



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 30, 2020 – 07:23 PM BST

PDB ID : 4U53
Title : Crystal structure of Deoxynivalenol bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-24
Resolution : 3.30 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), 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) : 2.13

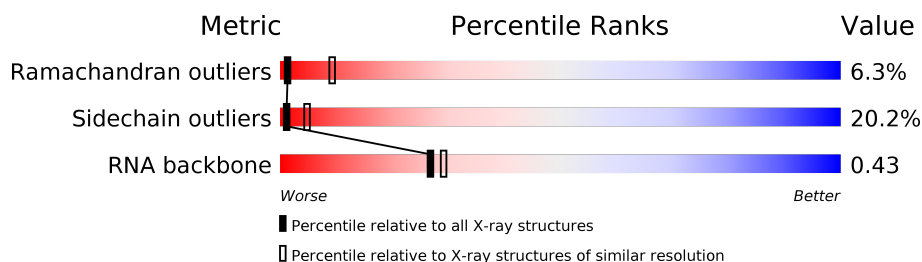
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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 | 1183 (3.34-3.26) |
| Sidechain outliers | 138945 | 1182 (3.34-3.26) |
| RNA backbone | 3102 | 1117 (3.70-2.90) |





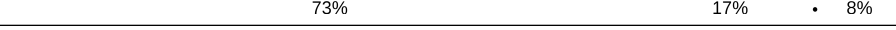
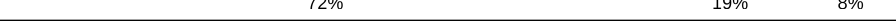

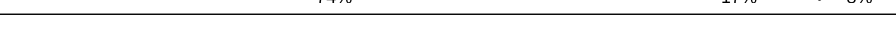
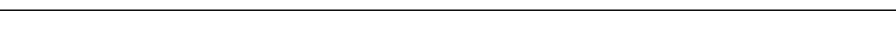
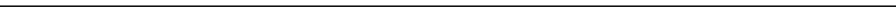















The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Note EDS failed to run properly.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 2 | 1800 | 63% 30% . . |
| 1 | 6 | 1800 | 62% 33% 5% |
| 2 | S0 | 251 | 62% 19% . 18% |
| 2 | s0 | 251 | 63% 17% . 18% |
| 3 | S1 | 254 | 60% 21% . 16% |
| 3 | s1 | 254 | 66% 18% . 15% |
| 4 | S2 | 253 | 65% 21% 14% |
| 4 | s2 | 253 | 62% 23% . 14% |















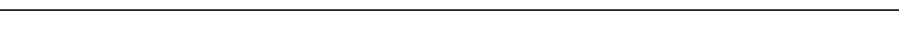




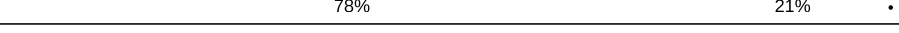
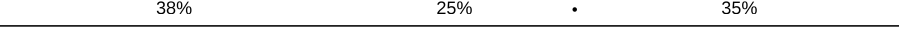




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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 5 | S3 | 239 |  |
| 5 | s3 | 239 |  |
| 6 | S4 | 260 |  |
| 6 | s4 | 260 |  |
| 7 | S5 | 224 |  |
| 7 | s5 | 224 |  |
| 8 | S6 | 236 |  |
| 8 | s6 | 236 |  |
| 9 | S7 | 189 |  |
| 9 | s7 | 189 |  |
| 10 | S8 | 200 |  |
| 10 | s8 | 200 |  |
| 11 | S9 | 196 |  |
| 11 | s9 | 196 |  |
| 12 | C0 | 105 |  |
| 12 | c0 | 105 |  |
| 13 | C1 | 155 |  |
| 13 | c1 | 155 |  |
| 14 | C2 | 142 |  |
| 14 | c2 | 142 |  |
| 15 | C3 | 150 |  |
| 15 | c3 | 150 |  |
| 16 | C4 | 136 |  |
| 16 | c4 | 136 |  |
| 17 | C5 | 141 |  |









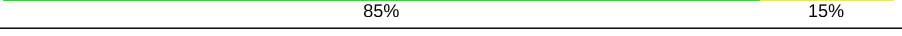
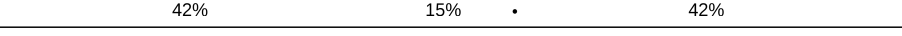

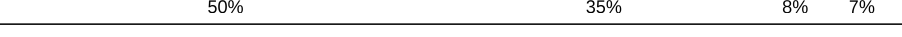

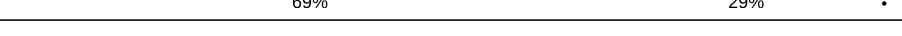


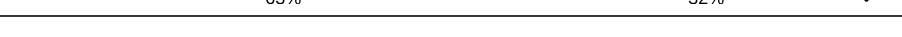

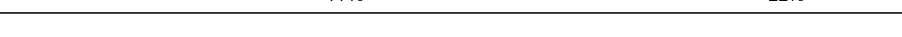
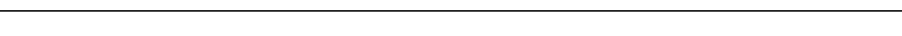

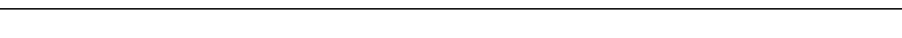
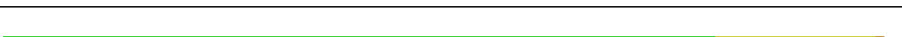


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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 17 | c5 | 141 |  |
| 18 | C6 | 142 |  |
| 18 | c6 | 142 |  |
| 19 | C7 | 136 |  |
| 19 | c7 | 136 |  |
| 20 | C8 | 145 |  |
| 20 | c8 | 145 |  |
| 21 | C9 | 143 |  |
| 21 | c9 | 143 |  |
| 22 | D0 | 120 |  |
| 22 | d0 | 120 |  |
| 23 | D1 | 87 |  |
| 23 | d1 | 87 |  |
| 24 | D2 | 129 |  |
| 24 | d2 | 129 |  |
| 25 | D3 | 144 |  |
| 25 | d3 | 144 |  |
| 26 | D4 | 134 |  |
| 26 | d4 | 134 |  |
| 27 | D5 | 107 |  |
| 27 | d5 | 107 |  |
| 28 | D6 | 97 |  |
| 28 | d6 | 97 |  |
| 29 | D7 | 81 |  |
| 29 | d7 | 81 |  |


























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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 30 | D8 | 66 |  |
| 30 | d8 | 66 |  |
| 31 | D9 | 55 |  |
| 31 | d9 | 55 |  |
| 32 | E0 | 60 |  |
| 33 | E1 | 76 |  |
| 33 | e1 | 76 |  |
| 34 | SR | 318 |  |
| 34 | sR | 318 |  |
| 35 | SM | 273 |  |
| 35 | sM | 273 |  |
| 36 | 1 | 3396 |  |
| 36 | 5 | 3396 |  |
| 37 | 3 | 121 |  |
| 37 | 7 | 121 |  |
| 38 | 4 | 158 |  |
| 38 | 8 | 158 |  |
| 39 | L2 | 253 |  |
| 39 | l2 | 253 |  |
| 40 | L3 | 386 |  |
| 40 | l3 | 386 |  |
| 41 | L4 | 361 |  |
| 41 | l4 | 361 |  |
| 42 | L5 | 296 |  |
| 42 | l5 | 296 |  |

















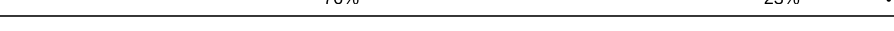

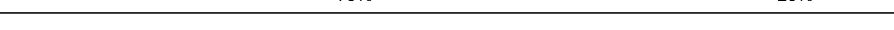
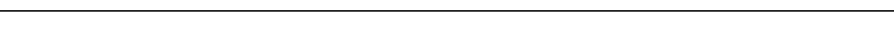
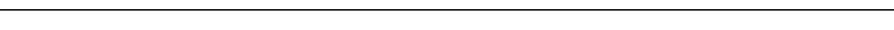
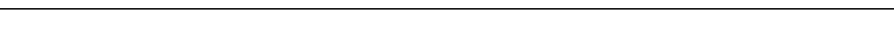
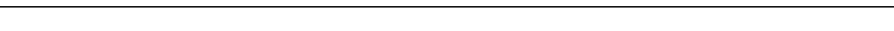
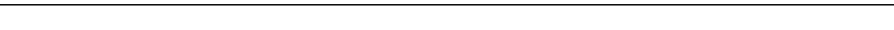

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 43 | L6 | 175 |  |
| 43 | l6 | 175 |  |
| 44 | L7 | 243 |  |
| 44 | l7 | 243 |  |
| 45 | L8 | 255 |  |
| 45 | l8 | 255 |  |
| 46 | L9 | 191 |  |
| 46 | l9 | 191 |  |
| 47 | M0 | 220 |  |
| 47 | m0 | 220 |  |
| 48 | M1 | 173 |  |
| 48 | m1 | 173 |  |
| 49 | M3 | 198 |  |
| 49 | m3 | 198 |  |
| 50 | M4 | 137 |  |
| 50 | m4 | 137 |  |
| 51 | M5 | 203 |  |
| 51 | m5 | 203 |  |
| 52 | M6 | 198 |  |
| 52 | m6 | 198 |  |
| 53 | M7 | 183 |  |
| 53 | m7 | 183 |  |
| 54 | M8 | 185 |  |
| 54 | m8 | 185 |  |
| 55 | M9 | 188 |  |











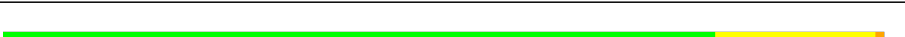


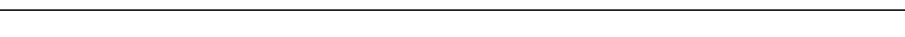











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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 55 | m9 | 188 |  |
| 56 | N0 | 172 |  |
| 56 | n0 | 172 |  |
| 57 | N1 | 159 |  |
| 57 | n1 | 159 |  |
| 58 | N2 | 120 |  |
| 58 | n2 | 120 |  |
| 59 | N3 | 136 |  |
| 59 | n3 | 136 |  |
| 60 | N4 | 155 |  |
| 60 | n4 | 155 |  |
| 61 | N5 | 141 |  |
| 61 | n5 | 141 |  |
| 62 | N6 | 126 |  |
| 62 | n6 | 126 |  |
| 63 | N7 | 135 |  |
| 63 | n7 | 135 |  |
| 64 | N8 | 148 |  |
| 64 | n8 | 148 |  |
| 65 | N9 | 58 |  |
| 65 | n9 | 58 |  |
| 66 | O0 | 104 |  |
| 66 | o0 | 104 |  |
| 67 | O1 | 112 |  |
| 67 | o1 | 112 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 68 | O2 | 129 |  |
| 68 | o2 | 129 |  |
| 69 | O3 | 106 |  |
| 69 | o3 | 106 |  |
| 70 | O4 | 119 |  |
| 70 | o4 | 119 |  |
| 71 | O5 | 119 |  |
| 71 | o5 | 119 |  |
| 72 | O6 | 99 |  |
| 72 | o6 | 99 |  |
| 73 | O7 | 87 |  |
| 73 | o7 | 87 |  |
| 74 | O8 | 77 |  |
| 74 | o8 | 77 |  |
| 75 | O9 | 50 |  |
| 75 | o9 | 50 |  |
| 76 | Q0 | 52 |  |
| 76 | q0 | 52 |  |
| 77 | Q1 | 25 |  |
| 77 | q1 | 25 |  |
| 78 | Q2 | 105 |  |
| 78 | q2 | 105 |  |
| 79 | Q3 | 91 |  |
| 79 | q3 | 91 |  |
| 80 | e0 | 62 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 81 | m2 | 160 | <div><div></div><div>93%</div><div>• 6%</div></div> |
| 82 | p0 | 311 | <div><div></div><div>38%</div><div>8%</div><div>54%</div></div> |
| 83 | p1 | 47 | <div><div></div><div>100%</div></div> |
| 84 | p2 | 46 | <div><div></div><div>100%</div></div> |

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 411183 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 |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1 | 2 | 1750 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 37283 | 16668 | 6591 | 12274 | 1750 | | | |
| 1 | 6 | 1795 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 38238 | 17095 | 6758 | 12590 | 1795 | | | |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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 |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | C1 | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1214 | 775 | 230 | 206 | 3 | | | |
| 13 | c1 | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1168 | 747 | 221 | 197 | 3 | | | |

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 |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14 | C2 | 124 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 892 | 562 | 156 | 172 | 2 | | | |
| 14 | c2 | 124 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 892 | 562 | 156 | 172 | 2 | | | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| C2 | 104 | ALA | GLY | conflict | UNP P48589 |
| C2 | 110 | ALA | GLY | conflict | UNP P48589 |
| c2 | 104 | ALA | GLY | conflict | UNP P48589 |
| c2 | 110 | ALA | GLY | conflict | UNP P48589 |

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 18 | C6 | 141 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 1105 | 708 | 203 | 194 | | | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 18 | c6 | 142 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1111 | 711 | 204 | 196 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | C7 | 120 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 926 | 577 | 177 | 170 | 2 | | | |
| 19 | c7 | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 906 | 563 | 174 | 167 | 2 | | | |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called Suppressor protein STM1.

