# wwPDB X-ray Structure Validation Summary Report (i)

Dec 12, 2023 – 08:00 pm GMT

| | | |
|---|---|---|
| PDB ID | : | 4U4R |
| Title | : | Crystal structure of Lactimidomycin bound to the yeast 80S ribosome |
| Authors | : | Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M. |
| Deposited on | : | 2014-07-24 |
| Resolution | : | 2.80 Å(reported) |

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

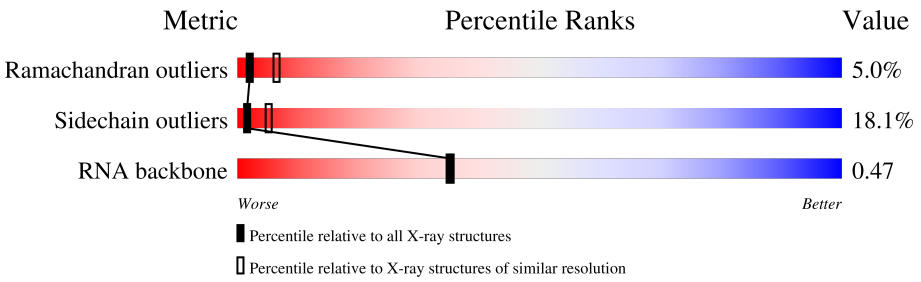
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | FAILED |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| Ramachandran outliers | 138981 | 3498 (2.80-2.80) |
| Sidechain outliers | 138945 | 3500 (2.80-2.80) |
| RNA backbone | 3102 | 1227 (3.10-2.50) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS failed to run properly.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | 2 | 1800 | 67% 25% 6% • |
| 1 | 6 | 1800 | 65% 29% 6% |
| 2 | S0 | 251 | 61% 20% • 18% |
| 2 | s0 | 251 | 64% 16% • 18% |
| 3 | S1 | 254 | 63% 20% • 16% |
| 3 | s1 | 254 | 70% 14% • 15% |
| 4 | S2 | 253 | 68% 17% • 14% |
| 4 | s2 | 253 | 68% 17% • 14% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 5 | S3 | 239 | 77% 16% • 7% |
| 5 | s3 | 239 | 75% 17% • 7% |
| 6 | S4 | 260 | 82% 16% • |
| 6 | s4 | 260 | 83% 17% • |
| 7 | S5 | 224 | 70% 20% • 8% |
| 7 | s5 | 224 | 70% 20% • 8% |
| 8 | S6 | 236 | 79% 17% • |
| 8 | s6 | 236 | 74% 18% 8% |
| 9 | S7 | 189 | 76% 20% • • |
| 9 | s7 | 189 | 76% 20% • • |
| 10 | S8 | 200 | 76% 16% • 6% |
| 10 | s8 | 200 | 80% 14% • 6% |
| 11 | S9 | 196 | 72% 21% • 6% |
| 11 | s9 | 196 | 76% 16% • 6% |
| 12 | C0 | 105 | 68% 23% • 9% |
| 12 | c0 | 105 | 68% 21% • 9% |
| 13 | C1 | 155 | 79% 20% • |
| 13 | c1 | 155 | 75% 19% • 6% |
| 14 | C2 | 142 | 58% 27% • 13% |
| 14 | c2 | 142 | 59% 25% • • 13% |
| 15 | C3 | 150 | 81% 19% • |
| 15 | c3 | 150 | 81% 18% • |
| 16 | C4 | 136 | 72% 18% • • 7% |
| 16 | c4 | 136 | 74% 15% • 6% |
| 17 | C5 | 141 | 71% 16% • 12% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 17 | c5 | 141 | 70% 23% |
| 18 | C6 | 142 | 80% 18% |
| 18 | c6 | 142 | 81% 18% |
| 19 | C7 | 136 | 66% 21% 12% |
| 19 | c7 | 136 | 71% 15% 14% |
| 20 | C8 | 145 | 78% 19% |
| 20 | c8 | 145 | 78% 20% |
| 21 | C9 | 143 | 83% 15% |
| 21 | c9 | 143 | 83% 16% |
| 22 | D0 | 120 | 67% 22% 11% |
| 22 | d0 | 120 | 68% 22% 8% |
| 23 | D1 | 87 | 77% 23% |
| 23 | d1 | 87 | 75% 25% |
| 24 | D2 | 129 | 87% 12% |
| 24 | d2 | 129 | 88% 12% |
| 25 | D3 | 144 | 79% 17% |
| 25 | d3 | 144 | 88% 10% |
| 26 | D4 | 134 | 82% 16% |
| 26 | d4 | 134 | 82% 16% |
| 27 | D5 | 107 | 42% 21% 35% |
| 27 | d5 | 107 | 52% 12% 36% |
| 28 | D6 | 97 | 74% 19% 5% |
| 28 | d6 | 97 | 78% 21% |
| 29 | D7 | 81 | 80% 16% |
| 29 | d7 | 81 | 78% 20% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 30 | D8 | 66 | 74% 20% • 5% |
| 30 | d8 | 66 | 79% 14% • 5% |
| 31 | D9 | 55 | 75% 20% • • |
| 31 | d9 | 55 | 73% 24% • |
| 32 | E0 | 60 | 83% 15% • |
| 33 | E1 | 76 | 55% 30% 8% 7% |
| 33 | e1 | 76 | 57% 37% 5% • |
| 34 | SR | 318 | 89% 10% • |
| 34 | sR | 318 | 89% 10% • |
| 35 | SM | 273 | 46% 10% • 42% |
| 35 | sM | 273 | 32% 5% • 62% |
| 36 | 1 | 3396 | 51% 34% 7% 7% |
| 36 | 5 | 3396 | 51% 35% 7% 7% |
| 37 | 3 | 121 | 70% 27% • |
| 37 | 7 | 121 | 63% 31% 6% |
| 38 | 4 | 158 | 58% 35% 7% |
| 38 | 8 | 158 | 63% 30% 7% |
| 39 | L2 | 253 | 84% 15% • |
| 39 | l2 | 253 | 81% 16% • |
| 40 | L3 | 386 | 81% 18% • |
| 40 | l3 | 386 | 81% 17% • |
| 41 | L4 | 361 | 80% 18% • |
| 41 | l4 | 361 | 81% 18% • |
| 42 | L5 | 296 | 78% 20% • |
| 42 | l5 | 296 | 79% 19% •• |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 43 | L6 | 175 | 76% 13% • 11% |
| 43 | l6 | 175 | 74% 15% • 10% |
| 44 | L7 | 243 | 80% 9% • 9% |
| 44 | l7 | 243 | 79% 11% • 8% |
| 45 | L8 | 255 | 75% 16% 9% |
| 45 | l8 | 255 | 70% 20% • 9% |
| 46 | L9 | 191 | 82% 17% • |
| 46 | l9 | 191 | 80% 20% • |
| 47 | M0 | 220 | 78% 17% • |
| 47 | m0 | 220 | 77% 20% • |
| 48 | M1 | 173 | 75% 20% • • |
| 48 | m1 | 173 | 79% 17% • • |
| 49 | M3 | 198 | 79% 17% • • |
| 49 | m3 | 198 | 80% 17% • • |
| 50 | M4 | 137 | 80% 18% • • |
| 50 | m4 | 137 | 87% 11% • |
| 51 | M5 | 203 | 83% 16% • |
| 51 | m5 | 203 | 85% 14% • |
| 52 | M6 | 198 | 84% 12% • • • |
| 52 | m6 | 198 | 82% 15% • • • |
| 53 | M7 | 183 | 82% 17% • |
| 53 | m7 | 183 | 74% 10% • 15% |
| 54 | M8 | 185 | 83% 16% • |
| 54 | m8 | 185 | 81% 18% • |
| 55 | M9 | 188 | 89% 10% • |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 55 | m9 | 188 | 81% 19% |
| 56 | N0 | 172 | 82% 17% |
| 56 | n0 | 172 | 84% 15% |
| 57 | N1 | 159 | 80% 19% |
| 57 | n1 | 159 | 86% 12% |
| 58 | N2 | 120 | 72% 11% 17% |
| 58 | n2 | 120 | 69% 12% 18% |
| 59 | N3 | 136 | 87% 12% |
| 59 | n3 | 136 | 90% 8% |
| 60 | N4 | 155 | 57% 5% 37% |
| 60 | n4 | 155 | 75% 10% 13% |
| 61 | N5 | 141 | 67% 18% 14% |
| 61 | n5 | 141 | 66% 18% 15% |
| 62 | N6 | 126 | 80% 17% |
| 62 | n6 | 126 | 76% 23% |
| 63 | N7 | 135 | 76% 23% |
| 63 | n7 | 135 | 78% 21% |
| 64 | N8 | 148 | 81% 16% |
| 64 | n8 | 148 | 80% 18% |
| 65 | N9 | 58 | 79% 21% |
| 65 | n9 | 58 | 69% 28% |
| 66 | O0 | 104 | 78% 14% 7% |
| 66 | o0 | 104 | 79% 17% |
| 67 | O1 | 112 | 76% 20% |
| 67 | o1 | 112 | 79% 17% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 68 | O2 | 129 | 85% 12% |
| 68 | o2 | 129 | 82% 14% |
| 69 | O3 | 106 | 85% 13% |
| 69 | o3 | 106 | 87% 12% |
| 70 | O4 | 119 | 77% 16% 6% |
| 70 | o4 | 119 | 81% 13% 6% |
| 71 | O5 | 119 | 78% 20% |
| 71 | o5 | 119 | 76% 23% |
| 72 | O6 | 99 | 71% 28% |
| 72 | o6 | 99 | 69% 27% |
| 73 | O7 | 87 | 79% 21% |
| 73 | o7 | 87 | 83% 17% |
| 74 | O8 | 77 | 79% 21% |
| 74 | o8 | 77 | 82% 17% |
| 75 | O9 | 50 | 80% 18% |
| 75 | o9 | 50 | 78% 22% |
| 76 | Q0 | 52 | 83% 15% |
| 76 | q0 | 52 | 85% 13% |
| 77 | Q1 | 25 | 68% 32% |
| 77 | q1 | 25 | 64% 32% |
| 78 | Q2 | 105 | 82% 17% |
| 78 | q2 | 105 | 79% 21% |
| 79 | Q3 | 91 | 87% 13% |
| 79 | q3 | 91 | 85% 15% |
| 80 | e0 | 62 | 76% 23% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 81 | m2 | 160 | 94% 6% |
| 82 | p0 | 311 | 39% 7% 54% |
| 83 | p1 | 47 | 100% |
| 84 | p2 | 46 | 100% |

# 2 Entry composition (i)

There are 88 unique types of molecules in this entry. The entry contains 411226 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 18S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 1 | 2 | 1750 | 37283 | 16668 | 6591 | 12274 | 1750 | 0 | 0 | 0 |
| 1 | 6 | 1795 | 38238 | 17095 | 6758 | 12590 | 1795 | 0 | 0 | 0 |

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 2 | S0 | 206 | 1577 | 1014 | 278 | 283 | 2 | 0 | 0 | 0 |
| 2 | s0 | 206 | 1583 | 1017 | 281 | 283 | 2 | 0 | 0 | 0 |

- Molecule 3 is a protein called 40S ribosomal protein S1-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 3 | S1 | 214 | 1709 | 1084 | 310 | 311 | 4 | 0 | 0 | 0 |
| 3 | s1 | 216 | 1722 | 1091 | 312 | 315 | 4 | 0 | 0 | 0 |

- Molecule 4 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 4 | S2 | 217 | 1635 | 1047 | 289 | 297 | 2 | 0 | 0 | 0 |
| 4 | s2 | 217 | 1635 | 1047 | 289 | 297 | 2 | 0 | 0 | 0 |

- Molecule 5 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 5 | S3 | 223 | 1734 | 1101 | 313 | 314 | 6 | 0 | 0 | 0 |
| 5 | s3 | 223 | 1734 | 1101 | 313 | 314 | 6 | 0 | 0 | 0 |

- Molecule 6 is a protein called 40S ribosomal protein S4-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 6 | S4 | 260 | 2068 | 1316 | 389 | 360 | 3 | 0 | 0 | 0 |
| 6 | s4 | 260 | 2068 | 1316 | 389 | 360 | 3 | 0 | 0 | 0 |

- Molecule 7 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 7 | S5 | 206 | 1609 | 1007 | 300 | 299 | 3 | 0 | 0 | 0 |
| 7 | s5 | 206 | 1609 | 1007 | 300 | 299 | 3 | 0 | 0 | 0 |

- Molecule 8 is a protein called 40S ribosomal protein S6-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 8 | S6 | 226 | 1799 | 1129 | 346 | 321 | 3 | 0 | 0 | 0 |
| 8 | s6 | 218 | 1755 | 1102 | 337 | 313 | 3 | 0 | 0 | 0 |

- Molecule 9 is a protein called 40S ribosomal protein S7-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 9 | S7 | 184 | 1481 | 951 | 265 | 265 | 0 | 0 | 0 |
| 9 | s7 | 186 | 1491 | 957 | 267 | 267 | 0 | 0 | 0 |

- Molecule 10 is a protein called 40S ribosomal protein S8-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 10 | S8 | 188 | 1489 | 925 | 298 | 264 | 2 | 0 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 10 | s8 | 188 | 1489 | 925 | 298 | 264 | 2 | 0 | 0 | 0 |

- Molecule 11 is a protein called 40S ribosomal protein S9-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 11 | S9 | 185 | 1494 | 943 | 289 | 261 | 1 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 11 | s9 | 185 | 1494 | 943 | 289 | 261 | 1 | 0 | 0 | 0 |

- Molecule 12 is a protein called 40S ribosomal protein S10-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 12 | C0 | 96 | 773 | 500 | 126 | 145 | 2 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 12 | c0 | 96 | 762 | 491 | 125 | 144 | 2 | 0 | 0 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| C0 | 89 | ALA | GLY | conflict | UNP Q08745 |
| c0 | 89 | ALA | GLY | conflict | UNP Q08745 |

- Molecule 13 is a protein called 40S ribosomal protein S11-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 13 | C1 | 155 | 1214 | 775 | 230 | 206 | 3 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 13 | c1 | 146 | 1168 | 747 | 221 | 197 | 3 | 0 | 0 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| C1 | 147 | ALA | GLY | conflict | UNP P0CX47 |
| c1 | 147 | ALA | GLY | conflict | UNP P0CX47 |

- Molecule 14 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 14 | C2 | 124 | 890 | 560 | 156 | 172 | 2 | 0 | 0 | 0 |
| 14 | c2 | 124 | 890 | 560 | 156 | 172 | 2 | 0 | 0 | 0 |

- Molecule 15 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 15 | C3 | 150 | 1192 | 759 | 224 | 207 | 2 | 0 | 0 | 0 |
| 15 | c3 | 150 | 1192 | 759 | 224 | 207 | 2 | 0 | 0 | 0 |

- Molecule 16 is a protein called 40S ribosomal protein S14-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 16 | C4 | 127 | 891 | 545 | 182 | 163 | 1 | 0 | 0 | 0 |
| 16 | c4 | 128 | 949 | 582 | 188 | 176 | 3 | 0 | 0 | 0 |

- Molecule 17 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 17 | C5 | 124 | 977 | 622 | 182 | 166 | 7 | 0 | 0 | 0 |
| 17 | c5 | 135 | 1039 | 658 | 196 | 178 | 7 | 0 | 0 | 0 |

- Molecule 18 is a protein called 40S ribosomal protein S16-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 18 | C6 | 141 | 1105 | 708 | 203 | 194 | 0 | 0 | 0 |
| 18 | c6 | 142 | 1111 | 711 | 204 | 196 | 0 | 0 | 0 |

- Molecule 19 is a protein called 40S ribosomal protein S17-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 19 | C7 | 120 | 926 | 577 | 177 | 170 | 2 | 0 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 19 | c7 | 117 | 906 | 563 | 174 | 167 | 2 | 0 | 0 | 0 |

- Molecule 20 is a protein called 40S ribosomal protein S18-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 20 | C8 | 145 | 1192 | 743 | 237 | 210 | 2 | 0 | 0 | 0 |
| 20 | c8 | 145 | 1192 | 743 | 237 | 210 | 2 | 0 | 0 | 0 |

- Molecule 21 is a protein called 40S ribosomal protein S19-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 21 | C9 | 143 | 1112 | 694 | 208 | 208 | 2 | 0 | 0 | 0 |
| 21 | c9 | 143 | 1112 | 694 | 208 | 208 | 2 | 0 | 0 | 0 |

- Molecule 22 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 22 | D0 | 107 | 855 | 539 | 156 | 159 | 1 | 0 | 0 | 0 |
| 22 | d0 | 110 | 882 | 554 | 161 | 166 | 1 | 0 | 0 | 0 |

- Molecule 23 is a protein called 40S ribosomal protein S21-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 23 | D1 | 87 | 684 | 420 | 125 | 137 | 2 | 0 | 0 | 0 |
| 23 | d1 | 87 | 684 | 420 | 125 | 137 | 2 | 0 | 0 | 0 |

- Molecule 24 is a protein called 40S ribosomal protein S22-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 24 | D2 | 129 | 1021 | 650 | 188 | 180 | 3 | 0 | 0 | 0 |
| 24 | d2 | 129 | 1021 | 650 | 188 | 180 | 3 | 0 | 0 | 0 |

- Molecule 25 is a protein called 40S ribosomal protein S23-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 25 | D3 | 144 | 1121 | 708 | 220 | 191 | 2 | 0 | 0 | 0 |
| 25 | d3 | 144 | 1121 | 708 | 220 | 191 | 2 | 0 | 0 | 0 |

- Molecule 26 is a protein called 40S ribosomal protein S24-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 26 | D4 | 134 | 1073 | 676 | 208 | 189 | 0 | 0 | 0 |
| 26 | d4 | 134 | 1073 | 676 | 208 | 189 | 0 | 0 | 0 |

- Molecule 27 is a protein called 40S ribosomal protein S25-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 27 | D5 | 70 | 563 | 360 | 104 | 99 | 0 | 0 | 0 |
| 27 | d5 | 69 | 558 | 357 | 103 | 98 | 0 | 0 | 0 |

- Molecule 28 is a protein called 40S ribosomal protein S26-B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 28 | D6 | 97 | 769 | 475 | 160 | 129 | 5 | 0 | 0 | 0 |
| 28 | d6 | 97 | 769 | 475 | 160 | 129 | 5 | 0 | 0 | 0 |

- Molecule 29 is a protein called 40S ribosomal protein S27-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 29 | D7 | 81 | 610 | 382 | 110 | 113 | 5 | 0 | 0 | 0 |
| 29 | d7 | 81 | 610 | 382 | 110 | 113 | 5 | 0 | 0 | 0 |

- Molecule 30 is a protein called 40S ribosomal protein S28-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 30 | D8 | 63 | 497 | 306 | 99 | 91 | 1 | 0 | 0 | 0 |
| 30 | d8 | 63 | 497 | 306 | 99 | 91 | 1 | 0 | 0 | 0 |

- Molecule 31 is a protein called 40S ribosomal protein S29-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 31 | D9 | 53 | 442 | 274 | 92 | 72 | 4 | 0 | 0 | 0 |
| 31 | d9 | 53 | 442 | 274 | 92 | 72 | 4 | 0 | 0 | 0 |

- Molecule 32 is a protein called 40S ribosomal protein S30-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 32 | E0 | 60 | 475 | 299 | 98 | 77 | 1 | 0 | 0 | 0 |

- Molecule 33 is a protein called Ubiquitin-40S ribosomal protein S31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 33 | E1 | 71 | 566 | 362 | 106 | 94 | 4 | 0 | 0 | 0 |
| 33 | e1 | 76 | 608 | 388 | 117 | 99 | 4 | 0 | 0 | 0 |

- Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 34 | SR | 318 | 2441 | 1544 | 419 | 470 | 8 | 0 | 0 | 0 |
| 34 | sR | 318 | 2442 | 1544 | 418 | 472 | 8 | 0 | 0 | 0 |

- Molecule 35 is a protein called Suppressor protein STM1.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 35 | SM | 159 | 1104 | 652 | 221 | 231 | 0 | 0 | 0 |
| 35 | sM | 104 | 680 | 403 | 140 | 137 | 0 | 0 | 0 |

- Molecule 36 is a RNA chain called 25S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 36 | 1 | 3149 | 67355 | 30086 | 12142 | 21978 | 3149 | 0 | 0 | 0 |
| 36 | 5 | 3150 | 67376 | 30095 | 12145 | 21987 | 3149 | 0 | 0 | 0 |

- Molecule 37 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 37 | 3 | 121 | 2579 | 1152 | 461 | 845 | 121 | 0 | 0 | 0 |
| 37 | 7 | 121 | 2579 | 1152 | 461 | 845 | 121 | 0 | 0 | 0 |

- Molecule 38 is a RNA chain called 5.8S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 38 | 4 | 158 | 3353 | 1500 | 586 | 1109 | 158 | 0 | 0 | 0 |
| 38 | 8 | 158 | 3353 | 1500 | 586 | 1109 | 158 | 0 | 0 | 0 |

- Molecule 39 is a protein called 60S ribosomal protein L2-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 39 | L2 | 252 | 1914 | 1191 | 388 | 334 | 1 | 0 | 0 | 0 |
| 39 | l2 | 252 | 1912 | 1190 | 388 | 333 | 1 | 0 | 0 | 0 |

- Molecule 40 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 40 | L3 | 386 | 3075 | 1950 | 584 | 533 | 8 | 0 | 0 | 0 |
| 40 | l3 | 386 | 3075 | 1950 | 584 | 533 | 8 | 0 | 0 | 0 |

- Molecule 41 is a protein called 60S ribosomal protein L4-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 41 | L4 | 361 | 2748 | 1729 | 522 | 494 | 3 | 0 | 0 | 0 |
| 41 | l4 | 361 | 2748 | 1729 | 522 | 494 | 3 | 0 | 0 | 0 |

- Molecule 42 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 42 | L5 | 296 | 2375 | 1501 | 414 | 458 | 2 | 0 | 0 | 0 |
| 42 | l5 | 294 | 2359 | 1489 | 412 | 456 | 2 | 0 | 0 | 0 |

- Molecule 43 is a protein called 60S ribosomal protein L6-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 43 | L6 | 156 | 1239 | 800 | 222 | 216 | 1 | 0 | 0 | 0 |
| 43 | l6 | 157 | 1248 | 806 | 224 | 217 | 1 | 0 | 0 | 0 |

- Molecule 44 is a protein called 60S ribosomal protein L7-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 44 | L7 | 222 | 1784 | 1151 | 324 | 308 | 1 | 0 | 0 | 0 |
| 44 | l7 | 223 | 1791 | 1155 | 325 | 310 | 1 | 0 | 0 | 0 |

- Molecule 45 is a protein called 60S ribosomal protein L8-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 45 | L8 | 233 | 1804 | 1151 | 323 | 327 | 3 | 0 | 0 | 0 |
| 45 | l8 | 231 | 1763 | 1130 | 316 | 314 | 3 | 0 | 0 | 0 |

- Molecule 46 is a protein called 60S ribosomal protein L9-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 46 | L9 | 191 | 1518 | 963 | 274 | 277 | 4 | 0 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 46 | l9 | 191 | 1518 | 963 | 274 | 277 | 4 | 0 | 0 | 0 |

- Molecule 47 is a protein called 60S ribosomal protein L10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 47 | M0 | 211 | 1705 | 1083 | 322 | 294 | 6 | 0 | 0 | 0 |
| 47 | m0 | 213 | 1722 | 1094 | 325 | 297 | 6 | 0 | 0 | 0 |

- Molecule 48 is a protein called 60S ribosomal protein L11-B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 48 | M1 | 169 | 1353 | 847 | 253 | 249 | 4 | 0 | 0 | 0 |
| 48 | m1 | 169 | 1353 | 847 | 253 | 249 | 4 | 0 | 0 | 0 |

- Molecule 49 is a protein called 60S ribosomal protein L13-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 49 | M3 | 193 | 1543 | 962 | 315 | 266 | 0 | 0 | 0 |
| 49 | m3 | 194 | 1548 | 965 | 316 | 267 | 0 | 0 | 0 |

- Molecule 50 is a protein called 60S ribosomal protein L14-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 50 | M4 | 136 | 1053 | 675 | 199 | 177 | 2 | 0 | 0 | 0 |
| 50 | m4 | 137 | 1059 | 678 | 200 | 179 | 2 | 0 | 0 | 0 |

- Molecule 51 is a protein called 60S ribosomal protein L15-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 51 | M5 | 203 | 1720 | 1077 | 361 | 281 | 1 | 0 | 0 | 0 |
| 51 | m5 | 203 | 1720 | 1077 | 361 | 281 | 1 | 0 | 0 | 0 |

- Molecule 52 is a protein called 60S ribosomal protein L16-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 52 | M6 | 197 | 1555 | 1003 | 289 | 262 | 1 | 0 | 0 | 0 |
| 52 | m6 | 197 | 1555 | 1003 | 289 | 262 | 1 | 0 | 0 | 0 |

- Molecule 53 is a protein called 60S ribosomal protein L17-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 53 | M7 | 183 | 1420 | 882 | 281 | 257 | 0 | 0 | 0 |
| 53 | m7 | 155 | 1227 | 764 | 238 | 225 | 0 | 0 | 0 |

- Molecule 54 is a protein called 60S ribosomal protein L18-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 54 | M8 | 185 | 1441 | 908 | 290 | 241 | 2 | 0 | 0 | 0 |
| 54 | m8 | 185 | 1441 | 908 | 290 | 241 | 2 | 0 | 0 | 0 |

- Molecule 55 is a protein called 60S ribosomal protein L19-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 55 | M9 | 188 | 1521 | 935 | 326 | 260 | 0 | 0 | 0 |
| 55 | m9 | 188 | 1521 | 935 | 326 | 260 | 0 | 0 | 0 |

- Molecule 56 is a protein called 60S ribosomal protein L20-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 56 | N0 | 172 | 1445 | 930 | 267 | 244 | 4 | 0 | 0 | 0 |
| 56 | n0 | 172 | 1445 | 930 | 267 | 244 | 4 | 0 | 0 | 0 |

- Molecule 57 is a protein called 60S ribosomal protein L21-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 57 | N1 | 159 | 1276 | 805 | 246 | 221 | 4 | 0 | 0 | 0 |
| 57 | n1 | 159 | 1276 | 805 | 246 | 221 | 4 | 0 | 0 | 0 |

- Molecule 58 is a protein called 60S ribosomal protein L22-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 58 | N2 | 100 | 796 | 516 | 131 | 149 | 0 | 0 | 0 |
| 58 | n2 | 98 | 778 | 505 | 127 | 146 | 0 | 0 | 0 |

- Molecule 59 is a protein called 60S ribosomal protein L23-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 59 | N3 | 136 | 1003 | 628 | 189 | 179 | 7 | 0 | 0 | 0 |
| 59 | n3 | 136 | 1003 | 628 | 189 | 179 | 7 | 0 | 0 | 0 |

- Molecule 60 is a protein called 60S ribosomal protein L24-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 60 | N4 | 98 | 699 | 443 | 137 | 118 | 1 | 0 | 0 | 0 |
| 60 | n4 | 135 | 1038 | 651 | 206 | 180 | 1 | 0 | 0 | 0 |

- Molecule 61 is a protein called 60S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 61 | N5 | 121 | 964 | 620 | 169 | 173 | 2 | 0 | 0 | 0 |
| 61 | n5 | 120 | 959 | 617 | 168 | 172 | 2 | 0 | 0 | 0 |

- Molecule 62 is a protein called 60S ribosomal protein L26-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 62 | N6 | 126 | 993 | 625 | 192 | 176 | 0 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 62 | n6 | 126 | 993 | 625 | 192 | 176 | 0 | 0 | 0 |

- Molecule 63 is a protein called 60S ribosomal protein L27-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 63 | N7 | 135 | 1092 | 710 | 202 | 180 | 0 | 0 | 0 |
| 63 | n7 | 135 | 1092 | 710 | 202 | 180 | 0 | 0 | 0 |

