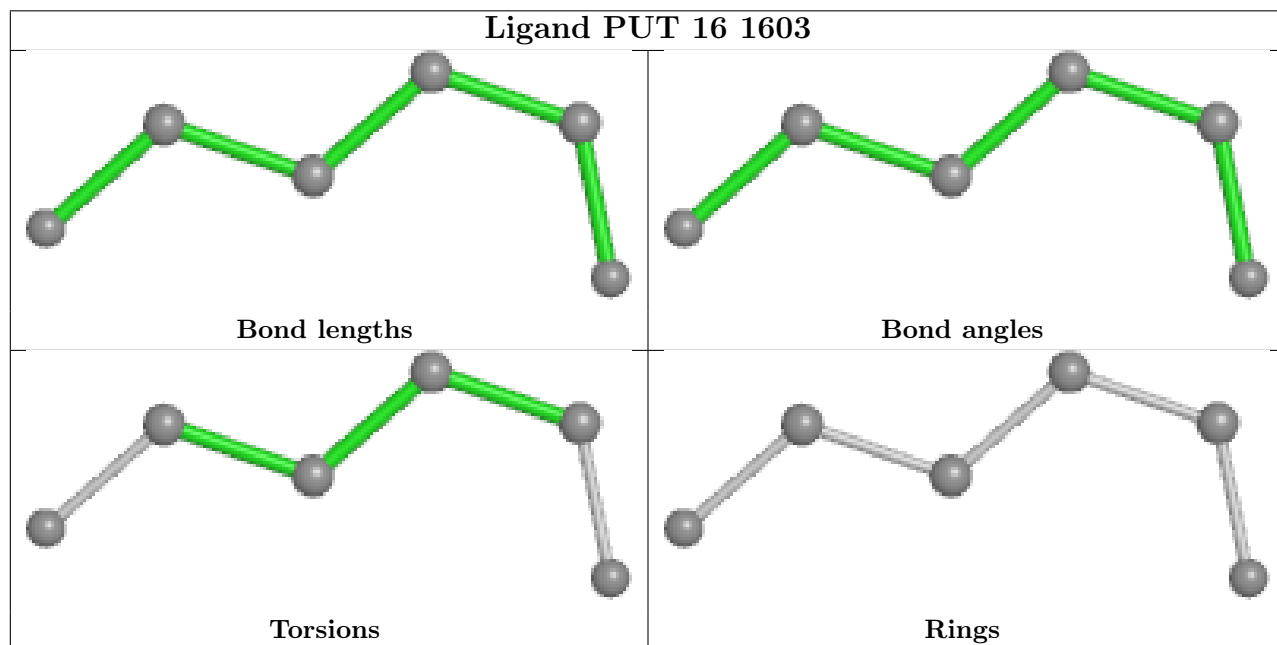
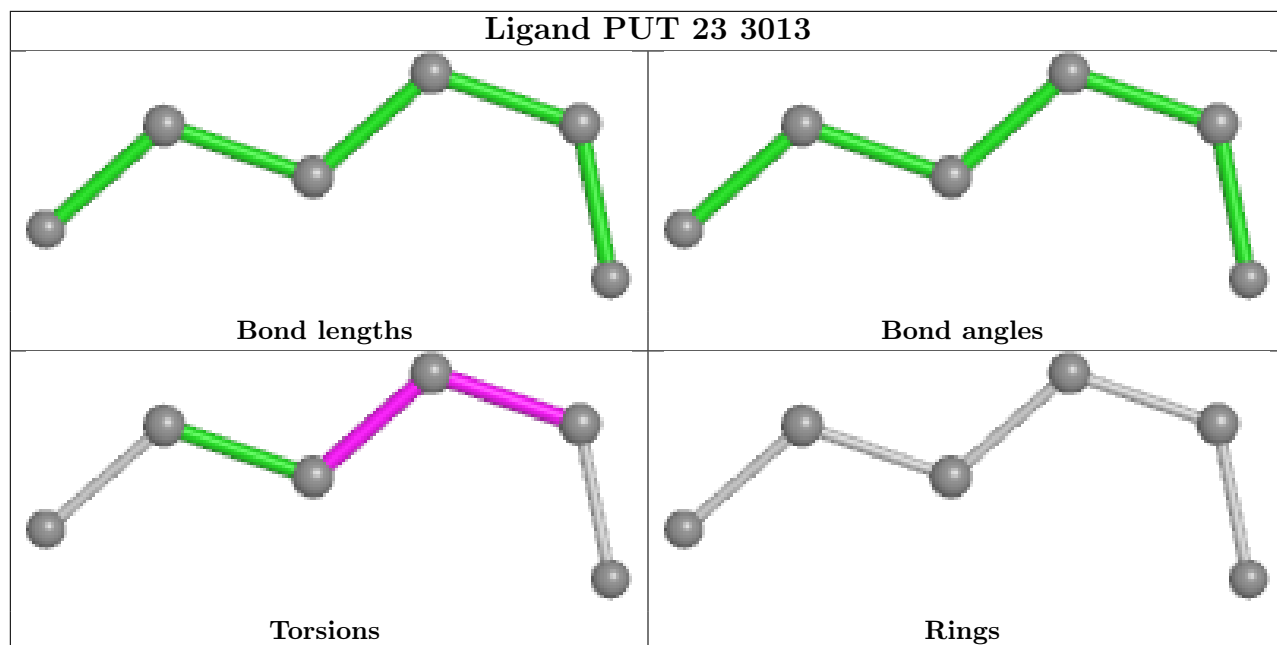