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 39 | L2 | 252 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1914 | 1191 | 388 | 334 | 1 | | | |
| 39 | 12 | 252 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1912 | 1190 | 388 | 333 | 1 | | | |

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 45 | L8 | 233 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1804 | 1151 | 323 | 327 | 3 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 45 | l8 | 231 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1763 | 1130 | 316 | 314 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46 | L9 | 191 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1518 | 963 | 274 | 277 | 4 | | | |
| 46 | l9 | 191 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1518 | 963 | 274 | 277 | 4 | | | |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 61 | N5 | 121 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 964 | 620 | 169 | 173 | 2 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 61 | n5 | 120 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 959 | 617 | 168 | 172 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 62 | N6 | 126 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 993 | 625 | 192 | 176 | | | | |
| 62 | n6 | 126 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 993 | 625 | 192 | 176 | | | | |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 78 | Q2 | 105 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 847 | 534 | 170 | 138 | 5 | | | |
| 78 | q2 | 105 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 847 | 534 | 170 | 138 | 5 | | | |

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

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

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

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

- Molecule 81 is a protein called Unknown Protein m2.

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

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

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

- Molecule 83 is a protein called Unknown Protein p1.

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

- Molecule 84 is a protein called Unknown Protein p2.

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

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

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 85 | L7 | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 85 | m6 | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 85 | n8 | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 85 | q3 | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 85 | o1 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 85 | N5 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 85 | 6 | 147 | Total | Mg | 0 | 0 |
| | | | 147 | 147 | | |
| 85 | sM | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 85 | m5 | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 85 | l3 | 3 | Total | Mg | 0 | 0 |
| | | | 3 | 3 | | |
| 85 | M1 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 85 | n0 | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 85 | d6 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 85 | 2 | 123 | Total | Mg | 0 | 0 |
| | | | 123 | 123 | | |
| 85 | O3 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 85 | L4 | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 85 | l7 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | M5 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | o0 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | S2 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | L8 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | D3 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | o4 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | M9 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | q0 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | c8 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | M0 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 85 | c1 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | 5 | 496 | Total 496 | Mg 496 | 0 | 0 |
| 85 | L5 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | O7 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | l4 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | n9 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | 1 | 471 | Total 471 | Mg 471 | 0 | 0 |
| 85 | D0 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | S8 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | m1 | 1 | Total 1 | Mg 1 | 0 | 0 |

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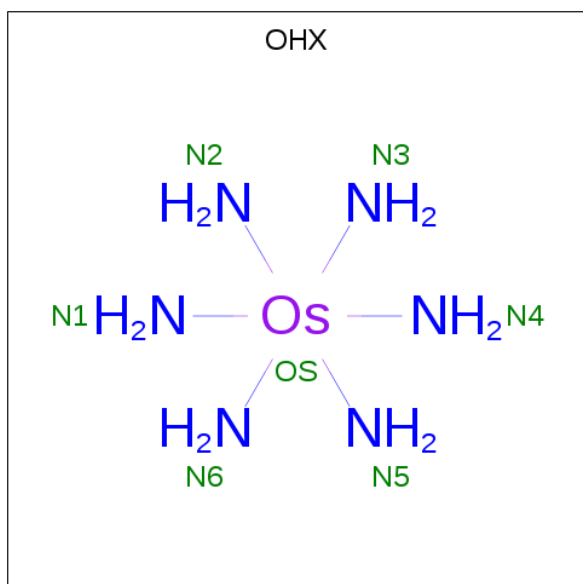
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 85 | O2 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | s9 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | o3 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | d3 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 85 | M3 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 85 | N3 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 85 | 4 | 20 | Total 20 | Mg 20 | 0 | 0 |
| 85 | n6 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | L2 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 85 | l5 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 85 | C3 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | M7 | 4 | Total 4 | Mg 4 | 0 | 0 |
| 85 | N8 | 5 | Total 5 | Mg 5 | 0 | 0 |
| 85 | s1 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | l9 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | s8 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | c7 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | 7 | 18 | Total 18 | Mg 18 | 0 | 0 |
| 85 | n3 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | L3 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 85 | l2 | 2 | Total 2 | Mg 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 85 | 8 | 15 | Total | Mg | 0 | 0 |
| | | | 15 | 15 | | |
| 85 | m0 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 85 | M6 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 85 | N0 | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 85 | 3 | 14 | Total | Mg | 0 | 0 |
| | | | 14 | 14 | | |
| 85 | m7 | 5 | Total | Mg | 0 | 0 |
| | | | 5 | 5 | | |

- Molecule 86 is osmium (III) hexammine (three-letter code: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



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

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

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

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

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

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 2 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | S6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | S8 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | C3 | 1 | Total | N | Os | 0 | 0 |
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| 86 | C5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | C8 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | D3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | D9 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | SR | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
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| | | | 7 | 6 | 1 | | |
| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |

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

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

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

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

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 4 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 4 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 4 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 4 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 4 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86 | 4 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 4 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 4 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 4 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 4 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 4 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 4 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 4 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | L3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | L3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | L4 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | M0 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | M5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | M7 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | M7 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | M9 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | N9 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | O1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | O3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86 | O4 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | O6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | O7 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | O9 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | Q2 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |

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

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

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

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

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | s1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | s1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | s8 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86 | c3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | c5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | c8 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | d4 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | d9 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | sR | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |

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

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

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

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

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

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

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

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

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

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86 | 8 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 8 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 8 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 8 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 8 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 8 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 13 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 13 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 14 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 14 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 15 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 15 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 15 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 15 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 19 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | m0 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | m0 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | m1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | m4 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | m5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86 | m6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | m7 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | m8 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | n3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | n3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | n6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | n9 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | o2 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | o3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | o7 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | o7 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | q2 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |

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

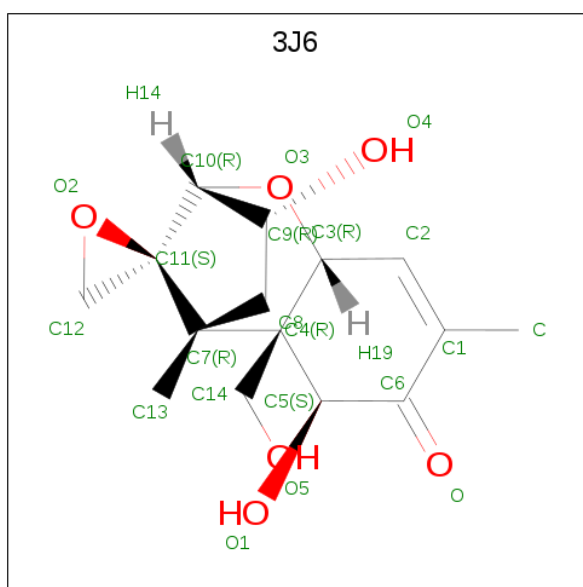
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 87 | q0 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 87 | D6 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 87 | Q2 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 87 | e1 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 87 | Q3 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 87 | D9 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 87 | E1 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 87 | Q0 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 87 | d7 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 87 | q3 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 87 | d9 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 87 | D7 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 87 | d6 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 87 | o7 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 87 | O7 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 87 | q2 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 88 is (3beta,7alpha)-3,7,15-trihydroxy-12,13-epoxytrichothec-9-en-8-one (three-letter code: 3J6) (formula: C₁₅H₂₀O₆).



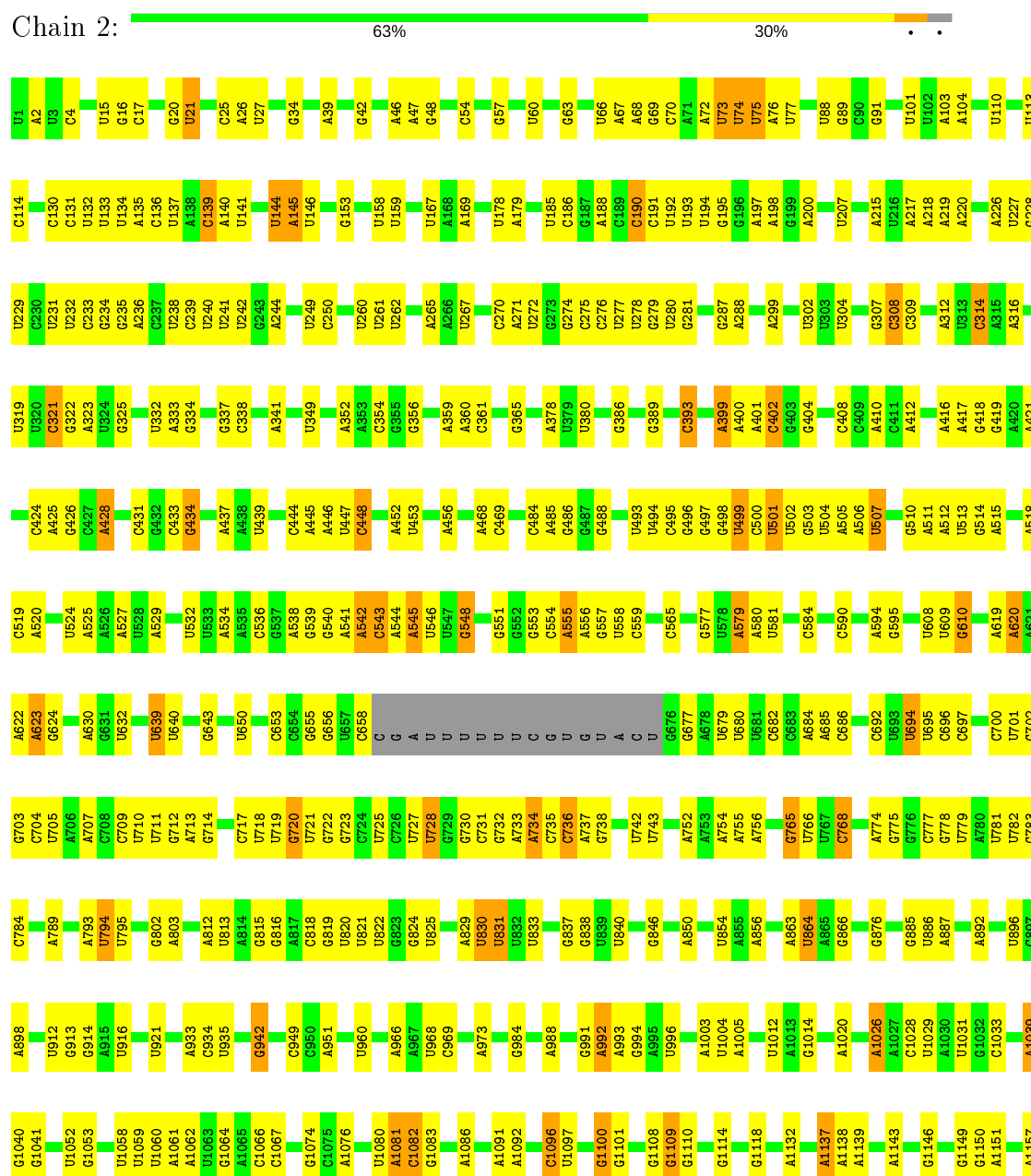
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 88 | 1 | 1 | Total | C | O | 0 | 0 |
| | | | 21 | 15 | 6 | | |
| 88 | 5 | 1 | Total | C | O | 0 | 0 |
| | | | 21 | 15 | 6 | | |

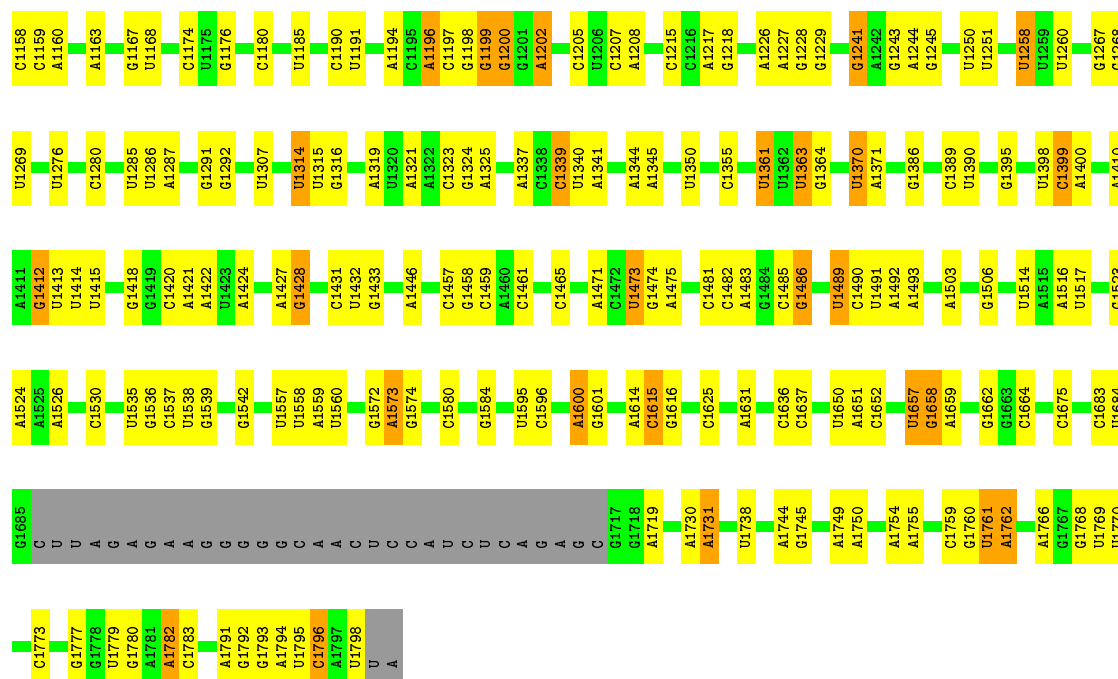
3 Residue-property plots

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

Note EDS failed to run properly.