- Molecule 64 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 64 | N8 | 148 | 1173 | 749 | 231 | 190 | 3 | 0 | 0 | 0 |
| 64 | n8 | 148 | 1173 | 749 | 231 | 190 | 3 | 0 | 0 | 0 |

- Molecule 65 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 65 | N9 | 58 | 462 | 289 | 100 | 73 | 0 | 0 | 0 |
| 65 | n9 | 58 | 462 | 289 | 100 | 73 | 0 | 0 | 0 |

- Molecule 66 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 66 | O0 | 97 | 743 | 479 | 124 | 139 | 1 | 0 | 0 | 0 |
| 66 | o0 | 100 | 767 | 492 | 128 | 146 | 1 | 0 | 0 | 0 |

- Molecule 67 is a protein called 60S ribosomal protein L31-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 67 | O1 | 109 | 876 | 556 | 167 | 152 | 1 | 0 | 0 | 0 |
| 67 | o1 | 109 | 883 | 559 | 167 | 156 | 1 | 0 | 0 | 0 |

- Molecule 68 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 68 | O2 | 127 | 1020 | 647 | 205 | 167 | 1 | 0 | 0 | 0 |
| 68 | o2 | 127 | 1020 | 647 | 205 | 167 | 1 | 0 | 0 | 0 |

- Molecule 69 is a protein called 60S ribosomal protein L33-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 69 | O3 | 106 | 850 | 540 | 165 | 144 | 1 | 0 | 0 | 0 |
| 69 | o3 | 106 | 850 | 540 | 165 | 144 | 1 | 0 | 0 | 0 |

- Molecule 70 is a protein called 60S ribosomal protein L34-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 70 | O4 | 112 | 880 | 545 | 179 | 152 | 4 | 0 | 0 | 0 |
| 70 | o4 | 112 | 880 | 545 | 179 | 152 | 4 | 0 | 0 | 0 |

- Molecule 71 is a protein called 60S ribosomal protein L35-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 71 | O5 | 119 | 969 | 615 | 186 | 167 | 1 | 0 | 0 | 0 |
| 71 | o5 | 119 | 965 | 612 | 185 | 167 | 1 | 0 | 0 | 0 |

- Molecule 72 is a protein called 60S ribosomal protein L36-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 72 | O6 | 99 | 771 | 481 | 156 | 132 | 2 | 0 | 0 | 0 |
| 72 | o6 | 99 | 770 | 481 | 156 | 131 | 2 | 0 | 0 | 0 |

- Molecule 73 is a protein called 60S ribosomal protein L37-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 73 | O7 | 87 | 681 | 414 | 148 | 114 | 5 | 0 | 0 | 0 |
| 73 | o7 | 87 | 681 | 414 | 148 | 114 | 5 | 0 | 0 | 0 |

- Molecule 74 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 74 | O8 | 77 | 612 | 391 | 115 | 106 | 0 | 0 | 0 |
| 74 | o8 | 77 | 608 | 388 | 114 | 106 | 0 | 0 | 0 |

- Molecule 75 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 75 | O9 | 50 | 436 | 272 | 97 | 65 | 2 | 0 | 0 | 0 |
| 75 | o9 | 50 | 436 | 272 | 97 | 65 | 2 | 0 | 0 | 0 |

- Molecule 76 is a protein called Ubiquitin-60S ribosomal protein L40.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 76 | Q0 | 52 | 417 | 259 | 86 | 67 | 5 | 0 | 0 | 0 |
| 76 | q0 | 52 | 417 | 259 | 86 | 67 | 5 | 0 | 0 | 0 |

- Molecule 77 is a protein called 60S ribosomal protein L41-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 77 | Q1 | 25 | 233 | 142 | 63 | 27 | 1 | 0 | 0 | 0 |
| 77 | q1 | 25 | 233 | 142 | 63 | 27 | 1 | 0 | 0 | 0 |

- Molecule 78 is a protein called 60S ribosomal protein L42-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 78 | Q2 | 105 | 847 | 534 | 170 | 138 | 5 | 0 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 78 | q2 | 105 | 847 | 534 | 170 | 138 | 5 | 0 | 0 | 0 |

- Molecule 79 is a protein called 60S ribosomal protein L43-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 79 | Q3 | 91 | 694 | 429 | 138 | 121 | 6 | 0 | 0 | 0 |
| 79 | q3 | 91 | 694 | 429 | 138 | 121 | 6 | 0 | 0 | 0 |

- Molecule 80 is a protein called 40S ribosomal protein S30-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 80 | e0 | 62 | 491 | 309 | 101 | 80 | 1 | 0 | 0 | 0 |

- Molecule 81 is a protein called Unknown protein m2.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 81 | m2 | 150 | 750 | 450 | 150 | 150 | 0 | 0 | 0 |

- Molecule 82 is a protein called 60S acidic ribosomal protein P0.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 82 | p0 | 143 | 1077 | 687 | 192 | 195 | 3 | 0 | 0 | 0 |

- Molecule 83 is a protein called Unknown protein p1.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 83 | p1 | 47 | 235 | 141 | 47 | 47 | 0 | 0 | 0 |

- Molecule 84 is a protein called Unknown protein p2.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 84 | p2 | 46 | 230 | 138 | 46 | 46 | 0 | 0 | 0 |

- Molecule 85 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Mg | | |
| 85 | 2 | 126 | 126 | 126 | 0 | 0 |
| 85 | S8 | 1 | 1 | 1 | 0 | 0 |
| 85 | C3 | 1 | 1 | 1 | 0 | 0 |
| 85 | SM | 1 | 1 | 1 | 0 | 0 |
| 85 | 1 | 475 | 475 | 475 | 0 | 0 |
| 85 | 3 | 14 | 14 | 14 | 0 | 0 |
| 85 | 4 | 21 | 21 | 21 | 0 | 0 |
| 85 | L2 | 1 | 1 | 1 | 0 | 0 |
| 85 | L3 | 2 | 2 | 2 | 0 | 0 |
| 85 | L4 | 3 | 3 | 3 | 0 | 0 |
| 85 | L5 | 1 | 1 | 1 | 0 | 0 |
| 85 | L6 | 1 | 1 | 1 | 0 | 0 |
| 85 | L7 | 2 | 2 | 2 | 0 | 0 |
| 85 | L8 | 1 | 1 | 1 | 0 | 0 |
| 85 | M0 | 2 | 2 | 2 | 0 | 0 |
| 85 | M1 | 1 | 1 | 1 | 0 | 0 |
| 85 | M3 | 4 | 4 | 4 | 0 | 0 |
| 85 | M5 | 2 | 2 | 2 | 0 | 0 |
| 85 | M6 | 1 | 1 | 1 | 0 | 0 |
| 85 | M7 | 6 | 6 | 6 | 0 | 0 |
| 85 | M9 | 1 | 1 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Mg | | |
| 85 | N0 | 1 | 1 | 1 | 0 | 0 |
| 85 | N3 | 3 | 3 | 3 | 0 | 0 |
| 85 | N5 | 1 | 1 | 1 | 0 | 0 |
| 85 | N8 | 2 | 2 | 2 | 0 | 0 |
| 85 | O3 | 1 | 1 | 1 | 0 | 0 |
| 85 | O4 | 1 | 1 | 1 | 0 | 0 |
| 85 | O7 | 1 | 1 | 1 | 0 | 0 |
| 85 | Q2 | 1 | 1 | 1 | 0 | 0 |
| 85 | 6 | 147 | 147 | 147 | 0 | 0 |
| 85 | s1 | 1 | 1 | 1 | 0 | 0 |
| 85 | s6 | 1 | 1 | 1 | 0 | 0 |
| 85 | s8 | 2 | 2 | 2 | 0 | 0 |
| 85 | c1 | 1 | 1 | 1 | 0 | 0 |
| 85 | c7 | 1 | 1 | 1 | 0 | 0 |
| 85 | c8 | 2 | 2 | 2 | 0 | 0 |
| 85 | d2 | 1 | 1 | 1 | 0 | 0 |
| 85 | d3 | 1 | 1 | 1 | 0 | 0 |
| 85 | d6 | 1 | 1 | 1 | 0 | 0 |
| 85 | sM | 2 | 2 | 2 | 0 | 0 |
| 85 | 5 | 504 | 504 | 504 | 0 | 0 |
| 85 | 7 | 15 | 15 | 15 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Mg | | |
| 85 | 8 | 13 | 13 | 13 | 0 | 0 |
| 85 | l2 | 2 | 2 | 2 | 0 | 0 |
| 85 | l3 | 1 | 1 | 1 | 0 | 0 |
| 85 | l4 | 1 | 1 | 1 | 0 | 0 |
| 85 | l5 | 3 | 3 | 3 | 0 | 0 |
| 85 | l7 | 1 | 1 | 1 | 0 | 0 |
| 85 | m1 | 2 | 2 | 2 | 0 | 0 |
| 85 | m4 | 1 | 1 | 1 | 0 | 0 |
| 85 | m5 | 1 | 1 | 1 | 0 | 0 |
| 85 | m6 | 1 | 1 | 1 | 0 | 0 |
| 85 | m7 | 5 | 5 | 5 | 0 | 0 |
| 85 | n0 | 2 | 2 | 2 | 0 | 0 |
| 85 | n3 | 2 | 2 | 2 | 0 | 0 |
| 85 | n6 | 2 | 2 | 2 | 0 | 0 |
| 85 | n8 | 4 | 4 | 4 | 0 | 0 |
| 85 | n9 | 2 | 2 | 2 | 0 | 0 |
| 85 | o1 | 1 | 1 | 1 | 0 | 0 |
| 85 | o3 | 2 | 2 | 2 | 0 | 0 |
| 85 | o4 | 2 | 2 | 2 | 0 | 0 |
| 85 | q0 | 1 | 1 | 1 | 0 | 0 |
| 85 | q1 | 1 | 1 | 1 | 0 | 0 |

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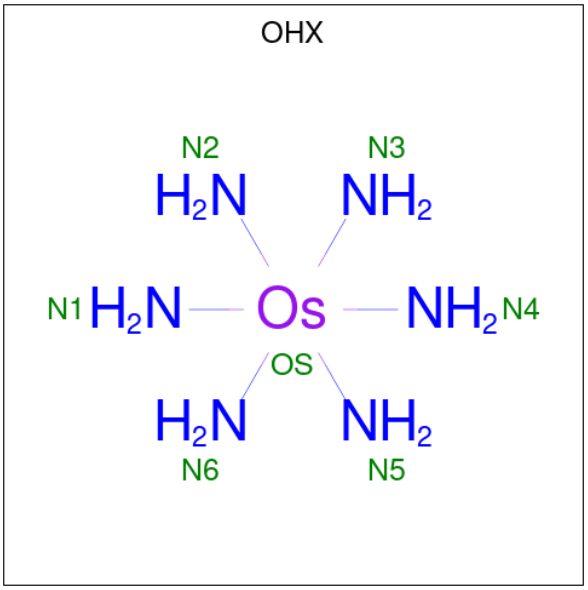
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Mg | | |
| 85 | q3 | 1 | 1 | 1 | 0 | 0 |

- Molecule 86 is osmium (III) hexammine (three-letter code: OHX) (formula: $H_{12}N_6Os$).




| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | N | Os | | |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| | | | Total | N | Os | | |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| | | | Total | N | Os | | |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
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| | | | Total | N | Os | | |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| | | | Total | N | Os | | |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| | | | Total | N | Os | | |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| | | | Total | N | Os | | |
| 86 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | S8 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | C1 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | C3 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | C5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | C8 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | D9 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | SR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 86 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 86 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 86 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| | | | Total | N | Os | | |
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| | | | Total | N | Os | | |
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| | | | Total | N | Os | | |
| 86 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 86 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 86 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 86 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |

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| 86 | 3 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 3 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 3 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 3 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | N | Os | | |
| 86 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | L3 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | L3 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | L4 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | L6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | M0 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | M5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | M5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | M6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | M7 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | M7 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | M9 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | N9 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | O2 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | O3 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | O7 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | O7 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | N | Os | | |
| 86 | O9 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | Q2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
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| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| | | | Total | N | Os | | |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | s1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | s1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | s4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | s8 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | s9 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | c1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | c3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | c5 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | N | Os | | |
| 86 | c8 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | d4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | d9 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| | | | Total | N | Os | | |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 86 | 5 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 86 | 7 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 7 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 7 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 7 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 7 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 8 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 8 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 8 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 8 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 8 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 8 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 8 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 8 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 8 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | N | Os | | |
| 86 | 8 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 8 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 8 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 8 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 8 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 8 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | 8 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | l3 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | l3 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | l3 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | l4 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | l4 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | l5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | l5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | l5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | l9 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | m0 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | m0 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | m1 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | m4 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 86 | m5 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | N | Os | | |
| 86 | m6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | m7 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | m8 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | n3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | n9 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | o2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | o3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | o4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | o7 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | q2 | 1 | 7 | 6 | 1 | 0 | 0 |

- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Zn | | |
| 87 | D6 | 1 | 1 | 1 | 0 | 0 |
| 87 | D7 | 1 | 1 | 1 | 0 | 0 |
| 87 | D9 | 1 | 1 | 1 | 0 | 0 |
| 87 | E1 | 1 | 1 | 1 | 0 | 0 |
| 87 | O7 | 1 | 1 | 1 | 0 | 0 |
| 87 | Q0 | 1 | 1 | 1 | 0 | 0 |
| 87 | Q2 | 1 | 1 | 1 | 0 | 0 |
| 87 | Q3 | 1 | 1 | 1 | 0 | 0 |
| 87 | d6 | 1 | 1 | 1 | 0 | 0 |

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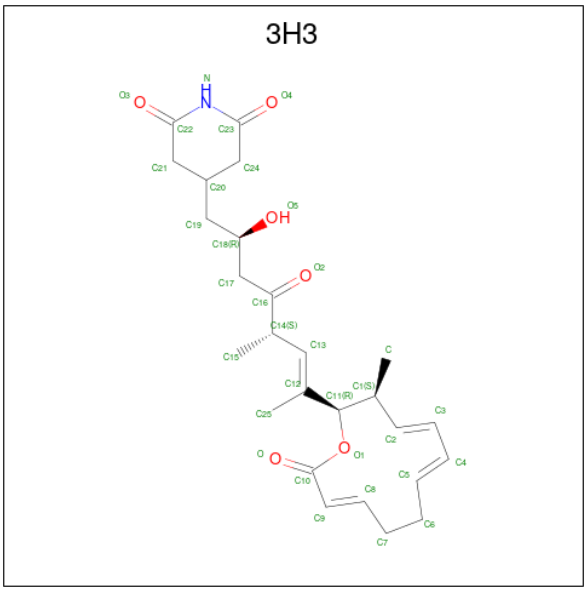
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 87 | d7 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 87 | d9 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 87 | e1 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 87 | o7 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 87 | q0 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 87 | q2 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 87 | q3 | 1 | Total Zn<br>1 1 | 0 | 0 |

- Molecule 88 is 4-{(2R,5S,6E)-2-hydroxy-5-methyl-7-[(2R,3S,4E,6Z,10E)-3-methyl-12-oxooxacyclododeca-4,6,10-trien-2-yl]-4-oxooct-6-en-1-yl}piperidine-2,6-dione (three-letter code: 3H3) (formula: $C_{26}H_{35}NO_6$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 88 | 1 | 1 | Total C N O<br>33 26 1 6 | 0 | 0 |
| 88 | 5 | 1 | Total C N O<br>33 26 1 6 | 0 | 0 |

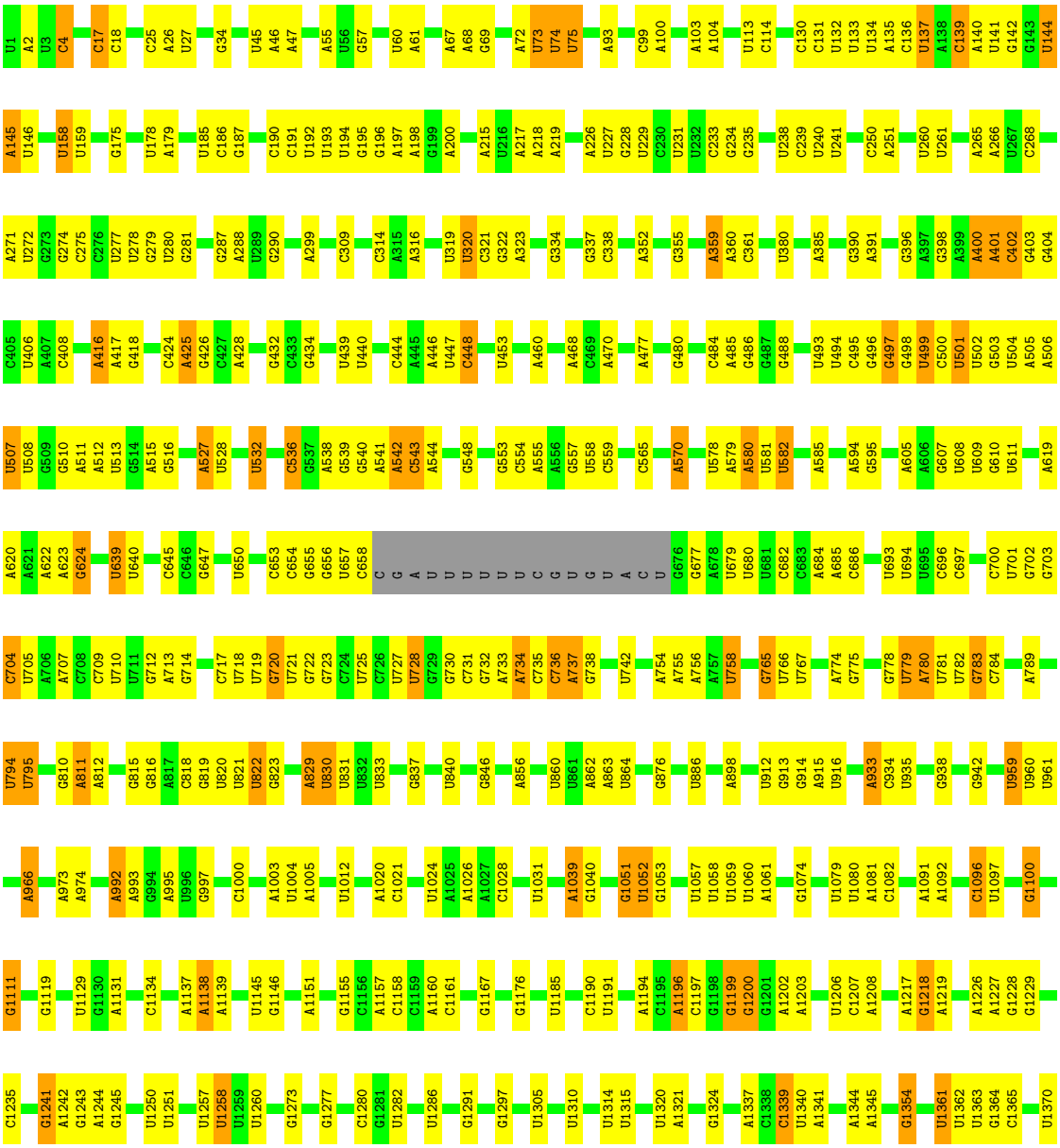
# 3 Residue-property plots (i)

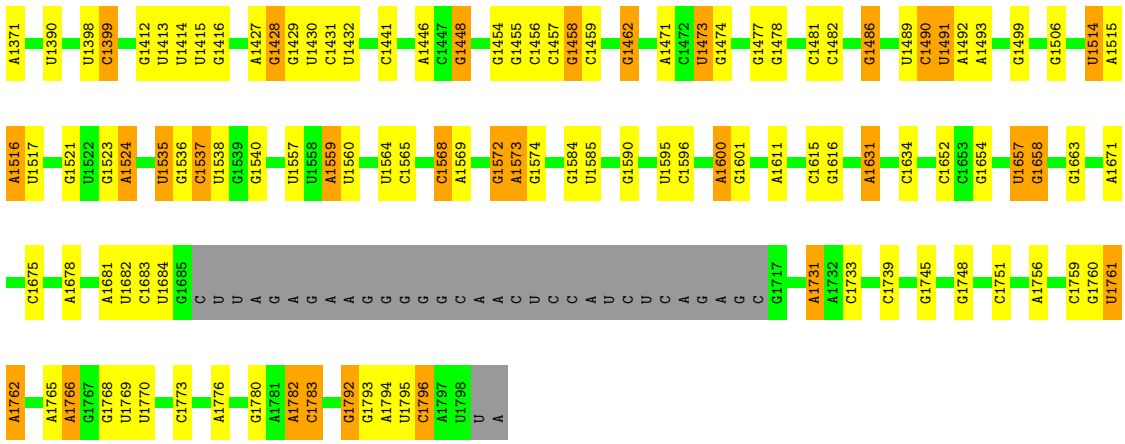
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS failed to run properly.

- Molecule 1: 18S ribosomal RNA

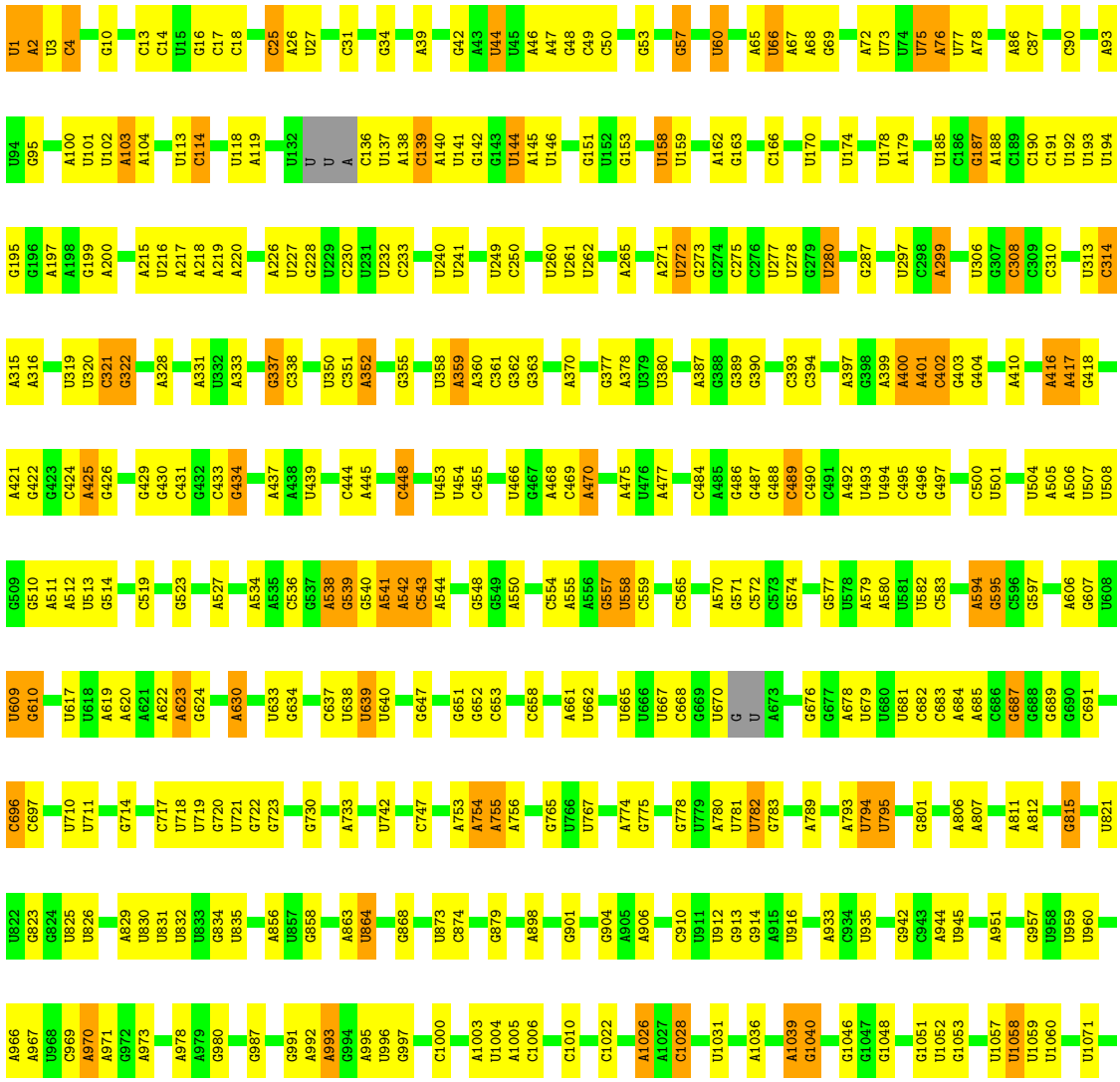
Chain 2: 67% 25% 6% •





• Molecule 1: 18S ribosomal RNA

Chain 6:



C1075 C1078 A1081 C1082 G1083 A1084 A1091 A1092 C1096 U1097 U1098 U1099 G1100 G1101 G1109 G1119 U1120 C1121 G1122 C1123 A1124 A1125 G1126 U1129 A1137 A1138 U1144 U1145 G1146 G1149 G1150 A1151 G1155 C1158 C1159 A1160 C1161 C1162 G1167 A1171 G1172 U1185 A1194 C1195

A1196 C1197 G1198 G1199 G1200 G1201 A1202 A1203 A1208 G1212 A1217 G1218 A1219 C1220 A1226 A1227 G1228 G1229 A1230 U1231 U1239 U1240 G1241 A1242 G1243 A1244 G1245 C1246 G1255 A1256 U1257 U1258 U1259 U1269 C1279 C1280 C1284 U1285 U1286 A1287 G1288 U1293 G1299 U1314 U1315 G1316 A1321

G1330 C1338 A1344 A1345 A1346 G1354 U1361 U1362 U1363 G1364 U1370 A1371 A1388 C1389 U1390 U1396 U1397 U1398 C1399 A1400 A1401 G1402 G1412 U1413 U1414 U1415 A1427 G1428 U1432 G1433 A1436 G1445 A1446 C1447 G1448 C1456 G1457 G1458 C1459 A1460 C1461 G1462 C1463 A1471 G1472

U1473 G1480 C1481 C1482 U1489 C1490 U1491 A1492 A1493 C1494 C1495 U1496 U1497 G1498 A1503 G1506 C1509 U1514 A1515 A1516 G1521 U1522 G1523 A1524 U1535 G1536 C1537 U1538 G1539 G1540 G1541 G1542 A1543 U1544 C1549 U1554 U1557 U1558 A1559 U1560 C1568 A1569 G1572 A1573 G1574 G1575 A1576

A1577 G1584 U1595 C1596 A1600 G1601 G1605 A1614 C1615 G1616 C1620 U1621 A1631 C1634 C1637 G1638 C1639 A1655 U1656 U1657 G1658 A1659 A1660 U1661 G1662 G1663 G1670 A1681 U1682 C1683 G1696 G1697 G1698 G1699 C1700 A1701 A1702 C1703 U1710 C1711 A1712 C1716 G1717 G1726

A1730 A1731 U1735 U1742 G1745 G1748 A1749 A1750 C1751 U1752 A1753 A1754 A1755 G1760 U1761 A1762 A1765 A1766 G1767 G1768 U1769 U1770 C1773 G1774 G1780 A1781 A1782 C1783 C1784 G1792 G1793 A1794 U1795 C1796 U1799 A1800

- Molecule 2: 40S ribosomal protein S0-A

Chain S0:

S2 L3 P4 A5 L24 R27 Q30 E34 P35 Y36 V37 F38 N39 D43 V50 R62 A66 T80 F81 R84 L87 K88 T93 G94 A95 T96 R101 F102 T103 I111 S114 R119 Q131 E135 V139 E154 F155 V156 D157 V158

N163 N164 S169 I170 G171 L172 L177 L184 R185 L188 V189 D190 R191 T192 Q193 P194 W195 S196 I197 M198 F203 Y204 R205 D206 P207 GLU GLU VAL GLU GLN GLN VAL ALA GLU GLU ALA THR THR GLU GLU ALA GLY GLU GLU GLU ALA LYS GLU GLU VAL THR GLU GLU GLN