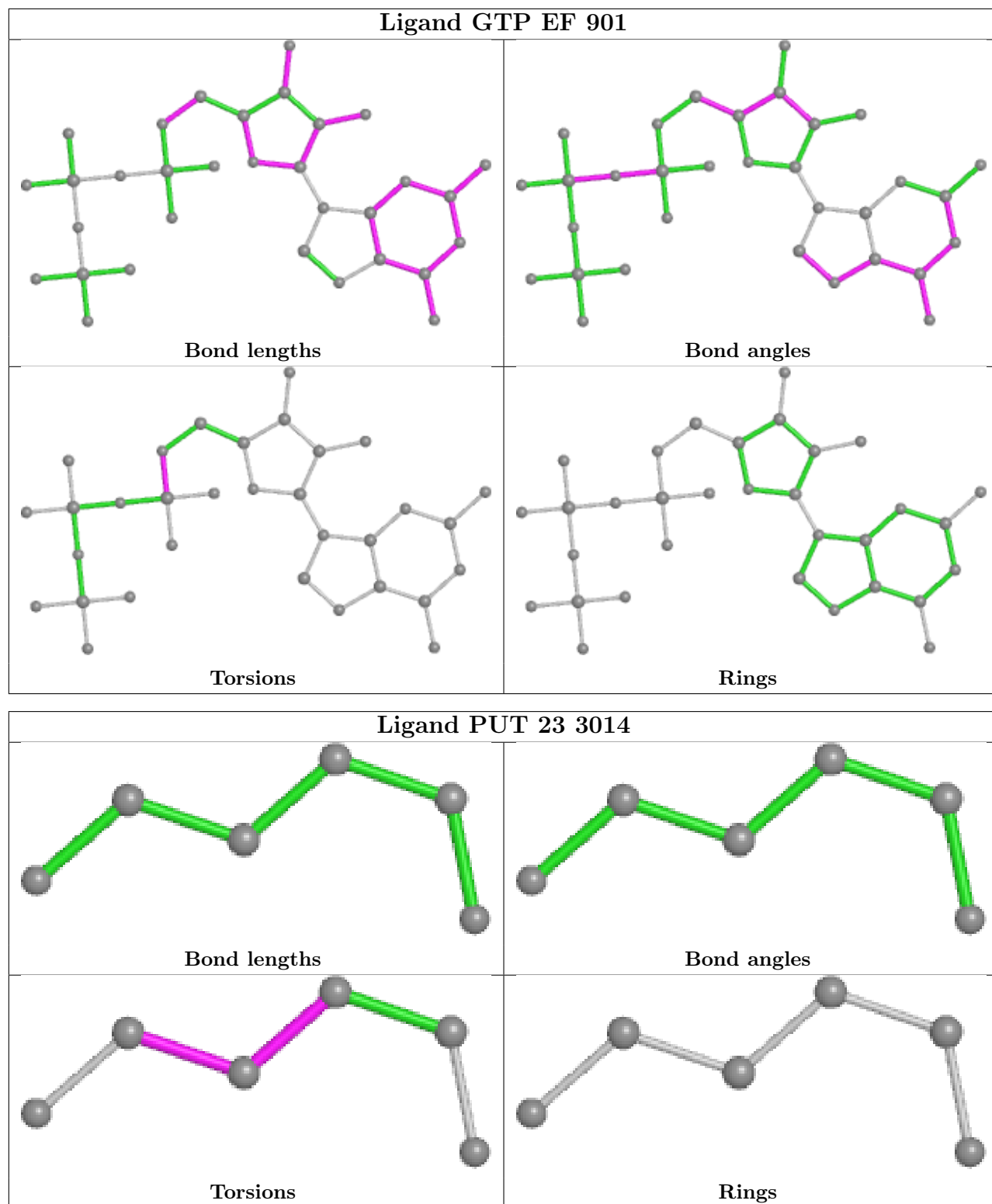


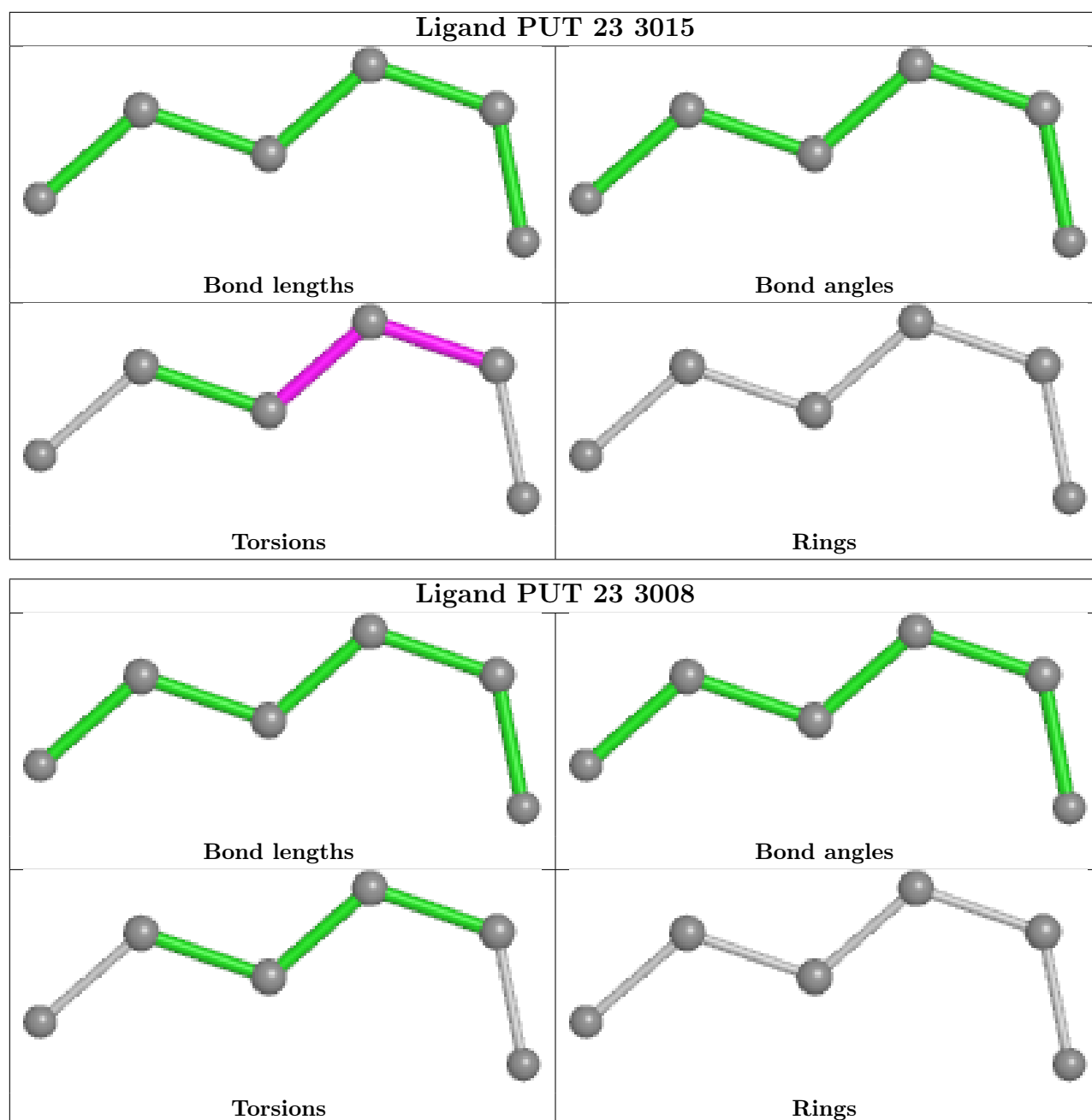












5.7 Other polymers [i](#)

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 |
|-----|-------|------------------|
| 28 | LE | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | LE | 93:GLY | C | 94:GLU | N | 1.14 |

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24134. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

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

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.