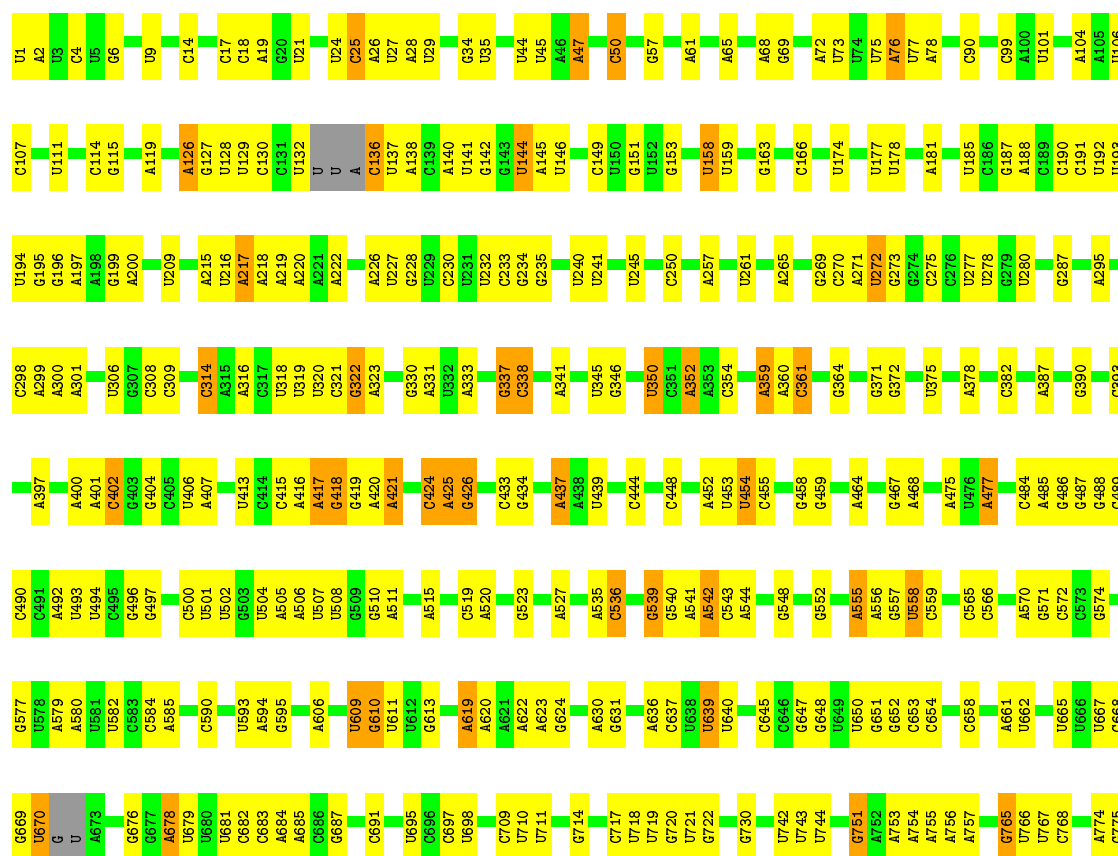
• Molecule 1: 18S ribosomal RNA

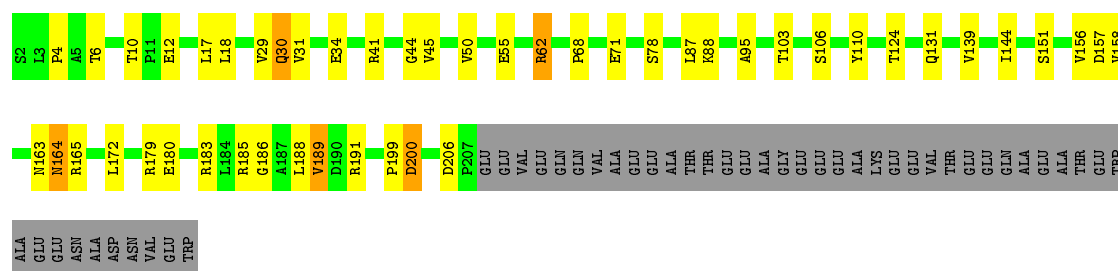




• Molecule 1: 18S ribosomal RNA

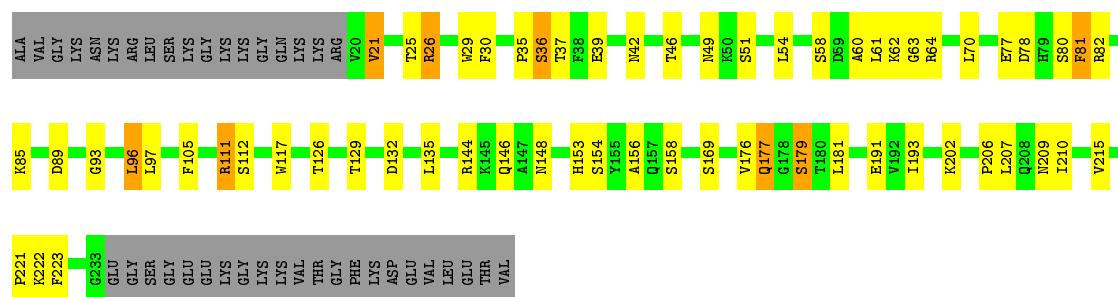
Chain 6: 62% 33% 5%





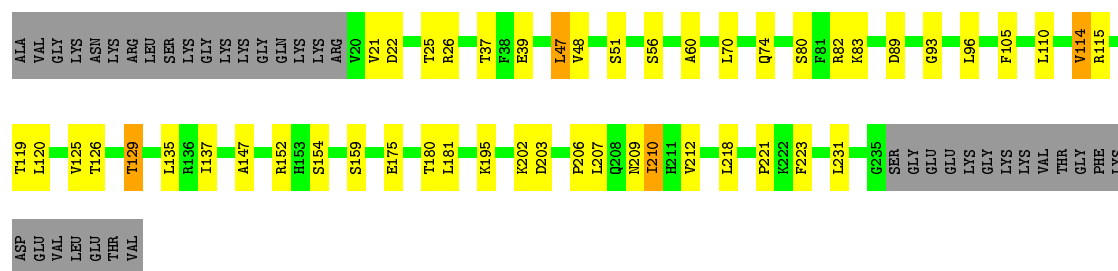
- Molecule 3: 40S ribosomal protein S1-A

Chain S1: 60% 21% 16%



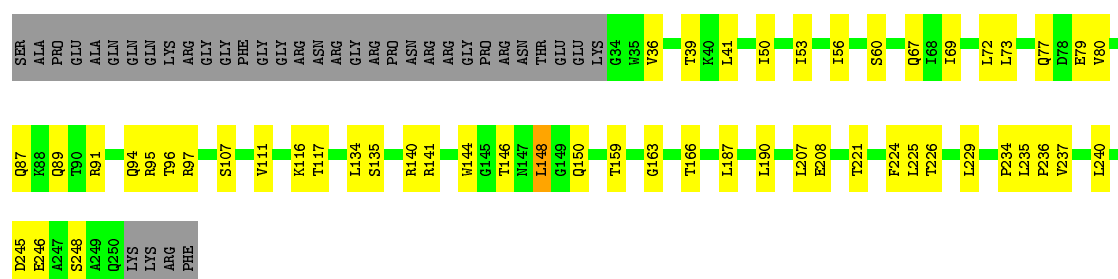
- Molecule 3: 40S ribosomal protein S1-A

Chain s1: 66% 18% 15%



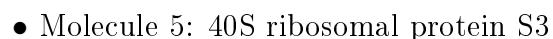
- Molecule 4: 40S ribosomal protein S2

Chain S2: 65% 21% 14%

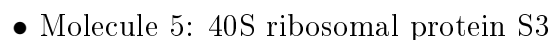


- Molecule 4: 40S ribosomal protein S2

| Category | Percentage |
|-----------|------------|
| Very good | 62% |
| Good | 23% |
| Not good | 1% |
| Very bad | 14% |



| Category | Percentage |
|-----------|------------|
| Very good | 72% |
| Good | 20% |
| Not good | 7% |
| Very bad | 3% |



| Response | Percentage |
|------------|------------|
| Yes | 71% |
| No | 21% |
| Don't know | 7% |



79% 19%



| Response | Percentage |
|----------------------|------------|
| Doing a good job | 80% |
| Not doing a good job | 18% |
| Don't know | 2% |







- Molecule 9: 40S ribosomal protein S7-A

Chain s7: 72% 24% • •



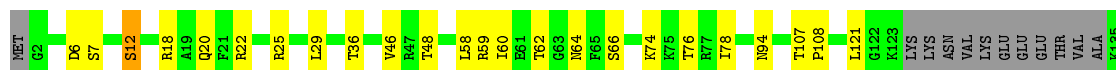
- Molecule 10: 40S ribosomal protein S8-A

Chain S8: 73% 19% • 6%



- Molecule 10: 40S ribosomal protein S8-A

Chain s8: 77% 17% • 6%



- Molecule 11: 40S ribosomal protein S9-A

Chain S9: 70% 23% • 6%



- Molecule 11: 40S ribosomal protein S9-A

Chain s9: 69% 23% • 6%



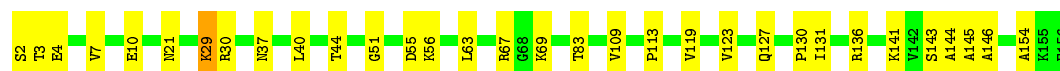
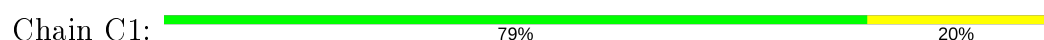
- Molecule 12: 40S ribosomal protein S10-A



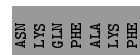
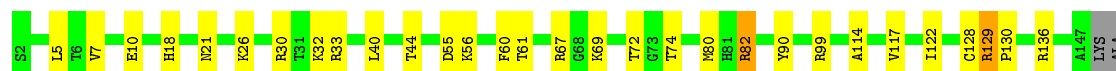
- Molecule 12: 40S ribosomal protein S10-A



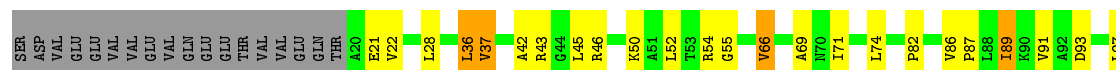
- Molecule 13: 40S ribosomal protein S11-A



- Molecule 13: 40S ribosomal protein S11-A



- Molecule 14: 40S ribosomal protein S12



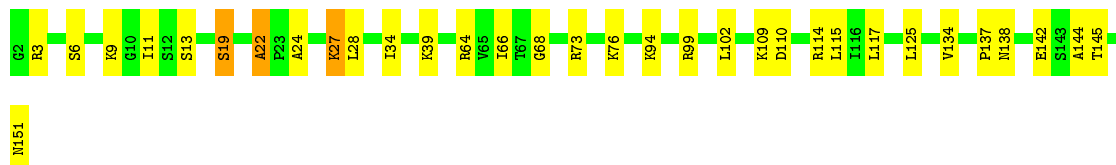
- Molecule 14: 40S ribosomal protein S12





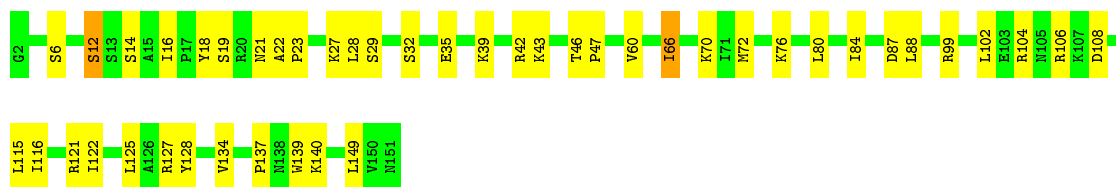
- Molecule 15: 40S ribosomal protein S13

Chain C3: 78% 20%



- Molecule 15: 40S ribosomal protein S13

Chain c3: 70% 29%



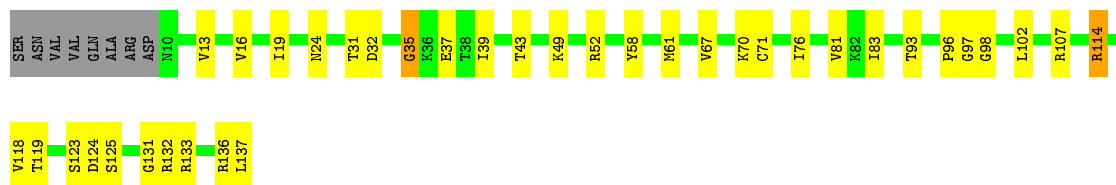
- Molecule 16: 40S ribosomal protein S14-A

Chain C4: 73% 17% 7%



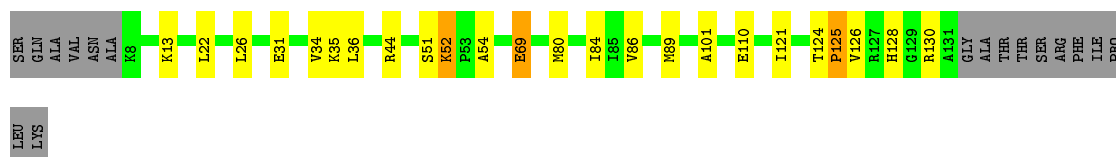
- Molecule 16: 40S ribosomal protein S14-A

Chain c4: 67% 26% 6%




- Molecule 17: 40S ribosomal protein S15

Chain C5: 71% 15% 12%



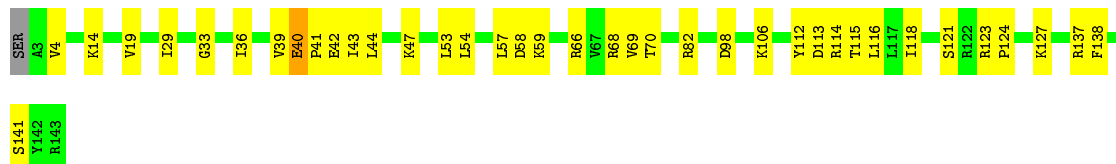
- Molecule 17: 40S ribosomal protein S15