ALA GLU ALA THR GLU TRP ALA GLU GLU ASN ALA ASP ASN VAL GLU TRP

- Molecule 2: 40S ribosomal protein S0-A

Chain s0:

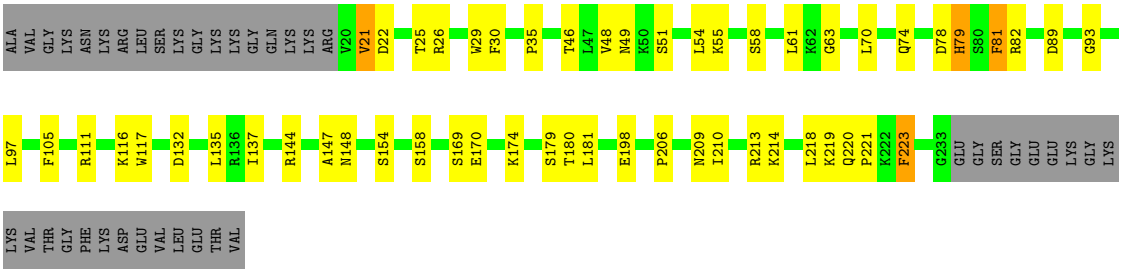
S2 L3 P4 A5 T6 T10 P11 E12 N21 N28 V29 Q30 V31 R41 P42 D43 G44 V45 L59 R62 P68 D72 L87 G94 A95 T96 R101 F102 T103 S106 I111 T112 T124 V139 I144 A145 L146 S153 D157 V158 N164

K167 H168 L172 R179 R183 L184 R185 G186 A187 L188 V189 D190 R191 M198 D206 P207 GLU GLU VAL GLU GLN GLN VAL ALA GLU GLU ALA THR THR GLU GLU ALA GLY GLU GLU GLU ALA LYS GLU GLU VAL THR GLU GLU GLN ALA GLU ALA THR GLU TRP ALA GLU GLU

ASN ALA ASP ASN VAL GLU TRP

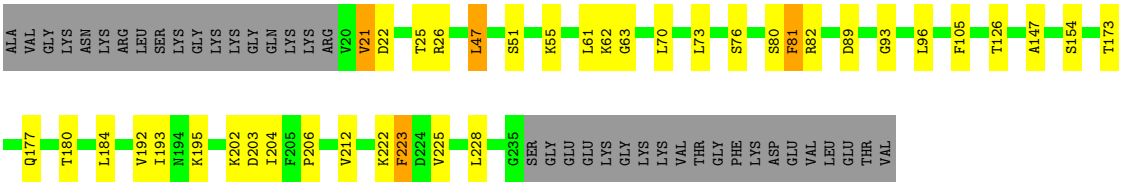
- Molecule 3: 40S ribosomal protein S1-A

Chain S1:



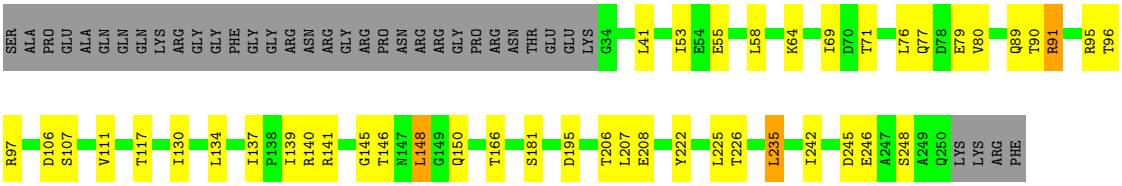

• Molecule 3: 40S ribosomal protein S1-A

Chain s1:



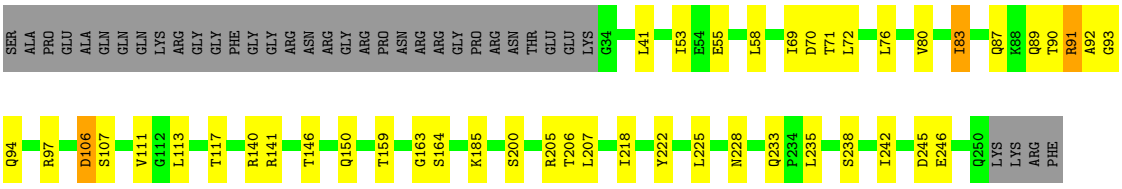

• Molecule 4: 40S ribosomal protein S2

Chain S2:



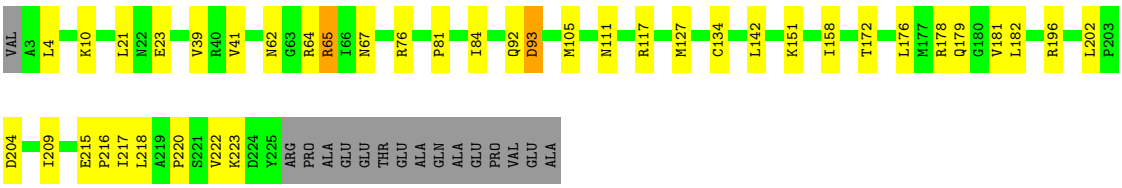

• Molecule 4: 40S ribosomal protein S2

Chain s2:




• Molecule 5: 40S ribosomal protein S3

Chain S3:




• Molecule 5: 40S ribosomal protein S3

Chain s3: 75% 17% • 7%

VAL A3 L4 K7 K8 R9 K10 V37 E38 V39 R40 L59 G60 E61 I66 L69 I84 E89 R90 Y91 Q92 D93 R94 N111 I115 R116 R117 E128 K132 L142 R143 A144 A145 R146 I158 Q162 P163 V164 D169 T172 Q179 G180 V181

R196 L202 P203 K212 P216 I217 L218 A219 P220 Y225 ARG PRO ALA GLU GLU THR GLU ALA GLN ALA GLU PRO VAL GLU ALA

• Molecule 6: 40S ribosomal protein S4-A

Chain S4: 82% 16% •

A2 K6 K7 H8 L9 L12 D21 K22 L23 C26 L38 I45 L48 K62 L65 M66 Q67 V70 K71 V72 R77 L92 V102 Y103 D104 V105 T115 D116 L123 V126 L131 G132 K133 N157 L164 L180 V181 Y182 R187

G193 T194 I195 V196 H197 K198 K211 D215 R221 L222 N223 V227 K233 K240 G241 K242 K245 I248 Q258 L261

• Molecule 6: 40S ribosomal protein S4-A

Chain s4: 83% 17% •

A2 K7 H8 L9 L12 L23 S24 R30 L38 L42 L48 R49 N50 R51 N57 Q67 V70 T78 I90 T91 T95 V102 Y103 D104 R113 D116 L123 V126 K127 K128 V129 Q130 L131 I147 R148 V160 D163 L164

K168 L180 V181 Y182 R187 I192 I195 V196 R221 L222 V227 S237 K245 R254 L261

• Molecule 7: 40S ribosomal protein S5

Chain S5: 70% 20% • 8%

SER ASP THR GLU ALA PRO VAL GLU VAL GLN GLU ASP PHE GLU VAL VAL GLU GLU F20 T21 P22 V23 V24 L25 A26 Q35 T38 E39 I40 K41 L42 F43 N44 K45 V51 E52 V53 L58 V59 D60 Q63 V64 R65 R76 N79 K84 P88 I89 L93 T94

M99 N100 G101 R112 D119 L124 Q127 N139 T146 T147 R148 V149 G150 G153 A154 A155 R156 R157 V160 D161 V162 R185 I190 T193 L194 G204 S205 S206 R225

• Molecule 7: 40S ribosomal protein S5

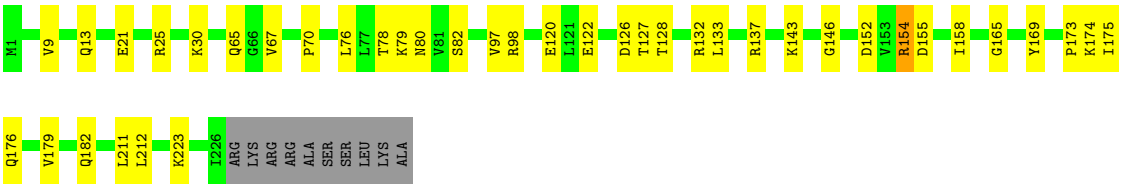
Chain s5: 70% 20% • 8%

SER ASP THR GLU ALA PRO VAL GLU VAL GLN GLU ASP PHE GLU VAL VAL GLU GLU F20 T21 P22 V23 V24 L25 A26 T27 P28 I29 E32 V33 A36 Q37 T38 E39 F43 N44 K45 K54 V59 D60 Q63 V64 I68 A71 R76 N79 R83 K84

I89 R92 L93 M99 N100 K109 I114 D119 T125 D126 Q127 T146 T147 R148 V149 G150 G151 G152 G153 R157 S163 R167 F184 I187 L194 K203 E216 R225

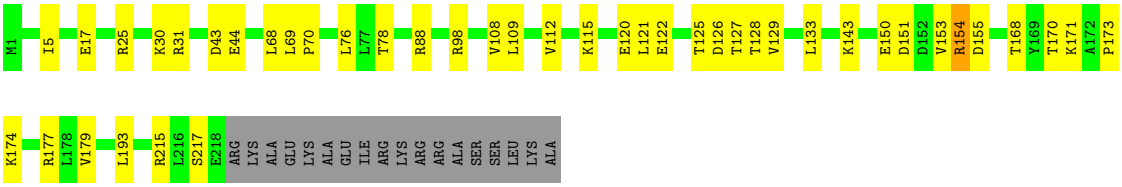
• Molecule 8: 40S ribosomal protein S6-A

Chain S6:



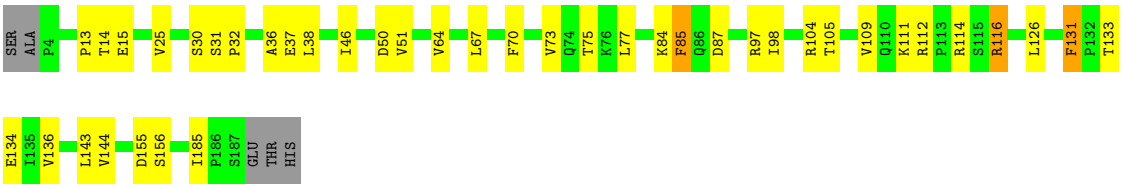

• Molecule 8: 40S ribosomal protein S6-A

Chain s6:



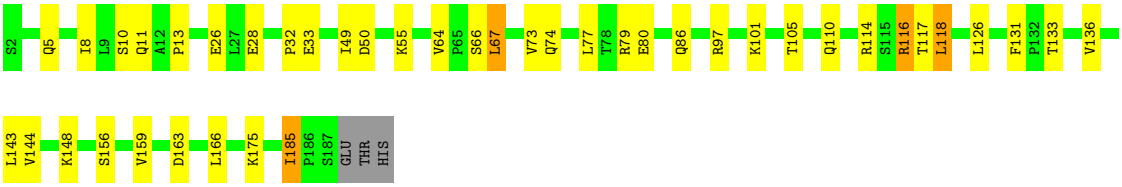

• Molecule 9: 40S ribosomal protein S7-A

Chain S7:



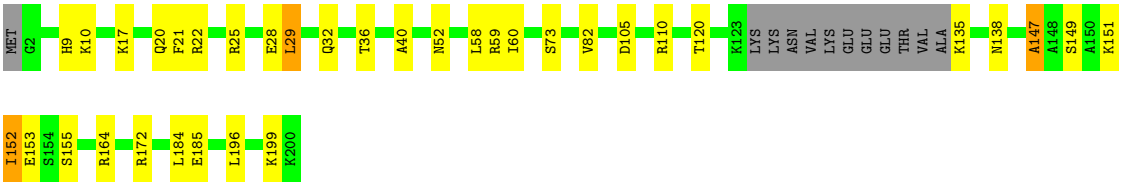

• Molecule 9: 40S ribosomal protein S7-A

Chain s7:



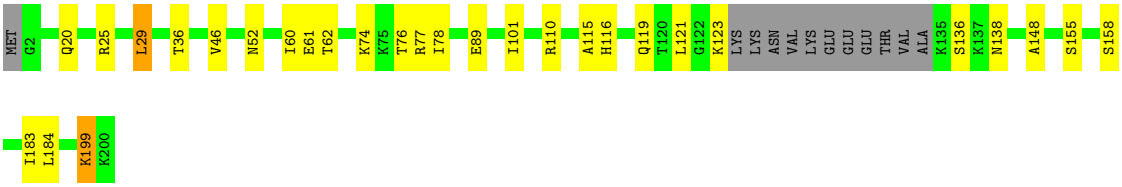

• Molecule 10: 40S ribosomal protein S8-A

Chain S8:



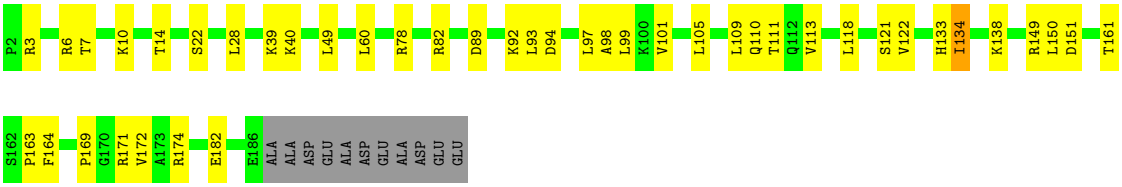

• Molecule 10: 40S ribosomal protein S8-A

Chain s8: 80% 14% • 6%



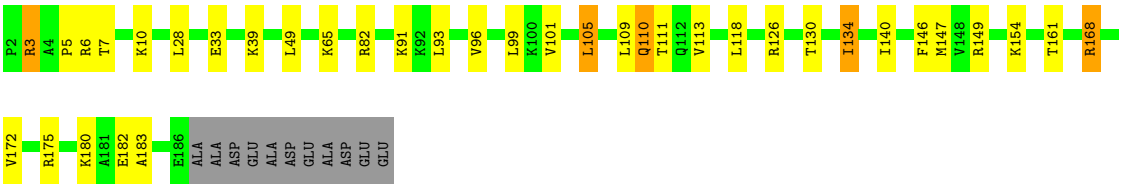

• Molecule 11: 40S ribosomal protein S9-A

Chain S9: 72% 21% • 6%




• Molecule 11: 40S ribosomal protein S9-A

Chain s9: 76% 16% • 6%

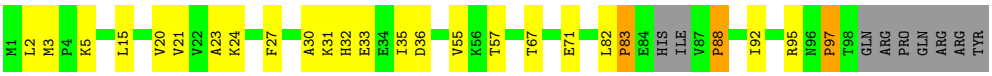



• Molecule 12: 40S ribosomal protein S10-A

Chain C0: 68% 23% • 9%

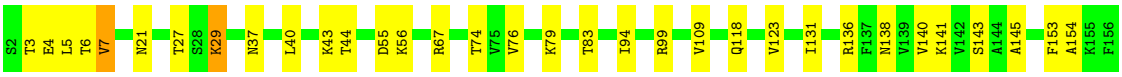
• Molecule 12: 40S ribosomal protein S10-A

Chain c0: 68% 21% • 9%




• Molecule 13: 40S ribosomal protein S11-A

Chain C1: 79% 20% •

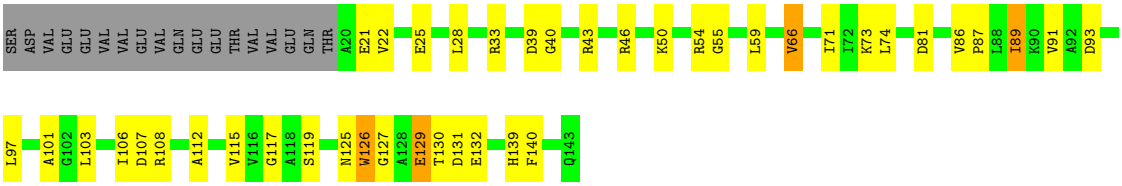


- Molecule 13: 40S ribosomal protein S11-A

Chain c1:

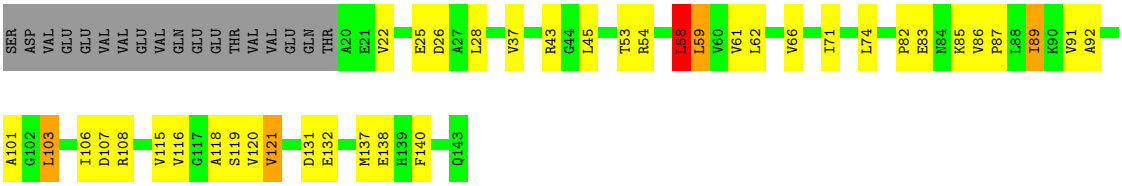
- Molecule 14: 40S ribosomal protein S12

Chain C2:




- Molecule 14: 40S ribosomal protein S12

Chain c2:

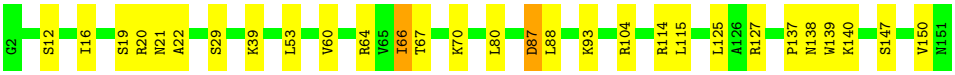



- Molecule 15: 40S ribosomal protein S13

Chain C3:

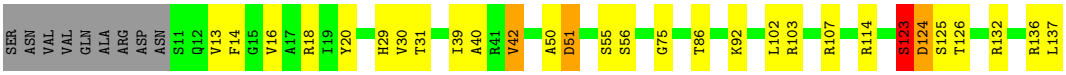
- Molecule 15: 40S ribosomal protein S13

Chain c3:



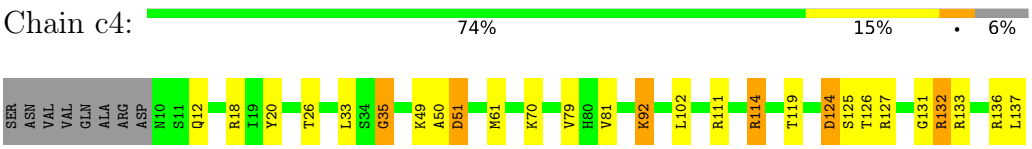

- Molecule 16: 40S ribosomal protein S14-A

Chain C4:



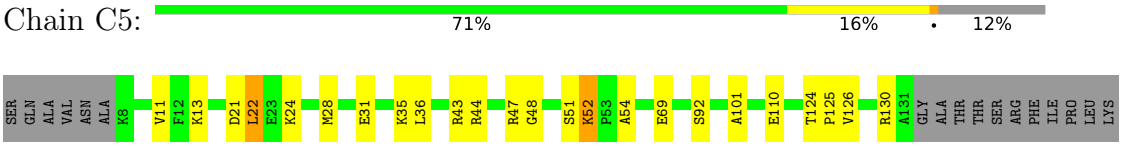
• Molecule 16: 40S ribosomal protein S14-A

Chain c4:



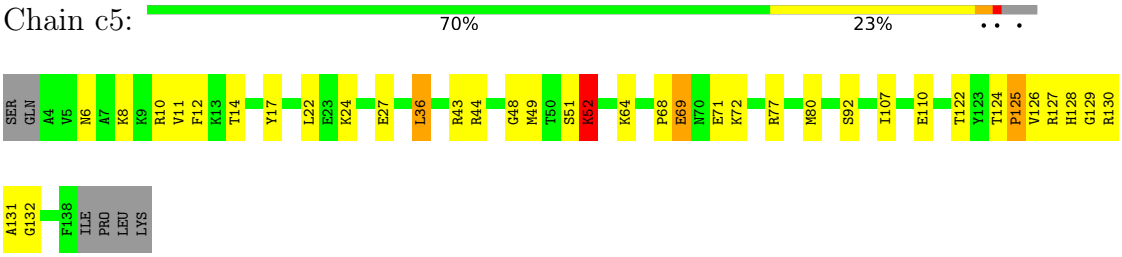

• Molecule 17: 40S ribosomal protein S15

Chain C5:



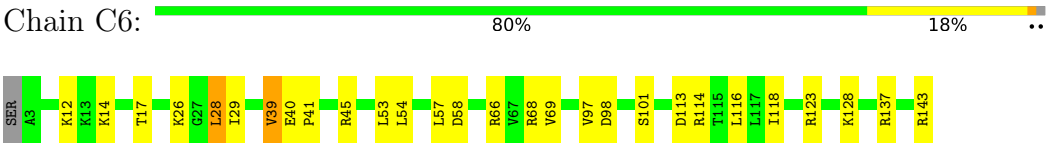

• Molecule 17: 40S ribosomal protein S15

Chain c5:



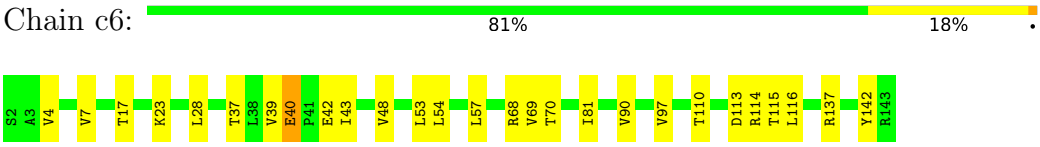

• Molecule 18: 40S ribosomal protein S16-A

Chain C6:



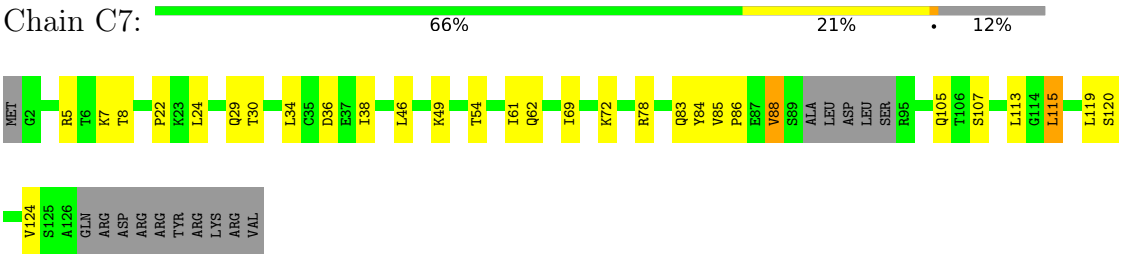

• Molecule 18: 40S ribosomal protein S16-A

Chain c6:



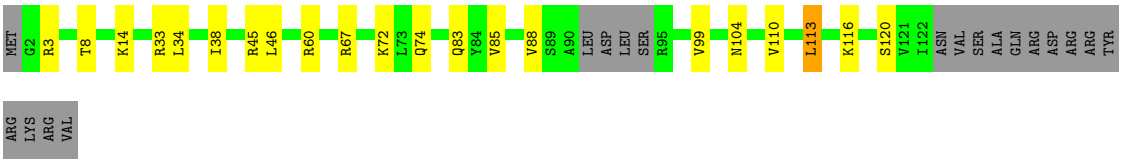

• Molecule 19: 40S ribosomal protein S17-A

Chain C7:



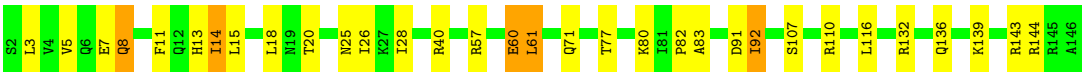

• Molecule 19: 40S ribosomal protein S17-A

Chain c7: 71% 15% • 14%



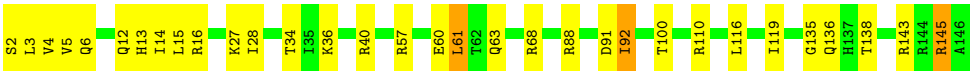

• Molecule 20: 40S ribosomal protein S18-A

Chain C8: 78% 19% •




• Molecule 20: 40S ribosomal protein S18-A

Chain c8: 78% 20% •

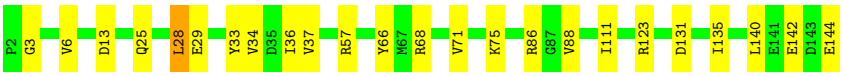



• Molecule 21: 40S ribosomal protein S19-A

Chain C9: 83% 15% •

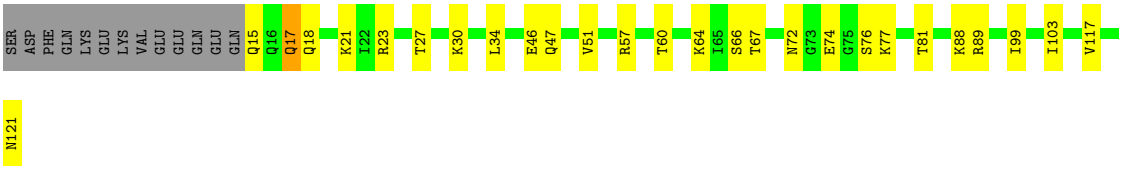
• Molecule 21: 40S ribosomal protein S19-A

Chain c9: 83% 16% •




• Molecule 22: 40S ribosomal protein S20

Chain D0: 67% 22% • 11%

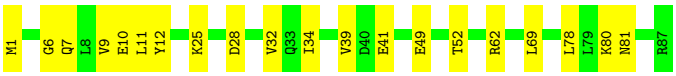



• Molecule 22: 40S ribosomal protein S20

Chain d0: 68% 22% • 8%

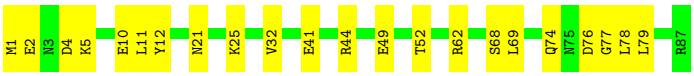
• Molecule 23: 40S ribosomal protein S21-A

Chain D1:




• Molecule 23: 40S ribosomal protein S21-A

Chain d1:




• Molecule 24: 40S ribosomal protein S22-A

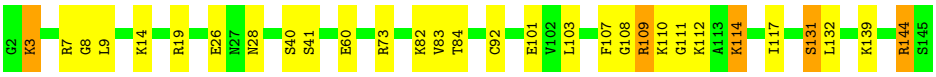
Chain D2:

• Molecule 24: 40S ribosomal protein S22-A

Chain d2:

• Molecule 25: 40S ribosomal protein S23-A

Chain D3:

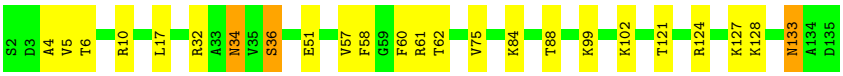



• Molecule 25: 40S ribosomal protein S23-A

Chain d3:

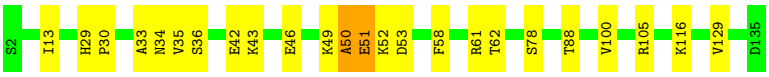
• Molecule 26: 40S ribosomal protein S24-A