Chain c5:  76% 17%



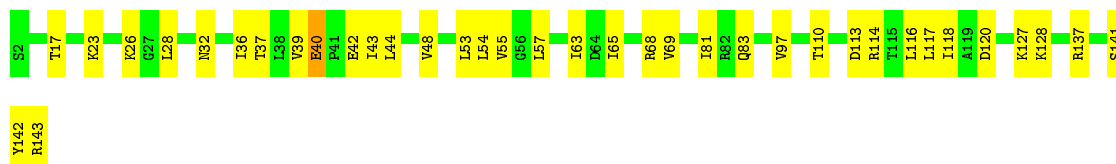
- Molecule 18: 40S ribosomal protein S16-A

Chain C6:  73% 26%



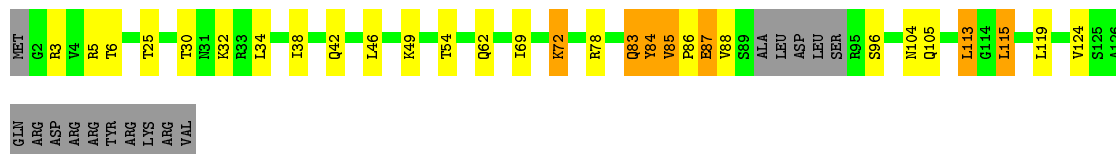
- Molecule 18: 40S ribosomal protein S16-A

Chain c6:  74% 25%



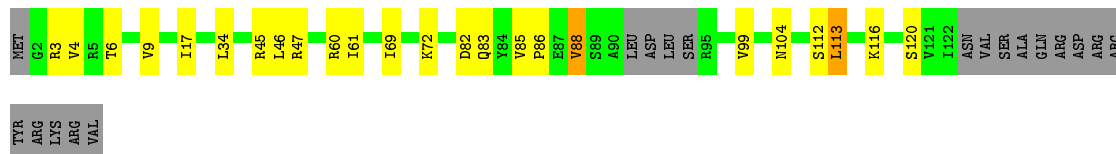
- Molecule 19: 40S ribosomal protein S17-A

Chain C7:  67% 16% 5% 12%




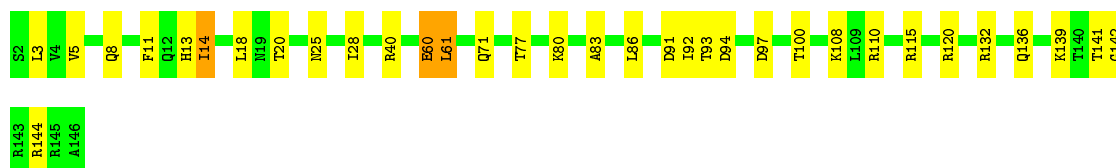
- Molecule 19: 40S ribosomal protein S17-A

Chain c7:  68% 16% 1% 14%

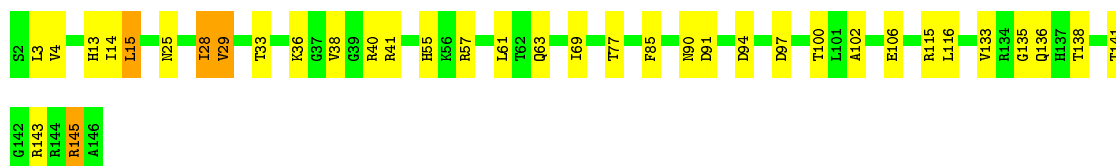


- Molecule 20: 40S ribosomal protein S18-A

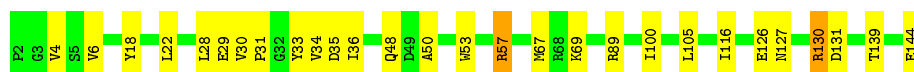
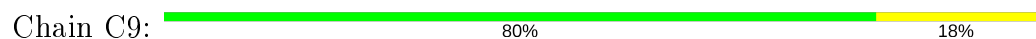
Chain C8:  77% 21%



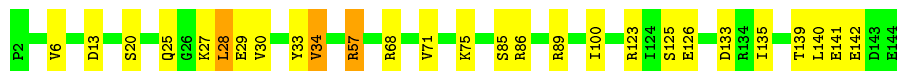
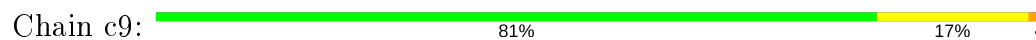
- Molecule 20: 40S ribosomal protein S18-A



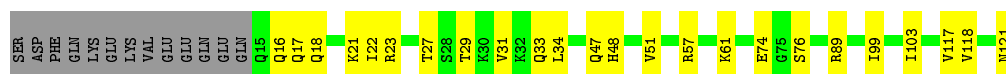
- Molecule 21: 40S ribosomal protein S19-A



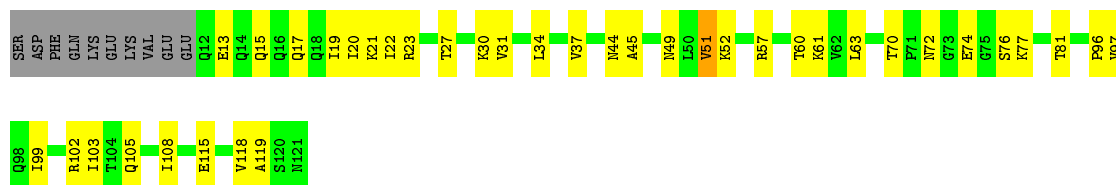
- Molecule 21: 40S ribosomal protein S19-A



- Molecule 22: 40S ribosomal protein S20

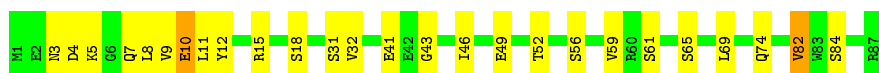


- Molecule 22: 40S ribosomal protein S20



- Molecule 23: 40S ribosomal protein S21-A

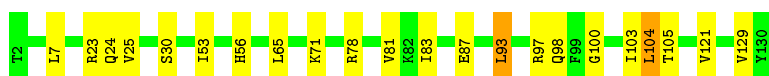
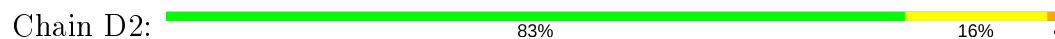




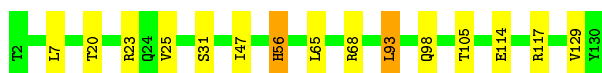
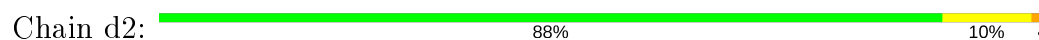
- Molecule 23: 40S ribosomal protein S21-A



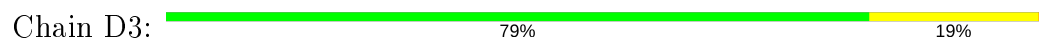
- Molecule 24: 40S ribosomal protein S22-A



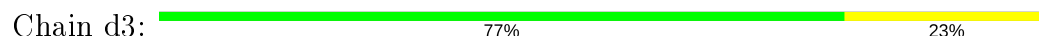
- Molecule 24: 40S ribosomal protein S22-A



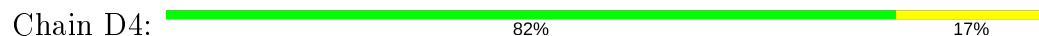
- Molecule 25: 40S ribosomal protein S23-A



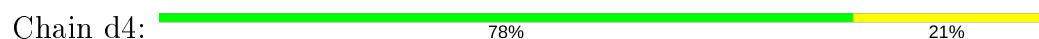
- Molecule 25: 40S ribosomal protein S23-A

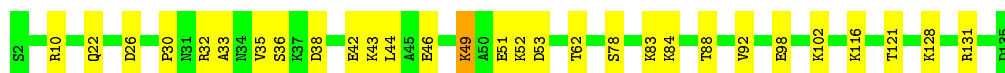


- Molecule 26: 40S ribosomal protein S24-A

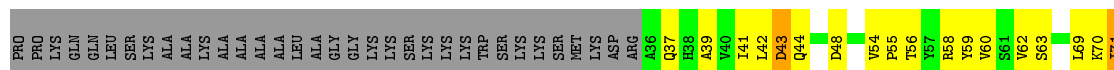


- Molecule 26: 40S ribosomal protein S24-A

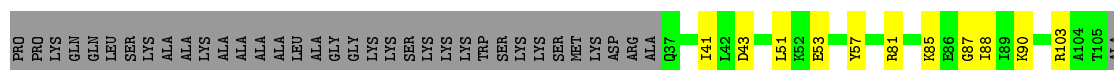




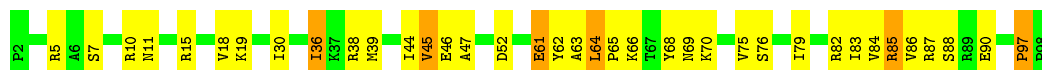
- Molecule 27: 40S ribosomal protein S25-A



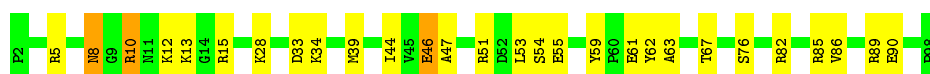
- Molecule 27: 40S ribosomal protein S25-A



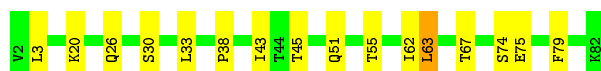
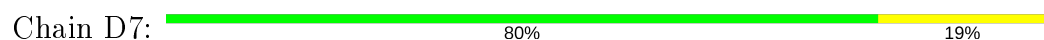
- Molecule 28: 40S ribosomal protein S26-B



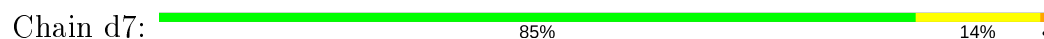
- Molecule 28: 40S ribosomal protein S26-B



- Molecule 29: 40S ribosomal protein S27-A

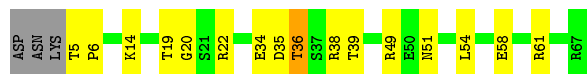


- Molecule 29: 40S ribosomal protein S27-A



- Molecule 30: 40S ribosomal protein S28-A

Chain D8:  71% 23% • 5%




- Molecule 30: 40S ribosomal protein S28-A

Chain d8:  73% 21% • 5%



- Molecule 31: 40S ribosomal protein S29-A

Chain D9:  80% 16% •




- Molecule 31: 40S ribosomal protein S29-A

Chain d9:  67% 25% • •



- Molecule 32: 40S ribosomal protein S30-A

Chain E0:  83% 13% •



- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1:  51% 34% 8% 7%



- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1:  57% 38% • •



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

| | |
|------|------|
| D266 | A2 |
| L270 | S3 |
| E277 | V6 |
| S291 | L7 |
| L292 | R10 |
| T300 | G28 |
| I308 | Q29 |
| Q314 | T48 |
| T317 | G49 |
| A318 | D50 |
| K319 | D51 |
| | Q52 |
| | S60 |
| | H66 |
| | D76 |
| | E98 |
| | T99 |
| | Y100 |
| | Q101 |
| | R102 |
| | K117 |
| | I136 |
| | T143 |
| | L144 |
| | L145 |
| | D149 |
| | E160 |
| | K161 |
| | I188 |
| | I193 |
| | G194 |
| | H195 |
| | P206 |
| | D207 |
| | Y232 |
| | Q237 |
| | D238 |
| | T256 |
| | A257 |
| | T258 |

- | | |
|------|------|
| I199 | A2 |
| L210 | S3 |
| K228 | N4 |
| Y232 | V8 |
| Q237 | L9 |
| Y250 | R10 |
| D266 | H16 |
| R275 | L23 |
| A279 | A24 |
| S282 | T25 |
| E286 | L32 |
| D297 | G49 |
| V309 | V58 |
| I310 | H64 |
| A318 | S65 |
| N319 | H66 |
| | T72 |
| | D76 |
| | S82 |
| | V94 |
| | A95 |
| | T96 |
| | G97 |
| | E98 |
| | T99 |
| | Y100 |
| | I123 |
| | L145 |
| | S152 |
| | E160 |
| | K161 |
| | A162 |
| | D163 |
| | D164 |
| | D165 |
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| | H178 |
| | V178 |
| | I188 |
| | A194 |

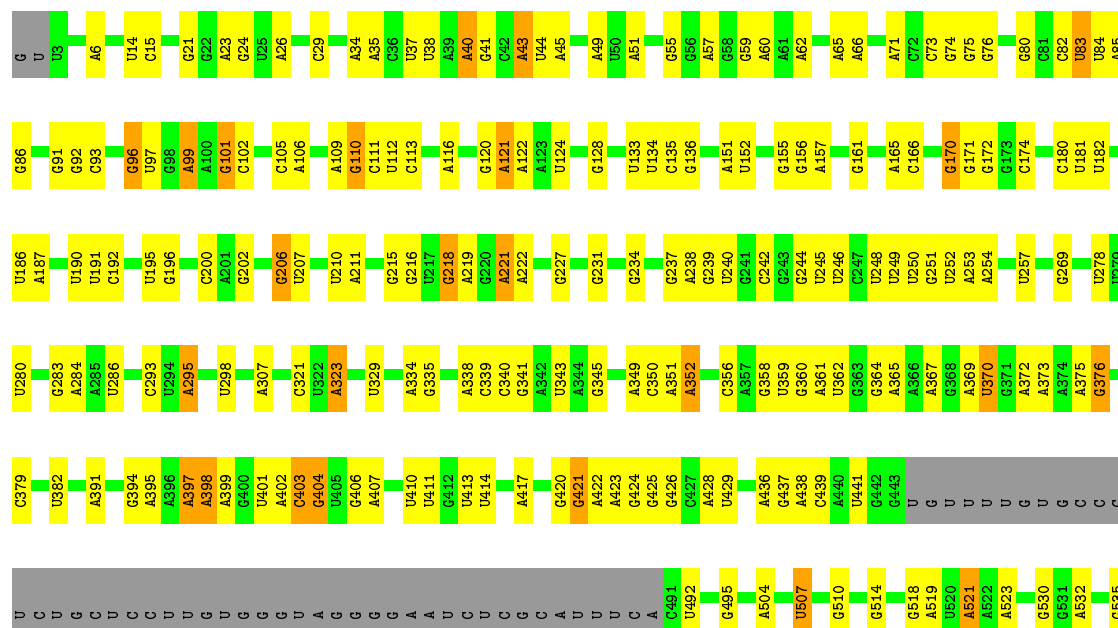
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|-----|-----|-------|------|
| ARG | LYS | EL16 | MT |
| ASN | THR | LI17 | ASN |
| ILE | LYS | | ASN |
| ASP | GLU | K121 | PRO |
| VAL | TVR | | PHE |
| SER | LEU | EL30 | ASP |
| ASN | GLU | | LEU |
| LEU | PHE | DI34 | LEU |
| PRO | ASP | AI135 | G9 |
| SER | ALA | | |
| LEU | THR | EL39 | V12 |
| ALA | PHE | DI40 | |
| | VAL | AI41 | L20 |
| | GLU | GLY | P21 |
| | SER | LYS | P22 |
| | ASN | PRO | K23 |
| | THR | LYS | E24 |
| | ARG | THR | |
| | LYS | ALA | S32 |
| | ASN | GLN | K33 |
| | PHE | LEU | K34 |
| | GLY | SER | |
| | ASP | LI151 | S45 |
| | ARG | Q152 | |
| | ASN | DI153 | R51 |
| | ASN | | P52 |
| | ASN | K165 | |
| | SER | V166 | I61 |
| | ARG | P167 | R62 |
| | ASN | | |
| | ASN | V172 | R68 |
| | PHE | EL73 | |
| | ASN | LI74 | R72 |
| | ASN | DI75 | |
| | ARG | AI76 | T77 |
| | ARG | GLU | |
| | GLY | ARG | T62 |
| | GLY | ILE | K83 |
| | ARG | GLU | K84 |
| | GLY | THR | S85 |
| | ALA | ALA | R86 |
| | ARG | GLU | T87 |
| | LYS | LYS | R88 |
| | GLY | GLU | R89 |
| | ASN | ALA | A90 |
| | ASN | TVR | T91 |
| | THR | VAL | |
| | ALA | PRO | S95 |
| | ASN | ALA | R96 |
| | ALA | THR | T97 |
| | THR | LYS | |
| | ASN | VAL | T100 |
| | SER | LYS | DI01 |
| | ALA | ASN | T102 |
| | ASN | VAL | |
| | THR | LYS | K105 |
| | VAL | SER | V106 |
| | GLN | LYS | |
| | LYS | GLN | G111 |
| | ASN | TVR | |

- [illegible]

- WORLDWIDE
PDB
PROTEIN DATA BANK

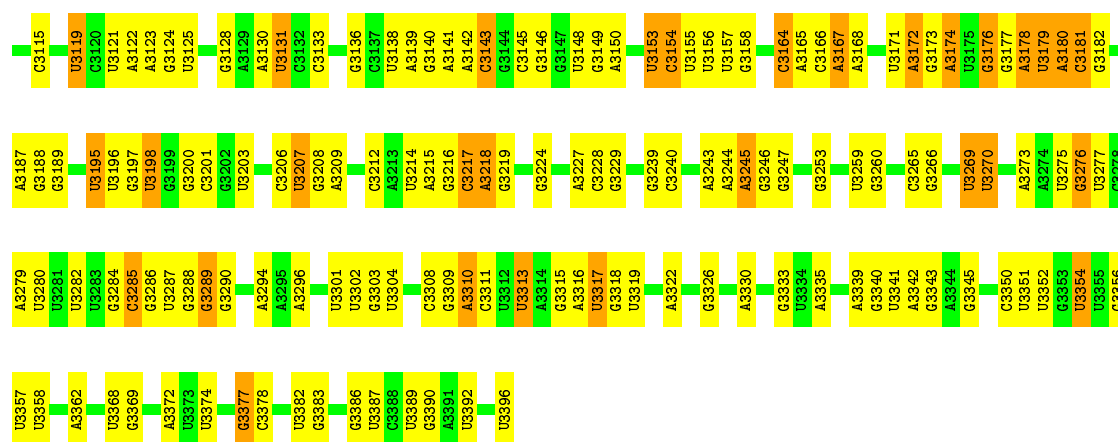




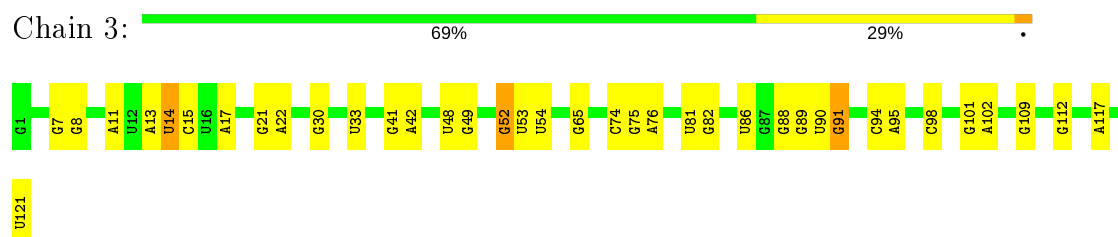


| | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|
| A1797 | C1885 | G1577 | A1490 | G1412 | C1333 | A1244 | C1160 | A1084 | G1001 | A926 | U834 | A746 | G639 | C542 |
| A1804 | U1686 | C1578 | G1493 | G1413 | U1334 | A1245 | G1161 | A1085 | A1002 | C927 | G835 | A747 | U640 | C543 |
| | U1687 | A1579 | U1493 | G1414 | C1335 | U1246 | U1162 | C1086 | A1003 | C928 | A836 | U748 | U641 | |
| G1808 | U1695 | C1580 | U1494 | G1415 | U1336 | U1247 | U1163 | G1087 | A1004 | A929 | A837 | G754 | U642 | C546 |
| A1809 | C1581 | C1582 | U1495 | A1418 | A1237 | C1248 | G1164 | U1088 | U1007 | A933 | G844 | | G644 | G547 |
| A1810 | U1496 | A1583 | C1496 | A1419 | C1338 | | A1165 | A1089 | U1008 | G934 | A645 | | A645 | G548 |
| | C1499 | | C1499 | A1420 | C1339 | A1252 | G1166 | U1094 | U1009 | U935 | A646 | | A646 | |
| A1813 | G1700 | A1587 | G1500 | G1421 | C1342 | U1258 | A1169 | U1095 | A1009 | U936 | A647 | | A647 | U555 |
| A1814 | C1588 | A1588 | A1503 | A1428 | A1343 | G1261 | G1171 | U1096 | A1010 | U937 | C758 | | A647 | U556 |
| U1815 | G1590 | A1589 | G1590 | G1429 | U1348 | G1262 | U1170 | U1097 | G1010 | U938 | | | A647 | A557 |
| A1816 | G1591 | G1590 | A1506 | U1430 | G1349 | A1263 | U1172 | U1098 | A1011 | G937 | G763 | | C648 | U558 |
| G1817 | G1592 | G1591 | G1507 | G1431 | U1350 | G1264 | U1173 | A1099 | G1012 | C938 | G764 | | A649 | A559 |
| U1818 | A1593 | A1592 | C1432 | A1432 | A1351 | U1265 | G1174 | U1100 | | U939 | A858 | | C650 | |
| A1819 | C1593 | A1593 | A1433 | G1433 | A1352 | G1266 | C1175 | U1101 | U1015 | U942 | G859 | | G651 | |
| U1820 | U1716 | A1594 | A1434 | G1434 | A1353 | A1274 | G1176 | A1102 | C1016 | U943 | G860 | | G652 | |
| U1821 | U1717 | | G1513 | | G1354 | A1274 | G1177 | G1104 | C1017 | U944 | C861 | | A653 | |
| | | C1597 | G1519 | C1437 | G1355 | | G1178 | G1104 | A866 | U945 | G867 | | A656 | |
| A1834 | U1724 | A1598 | G1520 | U1438 | A1356 | C1284 | A1179 | U1140 | G867 | U946 | G867 | | A657 | |
| A1835 | G1599 | G1599 | G1520 | U1438 | U1357 | G1285 | A1180 | | C868 | | C868 | | A657 | |
| C1836 | U1600 | U1600 | G1528 | U1443 | G1357 | G1289 | A1181 | U1114 | G869 | | U776 | | A660 | |
| G1838 | G1730 | A1605 | | U1443 | C1360 | G1289 | C1183 | G1115 | G870 | | U777 | | G661 | |
| U1839 | G1736 | U1606 | U1533 | A1446 | U1361 | C1292 | G1186 | G1116 | U871 | | U777 | | U662 | |
| A1841 | | U1607 | A1534 | G1447 | G1362 | U1293 | G1187 | G1117 | U872 | | U778 | | A665 | |
| A1842 | A1613 | C1614 | A1535 | U1448 | G1365 | A1294 | C1188 | C1119 | U873 | | A784 | | C667 | |
| C1843 | | | G1536 | A1449 | A1366 | A1294 | C1189 | | A1025 | | G785 | | G668 | |
| C1844 | G1618 | G1614 | A1539 | U1450 | G1367 | G1300 | C1189 | U1124 | A1026 | | G786 | | U669 | |
| G1845 | G1751 | U1619 | U1540 | C1451 | U1368 | A1301 | A1190 | U1125 | A1027 | | G787 | | A665 | |
| C1846 | A1619 | A1452 | G1541 | A1452 | A1369 | A1302 | C1192 | U1126 | U1028 | | A962 | | A666 | |
| A1847 | U1620 | | G1541 | A1453 | G1370 | A1303 | A1193 | G1127 | U1041 | | G878 | | C674 | |
| G1848 | C1547 | U1629 | G1547 | A1454 | A1373 | A1304 | G1194 | U1128 | U1042 | | U791 | | G675 | |
| A1849 | U1548 | C1548 | C1761 | U1455 | G1374 | U1305 | A1195 | G1127 | C1043 | | G792 | | C676 | |
| G1851 | U1549 | C1631 | A1456 | A1456 | G1375 | G1307 | C1196 | U1129 | C1044 | | C793 | | A677 | |
| | | | | | | A1308 | C1199 | A1130 | A1046 | | G890 | | U681 | |
| C1854 | | C1639 | G1552 | A1460 | G1379 | U1309 | A1200 | G1131 | A1047 | | G891 | | U682 | |
| | | | U1553 | A1461 | G1380 | G1310 | C1201 | A1135 | A1048 | | G897 | | U683 | |
| A1859 | U1765 | U1640 | U1554 | A1462 | A1381 | G1311 | A1202 | | C1049 | | U898 | | G684 | |
| | U1766 | U1641 | U1555 | U1463 | A1381 | C1312 | | U1138 | U1050 | | C802 | | A607 | |
| C1863 | C1767 | A1642 | C1556 | G1464 | C1385 | G1313 | G1207 | U1139 | U1052 | | C803 | | A608 | |
| A1864 | | A1643 | A1557 | G1465 | C1386 | G1314 | U1208 | A1053 | G975 | | C804 | | G609 | |
| A1865 | G1770 | C1644 | G1560 | A1466 | A1386 | U1315 | U1209 | A1054 | U976 | | A806 | | G610 | |
| C1866 | U1772 | U1645 | G1561 | A1467 | | C1316 | U1210 | A1055 | C977 | | A807 | | A611 | |
| A1868 | | A1656 | G1562 | A1468 | A1390 | A1317 | | U1142 | U1056 | | A808 | | U612 | |
| C1869 | G1775 | C1657 | C1563 | U1470 | C1391 | A1318 | U1215 | A1143 | | | C911 | | A705 | |
| C1870 | | G1658 | U1564 | U1471 | G1392 | G1319 | G1222 | U1144 | U1060 | | G813 | | A706 | |
| U1871 | G1780 | G1681 | G1565 | U1472 | C1396 | C1320 | G1236 | G1148 | A1064 | | U814 | | U707 | |
| | C1781 | G1682 | U1567 | G1473 | U1397 | G1321 | G1237 | G1149 | A980 | | G815 | | G708 | |
| | | | U1568 | A1474 | U1398 | U1322 | C1232 | A1150 | A983 | | A816 | | G712 | |
| A1874 | A1787 | C1685 | U1569 | A1475 | A1399 | G1323 | | U1151 | G984 | | G916 | | A715 | |
| | C1788 | G1686 | U1570 | G1476 | G1400 | U1324 | G1236 | G1152 | C993 | | C918 | | U629 | |
| U1877 | | A1687 | U1571 | G1480 | C1403 | C1327 | G1237 | A1153 | U919 | | G918 | | A716 | |
| A1878 | G1792 | | U1572 | A1481 | G1404 | G1328 | G1238 | A1154 | A920 | | G822 | | C717 | |
| U1880 | C1793 | G1677 | G1573 | A1482 | U1405 | U1329 | C1239 | A1155 | U995 | | C823 | | A920 | |
| A1881 | G1794 | | C1574 | A1483 | A1406 | A1330 | A1240 | C1156 | A996 | | C824 | | A720 | |
| | U1795 | A1683 | A1575 | G1483 | A1406 | U1331 | G1242 | G1157 | A998 | | A827 | | G725 | |
| A1884 | G1796 | U1684 | G1576 | A1489 | G1408 | A1332 | G1243 | A1159 | C1000 | | A830 | | G726 | |