Chain D4: 82% 16%



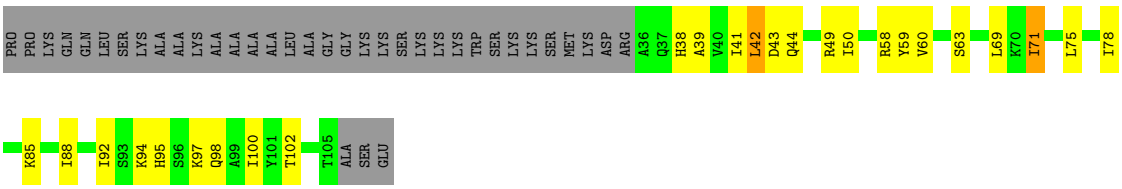

• Molecule 26: 40S ribosomal protein S24-A

Chain d4: 82% 16%



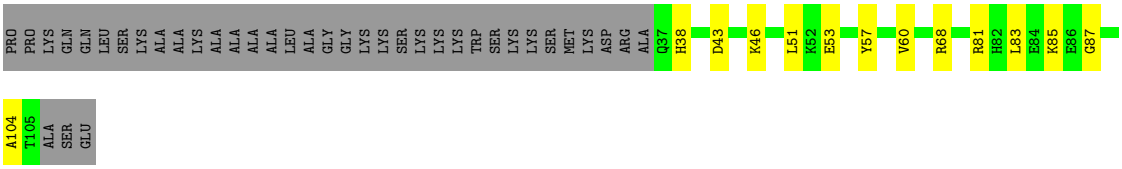

• Molecule 27: 40S ribosomal protein S25-A

Chain D5: 42% 21% 35%



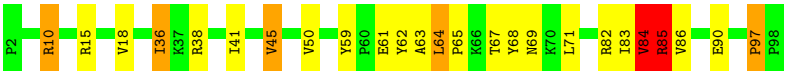

• Molecule 27: 40S ribosomal protein S25-A

Chain d5: 52% 12% 36%




• Molecule 28: 40S ribosomal protein S26-B

Chain D6: 74% 19% 5%

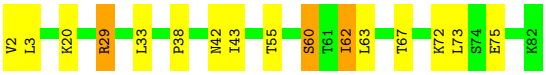



• Molecule 28: 40S ribosomal protein S26-B

Chain d6: 78% 21%

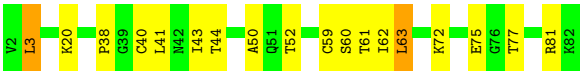
• Molecule 29: 40S ribosomal protein S27-A

Chain D7: 80% 16%




• Molecule 29: 40S ribosomal protein S27-A

Chain d7:




• Molecule 30: 40S ribosomal protein S28-A

Chain D8:

• Molecule 30: 40S ribosomal protein S28-A

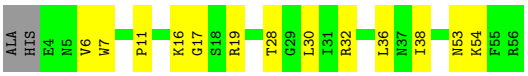
Chain d8:

• Molecule 31: 40S ribosomal protein S29-A

Chain D9:

• Molecule 31: 40S ribosomal protein S29-A

Chain d9:

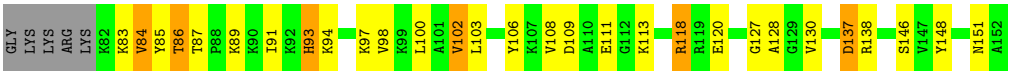



• Molecule 32: 40S ribosomal protein S30-A

Chain E0:

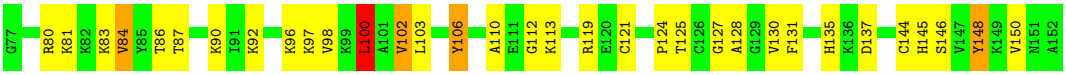
• Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1:



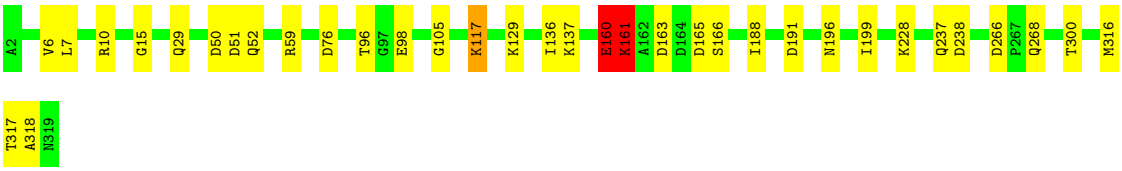

• Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1:



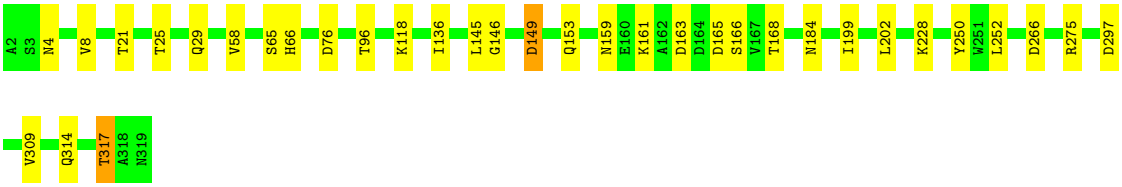

• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR:



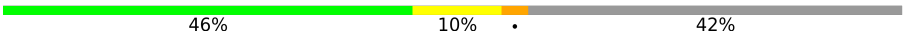

• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

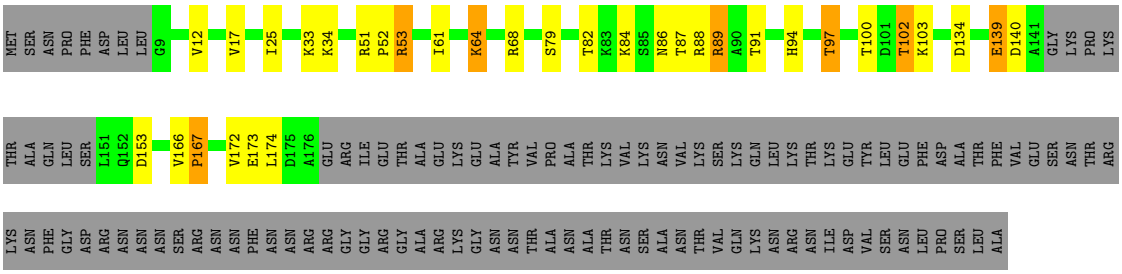
Chain sR:




• Molecule 35: Suppressor protein STM1

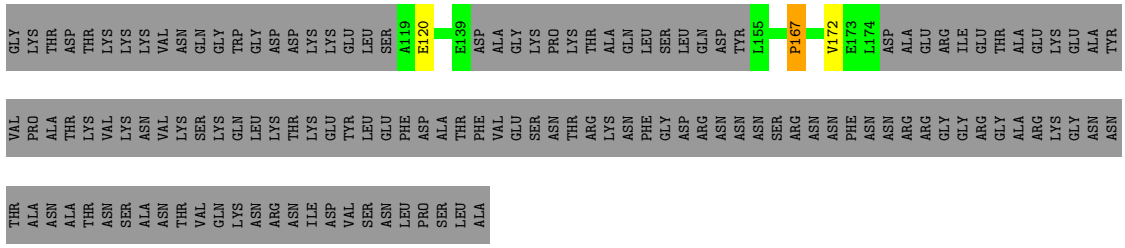
Chain SM:



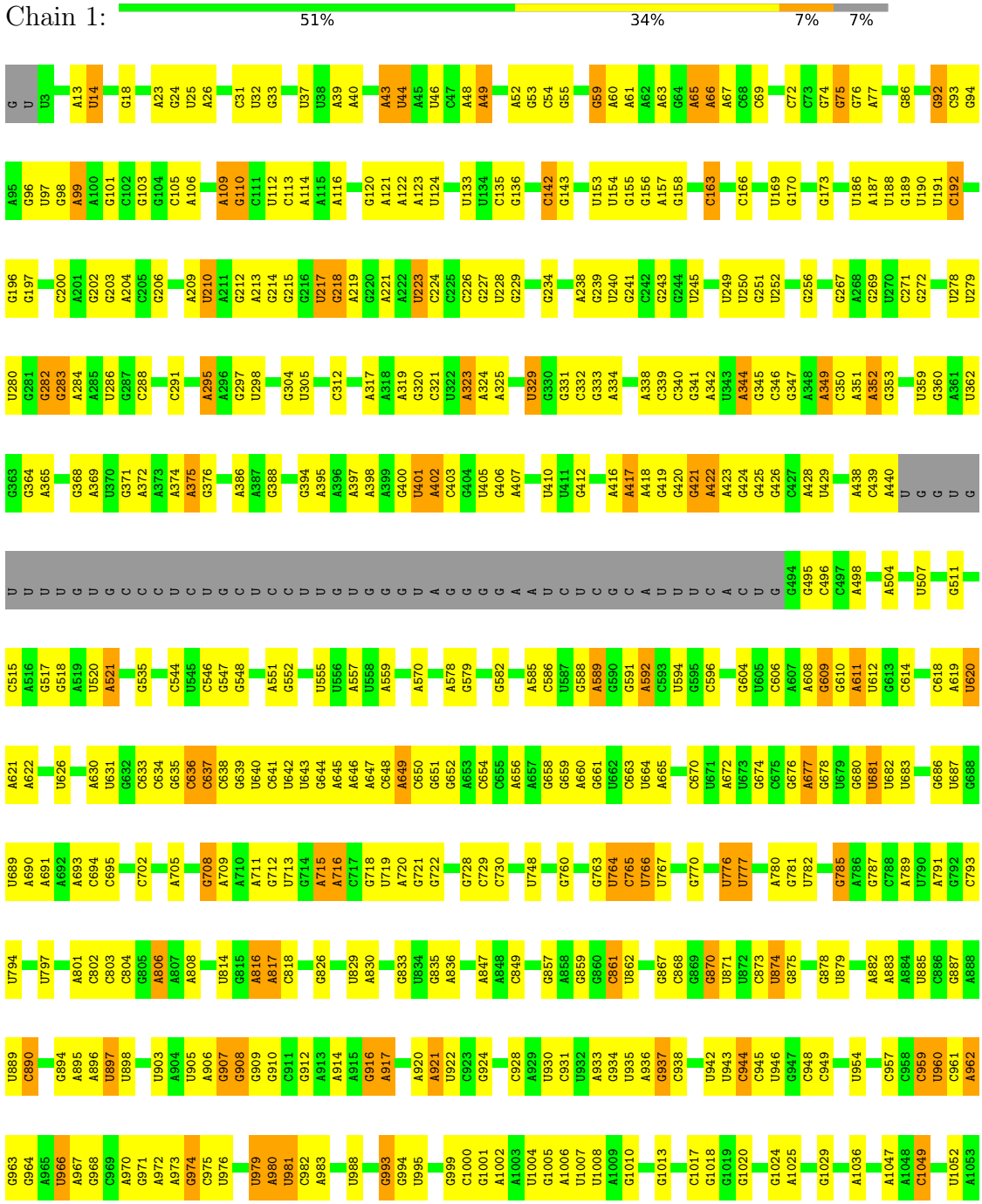

• Molecule 35: Suppressor protein STM1

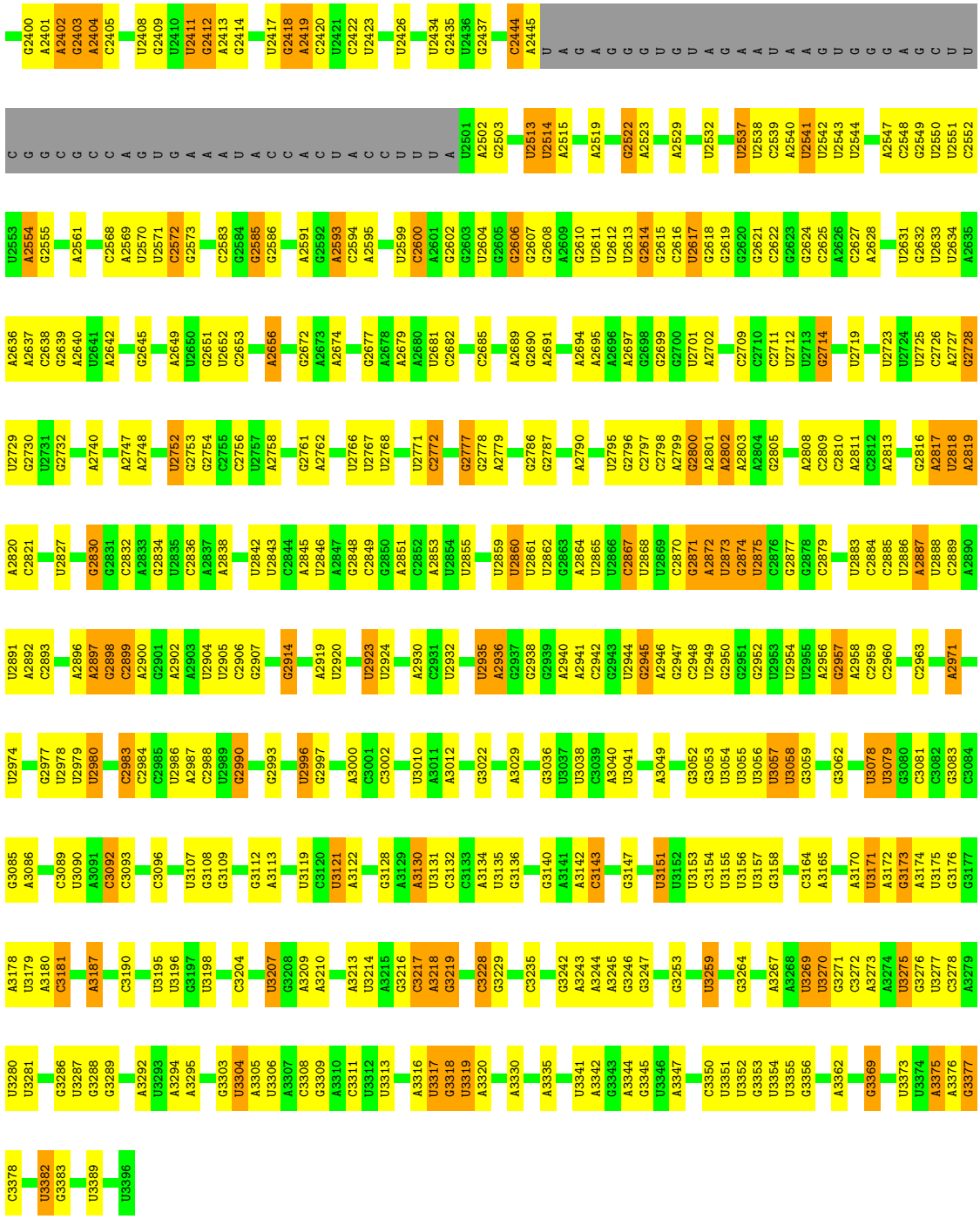
Chain sM:



• Molecule 36: 25S ribosomal RNA

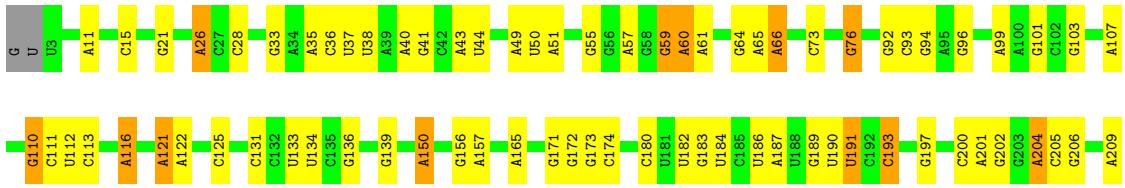
Chain 1:





• Molecule 36: 25S ribosomal RNA

Chain 5:



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C311 C312 A313 A318 A319 G320 C321 U322 A323 A324 A325 U326 U329 C339 C340 G341 G345 A348 A349 C350 A351 A352 G353 C356 U359 G360 A361 U362 G363 A366 G376 A385 A386 U393 A397 A398 A399 G400 U401 A402 C403 G404 U405 G406 U411 G412 U413
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U C G C A U U U C A C491 U492 G493 G494 G495 U506 U507 U508 U509 G513 A516 G517 G518 A519 U520 A521 A522 A532 G535 G542 C546 G547 G548 A551 U555 U556 A557 U558 A559 G560 A569 G575 C576 C577 A578 G579 C580 G583
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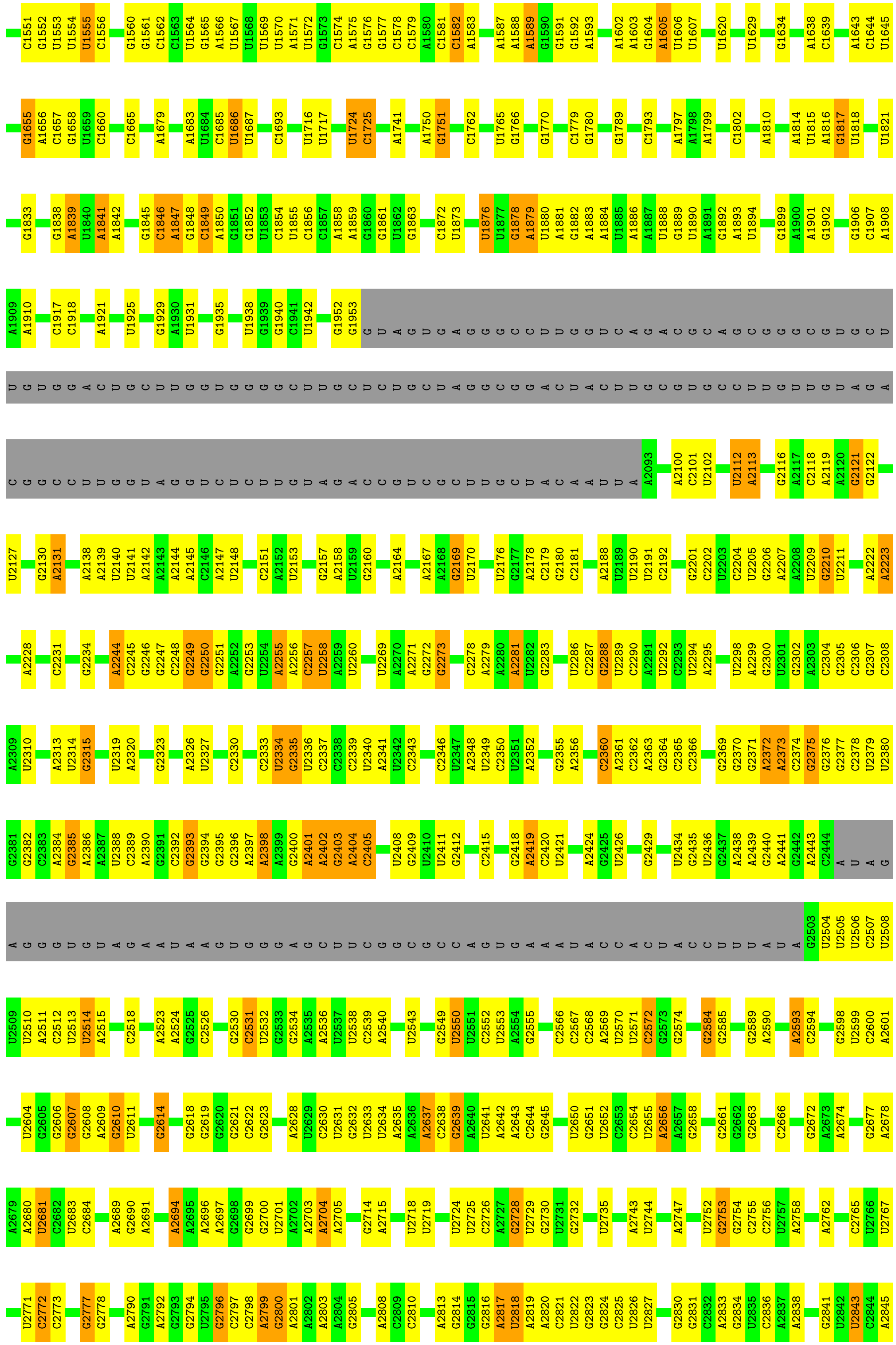
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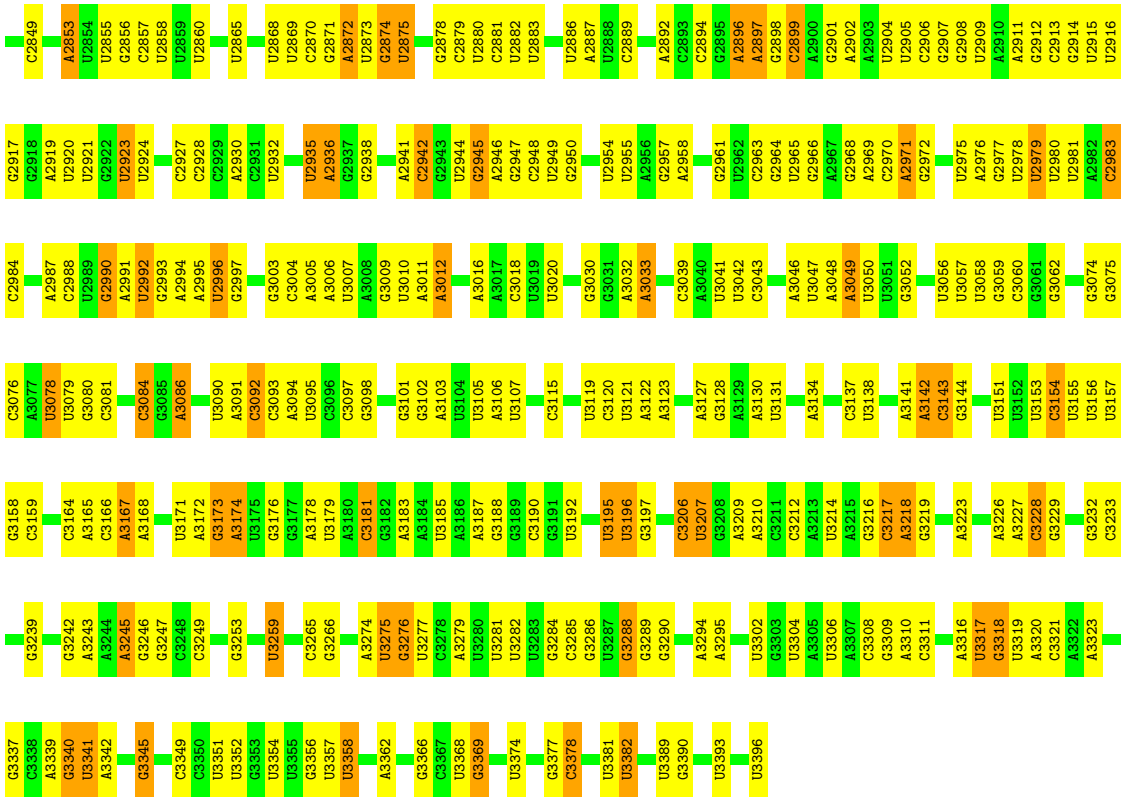
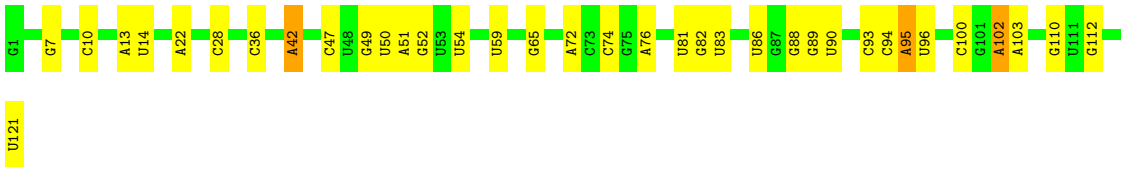
A1909 A1910 C1917 C1918 A1921 U1925 G1929 A1930 U1931 G1935 U1938 G1939 G1940 C1941 U1942 G1952 G1953 G U A G U G A G G G C C U U G G U C A G A C G C A G C G G G C G U G C U
U G U G G A C U G C U U G G U G G G G C U U G C U C U G C U A G G C G G A C U A C U U G C G U G C C U U G U U G U A G A
C G G C C U U G G U A G G U C U C U U G U A G A C C G U C G C U U G C U A C A A U U A A2093 A2100 C2101 U2102 U2112 A2113 G2116 A2117 C2118 A2119 A2120 G2121 G2122
U2127 G2130 A2131 A2138 A2139 U2140 U2141 A2142 A2143 A2144 A2145 C2146 A2147 U2148 C2151 A2152 U2153 G2157 A2158 U2159 G2160 A2164 A2167 A2168 G2169 U2170 U2176 G2177 A2178 C2179 G2180 C2181 A2188 U2189 U2190 U2191 C2192 G2201 C2202 U2203 C2204 U2205 G2206 A2207 A2208 U2209 G2210 U2211 A2222 A2223
A2228 C2231 G2234 A2244 C2245 G2246 G2247 C2248 G2249 G2250 G2251 A2252 G2253 U2254 A2255 A2256 C2257 U2258 A2259 U2260 U2269 A2270 A2271 G2272 G2273 C2278 A2279 A2280 A2281 U2282 G2283 U2286 C2287 G2288 U2289 C2290 A2291 U2292 C2293 U2294 A2295 U2298 A2299 G2300 U2301 G2302 A2303 C2304 G2305 C2306 G2307 C2308
A2309 U2310 A2313 U2314 G2315 U2319 A2320 G2323 A2326 U2327 C2330 C2333 U2334 G2335 U2336 C2337 C2338 C2339 U2340 A2341 U2342 C2343 C2346 U2347 A2348 U2349 C2350 U2351 A2352 G2355 A2356 C2360 A2361 C2362 A2363 G2364 C2365 C2366 G2369 G2370 G2371 A2372 A2373 C2374 G2375 G2376 G2377 C2378 U2379 U2380
G2381 G2382 C2383 A2384 G2385 A2386 A2387 U2388 C2389 A2390 G2391 C2392 G2393 G2394 G2395 G2396 A2397 A2398 A2399 G2400 A2401 A2402 G2403 A2404 C2405 U2408 G2409 U2410 U2411 G2412 C2415 G2418 A2419 C2420 U2421 A2424 G2425 U2426 G2429 U2434 G2435 U2436 G2437 A2438 A2439 G2440 A2441 G2442 A2443 C2444 A U A G
A G G G U G U A G A A U A A G U G G G A G C U U C G G C G C C A G U G A A A U A C C A C U A C C U U U A U A G2503 U2504 U2505 U2506 C2507 U2508
U2509 U2510 A2511 C2512 U2513 U2514 A2515 C2518 A2523 A2524 G2525 C2526 G2530 C2531 U2532 G2533 G2534 A2535 A2536 U2537 U2538 C2539 A2540 U2543 G2549 U2550 U2551 C2552 U2553 A2554 G2555 C2566 C2567 C2568 A2569 U2570 U2571 C2572 G2573 G2574 G2584 G2585 G2589 A2590 A2593 C2594 G2598 U2599 C2600 A2601
U2604 G2605 G2606 G2607 G2608 A2609 G2610 U2611 G2614 G2618 G2619 G2620 C2621 C2622 G2623 A2628 U2629 C2630 U2631 G2632 U2633 U2634 A2635 A2636 A2637 C2638 G2639 A2640 U2641 A2642 A2643 C2644 G2645 U2650 G2651 U2652 C2653 C2654 U2655 A2656 A2657 G2658 G2661 G2662 G2663 C2666 G2672 A2673 A2674 G2677 A2678
A2679 A2680 U2681 C2682 U2683 C2684 A2689 G2690 A2691 A2694 A2695 A2696 A2697 G2698 G2699 G2700 U2701 A2702 A2703 A2704 A2705 G2714 A2715 U2718 U2719 U2724 U2725 C2726 A2727 G2728 U2729 G2730 U2731 G2732 U2735 A2743 U2744 A2747 U2752 G2753 G2754 C2755 C2756 U2757 A2758 A2762 C2765 U2766 U2767
U2771 C2772 C2773 G2777 G2778 A2790 G2791 A2792 G2793 G2794 U2795 G2796 C2797 C2798 A2799 G2800 A2801 A2802 A2803 A2804 G2805 A2808 C2809 C2810 A2813 G2814 G2815 G2816 A2817 U2818 A2819 A2820 C2821 G2822 G2823 G2824 C2825 U2826 U2827 G2830 G2831 C2832 A2833 G2834 U2835 C2836 A2837 A2838 G2841 U2842 U2843 C2844 A2845



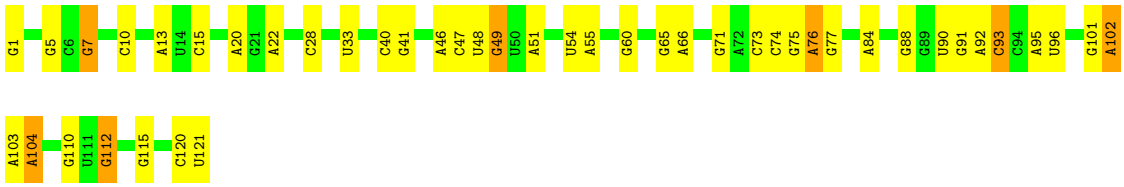

- Molecule 37: 5S ribosomal RNA

Chain 3:



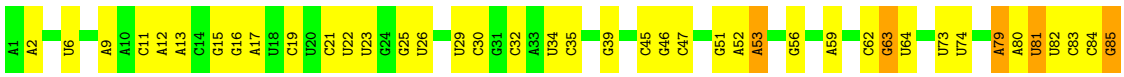

- Molecule 37: 5S ribosomal RNA

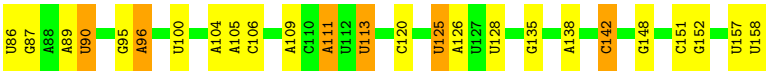
Chain 7:




- Molecule 38: 5.8S ribosomal RNA

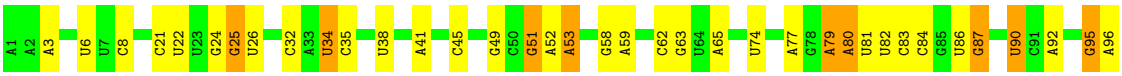
Chain 4:

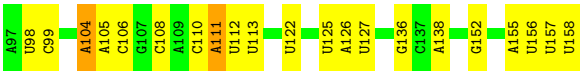





• Molecule 38: 5.8S ribosomal RNA

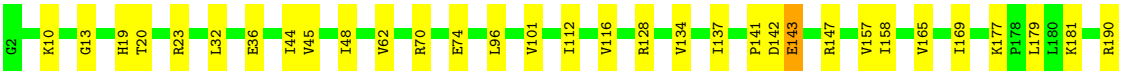
Chain 8:




• Molecule 39: 60S ribosomal protein L2-A

Chain L2:

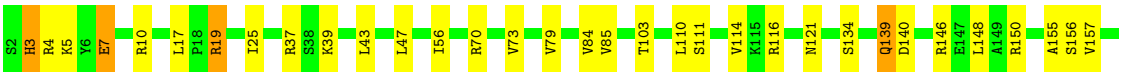


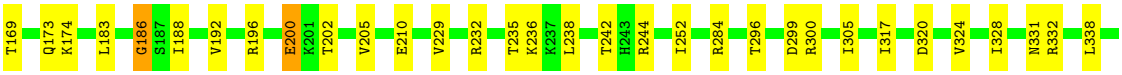
• Molecule 39: 60S ribosomal protein L2-A

Chain l2:

• Molecule 40: 60S ribosomal protein L3

Chain L3:



• Molecule 40: 60S ribosomal protein L3

Chain l3:

S2 H3 R4 R10 L17 P18 R19 K20 R21 K30 R37 S38 K39 L47 K50 I56 T77 V78 V79 D80 T81 V84 T103 V114 K120 K124 S134 A138 Q139 E145 R146 E147 L148 A149 R150 A155 S156 V157 V160 T169

L183 N184 G185 G186 S187 I188 R196 T202 V205 T221 V229 R232 T235 K236 K237 L238 T242 H243 R244 K248 V249 I252 M261 V264 A265 R266 R284 N293 T296 K302 M308 I317 V324 I328 R332 K333 R334 I335

L338 R339 K340 T346 S347 R348 K349 S355 T361 R369 T382 L387

- Molecule 41: 60S ribosomal protein L4-A

Chain L4: 80% 18%

S2 R3 P4 Q5 E14 A15 T16 L22 V25 T40 V52 S53 T60 R69 A70 V71 I74 M93 C94 R95 E117 K118 T122 A130 V131 L136 A137 R138 G139 K144 I145 P146 E147 I148 P149 L150 V151 V152 L156 K170 A171 V172 S176

D177 L178 L179 L182 K185 R188 A189 G190 K193 Y194 R197 R198 W199 T200 R203 L206 E211 R220 N221 V222 V230 A231 S232 L233 R246 L258 S270 T283 S292 S293 T306 Q307 H311 V312 L313 P317 L318 K319 N320 V323

L327 N328 L339 K346 T349 V354 T358 L359 D362

- Molecule 41: 60S ribosomal protein L4-A

Chain l4: 81% 18%

S2 Q5 E14 V25 V52 T60 T67 R76 F90 G91 N92 M93 R98 K112 Y120 A121 T122 E143 K144 I145 P146 L150 L156 Q160 K161 V172 S176 L179 K186 L187 R188 A189 G190 K191 R198 W199 T200 R203

L206 K217 R220 N221 V222 E226 N229 V230 L233 R246 L258 V267 V272 T283 S284 T287 I295 R300 P301 A302 A305 T306 Q307 H311 V312 L313 K319 V323 L327 N328 P329 Y330 L339 K342 E345 T358 L359 K360

H361 D362

- Molecule 42: 60S ribosomal protein L5

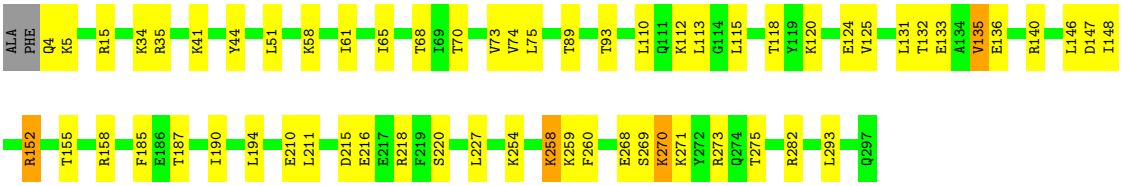
Chain L5: 78% 20%

A2 K5 D6 A7 S10 R23 R35 K41 N57 K58 I64 T68 I69 L75 L92 T101 I105 T109 K112 L113 G114 L115 T118 V122 V125 E128 L131 D137 R140 V144 F145 L146 D147 I148 Q151 R152

T155 L163 E177 F185 E186 T187 E188 L194 L195 R196 S205 E216 E217 E221 L222 D232 A233 D234 S235 L236 A252 F253 K254 E257 K258 K259 F260 T261 K262 E263 R273 Q274 T275 K279 I290 L293 A294 G295 Q296 Q297

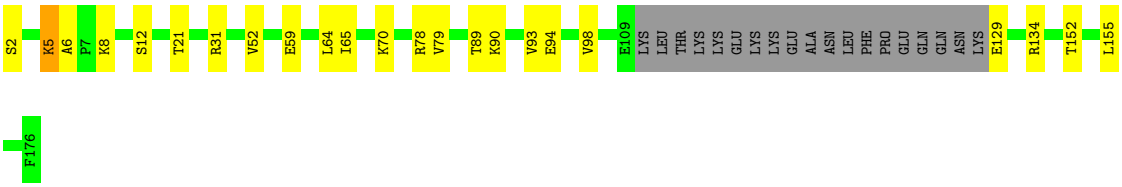
- Molecule 42: 60S ribosomal protein L5

Chain l5: 79% 19%



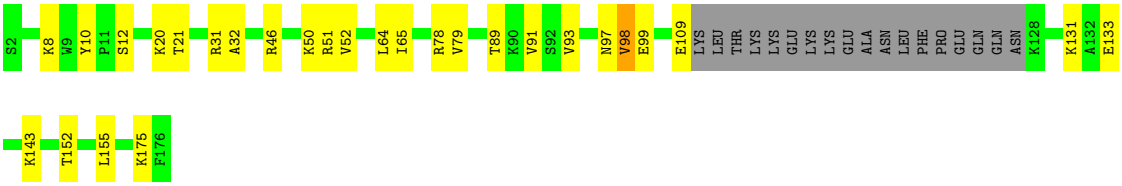

- Molecule 43: 60S ribosomal protein L6-A

Chain L6:



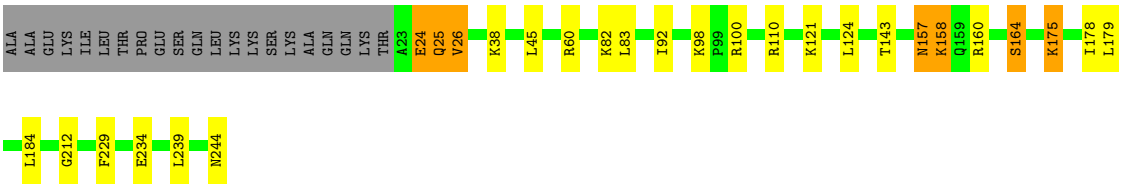

- Molecule 43: 60S ribosomal protein L6-A

Chain l6:



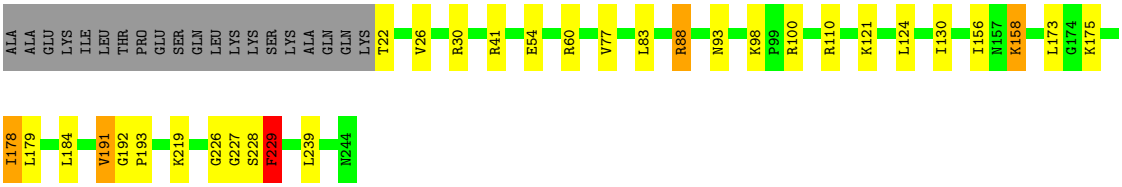

- Molecule 44: 60S ribosomal protein L7-A

Chain L7:




- Molecule 44: 60S ribosomal protein L7-A

Chain l7:




- Molecule 45: 60S ribosomal protein L8-A

Chain L8:

ALA PRO GLY LYS LYS VAL ALA PRO ALA PRO PHE GLY ALA LYS SER THR LYS SER ASN LYS THR ARG N24 P25 L26 T27 I36 A39 V40 Q41 S47 V50 Q61 K62 K63 V71 T74 F78 Q79 Y80 T81 R84 N95 T110 A117 E118 G119 K120

V132 L136 L150 D156 V157 I160 V163 L169 K172 M173 R185 L189 V203 R204 D219 L238 M246 D247 K248 K251 S255 A256

• Molecule 45: 60S ribosomal protein L8-A

Chain l8: 70% 20% • 9%

ALA PRO GLY LYS LYS VAL ALA PRO ALA PRO PHE GLY ALA LYS SER THR LYS SER ASN LYS THR ARG N24 P25 L26 N33 F34 A39 V40 Q41 V50 L65 S66 I67 R68 L69 K70 V71 T74 Q79 Y80 T81 E89 T90 N95 A114 A115 V116 A117 K120

S121 K122 Q123 D124 K128 K133 L136 N145 K146 K149 L150 I160 V163 V164 F165 L166 L169 K172 T188 L189 V190 V203 L211 L214 T217 K230 K231 I237 L238 G239 N240 K241 K248 D254 SER ALA

• Molecule 46: 60S ribosomal protein L9-A

Chain L9: 82% 17% •

M1 K2 Y3 I4 Q5 Q9 P13 E14 V18 S22 T33 I41 V48 L52 R62 A66 A67 L68 R69 T70 T80 G81 V82 R124 V132 E135 F136 S137 T138 N139 S150 V151 N157 L161 Q162 R173 D177 T188 E189 D190

L191

• Molecule 46: 60S ribosomal protein L9-A

Chain l9: 80% 20% •

M1 K2 Y3 I4 Q5 T6 V18 S19 I20 R31 G32 T33 K39 V43 T44 L52 V55 R62 L68 R69 T70 T80 G81 V82 E105 K106 D107 D120 D130 T133 I144 V151 N157 L161 Q162 V167 R168 N169 D177 G178 I179

I187 T188 L191

• Molecule 47: 60S ribosomal protein L10

Chain M0: 78% 17% •

A2 R3 R4 P18 R24 A25 V26 K30 I31 R32 I33 L36 K39 K40 A41 T42 L48 L52 L57 E63 K74 Y75 M76 T77 T78 L87 I99 M102 LEU SER CYS ALA GLY ALA ASP ARG LEU Q112 V129 D130 R139 T140 S143

Q163 K164 I165 K169 T174 R178 R185 E189 G194 V197 K203 R211 A219 Q220 A221

• Molecule 47: 60S ribosomal protein L10

Chain m0: 77% 20% •

A2 R3 R4 R24 D28 I31 R32 L36 T42 L48 L52 L57 K74 Y75 M76 T77 T78 R82 L87 I99 N100 K101 M102 L103 SER CYS ALA GLY ALA ASP ARG L111 R116 G117 V129 D130 R139 T140 S143 N144 K145 Q163

I166 L167 S168 K169 L182 R185 D193 G194 A195 F196 V197 G204 S205 L206 E207 R211 E212 E215 A219 Q220 A221

• Molecule 48: 60S ribosomal protein L11-B

Chain M1: 75% 20%

SER THR LYS ALA Q6 N7 P8 M9 R10 D11 L12 K13 K16 V23 G24 T31 L40 T44 P45 V46 R61 K64 I65 T70 L80 R94 N95 I106 D107 L112 G113 I114 K115 Y116 D117 I120 V130 V138 T139 R140 R141 K142 S151

D158 S161 Q165 K166 Y167 K174

• Molecule 48: 60S ribosomal protein L11-B

Chain m1: 79% 17%

SER THR LYS ALA Q6 N7 P8 M9 R10 D11 L12 L30 T31 T44 V54 R55 V71 L80 K85 R94 N95 N101 D107 L112 G113 I114 K115 Y116 D117 V129 R137 R140 R141 K142 K153 T159 V160 S161 Y167 D173 K174

• Molecule 49: 60S ribosomal protein L13-A

Chain M3: 79% 17%

A2 K5 K23 S34 R35 R42 I46 A47 L54 R55 V58 R59 V63 R67 K68 V69 T76 L85 I93 E107 Q114 K122 I123 I124 R128 N129 G130 K131 E134 A135 E136 T144 D153 E164 S165 R171 R180 G181

I182 K190 E194 ALA GLU LYS LYS LYS

• Molecule 49: 60S ribosomal protein L13-A

Chain m3: 80% 17%

A2 H13 Q19 I46 A47 P50 L51 L54 R55 P56 V57 V58 R59 V63 R67 K68 V69 R73 T76 L85 I93 R101 E107 Q114 R115 E118 K122 I123 I124 R128 N129 G130 K131 E134 A135 A141 E164 S165 E184

K190 E194 A195 GLU LYS LYS LYS

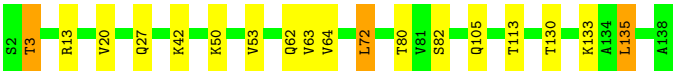
• Molecule 50: 60S ribosomal protein L14-A

Chain M4: 80% 18%

SER T3 I6 V7 K8 A9 V20 Q27 S28 K42 K43 K50 V53 P54 R55 N59 V64 L65 T66 L72 V90 C91 E92 K102 Q105 R108 T113 K125 Q126 T130 L135 A136 K137 A138

• Molecule 50: 60S ribosomal protein L14-A

Chain m4:




• Molecule 51: 60S ribosomal protein L15-A

Chain M5:

• Molecule 51: 60S ribosomal protein L15-A

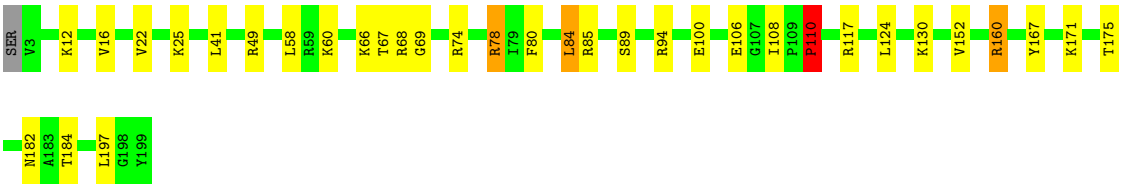
Chain m5:

• Molecule 52: 60S ribosomal protein L16-A

Chain M6:

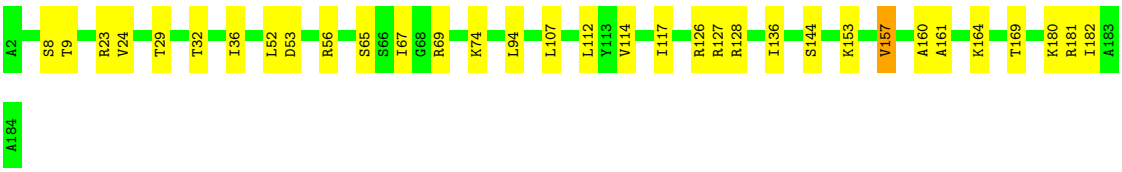
• Molecule 52: 60S ribosomal protein L16-A

Chain m6:



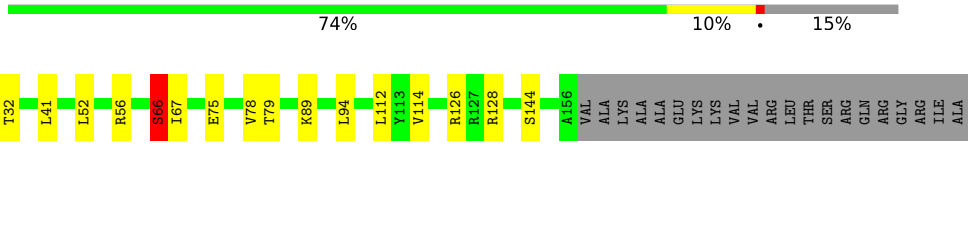

• Molecule 53: 60S ribosomal protein L17-A

Chain M7:



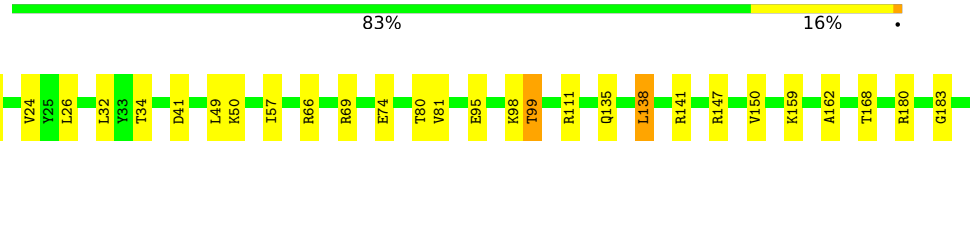
• Molecule 53: 60S ribosomal protein L17-A

Chain m7:



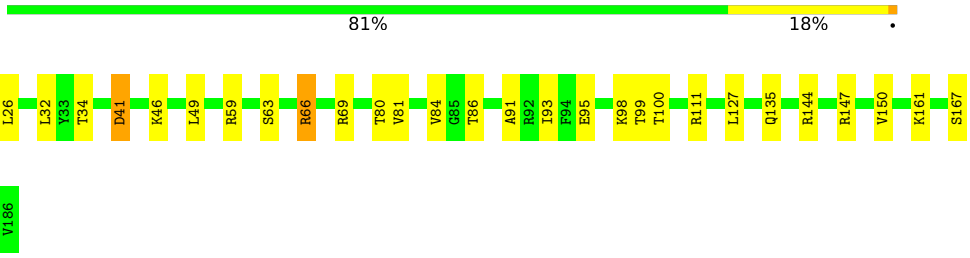

• Molecule 54: 60S ribosomal protein L18-A

Chain M8:



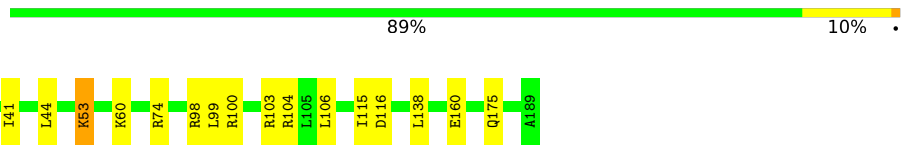

• Molecule 54: 60S ribosomal protein L18-A

Chain m8:



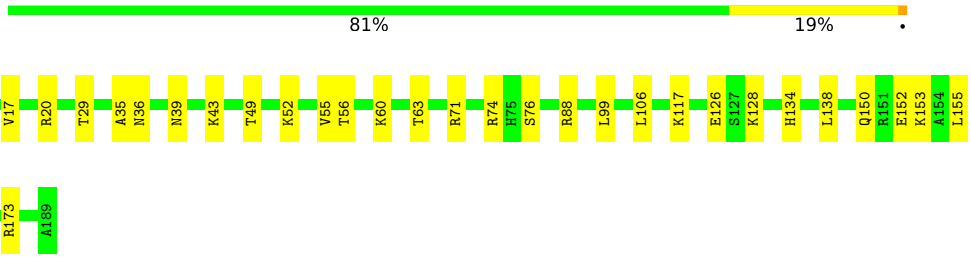

• Molecule 55: 60S ribosomal protein L19-A

Chain M9:



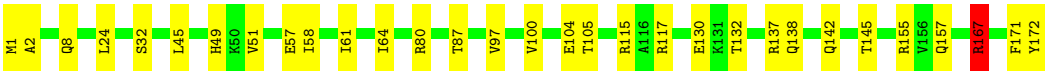

• Molecule 55: 60S ribosomal protein L19-A

Chain m9:



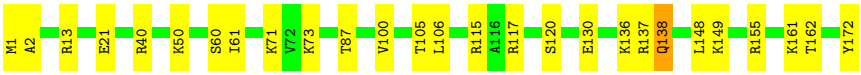

• Molecule 56: 60S ribosomal protein L20-A

Chain N0:




• Molecule 56: 60S ribosomal protein L20-A

Chain n0:

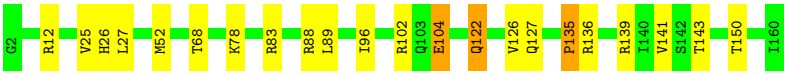



• Molecule 57: 60S ribosomal protein L21-A

Chain N1:

• Molecule 57: 60S ribosomal protein L21-A

Chain n1:

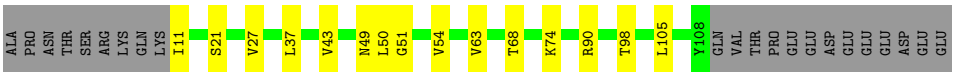



• Molecule 58: 60S ribosomal protein L22-A

Chain N2:

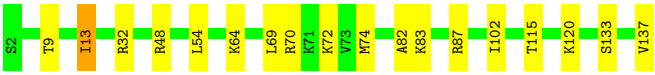
• Molecule 58: 60S ribosomal protein L22-A

Chain n2:




• Molecule 59: 60S ribosomal protein L23-A

Chain N3:

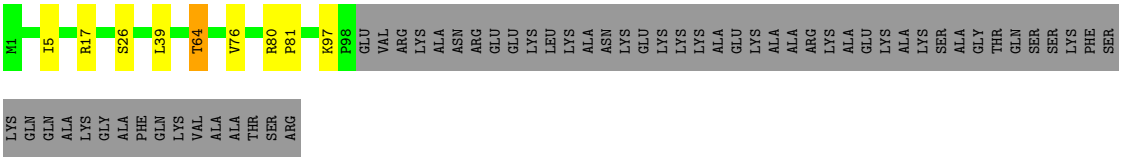



• Molecule 59: 60S ribosomal protein L23-A

Chain n3:

• Molecule 60: 60S ribosomal protein L24-A

Chain N4:

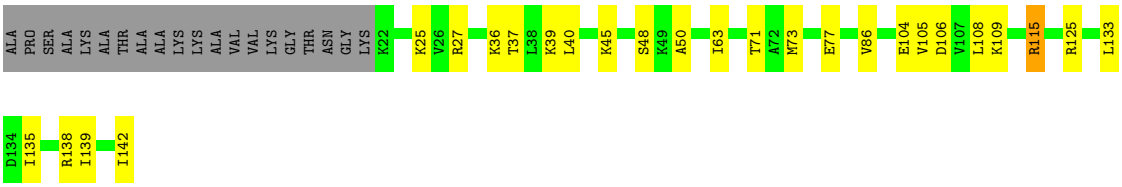



• Molecule 60: 60S ribosomal protein L24-A

Chain n4:

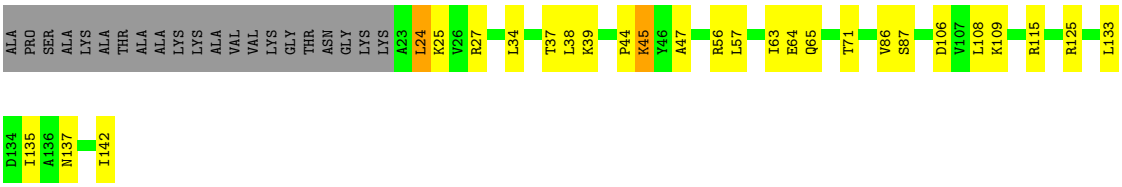
• Molecule 61: 60S ribosomal protein L25

Chain N5:



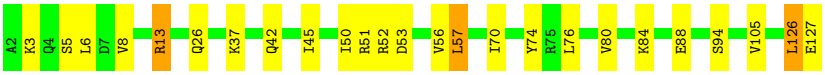

• Molecule 61: 60S ribosomal protein L25

Chain n5:




• Molecule 62: 60S ribosomal protein L26-A

Chain N6:

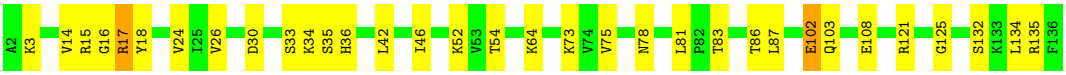



• Molecule 62: 60S ribosomal protein L26-A

Chain n6:

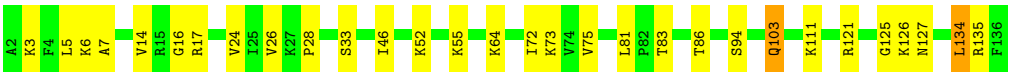
• Molecule 63: 60S ribosomal protein L27-A

Chain N7:



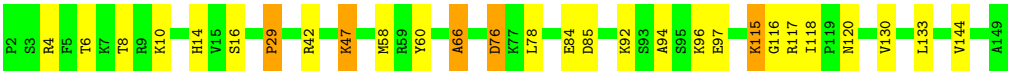

• Molecule 63: 60S ribosomal protein L27-A

Chain n7:



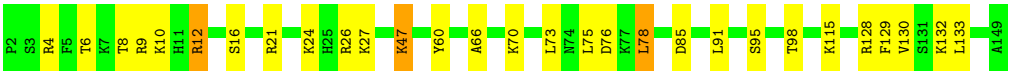

• Molecule 64: 60S ribosomal protein L28

Chain N8:



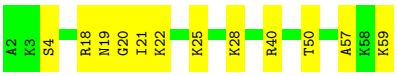

• Molecule 64: 60S ribosomal protein L28

Chain n8:



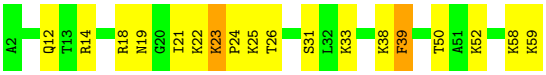

• Molecule 65: 60S ribosomal protein L29

Chain N9:



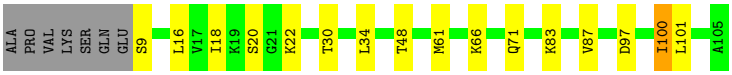

• Molecule 65: 60S ribosomal protein L29

Chain n9:




• Molecule 66: 60S ribosomal protein L30

Chain O0:

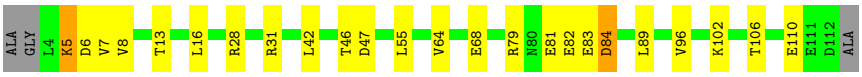



• Molecule 66: 60S ribosomal protein L30

Chain o0:

• Molecule 67: 60S ribosomal protein L31-A

Chain O1:

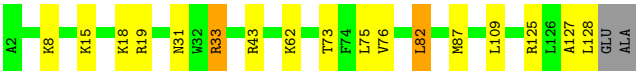



• Molecule 67: 60S ribosomal protein L31-A

Chain o1:

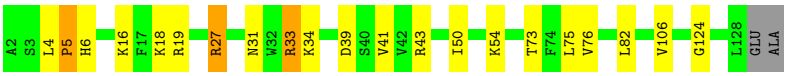
• Molecule 68: 60S ribosomal protein L32

Chain O2:



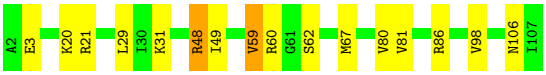

• Molecule 68: 60S ribosomal protein L32

Chain o2:



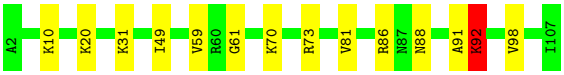

• Molecule 69: 60S ribosomal protein L33-A

Chain O3:



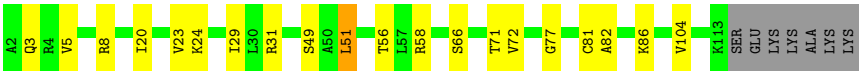

• Molecule 69: 60S ribosomal protein L33-A

Chain o3:



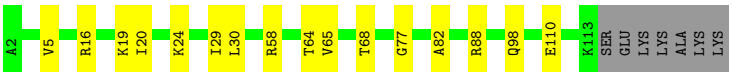

• Molecule 70: 60S ribosomal protein L34-A

Chain O4:



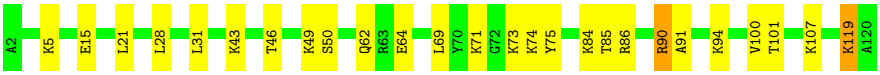

• Molecule 70: 60S ribosomal protein L34-A

Chain o4:



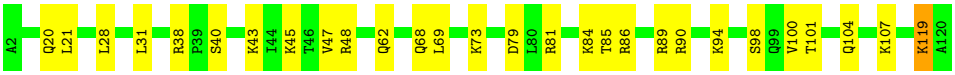

• Molecule 71: 60S ribosomal protein L35-A

Chain O5:



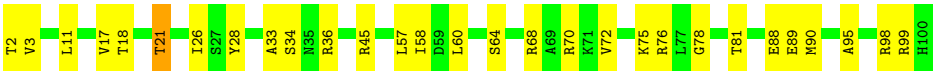

• Molecule 71: 60S ribosomal protein L35-A

Chain o5:



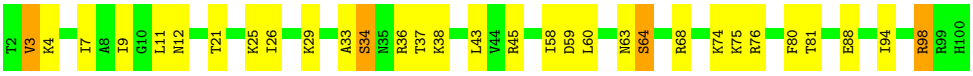

• Molecule 72: 60S ribosomal protein L36-A

Chain O6:



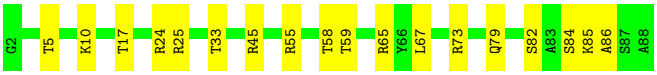

• Molecule 72: 60S ribosomal protein L36-A

Chain o6:




• Molecule 73: 60S ribosomal protein L37-A

Chain O7:




• Molecule 73: 60S ribosomal protein L37-A

Chain o7: 83% 17%

• Molecule 74: 60S ribosomal protein L38

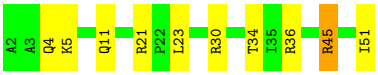
Chain O8: 79% 21%

• Molecule 74: 60S ribosomal protein L38

Chain o8: 82% 17%

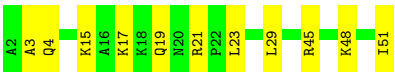
• Molecule 75: 60S ribosomal protein L39

Chain O9: 80% 18%



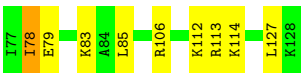

• Molecule 75: 60S ribosomal protein L39

Chain o9: 78% 22%




• Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0: 83% 15%




• Molecule 76: Ubiquitin-60S ribosomal protein L40

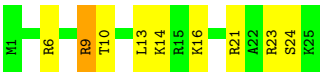
Chain q0: 85% 13%

• Molecule 77: 60S ribosomal protein L41-A

Chain Q1:


• Molecule 77: 60S ribosomal protein L41-A

Chain q1:


• Molecule 78: 60S ribosomal protein L42-A

Chain Q2:


• Molecule 78: 60S ribosomal protein L42-A

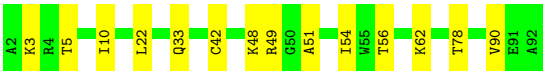
Chain q2:


• Molecule 79: 60S ribosomal protein L43-A

Chain Q3:

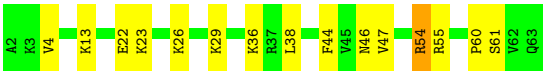

• Molecule 79: 60S ribosomal protein L43-A

Chain q3:

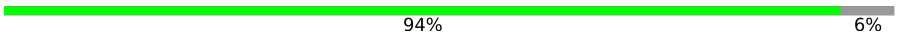

• Molecule 80: 40S ribosomal protein S30-A

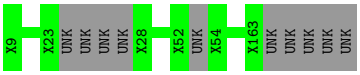
Chain e0:




• Molecule 81: Unknown protein m2

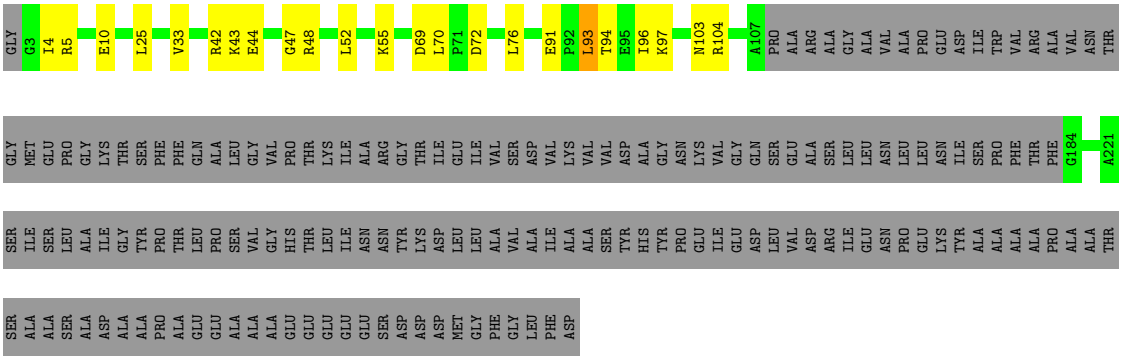
Chain m2:



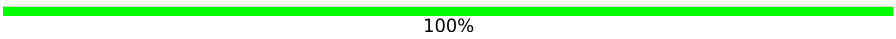

• Molecule 82: 60S acidic ribosomal protein P0

Chain p0:




• Molecule 83: Unknown protein p1

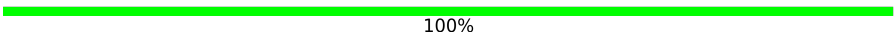
Chain p1:




There are no outlier residues recorded for this chain.

• Molecule 84: Unknown protein p2

Chain p2:




There are no outlier residues recorded for this chain.

# 4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 436.64Å 287.69Å 304.39Å<br>90.00° 98.98° 90.00° | Depositor |
| Resolution (Å) | 300.66 – 2.80 | Depositor |
| % Data completeness<br>(in resolution range) | 99.6 (300.66-2.80) | Depositor |
| $R_{merge}$ | 0.25 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.36 (at 2.82Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: dev_1702) | Depositor |
| R, $R_{free}$ | 0.208 , 0.246 | Depositor |
| Wilson B-factor (Å$^2$) | 60.5 | Xtriage |
| Anisotropy | 0.227 | Xtriage |
| L-test for twinning[2] | $< \|L\| > = 0.49$, $< L^2 > = 0.32$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 411226 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 57.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 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: OHX, MG, 3H3, 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 | 2 | 0.75 | 5/41698 (0.0%) | 1.30 | 337/64972 (0.5%) |
| 1 | 6 | 0.87 | 23/42765 (0.1%) | 1.40 | 490/66634 (0.7%) |
| 2 | S0 | 0.47 | 0/1617 | 0.67 | 0/2215 |
| 2 | s0 | 0.53 | 0/1623 | 0.76 | 2/2222 (0.1%) |
| 3 | S1 | 0.37 | 0/1735 | 0.62 | 0/2335 |
| 3 | s1 | 0.52 | 0/1748 | 0.71 | 1/2352 (0.0%) |
| 4 | S2 | 0.51 | 0/1665 | 0.67 | 0/2263 |
| 4 | s2 | 0.61 | 0/1665 | 0.79 | 0/2263 |
| 5 | S3 | 0.50 | 0/1759 | 0.65 | 0/2368 |
| 5 | s3 | 0.48 | 0/1759 | 0.62 | 0/2368 |
| 6 | S4 | 0.51 | 0/2109 | 0.74 | 2/2839 (0.1%) |
| 6 | s4 | 0.57 | 0/2109 | 0.79 | 1/2839 (0.0%) |
| 7 | S5 | 0.43 | 0/1629 | 0.60 | 0/2202 |
| 7 | s5 | 0.46 | 0/1629 | 0.66 | 1/2202 (0.0%) |
| 8 | S6 | 0.48 | 0/1823 | 0.65 | 0/2439 |
| 8 | s6 | 0.58 | 0/1779 | 0.72 | 1/2379 (0.0%) |
| 9 | S7 | 0.46 | 0/1506 | 0.65 | 0/2028 |
| 9 | s7 | 0.54 | 0/1516 | 0.70 | 1/2043 (0.0%) |
| 10 | S8 | 0.58 | 0/1514 | 0.79 | 3/2021 (0.1%) |
| 10 | s8 | 0.64 | 0/1514 | 0.77 | 1/2021 (0.0%) |
| 11 | S9 | 0.50 | 0/1519 | 0.69 | 0/2035 |
| 11 | s9 | 0.59 | 0/1519 | 0.74 | 0/2035 |
| 12 | C0 | 0.45 | 0/790 | 0.69 | 1/1069 (0.1%) |
| 12 | c0 | 0.40 | 0/777 | 0.63 | 3/1049 (0.3%) |
| 13 | C1 | 0.59 | 0/1240 | 0.71 | 0/1675 |
| 13 | c1 | 0.66 | 0/1194 | 0.86 | 0/1610 |
| 14 | C2 | 0.37 | 0/898 | 0.62 | 0/1220 |
| 14 | c2 | 0.31 | 0/898 | 0.58 | 1/1220 (0.1%) |
| 15 | C3 | 0.50 | 0/1215 | 0.71 | 2/1638 (0.1%) |
| 15 | c3 | 0.61 | 0/1215 | 0.77 | 0/1638 |
| 16 | C4 | 0.38 | 0/901 | 0.65 | 0/1217 |
| 16 | c4 | 0.54 | 0/960 | 0.77 | 1/1290 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 17 | C5 | 0.50 | 0/998 | 0.67 | 0/1341 |
| 17 | c5 | 0.51 | 0/1060 | 0.68 | 1/1426 (0.1%) |
| 18 | C6 | 0.47 | 0/1125 | 0.74 | 3/1510 (0.2%) |
| 18 | c6 | 0.50 | 0/1131 | 0.69 | 0/1518 |
| 19 | C7 | 0.46 | 0/935 | 0.65 | 0/1254 |
| 19 | c7 | 0.50 | 0/914 | 0.70 | 0/1224 |
| 20 | C8 | 0.49 | 0/1211 | 0.67 | 0/1628 |
| 20 | c8 | 0.51 | 0/1211 | 0.73 | 1/1628 (0.1%) |
| 21 | C9 | 0.48 | 0/1130 | 0.68 | 0/1517 |
| 21 | c9 | 0.51 | 0/1130 | 0.71 | 0/1517 |
| 22 | D0 | 0.48 | 0/865 | 0.66 | 0/1169 |
| 22 | d0 | 0.49 | 0/892 | 0.68 | 0/1205 |
| 23 | D1 | 0.47 | 0/693 | 0.66 | 0/935 |
| 23 | d1 | 0.57 | 0/693 | 0.80 | 0/935 |
| 24 | D2 | 0.55 | 0/1038 | 0.75 | 1/1395 (0.1%) |
| 24 | d2 | 0.68 | 0/1038 | 0.75 | 0/1395 |
| 25 | D3 | 0.63 | 0/1139 | 0.79 | 1/1518 (0.1%) |
| 25 | d3 | 0.73 | 0/1139 | 0.83 | 3/1518 (0.2%) |
| 26 | D4 | 0.48 | 0/1087 | 0.63 | 0/1449 |
| 26 | d4 | 0.53 | 0/1087 | 0.72 | 0/1449 |
| 27 | D5 | 0.42 | 0/571 | 0.71 | 0/768 |
| 27 | d5 | 0.45 | 0/566 | 0.63 | 0/761 |
| 28 | D6 | 0.47 | 0/782 | 0.67 | 0/1047 |
| 28 | d6 | 0.59 | 0/782 | 0.75 | 0/1047 |
| 29 | D7 | 0.46 | 0/620 | 0.68 | 1/838 (0.1%) |
| 29 | d7 | 0.52 | 0/620 | 0.73 | 0/838 |
| 30 | D8 | 0.36 | 0/499 | 0.56 | 0/670 |
| 30 | d8 | 0.44 | 0/499 | 0.67 | 0/670 |
| 31 | D9 | 0.56 | 0/452 | 0.82 | 1/600 (0.2%) |
| 31 | d9 | 0.58 | 0/452 | 0.72 | 0/600 |
| 32 | E0 | 0.49 | 0/483 | 0.65 | 0/643 |
| 33 | E1 | 0.49 | 0/577 | 0.83 | 0/770 |
| 33 | e1 | 0.43 | 0/619 | 0.75 | 1/822 (0.1%) |
| 34 | SR | 1.06 | 2/2494 (0.1%) | 1.50 | 6/3393 (0.2%) |
| 34 | sR | 0.41 | 0/2495 | 0.58 | 0/3395 |
| 35 | SM | 0.55 | 0/1113 | 0.71 | 2/1502 (0.1%) |
| 35 | sM | 0.51 | 0/683 | 0.68 | 1/923 (0.1%) |
| 36 | 1 | 1.16 | 152/75394 (0.2%) | 1.67 | 1955/117545 (1.7%) |
| 36 | 5 | 1.20 | 176/75414 (0.2%) | 1.69 | 1938/117575 (1.6%) |
| 37 | 3 | 0.96 | 4/2883 (0.1%) | 1.42 | 33/4491 (0.7%) |
| 37 | 7 | 1.13 | 7/2883 (0.2%) | 1.63 | 50/4491 (1.1%) |
| 38 | 4 | 1.11 | 2/3746 (0.1%) | 1.60 | 70/5832 (1.2%) |
| 38 | 8 | 1.00 | 5/3746 (0.1%) | 1.51 | 46/5832 (0.8%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 39 | L2 | 0.75 | 0/1948 | 0.87 | 2/2617 (0.1%) |
| 39 | l2 | 0.82 | 1/1946 (0.1%) | 0.95 | 5/2614 (0.2%) |
| 40 | L3 | 0.77 | 2/3146 (0.1%) | 0.88 | 2/4228 (0.0%) |
| 40 | l3 | 0.85 | 1/3146 (0.0%) | 0.96 | 11/4228 (0.3%) |
| 41 | L4 | 0.86 | 3/2800 (0.1%) | 1.02 | 10/3790 (0.3%) |
| 41 | l4 | 0.79 | 0/2800 | 0.94 | 6/3790 (0.2%) |
| 42 | L5 | 0.59 | 0/2425 | 0.72 | 0/3271 |
| 42 | l5 | 0.78 | 0/2408 | 0.83 | 3/3248 (0.1%) |
| 43 | L6 | 0.77 | 0/1260 | 0.85 | 3/1694 (0.2%) |
| 43 | l6 | 0.78 | 0/1269 | 0.85 | 0/1705 |
| 44 | L7 | 0.85 | 1/1821 (0.1%) | 0.90 | 0/2451 |
| 44 | l7 | 0.86 | 1/1828 (0.1%) | 0.91 | 5/2461 (0.2%) |
| 45 | L8 | 0.59 | 0/1836 | 0.69 | 1/2481 (0.0%) |
| 45 | l8 | 0.57 | 0/1795 | 0.69 | 0/2429 |
| 46 | L9 | 0.70 | 0/1539 | 0.79 | 0/2073 |
| 46 | l9 | 0.80 | 0/1539 | 0.85 | 0/2073 |
| 47 | M0 | 0.76 | 0/1741 | 0.88 | 3/2335 (0.1%) |
| 47 | m0 | 0.82 | 0/1758 | 0.89 | 0/2358 |
| 48 | M1 | 0.55 | 0/1374 | 0.74 | 1/1842 (0.1%) |
| 48 | m1 | 0.67 | 0/1374 | 0.83 | 2/1842 (0.1%) |
| 49 | M3 | 0.77 | 0/1568 | 0.91 | 3/2106 (0.1%) |
| 49 | m3 | 0.75 | 0/1573 | 0.89 | 4/2113 (0.2%) |
| 50 | M4 | 0.79 | 0/1068 | 0.87 | 2/1438 (0.1%) |
| 50 | m4 | 0.81 | 0/1074 | 0.84 | 1/1446 (0.1%) |
| 51 | M5 | 0.78 | 0/1757 | 0.97 | 3/2354 (0.1%) |
| 51 | m5 | 0.72 | 0/1757 | 0.83 | 0/2354 |
| 52 | M6 | 0.93 | 3/1585 (0.2%) | 1.00 | 7/2128 (0.3%) |
| 52 | m6 | 1.06 | 2/1585 (0.1%) | 1.04 | 9/2128 (0.4%) |
| 53 | M7 | 0.84 | 0/1443 | 0.87 | 0/1944 |
| 53 | m7 | 0.93 | 1/1250 (0.1%) | 0.89 | 0/1683 |
| 54 | M8 | 0.84 | 0/1465 | 0.95 | 4/1965 (0.2%) |
| 54 | m8 | 0.76 | 0/1465 | 0.94 | 2/1965 (0.1%) |
| 55 | M9 | 0.58 | 0/1538 | 0.68 | 0/2050 |
| 55 | m9 | 0.65 | 0/1538 | 0.72 | 0/2050 |
| 56 | N0 | 0.81 | 0/1481 | 0.87 | 3/1990 (0.2%) |
| 56 | n0 | 0.84 | 0/1481 | 0.92 | 1/1990 (0.1%) |
| 57 | N1 | 0.81 | 0/1300 | 0.86 | 0/1743 |
| 57 | n1 | 0.86 | 1/1300 (0.1%) | 0.86 | 0/1743 |
| 58 | N2 | 0.46 | 0/812 | 0.61 | 0/1099 |
| 58 | n2 | 0.53 | 0/794 | 0.66 | 0/1076 |
| 59 | N3 | 0.78 | 0/1018 | 0.94 | 5/1369 (0.4%) |
| 59 | n3 | 0.85 | 0/1018 | 0.93 | 4/1369 (0.3%) |
| 60 | N4 | 0.61 | 0/712 | 0.69 | 0/958 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 60 | n4 | 0.68 | 0/1052 | 0.72 | 0/1398 |
| 61 | N5 | 0.65 | 0/979 | 0.82 | 1/1321 (0.1%) |
| 61 | n5 | 0.68 | 0/974 | 0.84 | 0/1314 |
| 62 | N6 | 0.76 | 0/1004 | 0.94 | 4/1341 (0.3%) |
| 62 | n6 | 0.68 | 0/1004 | 0.82 | 0/1341 |
| 63 | N7 | 0.54 | 0/1118 | 0.72 | 0/1497 |
| 63 | n7 | 0.52 | 0/1118 | 0.66 | 0/1497 |
| 64 | N8 | 0.86 | 0/1204 | 0.97 | 4/1612 (0.2%) |
| 64 | n8 | 0.84 | 0/1204 | 0.97 | 4/1612 (0.2%) |
| 65 | N9 | 0.85 | 0/473 | 0.81 | 1/629 (0.2%) |
| 65 | n9 | 0.90 | 0/473 | 0.93 | 2/629 (0.3%) |
| 66 | O0 | 0.53 | 0/751 | 0.68 | 0/1008 |
| 66 | o0 | 0.55 | 0/775 | 0.67 | 0/1040 |
| 67 | O1 | 0.68 | 0/890 | 0.75 | 0/1196 |
| 67 | o1 | 0.85 | 1/897 (0.1%) | 0.86 | 0/1205 |
| 68 | O2 | 0.87 | 0/1041 | 0.95 | 4/1394 (0.3%) |
| 68 | o2 | 0.89 | 0/1041 | 1.02 | 5/1394 (0.4%) |
| 69 | O3 | 0.92 | 0/868 | 0.90 | 3/1168 (0.3%) |
| 69 | o3 | 0.98 | 1/868 (0.1%) | 0.92 | 2/1168 (0.2%) |
| 70 | O4 | 0.62 | 0/890 | 0.80 | 1/1189 (0.1%) |
| 70 | o4 | 0.67 | 0/890 | 0.74 | 0/1189 |
| 71 | O5 | 0.71 | 1/978 (0.1%) | 0.84 | 2/1301 (0.2%) |
| 71 | o5 | 0.62 | 0/974 | 0.71 | 0/1297 |
| 72 | O6 | 0.68 | 0/778 | 0.84 | 0/1034 |
| 72 | o6 | 0.60 | 0/777 | 0.74 | 0/1033 |
| 73 | O7 | 0.89 | 1/696 (0.1%) | 1.00 | 2/923 (0.2%) |
| 73 | o7 | 0.75 | 0/696 | 0.88 | 1/923 (0.1%) |
| 74 | O8 | 0.52 | 0/618 | 0.64 | 0/826 |
| 74 | o8 | 0.49 | 0/614 | 0.67 | 0/822 |
| 75 | O9 | 0.89 | 1/443 (0.2%) | 0.96 | 1/588 (0.2%) |
| 75 | o9 | 0.81 | 0/443 | 0.95 | 0/588 |
| 76 | Q0 | 0.73 | 0/423 | 0.90 | 1/562 (0.2%) |
| 76 | q0 | 0.89 | 0/423 | 0.92 | 1/562 (0.2%) |
| 77 | Q1 | 0.70 | 0/234 | 0.93 | 0/300 |
| 77 | q1 | 0.94 | 0/234 | 1.05 | 1/300 (0.3%) |
| 78 | Q2 | 1.00 | 1/860 (0.1%) | 0.99 | 2/1136 (0.2%) |
| 78 | q2 | 0.83 | 2/860 (0.2%) | 0.87 | 0/1136 |
| 79 | Q3 | 0.73 | 0/701 | 0.84 | 0/934 |
| 79 | q3 | 0.78 | 0/701 | 0.88 | 0/934 |
| 80 | e0 | 0.58 | 0/499 | 0.77 | 0/665 |
| 82 | p0 | 0.46 | 0/1092 | 0.62 | 0/1474 |
| All | All | 0.92 | 400/430070 (0.1%) | 1.33 | 5106/631356 (0.8%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 2 | S0 | 0 | 1 |
| 7 | s5 | 0 | 2 |
| 9 | S7 | 0 | 1 |
| 10 | S8 | 0 | 1 |
| 16 | C4 | 0 | 2 |
| 17 | c5 | 0 | 1 |
| 19 | C7 | 0 | 1 |
| 22 | d0 | 0 | 1 |
| 25 | D3 | 0 | 1 |
| 25 | d3 | 0 | 1 |
| 26 | d4 | 0 | 2 |
| 27 | D5 | 0 | 1 |
| 28 | D6 | 0 | 3 |
| 31 | d9 | 0 | 1 |
| 33 | E1 | 0 | 1 |
| 34 | SR | 0 | 2 |
| 39 | L2 | 0 | 1 |
| 39 | l2 | 0 | 2 |
| 40 | l3 | 0 | 2 |
| 41 | L4 | 0 | 2 |
| 41 | l4 | 0 | 1 |
| 42 | L5 | 0 | 1 |
| 42 | l5 | 0 | 2 |
| 43 | l6 | 0 | 1 |
| 44 | L7 | 0 | 1 |
| 44 | l7 | 0 | 2 |
| 51 | M5 | 0 | 1 |
| 52 | M6 | 0 | 2 |
| 52 | m6 | 0 | 1 |
| 53 | M7 | 0 | 1 |
| 53 | m7 | 0 | 1 |
| 57 | N1 | 0 | 1 |
| 59 | n3 | 0 | 1 |
| 62 | n6 | 0 | 1 |
| 63 | N7 | 0 | 1 |
| 63 | n7 | 0 | 1 |
| 64 | n8 | 0 | 2 |
| 65 | N9 | 0 | 1 |
| 65 | n9 | 0 | 3 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 67 | O1 | 0 | 1 |
| 67 | o1 | 0 | 1 |
| 72 | O6 | 0 | 1 |
| All | All | 0 | 57 |

The worst 5 of 400 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 34 | SR | 160 | GLU | C-N | -38.52 | 0.45 | 1.34 |
| 34 | SR | 161 | LYS | C-N | -29.42 | 0.66 | 1.34 |
| 78 | Q2 | 17 | CYS | CB-SG | 16.03 | 2.09 | 1.82 |
| 36 | 5 | 1152 | G | N9-C4 | -13.26 | 1.27 | 1.38 |
| 39 | l2 | 213 | GLY | C-O | 9.71 | 1.39 | 1.23 |

The worst 5 of 5106 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | SR | 161 | LYS | O-C-N | -48.73 | 44.74 | 122.70 |
| 34 | SR | 160 | GLU | C-N-CA | -43.07 | 14.02 | 121.70 |
| 34 | SR | 160 | GLU | CA-C-N | -38.98 | 31.43 | 117.20 |
| 36 | 5 | 1152 | G | N3-C4-C5 | 26.73 | 141.96 | 128.60 |
| 36 | 5 | 1152 | G | N3-C4-N9 | -24.27 | 111.44 | 126.00 |

There are no chirality outliers.

5 of 57 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 16 | C4 | 123 | SER | Peptide |
| 16 | C4 | 124 | ASP | Peptide |
| 2 | S0 | 188 | LEU | Peptide |
| 9 | S7 | 131 | PHE | Peptide |
| 10 | S8 | 147 | ALA | 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 X-ray entries followed by that with respect to entries of similar resolution.