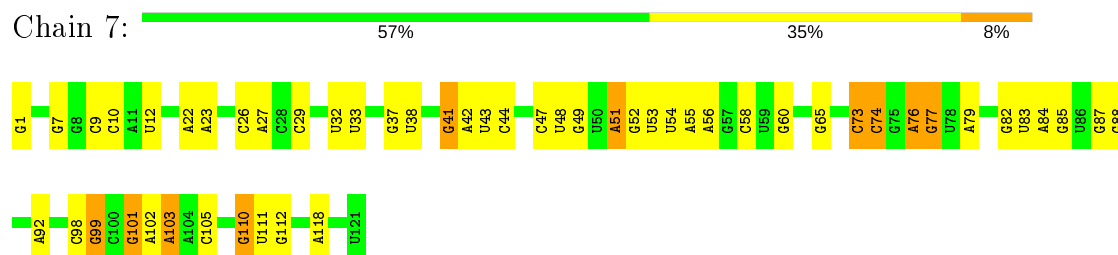




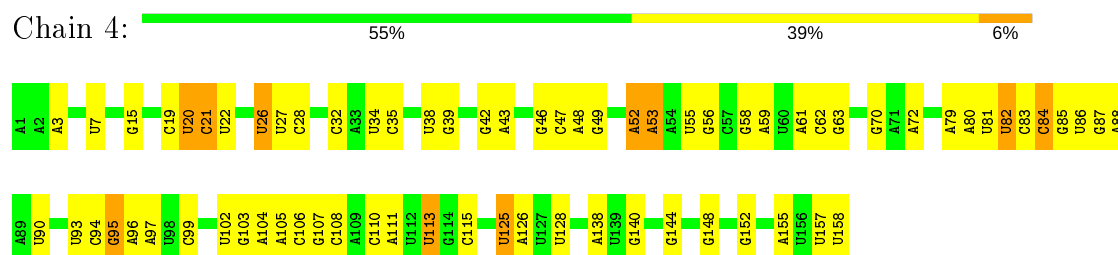
• Molecule 37: 5S ribosomal RNA



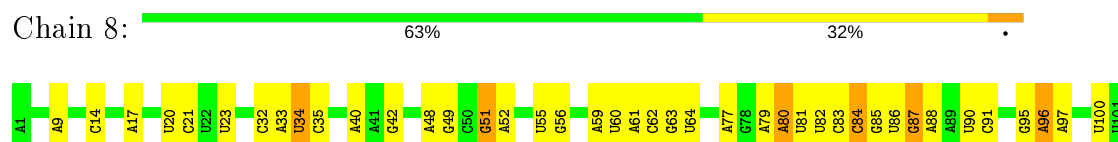
• Molecule 37: 5S ribosomal RNA

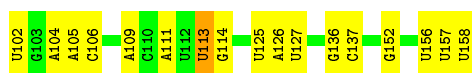


• Molecule 38: 5.8S ribosomal RNA



• Molecule 38: 5.8S ribosomal RNA





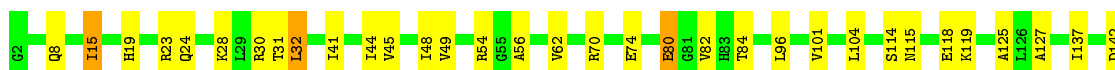
• Molecule 39: 60S ribosomal protein L2-A

Chain L2: 79% 19%



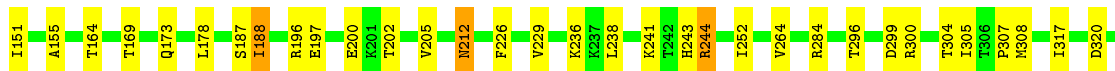
• Molecule 39: 60S ribosomal protein L2-A

Chain L2: 77% 22%



• Molecule 40: 60S ribosomal protein L3

Chain L3: 78% 20%

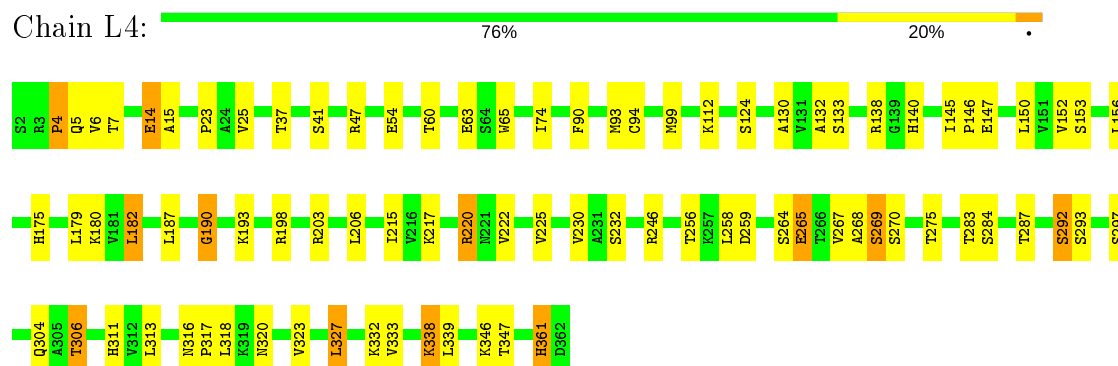


• Molecule 40: 60S ribosomal protein L3

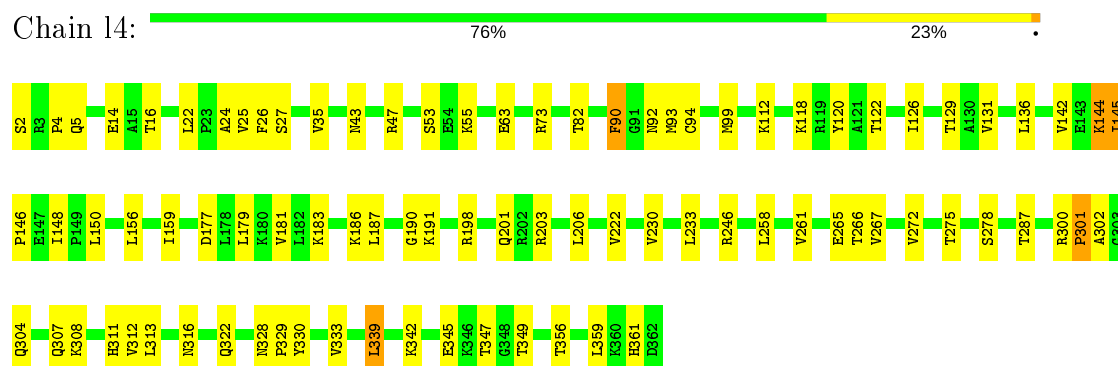
Chain L3: 78% 20%



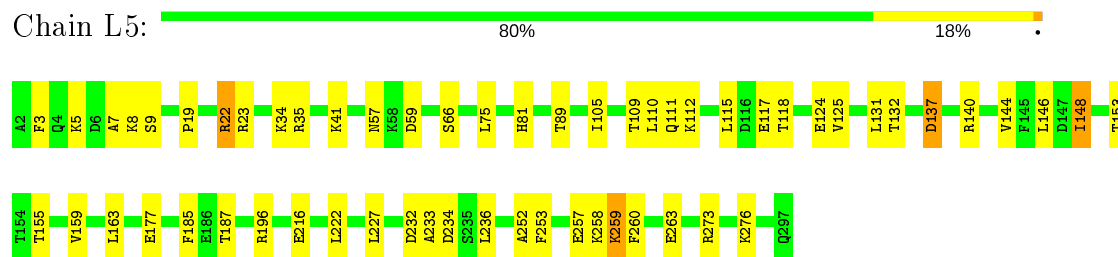
- Molecule 41: 60S ribosomal protein L4-A



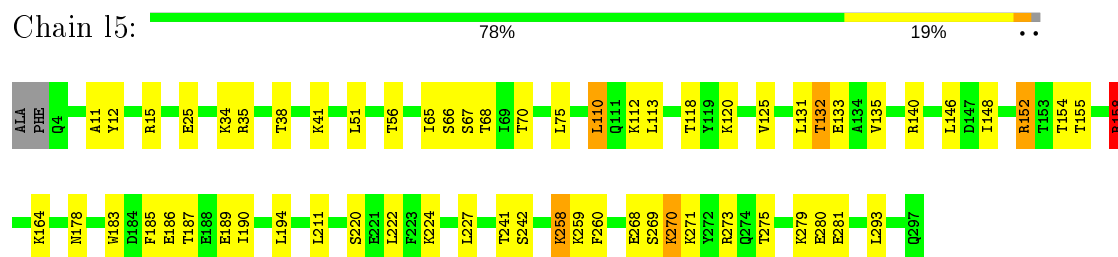
- Molecule 41: 60S ribosomal protein L4-A



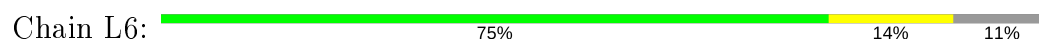
- Molecule 42: 60S ribosomal protein L5



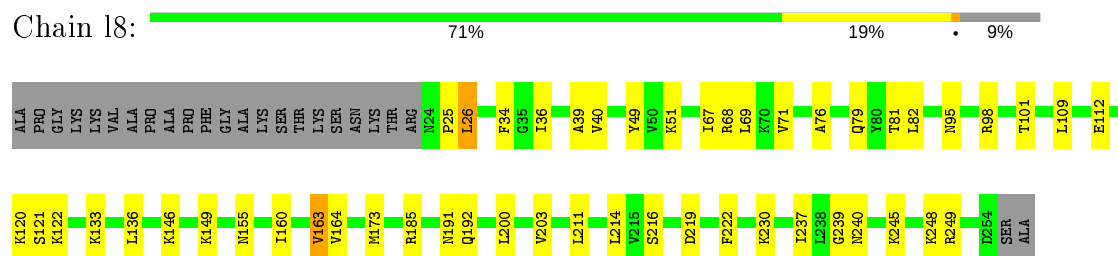
- Molecule 42: 60S ribosomal protein L5



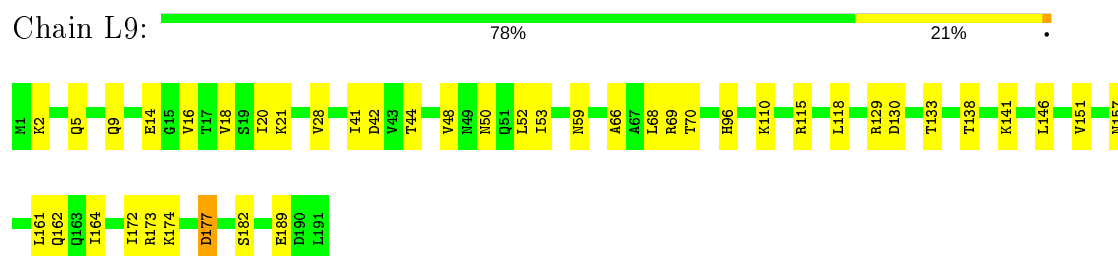
- Molecule 43: 60S ribosomal protein L6-A



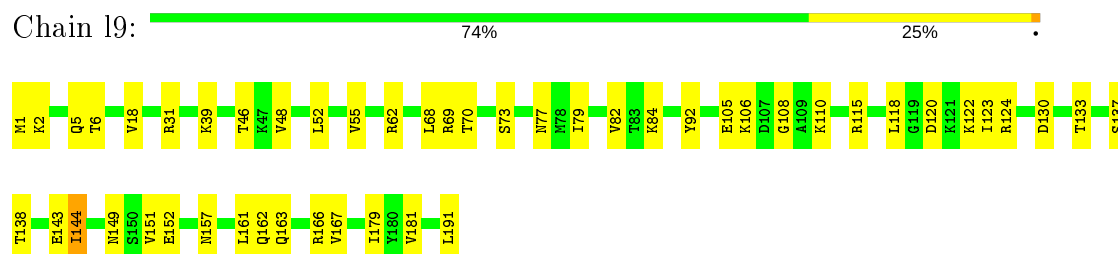
- Molecule 45: 60S ribosomal protein L8-A



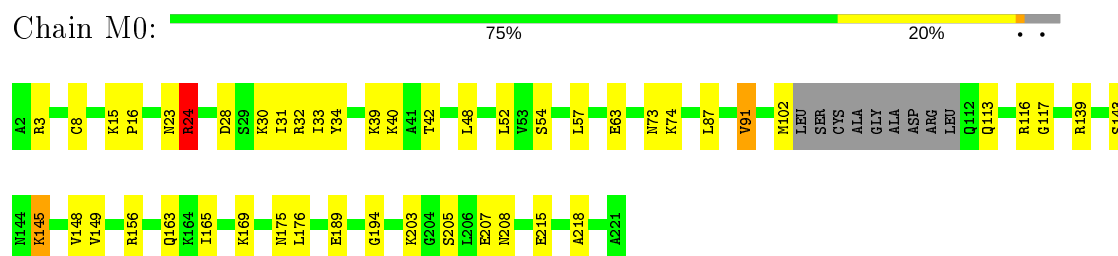
- Molecule 46: 60S ribosomal protein L9-A



- Molecule 46: 60S ribosomal protein L9-A



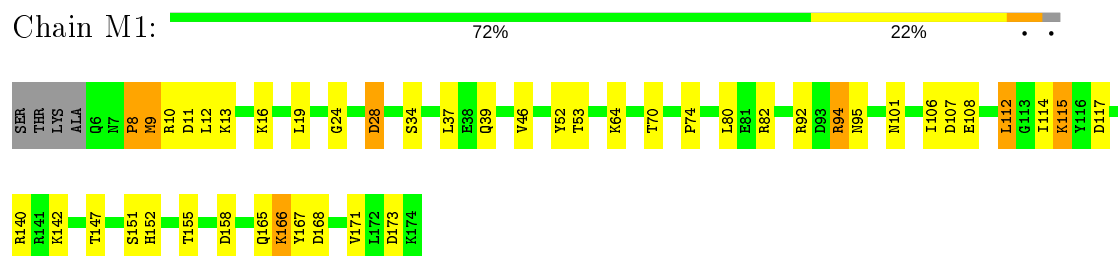
- Molecule 47: 60S ribosomal protein L10



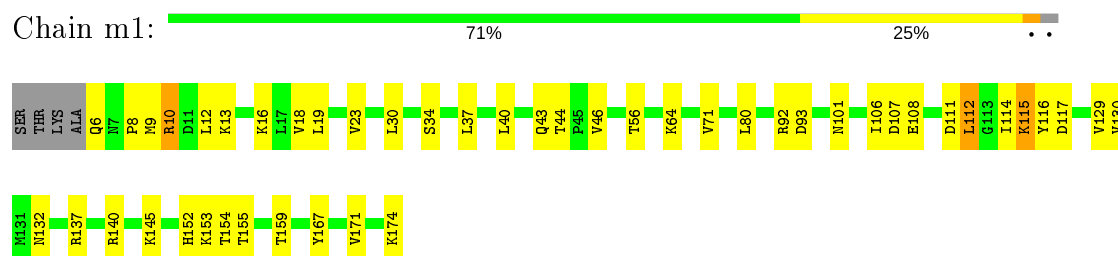
- Molecule 47: 60S ribosomal protein L10



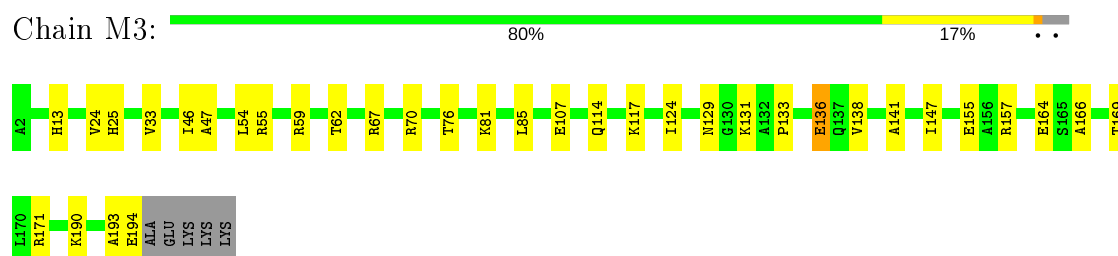
- Molecule 48: 60S ribosomal protein L11-B



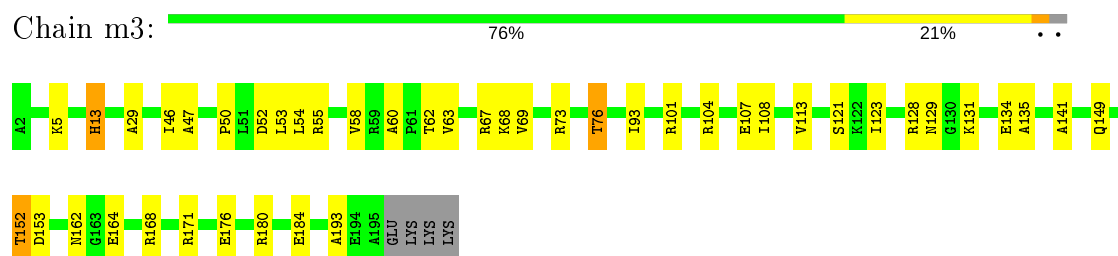
- Molecule 48: 60S ribosomal protein L11-B



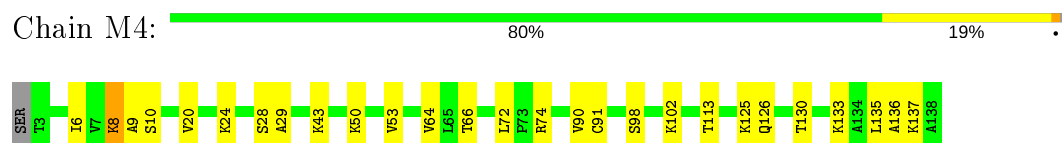
- Molecule 49: 60S ribosomal protein L13-A




- Molecule 49: 60S ribosomal protein L13-A



- Molecule 50: 60S ribosomal protein L14-A




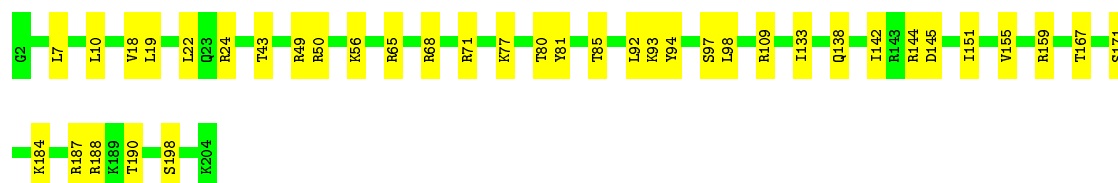
- Molecule 50: 60S ribosomal protein L14-A

Chain m4:  82% 18%



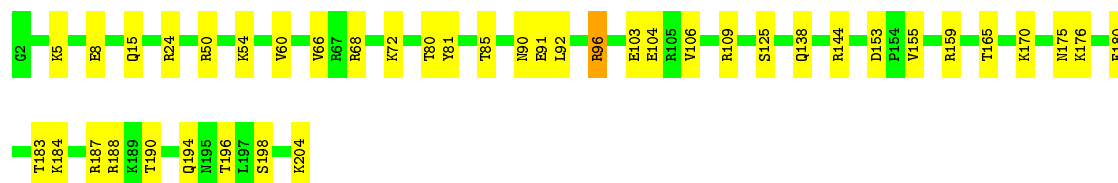
- Molecule 51: 60S ribosomal protein L15-A

Chain M5:  81% 19%




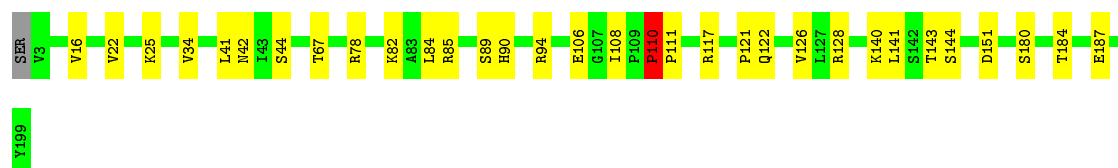
- Molecule 51: 60S ribosomal protein L15-A

Chain m5:  80% 20%




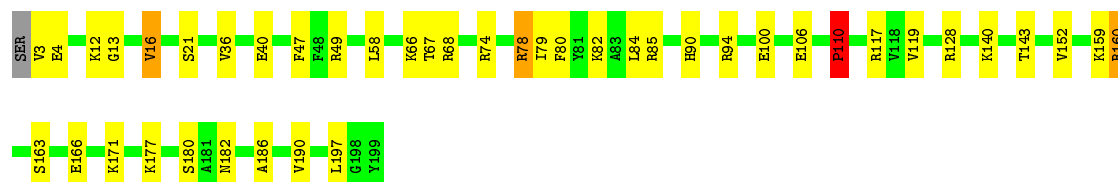
- Molecule 52: 60S ribosomal protein L16-A

Chain M6:  83% 16% ..




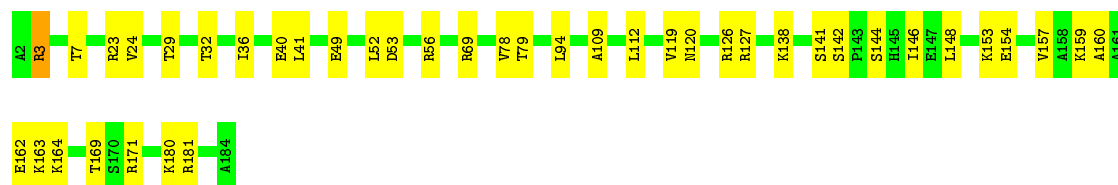
- Molecule 52: 60S ribosomal protein L16-A

Chain m6:  78% 20% ...



- Molecule 53: 60S ribosomal protein L17-A

Chain M7:  78% 22% .



- Molecule 53: 60S ribosomal protein L17-A

Chain m7: 70% 15% 15%



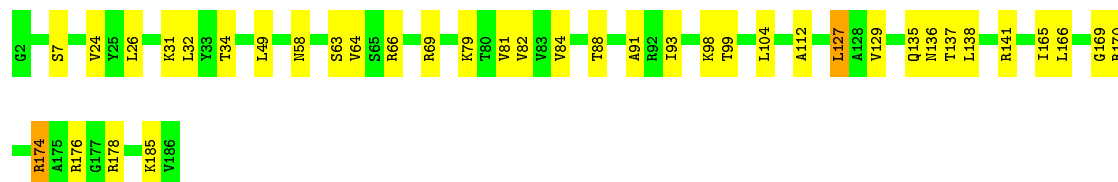
- Molecule 54: 60S ribosomal protein L18-A

Chain M8: 87% 13%



- Molecule 54: 60S ribosomal protein L18-A

Chain m8: 79% 19% .



- Molecule 55: 60S ribosomal protein L19-A


Chain M9: 83% 17%



- Molecule 55: 60S ribosomal protein L19-A

Chain m9: 84% 16%



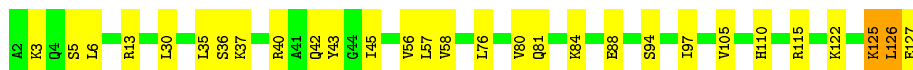
- Chain n2: 

Chain n5:



- Molecule 62: 60S ribosomal protein L26-A

Chain N6: 77% 21%



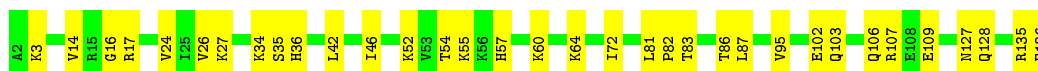
- Molecule 62: 60S ribosomal protein L26-A

Chain n6: 79% 21%



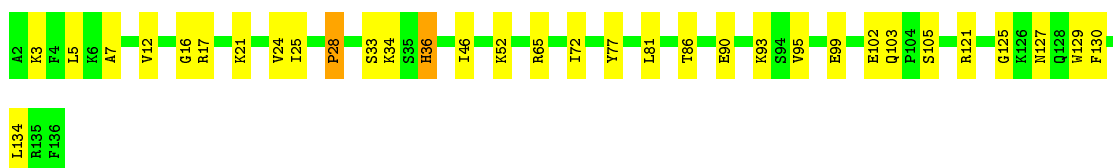
- Molecule 63: 60S ribosomal protein L27-A

Chain N7: 75% 25%



- Molecule 63: 60S ribosomal protein L27-A

Chain n7: 76% 23%



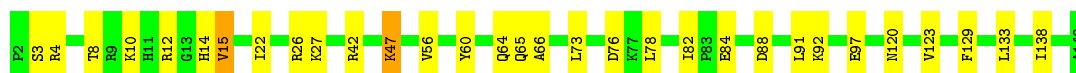
- Molecule 64: 60S ribosomal protein L28

Chain N8: 81% 17%

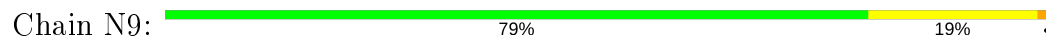


- Molecule 64: 60S ribosomal protein L28

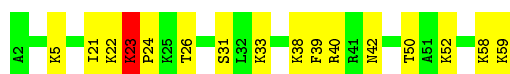
Chain n8: 79% 20%



- Molecule 65: 60S ribosomal protein L29



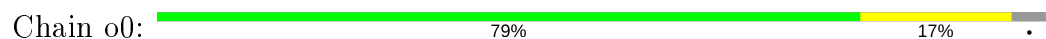
- Molecule 65: 60S ribosomal protein L29



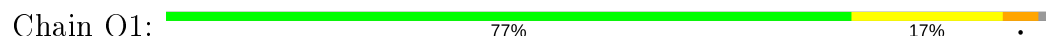
- Molecule 66: 60S ribosomal protein L30



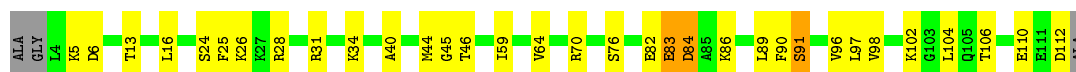
- Molecule 66: 60S ribosomal protein L30



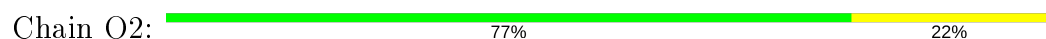
- Molecule 67: 60S ribosomal protein L31-A



- Molecule 67: 60S ribosomal protein L31-A



- Molecule 68: 60S ribosomal protein L32





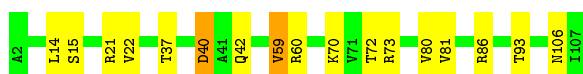
- Molecule 68: 60S ribosomal protein L32

Chain o2: 76% 20% ...