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 | S0 | 204/251 (81%) | 154 (76%) | 27 (13%) | 23 (11%) | 0 | 1 |
| 2 | s0 | 204/251 (81%) | 161 (79%) | 27 (13%) | 16 (8%) | 1 | 2 |
| 3 | S1 | 212/254 (84%) | 152 (72%) | 31 (15%) | 29 (14%) | 0 | 0 |
| 3 | s1 | 214/254 (84%) | 179 (84%) | 23 (11%) | 12 (6%) | 2 | 5 |
| 4 | S2 | 215/253 (85%) | 181 (84%) | 25 (12%) | 9 (4%) | 3 | 9 |
| 4 | s2 | 215/253 (85%) | 187 (87%) | 16 (7%) | 12 (6%) | 2 | 5 |
| 5 | S3 | 221/239 (92%) | 198 (90%) | 14 (6%) | 9 (4%) | 3 | 9 |
| 5 | s3 | 221/239 (92%) | 193 (87%) | 15 (7%) | 13 (6%) | 1 | 4 |
| 6 | S4 | 258/260 (99%) | 219 (85%) | 27 (10%) | 12 (5%) | 2 | 7 |
| 6 | s4 | 258/260 (99%) | 223 (86%) | 23 (9%) | 12 (5%) | 2 | 7 |
| 7 | S5 | 204/224 (91%) | 162 (79%) | 21 (10%) | 21 (10%) | 0 | 1 |
| 7 | s5 | 204/224 (91%) | 164 (80%) | 23 (11%) | 17 (8%) | 1 | 2 |
| 8 | S6 | 224/236 (95%) | 195 (87%) | 21 (9%) | 8 (4%) | 3 | 11 |
| 8 | s6 | 216/236 (92%) | 194 (90%) | 14 (6%) | 8 (4%) | 3 | 11 |
| 9 | S7 | 182/189 (96%) | 143 (79%) | 21 (12%) | 18 (10%) | 0 | 1 |
| 9 | s7 | 184/189 (97%) | 148 (80%) | 22 (12%) | 14 (8%) | 1 | 2 |
| 10 | S8 | 184/200 (92%) | 159 (86%) | 12 (6%) | 13 (7%) | 1 | 2 |
| 10 | s8 | 184/200 (92%) | 164 (89%) | 11 (6%) | 9 (5%) | 2 | 7 |
| 11 | S9 | 183/196 (93%) | 159 (87%) | 15 (8%) | 9 (5%) | 2 | 7 |
| 11 | s9 | 183/196 (93%) | 148 (81%) | 23 (13%) | 12 (7%) | 1 | 3 |
| 12 | C0 | 94/105 (90%) | 74 (79%) | 14 (15%) | 6 (6%) | 1 | 3 |
| 12 | c0 | 92/105 (88%) | 63 (68%) | 16 (17%) | 13 (14%) | 0 | 0 |
| 13 | C1 | 153/155 (99%) | 125 (82%) | 18 (12%) | 10 (6%) | 1 | 3 |
| 13 | c1 | 144/155 (93%) | 117 (81%) | 18 (12%) | 9 (6%) | 1 | 3 |
| 14 | C2 | 122/142 (86%) | 70 (57%) | 26 (21%) | 26 (21%) | 0 | 0 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 14 | c2 | 122/142 (86%) | 71 (58%) | 29 (24%) | 22 (18%) | 0 | 0 |
| 15 | C3 | 148/150 (99%) | 132 (89%) | 13 (9%) | 3 (2%) | 7 | 24 |
| 15 | c3 | 148/150 (99%) | 123 (83%) | 16 (11%) | 9 (6%) | 1 | 4 |
| 16 | C4 | 125/136 (92%) | 97 (78%) | 16 (13%) | 12 (10%) | 0 | 1 |
| 16 | c4 | 126/136 (93%) | 101 (80%) | 15 (12%) | 10 (8%) | 1 | 2 |
| 17 | C5 | 122/141 (86%) | 95 (78%) | 16 (13%) | 11 (9%) | 1 | 1 |
| 17 | c5 | 133/141 (94%) | 97 (73%) | 16 (12%) | 20 (15%) | 0 | 0 |
| 18 | C6 | 139/142 (98%) | 121 (87%) | 13 (9%) | 5 (4%) | 3 | 11 |
| 18 | c6 | 140/142 (99%) | 121 (86%) | 11 (8%) | 8 (6%) | 1 | 5 |
| 19 | C7 | 116/136 (85%) | 87 (75%) | 22 (19%) | 7 (6%) | 1 | 4 |
| 19 | c7 | 113/136 (83%) | 96 (85%) | 11 (10%) | 6 (5%) | 2 | 6 |
| 20 | C8 | 143/145 (99%) | 121 (85%) | 11 (8%) | 11 (8%) | 1 | 2 |
| 20 | c8 | 143/145 (99%) | 115 (80%) | 21 (15%) | 7 (5%) | 2 | 7 |
| 21 | C9 | 141/143 (99%) | 122 (86%) | 14 (10%) | 5 (4%) | 3 | 12 |
| 21 | c9 | 141/143 (99%) | 122 (86%) | 14 (10%) | 5 (4%) | 3 | 12 |
| 22 | D0 | 105/120 (88%) | 88 (84%) | 15 (14%) | 2 (2%) | 8 | 26 |
| 22 | d0 | 108/120 (90%) | 85 (79%) | 15 (14%) | 8 (7%) | 1 | 2 |
| 23 | D1 | 85/87 (98%) | 69 (81%) | 10 (12%) | 6 (7%) | 1 | 2 |
| 23 | d1 | 85/87 (98%) | 75 (88%) | 5 (6%) | 5 (6%) | 1 | 4 |
| 24 | D2 | 127/129 (98%) | 113 (89%) | 13 (10%) | 1 (1%) | 19 | 49 |
| 24 | d2 | 127/129 (98%) | 116 (91%) | 10 (8%) | 1 (1%) | 19 | 49 |
| 25 | D3 | 142/144 (99%) | 117 (82%) | 14 (10%) | 11 (8%) | 1 | 2 |
| 25 | d3 | 142/144 (99%) | 131 (92%) | 10 (7%) | 1 (1%) | 22 | 53 |
| 26 | D4 | 132/134 (98%) | 110 (83%) | 14 (11%) | 8 (6%) | 1 | 4 |
| 26 | d4 | 132/134 (98%) | 106 (80%) | 15 (11%) | 11 (8%) | 1 | 2 |
| 27 | D5 | 68/107 (64%) | 51 (75%) | 9 (13%) | 8 (12%) | 0 | 1 |
| 27 | d5 | 67/107 (63%) | 48 (72%) | 13 (19%) | 6 (9%) | 1 | 1 |
| 28 | D6 | 95/97 (98%) | 69 (73%) | 12 (13%) | 14 (15%) | 0 | 0 |
| 28 | d6 | 95/97 (98%) | 73 (77%) | 14 (15%) | 8 (8%) | 1 | 2 |
| 29 | D7 | 79/81 (98%) | 62 (78%) | 12 (15%) | 5 (6%) | 1 | 3 |
| 29 | d7 | 79/81 (98%) | 60 (76%) | 10 (13%) | 9 (11%) | 0 | 1 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 30 | D8 | 61/66 (92%) | 51 (84%) | 7 (12%) | 3 (5%) | 2 | 7 |
| 30 | d8 | 61/66 (92%) | 46 (75%) | 10 (16%) | 5 (8%) | 1 | 2 |
| 31 | D9 | 51/55 (93%) | 41 (80%) | 7 (14%) | 3 (6%) | 1 | 4 |
| 31 | d9 | 51/55 (93%) | 42 (82%) | 5 (10%) | 4 (8%) | 1 | 2 |
| 32 | E0 | 58/60 (97%) | 45 (78%) | 12 (21%) | 1 (2%) | 9 | 29 |
| 33 | E1 | 69/76 (91%) | 36 (52%) | 14 (20%) | 19 (28%) | 0 | 0 |
| 33 | e1 | 74/76 (97%) | 38 (51%) | 16 (22%) | 20 (27%) | 0 | 0 |
| 34 | SR | 316/318 (99%) | 274 (87%) | 29 (9%) | 13 (4%) | 3 | 9 |
| 34 | sR | 316/318 (99%) | 268 (85%) | 40 (13%) | 8 (2%) | 5 | 19 |
| 35 | SM | 155/273 (57%) | 109 (70%) | 26 (17%) | 20 (13%) | 0 | 1 |
| 35 | sM | 98/273 (36%) | 61 (62%) | 24 (24%) | 13 (13%) | 0 | 0 |
| 39 | L2 | 250/253 (99%) | 226 (90%) | 20 (8%) | 4 (2%) | 9 | 31 |
| 39 | l2 | 250/253 (99%) | 214 (86%) | 27 (11%) | 9 (4%) | 3 | 11 |
| 40 | L3 | 384/386 (100%) | 340 (88%) | 31 (8%) | 13 (3%) | 3 | 13 |
| 40 | l3 | 384/386 (100%) | 350 (91%) | 25 (6%) | 9 (2%) | 6 | 21 |
| 41 | L4 | 359/361 (99%) | 315 (88%) | 23 (6%) | 21 (6%) | 1 | 4 |
| 41 | l4 | 359/361 (99%) | 308 (86%) | 38 (11%) | 13 (4%) | 3 | 11 |
| 42 | L5 | 294/296 (99%) | 253 (86%) | 23 (8%) | 18 (6%) | 1 | 4 |
| 42 | l5 | 292/296 (99%) | 262 (90%) | 21 (7%) | 9 (3%) | 4 | 14 |
| 43 | L6 | 152/175 (87%) | 141 (93%) | 8 (5%) | 3 (2%) | 7 | 24 |
| 43 | l6 | 153/175 (87%) | 132 (86%) | 17 (11%) | 4 (3%) | 5 | 18 |
| 44 | L7 | 220/243 (90%) | 205 (93%) | 6 (3%) | 9 (4%) | 3 | 9 |
| 44 | l7 | 221/243 (91%) | 203 (92%) | 15 (7%) | 3 (1%) | 11 | 34 |
| 45 | L8 | 231/255 (91%) | 193 (84%) | 30 (13%) | 8 (4%) | 3 | 12 |
| 45 | l8 | 229/255 (90%) | 184 (80%) | 25 (11%) | 20 (9%) | 1 | 1 |
| 46 | L9 | 189/191 (99%) | 170 (90%) | 14 (7%) | 5 (3%) | 5 | 18 |
| 46 | l9 | 189/191 (99%) | 173 (92%) | 10 (5%) | 6 (3%) | 4 | 13 |
| 47 | M0 | 207/220 (94%) | 185 (89%) | 17 (8%) | 5 (2%) | 6 | 20 |
| 47 | m0 | 209/220 (95%) | 181 (87%) | 20 (10%) | 8 (4%) | 3 | 10 |
| 48 | M1 | 167/173 (96%) | 133 (80%) | 20 (12%) | 14 (8%) | 1 | 2 |
| 48 | m1 | 167/173 (96%) | 146 (87%) | 11 (7%) | 10 (6%) | 1 | 4 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 49 | M3 | 191/198 (96%) | 164 (86%) | 19 (10%) | 8 (4%) | 3 | 9 |
| 49 | m3 | 192/198 (97%) | 164 (85%) | 17 (9%) | 11 (6%) | 1 | 5 |
| 50 | M4 | 134/137 (98%) | 118 (88%) | 11 (8%) | 5 (4%) | 3 | 11 |
| 50 | m4 | 135/137 (98%) | 127 (94%) | 6 (4%) | 2 (2%) | 10 | 33 |
| 51 | M5 | 201/203 (99%) | 188 (94%) | 7 (4%) | 6 (3%) | 4 | 15 |
| 51 | m5 | 201/203 (99%) | 180 (90%) | 14 (7%) | 7 (4%) | 3 | 12 |
| 52 | M6 | 195/198 (98%) | 185 (95%) | 6 (3%) | 4 (2%) | 7 | 23 |
| 52 | m6 | 195/198 (98%) | 185 (95%) | 8 (4%) | 2 (1%) | 15 | 44 |
| 53 | M7 | 181/183 (99%) | 159 (88%) | 16 (9%) | 6 (3%) | 4 | 13 |
| 53 | m7 | 153/183 (84%) | 140 (92%) | 10 (6%) | 3 (2%) | 7 | 24 |
| 54 | M8 | 183/185 (99%) | 169 (92%) | 10 (6%) | 4 (2%) | 6 | 22 |
| 54 | m8 | 183/185 (99%) | 165 (90%) | 11 (6%) | 7 (4%) | 3 | 10 |
| 55 | M9 | 186/188 (99%) | 173 (93%) | 12 (6%) | 1 (0%) | 29 | 61 |
| 55 | m9 | 186/188 (99%) | 175 (94%) | 8 (4%) | 3 (2%) | 9 | 31 |
| 56 | N0 | 170/172 (99%) | 157 (92%) | 11 (6%) | 2 (1%) | 13 | 39 |
| 56 | n0 | 170/172 (99%) | 158 (93%) | 9 (5%) | 3 (2%) | 8 | 28 |
| 57 | N1 | 157/159 (99%) | 138 (88%) | 14 (9%) | 5 (3%) | 4 | 13 |
| 57 | n1 | 157/159 (99%) | 143 (91%) | 10 (6%) | 4 (2%) | 5 | 19 |
| 58 | N2 | 98/120 (82%) | 79 (81%) | 15 (15%) | 4 (4%) | 3 | 9 |
| 58 | n2 | 96/120 (80%) | 84 (88%) | 9 (9%) | 3 (3%) | 4 | 14 |
| 59 | N3 | 134/136 (98%) | 126 (94%) | 7 (5%) | 1 (1%) | 22 | 53 |
| 59 | n3 | 134/136 (98%) | 125 (93%) | 8 (6%) | 1 (1%) | 22 | 53 |
| 60 | N4 | 96/155 (62%) | 77 (80%) | 14 (15%) | 5 (5%) | 2 | 6 |
| 60 | n4 | 133/155 (86%) | 113 (85%) | 12 (9%) | 8 (6%) | 1 | 4 |
| 61 | N5 | 119/141 (84%) | 110 (92%) | 8 (7%) | 1 (1%) | 19 | 49 |
| 61 | n5 | 118/141 (84%) | 100 (85%) | 13 (11%) | 5 (4%) | 3 | 9 |
| 62 | N6 | 124/126 (98%) | 114 (92%) | 6 (5%) | 4 (3%) | 4 | 13 |
| 62 | n6 | 124/126 (98%) | 113 (91%) | 6 (5%) | 5 (4%) | 3 | 9 |
| 63 | N7 | 133/135 (98%) | 111 (84%) | 12 (9%) | 10 (8%) | 1 | 2 |
| 63 | n7 | 133/135 (98%) | 111 (84%) | 14 (10%) | 8 (6%) | 1 | 4 |
| 64 | N8 | 146/148 (99%) | 122 (84%) | 16 (11%) | 8 (6%) | 2 | 5 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 64 | n8 | 146/148 (99%) | 126 (86%) | 16 (11%) | 4 (3%) | 5 | 17 |
| 65 | N9 | 56/58 (97%) | 49 (88%) | 5 (9%) | 2 (4%) | 3 | 11 |
| 65 | n9 | 56/58 (97%) | 43 (77%) | 9 (16%) | 4 (7%) | 1 | 2 |
| 66 | O0 | 95/104 (91%) | 87 (92%) | 6 (6%) | 2 (2%) | 7 | 23 |
| 66 | o0 | 98/104 (94%) | 89 (91%) | 7 (7%) | 2 (2%) | 7 | 24 |
| 67 | O1 | 107/112 (96%) | 95 (89%) | 7 (6%) | 5 (5%) | 2 | 7 |
| 67 | o1 | 107/112 (96%) | 98 (92%) | 5 (5%) | 4 (4%) | 3 | 11 |
| 68 | O2 | 125/129 (97%) | 116 (93%) | 8 (6%) | 1 (1%) | 19 | 49 |
| 68 | o2 | 125/129 (97%) | 111 (89%) | 11 (9%) | 3 (2%) | 6 | 20 |
| 69 | O3 | 104/106 (98%) | 101 (97%) | 2 (2%) | 1 (1%) | 15 | 44 |
| 69 | o3 | 104/106 (98%) | 92 (88%) | 7 (7%) | 5 (5%) | 2 | 7 |
| 70 | O4 | 110/119 (92%) | 103 (94%) | 4 (4%) | 3 (3%) | 5 | 17 |
| 70 | o4 | 110/119 (92%) | 100 (91%) | 8 (7%) | 2 (2%) | 8 | 28 |
| 71 | O5 | 117/119 (98%) | 108 (92%) | 5 (4%) | 4 (3%) | 3 | 13 |
| 71 | o5 | 117/119 (98%) | 106 (91%) | 9 (8%) | 2 (2%) | 9 | 29 |
| 72 | O6 | 97/99 (98%) | 78 (80%) | 11 (11%) | 8 (8%) | 1 | 2 |
| 72 | o6 | 97/99 (98%) | 81 (84%) | 9 (9%) | 7 (7%) | 1 | 2 |
| 73 | O7 | 85/87 (98%) | 76 (89%) | 6 (7%) | 3 (4%) | 3 | 12 |
| 73 | o7 | 85/87 (98%) | 72 (85%) | 10 (12%) | 3 (4%) | 3 | 12 |
| 74 | O8 | 75/77 (97%) | 62 (83%) | 10 (13%) | 3 (4%) | 3 | 9 |
| 74 | o8 | 75/77 (97%) | 66 (88%) | 6 (8%) | 3 (4%) | 3 | 9 |
| 75 | O9 | 48/50 (96%) | 44 (92%) | 4 (8%) | 0 | 100 | 100 |
| 75 | o9 | 48/50 (96%) | 44 (92%) | 3 (6%) | 1 (2%) | 7 | 23 |
| 76 | Q0 | 50/52 (96%) | 48 (96%) | 0 | 2 (4%) | 3 | 9 |
| 76 | q0 | 50/52 (96%) | 49 (98%) | 0 | 1 (2%) | 7 | 24 |
| 77 | Q1 | 23/25 (92%) | 22 (96%) | 1 (4%) | 0 | 100 | 100 |
| 77 | q1 | 23/25 (92%) | 23 (100%) | 0 | 0 | 100 | 100 |
| 78 | Q2 | 103/105 (98%) | 90 (87%) | 10 (10%) | 3 (3%) | 4 | 15 |
| 78 | q2 | 103/105 (98%) | 92 (89%) | 8 (8%) | 3 (3%) | 4 | 15 |
| 79 | Q3 | 89/91 (98%) | 80 (90%) | 7 (8%) | 2 (2%) | 6 | 22 |
| 79 | q3 | 89/91 (98%) | 80 (90%) | 8 (9%) | 1 (1%) | 14 | 41 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 80 | e0 | 60/62 (97%) | 47 (78%) | 9 (15%) | 4 (7%) | 1 3 |
| 82 | p0 | 139/311 (45%) | 117 (84%) | 19 (14%) | 3 (2%) | 6 22 |
| All | All | 22333/24141 (92%) | 19119 (86%) | 2092 (9%) | 1122 (5%) | 2 6 |

5 of 1122 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | S0 | 39 | ASN |
| 2 | S0 | 66 | ALA |
| 2 | S0 | 103 | THR |
| 2 | S0 | 158 | VAL |
| 2 | S0 | 163 | 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 X-ray entries followed by that with respect to entries of similar resolution.

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 | S0 | 164/209 (78%) | 134 (82%) | 30 (18%) | 1 5 |
| 2 | s0 | 165/209 (79%) | 131 (79%) | 34 (21%) | 1 3 |
| 3 | S1 | 191/223 (86%) | 162 (85%) | 29 (15%) | 3 8 |
| 3 | s1 | 192/223 (86%) | 162 (84%) | 30 (16%) | 2 8 |
| 4 | S2 | 176/204 (86%) | 137 (78%) | 39 (22%) | 1 2 |
| 4 | s2 | 176/204 (86%) | 139 (79%) | 37 (21%) | 1 3 |
| 5 | S3 | 182/194 (94%) | 149 (82%) | 33 (18%) | 1 5 |
| 5 | s3 | 182/194 (94%) | 149 (82%) | 33 (18%) | 1 5 |
| 6 | S4 | 221/221 (100%) | 182 (82%) | 39 (18%) | 2 5 |
| 6 | s4 | 221/221 (100%) | 187 (85%) | 34 (15%) | 2 8 |
| 7 | S5 | 173/190 (91%) | 140 (81%) | 33 (19%) | 1 4 |
| 7 | s5 | 173/190 (91%) | 138 (80%) | 35 (20%) | 1 4 |
| 8 | S6 | 188/201 (94%) | 155 (82%) | 33 (18%) | 2 5 |
| 8 | s6 | 187/201 (93%) | 152 (81%) | 35 (19%) | 1 5 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 9 | S7 | 165/169 (98%) | 140 (85%) | 25 (15%) | 3 | 8 |
| 9 | s7 | 165/169 (98%) | 134 (81%) | 31 (19%) | 1 | 5 |
| 10 | S8 | 150/161 (93%) | 128 (85%) | 22 (15%) | 3 | 9 |
| 10 | s8 | 150/161 (93%) | 129 (86%) | 21 (14%) | 3 | 11 |
| 11 | S9 | 158/165 (96%) | 123 (78%) | 35 (22%) | 1 | 2 |
| 11 | s9 | 158/165 (96%) | 128 (81%) | 30 (19%) | 1 | 4 |
| 12 | C0 | 77/98 (79%) | 58 (75%) | 19 (25%) | 0 | 2 |
| 12 | c0 | 73/98 (74%) | 61 (84%) | 12 (16%) | 2 | 7 |
| 13 | C1 | 129/136 (95%) | 104 (81%) | 25 (19%) | 1 | 4 |
| 13 | c1 | 129/136 (95%) | 107 (83%) | 22 (17%) | 2 | 6 |
| 14 | C2 | 88/118 (75%) | 68 (77%) | 20 (23%) | 1 | 2 |
| 14 | c2 | 88/118 (75%) | 65 (74%) | 23 (26%) | 0 | 1 |
| 15 | C3 | 127/127 (100%) | 101 (80%) | 26 (20%) | 1 | 3 |
| 15 | c3 | 127/127 (100%) | 105 (83%) | 22 (17%) | 2 | 6 |
| 16 | C4 | 81/104 (78%) | 61 (75%) | 20 (25%) | 0 | 2 |
| 16 | c4 | 97/104 (93%) | 75 (77%) | 22 (23%) | 1 | 2 |
| 17 | C5 | 101/117 (86%) | 86 (85%) | 15 (15%) | 3 | 9 |
| 17 | c5 | 103/117 (88%) | 83 (81%) | 20 (19%) | 1 | 4 |
| 18 | C6 | 117/118 (99%) | 94 (80%) | 23 (20%) | 1 | 4 |
| 18 | c6 | 118/118 (100%) | 98 (83%) | 20 (17%) | 2 | 6 |
| 19 | C7 | 94/124 (76%) | 70 (74%) | 24 (26%) | 0 | 1 |
| 19 | c7 | 92/124 (74%) | 76 (83%) | 16 (17%) | 2 | 6 |
| 20 | C8 | 128/128 (100%) | 102 (80%) | 26 (20%) | 1 | 4 |
| 20 | c8 | 128/128 (100%) | 101 (79%) | 27 (21%) | 1 | 3 |
| 21 | C9 | 115/115 (100%) | 93 (81%) | 22 (19%) | 1 | 4 |
| 21 | c9 | 115/115 (100%) | 95 (83%) | 20 (17%) | 2 | 6 |
| 22 | D0 | 100/113 (88%) | 74 (74%) | 26 (26%) | 0 | 1 |
| 22 | d0 | 103/113 (91%) | 80 (78%) | 23 (22%) | 1 | 2 |
| 23 | D1 | 74/74 (100%) | 60 (81%) | 14 (19%) | 1 | 5 |
| 23 | d1 | 74/74 (100%) | 57 (77%) | 17 (23%) | 1 | 2 |
| 24 | D2 | 110/110 (100%) | 94 (86%) | 16 (14%) | 3 | 9 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 24 | d2 | 110/110 (100%) | 96 (87%) | 14 (13%) | 4 | 14 |
| 25 | D3 | 119/119 (100%) | 97 (82%) | 22 (18%) | 1 | 5 |
| 25 | d3 | 119/119 (100%) | 104 (87%) | 15 (13%) | 4 | 14 |
| 26 | D4 | 112/112 (100%) | 93 (83%) | 19 (17%) | 2 | 6 |
| 26 | d4 | 112/112 (100%) | 99 (88%) | 13 (12%) | 5 | 17 |
| 27 | D5 | 61/88 (69%) | 43 (70%) | 18 (30%) | 0 | 1 |
| 27 | d5 | 61/88 (69%) | 54 (88%) | 7 (12%) | 5 | 17 |
| 28 | D6 | 83/83 (100%) | 66 (80%) | 17 (20%) | 1 | 3 |
| 28 | d6 | 83/83 (100%) | 69 (83%) | 14 (17%) | 2 | 6 |
| 29 | D7 | 70/70 (100%) | 57 (81%) | 13 (19%) | 1 | 5 |
| 29 | d7 | 70/70 (100%) | 59 (84%) | 11 (16%) | 2 | 8 |
| 30 | D8 | 56/59 (95%) | 44 (79%) | 12 (21%) | 1 | 3 |
| 30 | d8 | 56/59 (95%) | 48 (86%) | 8 (14%) | 3 | 10 |
| 31 | D9 | 47/48 (98%) | 38 (81%) | 9 (19%) | 1 | 4 |
| 31 | d9 | 47/48 (98%) | 39 (83%) | 8 (17%) | 2 | 6 |
| 32 | E0 | 51/51 (100%) | 41 (80%) | 10 (20%) | 1 | 4 |
| 33 | E1 | 62/66 (94%) | 47 (76%) | 15 (24%) | 0 | 2 |
| 33 | e1 | 66/66 (100%) | 48 (73%) | 18 (27%) | 0 | 1 |
| 34 | SR | 260/261 (100%) | 237 (91%) | 23 (9%) | 10 | 29 |
| 34 | sR | 260/261 (100%) | 232 (89%) | 28 (11%) | 6 | 19 |
| 35 | SM | 97/228 (42%) | 79 (81%) | 18 (19%) | 1 | 5 |
| 35 | sM | 54/228 (24%) | 47 (87%) | 7 (13%) | 4 | 13 |
| 39 | L2 | 193/195 (99%) | 157 (81%) | 36 (19%) | 1 | 5 |
| 39 | l2 | 192/195 (98%) | 155 (81%) | 37 (19%) | 1 | 4 |
| 40 | L3 | 321/322 (100%) | 258 (80%) | 63 (20%) | 1 | 4 |
| 40 | l3 | 320/322 (99%) | 255 (80%) | 65 (20%) | 1 | 4 |
| 41 | L4 | 288/288 (100%) | 239 (83%) | 49 (17%) | 2 | 6 |
| 41 | l4 | 288/288 (100%) | 235 (82%) | 53 (18%) | 1 | 5 |
| 42 | L5 | 244/244 (100%) | 194 (80%) | 50 (20%) | 1 | 3 |
| 42 | l5 | 243/244 (100%) | 192 (79%) | 51 (21%) | 1 | 3 |
| 43 | L6 | 134/152 (88%) | 115 (86%) | 19 (14%) | 3 | 10 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 43 | l6 | 135/152 (89%) | 111 (82%) | 24 (18%) | 2 5 |
| 44 | L7 | 186/204 (91%) | 162 (87%) | 24 (13%) | 4 13 |
| 44 | l7 | 187/204 (92%) | 159 (85%) | 28 (15%) | 3 9 |
| 45 | L8 | 187/207 (90%) | 154 (82%) | 33 (18%) | 2 5 |
| 45 | l8 | 177/207 (86%) | 143 (81%) | 34 (19%) | 1 4 |
| 46 | L9 | 171/171 (100%) | 139 (81%) | 32 (19%) | 1 5 |
| 46 | l9 | 171/171 (100%) | 137 (80%) | 34 (20%) | 1 4 |
| 47 | M0 | 177/186 (95%) | 144 (81%) | 33 (19%) | 1 5 |
| 47 | m0 | 179/186 (96%) | 142 (79%) | 37 (21%) | 1 3 |
| 48 | M1 | 147/150 (98%) | 119 (81%) | 28 (19%) | 1 4 |
| 48 | m1 | 147/150 (98%) | 125 (85%) | 22 (15%) | 3 9 |
| 49 | M3 | 154/158 (98%) | 126 (82%) | 28 (18%) | 1 5 |
| 49 | m3 | 154/158 (98%) | 130 (84%) | 24 (16%) | 2 8 |
| 50 | M4 | 107/108 (99%) | 86 (80%) | 21 (20%) | 1 4 |
| 50 | m4 | 108/108 (100%) | 90 (83%) | 18 (17%) | 2 6 |
| 51 | M5 | 175/175 (100%) | 146 (83%) | 29 (17%) | 2 7 |
| 51 | m5 | 175/175 (100%) | 148 (85%) | 27 (15%) | 2 8 |
| 52 | M6 | 160/161 (99%) | 137 (86%) | 23 (14%) | 3 10 |
| 52 | m6 | 160/161 (99%) | 132 (82%) | 28 (18%) | 2 6 |
| 53 | M7 | 140/145 (97%) | 113 (81%) | 27 (19%) | 1 4 |
| 53 | m7 | 125/145 (86%) | 108 (86%) | 17 (14%) | 3 11 |
| 54 | M8 | 150/150 (100%) | 125 (83%) | 25 (17%) | 2 6 |
| 54 | m8 | 150/150 (100%) | 122 (81%) | 28 (19%) | 1 5 |
| 55 | M9 | 153/153 (100%) | 133 (87%) | 20 (13%) | 4 12 |
| 55 | m9 | 153/153 (100%) | 119 (78%) | 34 (22%) | 1 2 |
| 56 | N0 | 156/156 (100%) | 128 (82%) | 28 (18%) | 2 5 |
| 56 | n0 | 156/156 (100%) | 132 (85%) | 24 (15%) | 2 8 |
| 57 | N1 | 136/136 (100%) | 108 (79%) | 28 (21%) | 1 3 |
| 57 | n1 | 136/136 (100%) | 116 (85%) | 20 (15%) | 3 9 |
| 58 | N2 | 87/106 (82%) | 76 (87%) | 11 (13%) | 4 14 |
| 58 | n2 | 85/106 (80%) | 73 (86%) | 12 (14%) | 3 10 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 59 | N3 | 104/104 (100%) | 90 (86%) | 14 (14%) | 4 | 11 |
| 59 | n3 | 104/104 (100%) | 95 (91%) | 9 (9%) | 10 | 30 |
| 60 | N4 | 57/129 (44%) | 52 (91%) | 5 (9%) | 10 | 29 |
| 60 | n4 | 100/129 (78%) | 88 (88%) | 12 (12%) | 5 | 15 |
| 61 | N5 | 104/117 (89%) | 79 (76%) | 25 (24%) | 0 | 2 |
| 61 | n5 | 104/117 (89%) | 80 (77%) | 24 (23%) | 1 | 2 |
| 62 | N6 | 109/109 (100%) | 88 (81%) | 21 (19%) | 1 | 4 |
| 62 | n6 | 109/109 (100%) | 84 (77%) | 25 (23%) | 1 | 2 |
| 63 | N7 | 115/115 (100%) | 91 (79%) | 24 (21%) | 1 | 3 |
| 63 | n7 | 115/115 (100%) | 92 (80%) | 23 (20%) | 1 | 4 |
| 64 | N8 | 118/118 (100%) | 97 (82%) | 21 (18%) | 2 | 5 |
| 64 | n8 | 118/118 (100%) | 95 (80%) | 23 (20%) | 1 | 4 |
| 65 | N9 | 46/46 (100%) | 38 (83%) | 8 (17%) | 2 | 6 |
| 65 | n9 | 46/46 (100%) | 35 (76%) | 11 (24%) | 0 | 2 |
| 66 | O0 | 81/87 (93%) | 66 (82%) | 15 (18%) | 1 | 5 |
| 66 | o0 | 84/87 (97%) | 68 (81%) | 16 (19%) | 1 | 4 |
| 67 | O1 | 92/96 (96%) | 72 (78%) | 20 (22%) | 1 | 3 |
| 67 | o1 | 94/96 (98%) | 77 (82%) | 17 (18%) | 1 | 5 |
| 68 | O2 | 109/110 (99%) | 94 (86%) | 15 (14%) | 3 | 11 |
| 68 | o2 | 109/110 (99%) | 92 (84%) | 17 (16%) | 2 | 8 |
| 69 | O3 | 90/90 (100%) | 76 (84%) | 14 (16%) | 2 | 8 |
| 69 | o3 | 90/90 (100%) | 82 (91%) | 8 (9%) | 9 | 28 |
| 70 | O4 | 95/101 (94%) | 78 (82%) | 17 (18%) | 2 | 5 |
| 70 | o4 | 95/101 (94%) | 81 (85%) | 14 (15%) | 3 | 9 |
| 71 | O5 | 104/104 (100%) | 83 (80%) | 21 (20%) | 1 | 4 |
| 71 | o5 | 103/104 (99%) | 76 (74%) | 27 (26%) | 0 | 1 |
| 72 | O6 | 81/81 (100%) | 60 (74%) | 21 (26%) | 0 | 1 |
| 72 | o6 | 80/81 (99%) | 52 (65%) | 28 (35%) | 0 | 0 |
| 73 | O7 | 70/70 (100%) | 58 (83%) | 12 (17%) | 2 | 6 |
| 73 | o7 | 70/70 (100%) | 59 (84%) | 11 (16%) | 2 | 8 |
| 74 | O8 | 68/68 (100%) | 55 (81%) | 13 (19%) | 1 | 4 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 74 | o8 | 67/68 (98%) | 55 (82%) | 12 (18%) | 2 5 |
| 75 | O9 | 45/45 (100%) | 36 (80%) | 9 (20%) | 1 4 |
| 75 | o9 | 45/45 (100%) | 35 (78%) | 10 (22%) | 1 2 |
| 76 | Q0 | 47/47 (100%) | 40 (85%) | 7 (15%) | 3 9 |
| 76 | q0 | 47/47 (100%) | 40 (85%) | 7 (15%) | 3 9 |
| 77 | Q1 | 23/23 (100%) | 15 (65%) | 8 (35%) | 0 0 |
| 77 | q1 | 23/23 (100%) | 14 (61%) | 9 (39%) | 0 0 |
| 78 | Q2 | 90/90 (100%) | 76 (84%) | 14 (16%) | 2 8 |
| 78 | q2 | 90/90 (100%) | 73 (81%) | 17 (19%) | 1 5 |
| 79 | Q3 | 71/71 (100%) | 61 (86%) | 10 (14%) | 3 10 |
| 79 | q3 | 71/71 (100%) | 58 (82%) | 13 (18%) | 1 5 |
| 80 | e0 | 53/53 (100%) | 41 (77%) | 12 (23%) | 1 2 |
| 82 | p0 | 105/253 (42%) | 84 (80%) | 21 (20%) | 1 4 |
| All | All | 18729/20239 (92%) | 15348 (82%) | 3381 (18%) | 1 5 |

5 of 3381 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | s4 | 187 | ARG |
| 26 | d4 | 62 | THR |
| 68 | o2 | 73 | THR |
| 8 | s6 | 112 | VAL |
| 6 | s4 | 180 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 69 | O3 | 42 | GLN |
| 15 | c3 | 62 | GLN |
| 2 | s0 | 140 | ASN |
| 12 | c0 | 29 | GLN |
| 24 | d2 | 56 | HIS |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | 2 | 1747/1800 (97%) | 449 (25%) | 63 (3%) |
| 1 | 6 | 1794/1800 (99%) | 430 (23%) | 59 (3%) |
| 36 | 1 | 3145/3396 (92%) | 609 (19%) | 99 (3%) |
| 36 | 5 | 3145/3396 (92%) | 613 (19%) | 101 (3%) |
| 37 | 3 | 120/121 (99%) | 17 (14%) | 2 (1%) |
| 37 | 7 | 120/121 (99%) | 15 (12%) | 1 (0%) |
| 38 | 4 | 157/158 (99%) | 35 (22%) | 3 (1%) |
| 38 | 8 | 157/158 (99%) | 37 (23%) | 2 (1%) |
| All | All | 10385/10950 (94%) | 2205 (21%) | 330 (3%) |

5 of 2205 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2 | 2 | A |
| 1 | 2 | 4 | C |
| 1 | 2 | 17 | C |
| 1 | 2 | 25 | C |
| 1 | 2 | 26 | A |

5 of 330 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 36 | 5 | 217 | U |
| 36 | 5 | 2255 | A |
| 36 | 5 | 647 | A |
| 36 | 5 | 1307 | G |
| 36 | 5 | 2585 | G |

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 2559 ligands modelled in this entry, 1424 are monoatomic - leaving 1135 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 | $\#\|Z\| > 2$ |
| 86 | OHX | 5 | 4181 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4043 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2084 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2166 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4213 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4225 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4036 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4076 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2060 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 7 | 217 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4032 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 7 | 216 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3877 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2113 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2088 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | L6 | 202 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2149 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4012 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4205 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4122 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4196 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3963 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4116 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | L3 | 404 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | m1 | 203 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3894 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3980 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4116 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2042 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2064 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3947 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4067 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3980 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | C1 | 201 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3904 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2147 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4010 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 86 | OHX | 6 | 2068 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2197 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2130 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3947 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2048 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2056 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4103 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4189 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2156 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3934 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | l3 | 404 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2164 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2074 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2096 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2173 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2033 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2110 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2144 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4075 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2098 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4119 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4127 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4159 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4210 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4104 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | d9 | 102 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4090 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2180 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4038 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3956 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4052 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3919 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2142 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4038 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2132 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2025 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4237 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4153 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2095 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2046 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3981 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4089 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4155 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 86 | OHX | 1 | 3875 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4089 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4143 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2106 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 3 | 222 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3974 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2163 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2201 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3927 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4067 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3920 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3974 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4065 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4109 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4204 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2152 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2144 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2130 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2126 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2100 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4000 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4109 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3954 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2193 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4221 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4025 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4025 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2180 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2138 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4091 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2143 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4133 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | m0 | 302 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2133 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 7 | 220 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2057 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4100 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3987 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3997 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2188 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3905 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 4 | 236 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4159 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 86 | OHX | O2 | 201 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4188 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 7 | 227 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4179 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2162 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | l3 | 402 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4181 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 3 | 225 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4085 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2092 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3956 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4018 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | O7 | 103 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4248 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3902 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3912 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3979 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4118 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4008 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4114 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4005 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2163 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2081 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4207 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2082 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4156 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | s8 | 303 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4047 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4021 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4206 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2165 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2186 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2049 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2088 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2195 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3995 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4071 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4176 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4194 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2052 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4013 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3961 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4176 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 86 | OHX | 1 | 3958 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4065 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4098 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2127 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4062 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3934 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | c8 | 203 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4093 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3958 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2100 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | s9 | 201 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2047 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4098 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4231 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2077 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4041 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2127 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3919 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3891 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2171 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2050 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2086 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4141 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2097 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4092 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2070 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4096 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3932 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4020 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2132 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3941 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2091 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2107 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2075 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2068 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2119 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3982 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2185 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4149 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4154 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4208 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4039 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3890 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 86 | OHX | 1 | 4090 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3949 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2091 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 3 | 215 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3979 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4150 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | O3 | 202 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4094 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2136 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3907 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4150 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3964 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4047 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4169 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4140 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2129 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4071 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4239 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 8 | 219 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4110 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4140 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4035 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4199 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3971 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2050 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3869 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3888 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | c1 | 202 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2159 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | C8 | 201 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3889 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2054 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4205 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4187 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2093 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4117 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 3 | 218 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3892 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4148 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4192 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4187 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2104 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4246 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 86 | OHX | 8 | 215 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3906 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2026 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 3 | 226 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | m5 | 302 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2085 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2183 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3899 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4149 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2145 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4191 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4030 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3952 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2117 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4180 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4030 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2056 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3957 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4180 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2073 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4229 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 8 | 225 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2053 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3938 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 3 | 223 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3887 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4210 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4127 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3973 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4064 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2090 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2114 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4146 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3973 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4024 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4084 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3999 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4115 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 4 | 232 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3917 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4094 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2116 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4193 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 86 | OHX | 5 | 4147 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4032 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3971 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3993 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3924 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4004 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4081 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2038 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2179 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4171 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2085 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3967 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2080 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4019 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3911 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4049 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3975 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2151 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4081 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2040 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4019 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4052 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3893 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4011 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | m7 | 206 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3959 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3926 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4070 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3901 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3959 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4189 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2063 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2048 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4070 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4232 | 86 | 0,6,6 | - | - | - | | |
| 86 | OHX | 4 | 222 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4001 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2129 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4191 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | q2 | 502 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4108 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4123 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2200 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 86 | OHX | 5 | 3966 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4080 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2084 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2202 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3936 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2054 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3969 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3943 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4004 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4138 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4141 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2161 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4002 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2150 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4111 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | M6 | 202 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3910 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2156 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4115 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2169 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | m0 | 301 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4111 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3917 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3906 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2174 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 8 | 220 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4193 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4241 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4208 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4086 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3972 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | o7 | 502 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3993 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4211 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4185 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4218 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4086 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3972 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3914 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2079 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4183 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3978 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2115 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 86 | OHX | 5 | 4152 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2051 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3914 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3967 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4050 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4172 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2106 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4062 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2063 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2108 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3963 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2123 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4186 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2082 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2173 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2089 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 3 | 221 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3901 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4033 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2152 | - | 0,6,6 | - | - | - | | |
| 88 | 3H3 | 5 | 4251 | - | 33,34,34 | 0.97 | 2 (6%) | 34,45,45 | 1.42 | 4 (11%) |
| 86 | OHX | 1 | 3970 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4136 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4124 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4236 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | l5 | 306 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3970 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4226 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4142 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4080 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3896 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4027 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2133 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | s1 | 303 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3941 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2062 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4138 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4192 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4196 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2096 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4007 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3910 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2157 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 86 | OHX | 5 | 4108 | - | 0,6,6 | - | - | - | | |
| 88 | 3H3 | 1 | 4216 | - | 33,34,34 | 1.01 | 3 (9%) | 34,45,45 | 1.65 | 7 (20%) |
| 86 | OHX | 1 | 4177 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3962 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4213 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4002 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4161 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | l9 | 600 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2146 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4029 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4088 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2032 | 86 | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4177 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4034 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 4 | 226 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4161 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 3 | 220 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4029 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4211 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4096 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 7 | 219 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | m6 | 202 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 4 | 234 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3913 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2146 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4224 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4219 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3948 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4053 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4104 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4167 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3880 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4164 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3873 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4198 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3933 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2101 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2139 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2141 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2052 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2189 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2055 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3886 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 86 | OHX | 1 | 4048 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | sR | 401 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4097 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 4 | 225 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3955 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2161 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4201 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4183 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | s4 | 301 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4061 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4136 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4087 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 7 | 218 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3898 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4040 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4121 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2078 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4142 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4165 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4247 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | l4 | 402 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4001 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2095 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2071 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2111 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2037 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3997 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | Q2 | 503 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3962 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | D9 | 102 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2119 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3916 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3915 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3964 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2079 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | d4 | 201 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4151 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2043 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3916 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2160 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4023 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3897 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4216 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 86 | OHX | 5 | 4230 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4243 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4078 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4197 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4106 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4123 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2179 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4078 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3951 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3918 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2166 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4005 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4197 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4158 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 7 | 224 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2061 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4158 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | S8 | 302 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2049 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2051 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3928 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4058 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2105 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3907 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | O7 | 104 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2187 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4170 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4106 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3872 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4201 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4087 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4015 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2062 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3911 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3991 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4015 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4099 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3935 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3930 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2198 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 8 | 216 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4132 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2065 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 86 | OHX | 1 | 3868 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2120 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | C5 | 201 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4164 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2072 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4132 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2067 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2139 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2149 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4157 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2103 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4064 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2053 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2083 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4016 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4083 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2145 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4190 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4083 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3874 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4010 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2116 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4168 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3924 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 8 | 214 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2087 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3903 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3976 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2181 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3942 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 8 | 222 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3944 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | s1 | 302 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4113 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3942 | 86 | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3928 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4135 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2086 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4173 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2137 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4134 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4028 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4249 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 86 | OHX | 2 | 2111 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4134 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3885 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2135 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4118 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2109 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3925 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4155 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3871 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2102 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4021 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3935 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4222 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | C3 | 202 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4112 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 8 | 218 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3968 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4194 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2066 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4112 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2123 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4215 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3968 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4139 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2069 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2094 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 4 | 230 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4143 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4044 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4041 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4215 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3945 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4190 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2143 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2099 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3977 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4054 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3929 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3976 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4054 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2137 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4074 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3989 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 86 | OHX | 1 | 4000 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3921 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4113 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4130 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2121 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4168 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | M5 | 304 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3982 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2109 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2170 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3943 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4235 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4110 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2108 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4107 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | l5 | 304 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2107 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2128 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2118 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2167 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4186 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2115 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 4 | 223 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2162 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2168 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4160 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4011 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4223 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2150 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2055 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2089 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4073 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2125 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3988 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4036 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2067 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4160 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3913 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3926 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4244 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4077 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4165 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2101 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 86 | OHX | 5 | 4073 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3900 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2141 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4077 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3923 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4238 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | m4 | 202 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3922 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3931 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4139 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4045 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4055 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2029 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 3 | 216 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4131 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4003 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2098 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4045 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | l3 | 403 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2121 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2039 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4003 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4169 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3939 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4059 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2204 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 7 | 222 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2135 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | l4 | 403 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3881 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4163 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2177 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3977 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2058 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 4 | 227 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2169 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4069 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4163 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4023 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4085 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4069 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3925 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3921 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 86 | OHX | 1 | 4097 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4128 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3998 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3918 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4105 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2097 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4033 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2074 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3905 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2076 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4048 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2027 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3953 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3938 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2174 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4212 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4145 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3884 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2028 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3988 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3909 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3900 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4050 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3909 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2080 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4170 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2036 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4013 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2081 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4178 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2153 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3992 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 4 | 233 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2199 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2176 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4031 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2131 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4178 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4060 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4167 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3908 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2078 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2073 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 86 | OHX | 6 | 2192 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3908 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4042 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3936 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3876 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3960 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4042 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4217 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2171 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4088 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4082 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2071 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2072 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3998 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4242 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4058 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4017 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4035 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4044 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2041 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4156 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2076 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4179 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4072 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3931 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3965 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3996 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3915 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4017 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4008 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2102 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2154 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4121 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4154 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2134 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3994 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4120 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3933 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4072 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4145 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | l5 | 305 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4120 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2155 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 86 | OHX | 1 | 4099 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2124 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3986 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2158 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4153 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4162 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4063 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 4 | 224 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2196 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3930 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4184 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4175 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3975 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4049 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2140 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3955 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2158 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4199 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4147 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2110 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2065 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4122 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3987 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2120 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4129 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4102 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 8 | 223 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 8 | 226 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | n3 | 203 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4006 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4107 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4129 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3957 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4102 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 7 | 225 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4228 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 8 | 228 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2175 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2191 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | L3 | 403 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2181 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4240 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3937 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 86 | OHX | 6 | 2203 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4200 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2059 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3920 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4027 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2122 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2160 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3944 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4133 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3996 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4137 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4018 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3983 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4034 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4200 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3994 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3878 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4051 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4126 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4074 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2153 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 3 | 217 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2034 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4130 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3945 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | c3 | 201 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4166 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | M7 | 208 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2155 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2172 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3937 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4063 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2182 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4214 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3978 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2140 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4233 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3989 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | o4 | 203 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2077 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4100 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2045 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2142 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 86 | OHX | 1 | 4043 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3927 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4171 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4174 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2128 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2060 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3985 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4114 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2113 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4006 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 8 | 221 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2030 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3992 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4093 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 8 | 217 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2064 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4082 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2044 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2148 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4028 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4144 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3882 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3969 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3984 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4124 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4057 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3961 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4061 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | n9 | 3803 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4188 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2148 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4014 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3991 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4057 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4245 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2069 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3903 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2126 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4051 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4022 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | SR | 401 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4126 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3946 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 86 | OHX | 1 | 4146 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2170 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3904 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2070 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2112 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 4 | 231 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4173 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4037 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | m8 | 201 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | c5 | 201 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4250 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3932 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4037 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2118 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2057 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2061 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2075 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2157 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2175 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4162 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | M9 | 202 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4039 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | o2 | 201 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2094 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3952 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2092 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 3 | 219 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4182 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4166 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3922 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4055 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3939 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4182 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4046 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4198 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2105 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4046 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2190 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4148 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3951 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 4 | 228 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2122 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4157 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 86 | OHX | o3 | 203 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4068 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4214 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2151 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4103 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2047 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 8 | 229 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4014 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | M7 | 207 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3984 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4016 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4092 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2172 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4026 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4206 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4117 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2099 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4022 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2083 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4184 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4026 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4131 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2138 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | M0 | 303 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4209 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2168 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3946 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2035 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4007 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4220 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2117 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3950 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4068 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2125 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4009 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4209 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | N9 | 101 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4056 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3950 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3899 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4009 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2178 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4066 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 86 | OHX | 5 | 3965 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3966 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4152 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3912 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2114 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4020 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2134 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2087 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2112 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 7 | 221 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2194 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3983 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4202 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2165 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3948 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4053 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2066 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3902 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2147 | 86 | 0,6,6 | - | - | - | | |
| 86 | OHX | M5 | 303 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3954 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4060 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4202 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4227 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 8 | 224 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3883 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 7 | 223 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 7 | 226 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2136 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4105 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3986 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3990 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4135 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4031 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 3 | 224 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 8 | 227 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3870 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4059 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3999 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2176 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2164 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3995 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4040 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 86 | OHX | 1 | 4125 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2031 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | L4 | 404 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | O9 | 101 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3898 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4125 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4076 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2167 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2177 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3923 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4091 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4174 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3940 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4012 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2093 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2059 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4151 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4185 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3895 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4144 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2103 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4128 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2184 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4095 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3940 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3879 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3960 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4095 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4079 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4203 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4234 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4056 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4079 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2178 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2104 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4203 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2154 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3953 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4066 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4084 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3985 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2131 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4195 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 86 | OHX | 2 | 2024 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4137 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3949 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 4 | 235 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3981 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4204 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4101 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4024 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 3929 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4207 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 4 | 229 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4195 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2124 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4101 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 4175 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4212 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4075 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4119 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2058 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 2 | 2090 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 5 | 3990 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 6 | 2159 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | 1 | 4172 | - | 0,6,6 | - | - | - | | |

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 |
|---|---|---|---|---|---|---|---|
| 88 | 3H3 | 5 | 4251 | - | - | 7/39/51/51 | 0/1/2/2 |
| 88 | 3H3 | 1 | 4216 | - | - | 7/39/51/51 | 0/1/2/2 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 88 | 1 | 4216 | 3H3 | C3-C2 | 3.57 | 1.47 | 1.33 |
| 88 | 5 | 4251 | 3H3 | C14-C16 | 3.36 | 1.56 | 1.53 |
| 88 | 5 | 4251 | 3H3 | C15-C14 | -2.77 | 1.50 | 1.54 |
| 88 | 1 | 4216 | 3H3 | C15-C14 | -2.77 | 1.50 | 1.54 |
| 88 | 1 | 4216 | 3H3 | C14-C13 | 2.16 | 1.54 | 1.51 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 88 | 5 | 4251 | 3H3 | C15-C14-C16 | 4.81 | 116.50 | 109.19 |
| 88 | 1 | 4216 | 3H3 | C15-C14-C16 | 4.77 | 116.44 | 109.19 |
| 88 | 1 | 4216 | 3H3 | C1-C11-C12 | 4.38 | 122.64 | 113.89 |
| 88 | 5 | 4251 | 3H3 | C1-C11-C12 | 3.40 | 120.67 | 113.89 |
| 88 | 1 | 4216 | 3H3 | C-C1-C2 | -3.30 | 102.02 | 109.99 |

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

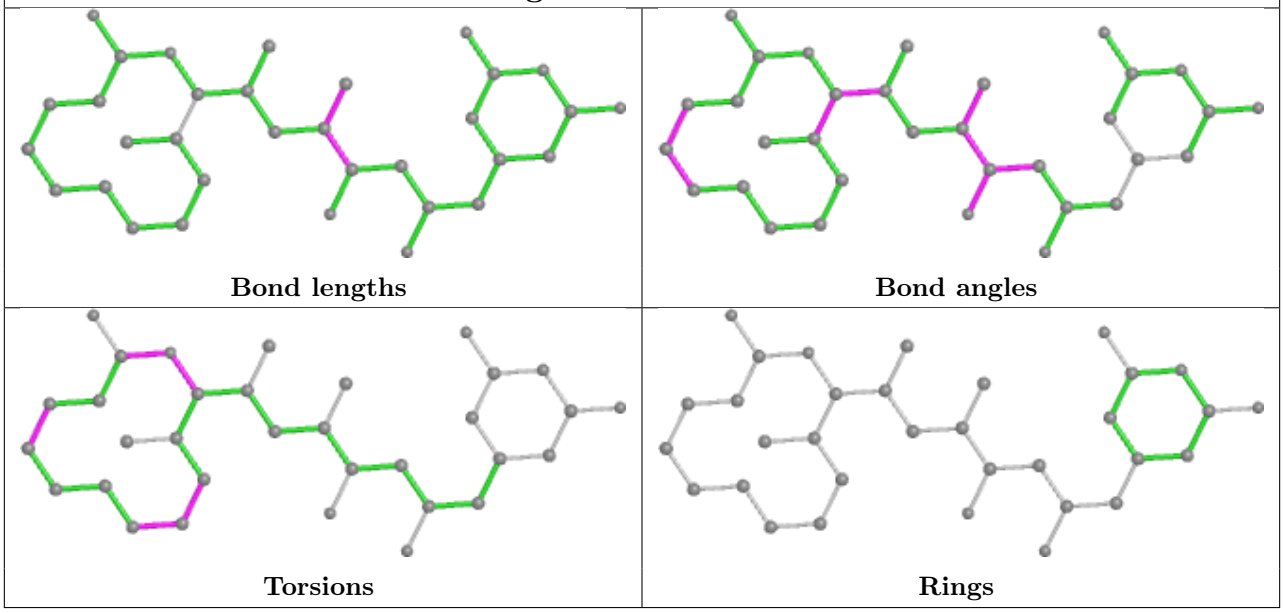
| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 88 | 1 | 4216 | 3H3 | C2-C1-C11-O1 |
| 88 | 1 | 4216 | 3H3 | C2-C1-C11-C12 |
| 88 | 1 | 4216 | 3H3 | C-C1-C11-O1 |
| 88 | 1 | 4216 | 3H3 | C-C1-C11-C12 |
| 88 | 1 | 4216 | 3H3 | C12-C13-C14-C16 |

There are no ring outliers.

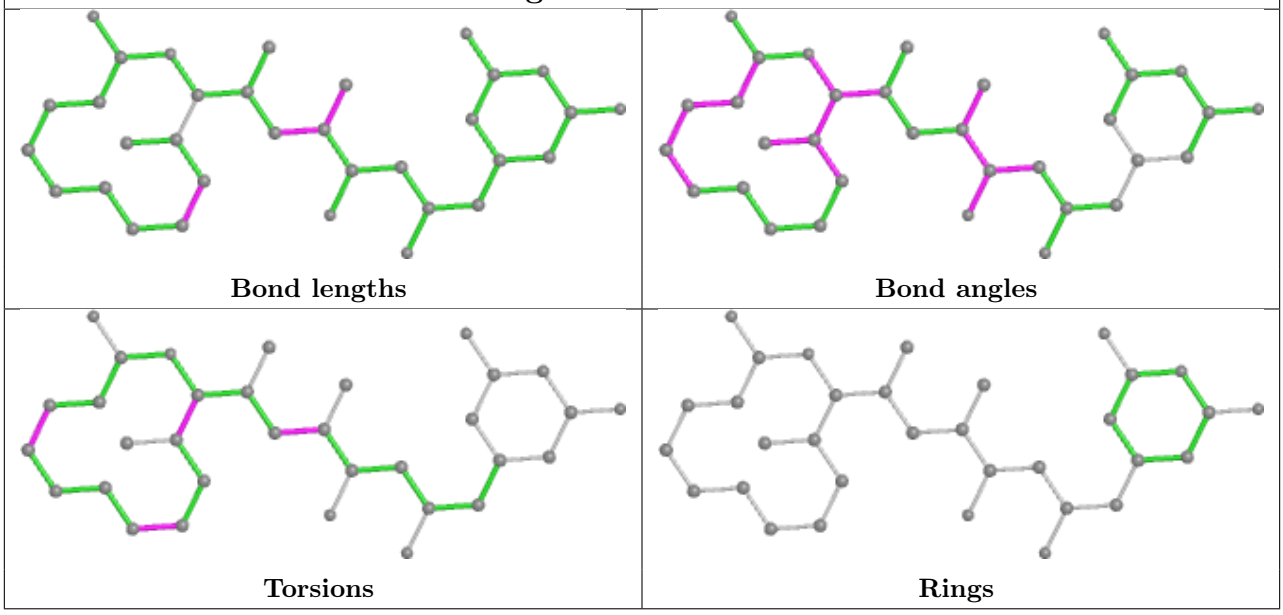
No monomer is involved in short contacts.

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 then 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.

**Ligand 3H3 5 4251**




**Ligand 3H3 1 4216**




## 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 |
|---|---|---|
| 34 | SR | 2 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | SR | 161:LYS | C | 162:ALA | N | 0.66 |
| 1 | SR | 160:GLU | C | 161:LYS | N | 0.45 |

# 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

## 6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

## 6.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

## 6.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

## 6.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.