- Molecule 69: 60S ribosomal protein L33-A

Chain O3: 84% 14% .



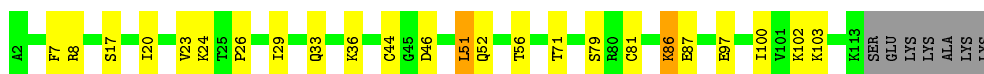
- Molecule 69: 60S ribosomal protein L33-A

Chain o3: 80% 17% .



- Molecule 70: 60S ribosomal protein L34-A

Chain O4: 74% 18% 6%



- Molecule 70: 60S ribosomal protein L34-A

Chain o4: 72% 22% 6%



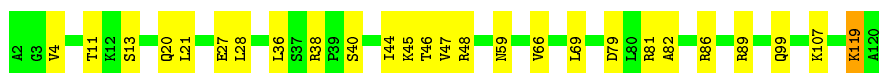
- Molecule 71: 60S ribosomal protein L35-A

Chain O5: 82% 17% .

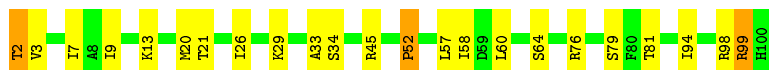
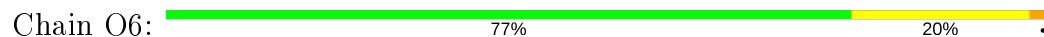


- Molecule 71: 60S ribosomal protein L35-A

Chain o5: 78% 21% .



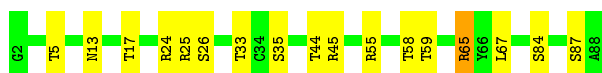
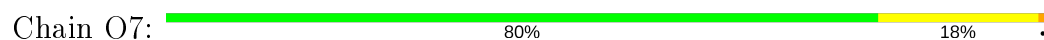
- Molecule 72: 60S ribosomal protein L36-A



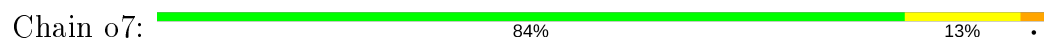
- Molecule 72: 60S ribosomal protein L36-A



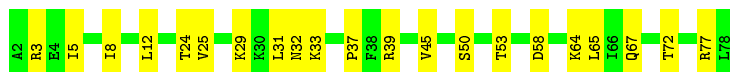
- Molecule 73: 60S ribosomal protein L37-A



- Molecule 73: 60S ribosomal protein L37-A



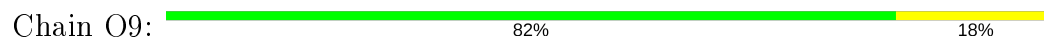
- Molecule 74: 60S ribosomal protein L38



- Molecule 74: 60S ribosomal protein L38



- Molecule 75: 60S ribosomal protein L39





- Molecule 75: 60S ribosomal protein L39

Chain o9: 84% 16%



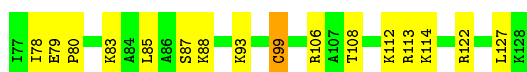
- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0: 85% 13%



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0: 69% 29%



- Molecule 77: 60S ribosomal protein L41-A

Chain Q1: 72% 28%



- Molecule 77: 60S ribosomal protein L41-A

Chain q1: 64% 32%



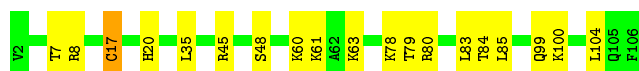
- Molecule 78: 60S ribosomal protein L42-A

Chain Q2: 72% 26%

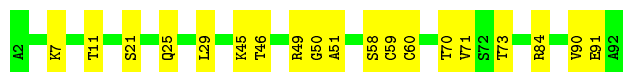
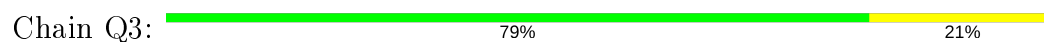


- Molecule 78: 60S ribosomal protein L42-A

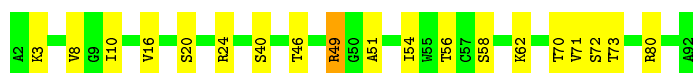
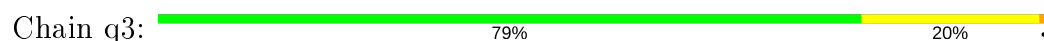
Chain q2: 82% 17%



- Molecule 79: 60S ribosomal protein L43-A



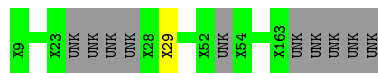
- Molecule 79: 60S ribosomal protein L43-A



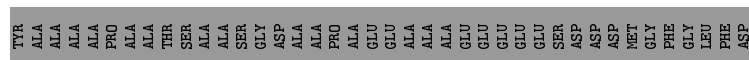
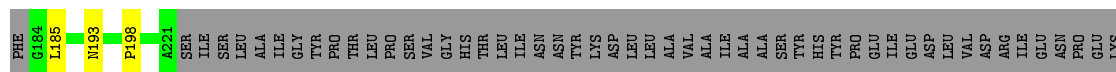
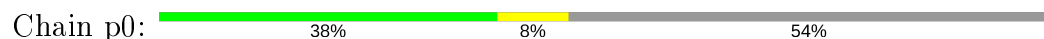
- Molecule 80: 40S ribosomal protein S30-A



- Molecule 81: Unknown Protein m2



- Molecule 82: 60S acidic ribosomal protein P0



- Molecule 83: Unknown Protein p1



There are no outlier residues recorded for this chain.

- Molecule 84: Unknown Protein p2

Chain p2:



100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

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

| Property | Value | Source |
|--|---|-----------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 435.84Å 286.77Å 303.77Å 90.00° 99.03° 90.00° | Depositor |
| Resolution (Å) | 49.70 – 3.30 | Depositor |
| % Data completeness (in resolution range) | 99.4 (49.70-3.30) | Depositor |
| R_{merge} | 0.31 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.34 (at 3.33Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: dev_1702) | Depositor |
| R, R_{free} | 0.202 , 0.255 | Depositor |
| Wilson B-factor (Å ²) | 90.1 | Xtriage |
| Anisotropy | 0.099 | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 411183 | wwPDB-VP |
| Average B, all atoms (Å ²) | 79.0 | 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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 3J6, ZN, OHX, MG

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 | 0.74 | 6/41698 (0.0%) | 1.29 | 289/64972 (0.4%) |
| 1 | 6 | 0.88 | 18/42765 (0.0%) | 1.38 | 477/66634 (0.7%) |
| 2 | S0 | 0.46 | 0/1617 | 0.66 | 0/2215 |
| 2 | s0 | 0.48 | 0/1623 | 0.69 | 0/2222 |
| 3 | S1 | 0.39 | 0/1735 | 0.65 | 1/2335 (0.0%) |
| 3 | s1 | 0.50 | 0/1748 | 0.70 | 1/2352 (0.0%) |
| 4 | S2 | 0.50 | 0/1665 | 0.66 | 0/2263 |
| 4 | s2 | 0.58 | 0/1665 | 0.72 | 0/2263 |
| 5 | S3 | 0.50 | 0/1759 | 0.66 | 0/2368 |
| 5 | s3 | 0.42 | 0/1759 | 0.60 | 0/2368 |
| 6 | S4 | 0.47 | 0/2109 | 0.70 | 1/2839 (0.0%) |
| 6 | s4 | 0.53 | 0/2109 | 0.73 | 0/2839 |
| 7 | S5 | 0.40 | 0/1629 | 0.59 | 0/2202 |
| 7 | s5 | 0.46 | 0/1629 | 0.69 | 0/2202 |
| 8 | S6 | 0.44 | 0/1823 | 0.64 | 0/2439 |
| 8 | s6 | 0.55 | 0/1779 | 0.70 | 0/2379 |
| 9 | S7 | 0.43 | 0/1506 | 0.65 | 0/2028 |
| 9 | s7 | 0.44 | 0/1516 | 0.65 | 0/2043 |
| 10 | S8 | 0.54 | 0/1514 | 0.71 | 2/2021 (0.1%) |
| 10 | s8 | 0.60 | 0/1514 | 0.74 | 0/2021 |
| 11 | S9 | 0.47 | 0/1519 | 0.65 | 0/2035 |
| 11 | s9 | 0.56 | 0/1519 | 0.78 | 1/2035 (0.0%) |
| 12 | C0 | 0.42 | 0/790 | 0.64 | 1/1069 (0.1%) |
| 12 | c0 | 0.37 | 0/777 | 0.66 | 3/1049 (0.3%) |
| 13 | C1 | 0.58 | 0/1240 | 0.70 | 0/1675 |
| 13 | c1 | 0.63 | 0/1194 | 0.76 | 0/1610 |
| 14 | C2 | 0.38 | 0/900 | 0.64 | 1/1224 (0.1%) |
| 14 | c2 | 0.29 | 0/900 | 0.57 | 0/1224 |
| 15 | C3 | 0.47 | 0/1215 | 0.68 | 2/1638 (0.1%) |
| 15 | c3 | 0.54 | 0/1215 | 0.71 | 0/1638 |
| 16 | C4 | 0.40 | 0/901 | 0.68 | 0/1217 |
| 16 | c4 | 0.52 | 0/960 | 0.74 | 1/1290 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | C5 | 0.46 | 0/998 | 0.65 | 0/1341 |
| 17 | c5 | 0.48 | 0/1060 | 0.70 | 1/1426 (0.1%) |
| 18 | C6 | 0.45 | 0/1125 | 0.68 | 1/1510 (0.1%) |
| 18 | c6 | 0.51 | 0/1131 | 0.70 | 0/1518 |
| 19 | C7 | 0.44 | 0/935 | 0.63 | 0/1254 |
| 19 | c7 | 0.47 | 0/914 | 0.69 | 0/1224 |
| 20 | C8 | 0.42 | 0/1211 | 0.64 | 0/1628 |
| 20 | c8 | 0.50 | 0/1211 | 0.71 | 1/1628 (0.1%) |
| 21 | C9 | 0.45 | 0/1130 | 0.65 | 1/1517 (0.1%) |
| 21 | c9 | 0.50 | 0/1130 | 0.67 | 1/1517 (0.1%) |
| 22 | D0 | 0.46 | 0/865 | 0.65 | 0/1169 |
| 22 | d0 | 0.48 | 0/892 | 0.68 | 0/1205 |
| 23 | D1 | 0.46 | 0/693 | 0.65 | 0/935 |
| 23 | d1 | 0.52 | 0/693 | 0.68 | 0/935 |
| 24 | D2 | 0.50 | 0/1038 | 0.75 | 2/1395 (0.1%) |
| 24 | d2 | 0.61 | 0/1038 | 0.76 | 1/1395 (0.1%) |
| 25 | D3 | 0.61 | 0/1139 | 0.75 | 0/1518 |
| 25 | d3 | 0.75 | 0/1139 | 0.86 | 2/1518 (0.1%) |
| 26 | D4 | 0.45 | 0/1087 | 0.61 | 0/1449 |
| 26 | d4 | 0.51 | 0/1087 | 0.71 | 0/1449 |
| 27 | D5 | 0.40 | 0/571 | 0.72 | 0/768 |
| 27 | d5 | 0.46 | 0/566 | 0.71 | 0/761 |
| 28 | D6 | 0.48 | 0/782 | 0.71 | 0/1047 |
| 28 | d6 | 0.65 | 0/782 | 0.79 | 1/1047 (0.1%) |
| 29 | D7 | 0.43 | 0/620 | 0.67 | 0/838 |
| 29 | d7 | 0.49 | 0/620 | 0.64 | 0/838 |
| 30 | D8 | 0.36 | 0/499 | 0.56 | 0/670 |
| 30 | d8 | 0.46 | 0/499 | 0.63 | 0/670 |
| 31 | D9 | 0.54 | 0/452 | 0.70 | 1/600 (0.2%) |
| 31 | d9 | 0.48 | 0/452 | 0.65 | 0/600 |
| 32 | E0 | 0.48 | 0/483 | 0.61 | 0/643 |
| 33 | E1 | 0.43 | 0/577 | 0.77 | 0/770 |
| 33 | e1 | 0.39 | 0/619 | 0.69 | 1/822 (0.1%) |
| 34 | SR | 0.37 | 0/2494 | 0.58 | 0/3393 |
| 34 | sR | 0.42 | 0/2495 | 0.59 | 0/3395 |
| 35 | SM | 0.53 | 0/1113 | 0.80 | 4/1502 (0.3%) |
| 35 | sM | 0.50 | 0/683 | 0.73 | 1/923 (0.1%) |
| 36 | 1 | 1.15 | 144/75394 (0.2%) | 1.64 | 1754/117545 (1.5%) |
| 36 | 5 | 1.19 | 180/75414 (0.2%) | 1.67 | 1900/117575 (1.6%) |
| 37 | 3 | 0.94 | 1/2883 (0.0%) | 1.44 | 31/4491 (0.7%) |
| 37 | 7 | 1.14 | 3/2883 (0.1%) | 1.67 | 68/4491 (1.5%) |
| 38 | 4 | 1.06 | 2/3746 (0.1%) | 1.55 | 59/5832 (1.0%) |
| 38 | 8 | 0.98 | 1/3746 (0.0%) | 1.42 | 27/5832 (0.5%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 39 | L2 | 0.70 | 0/1948 | 0.85 | 4/2617 (0.2%) |
| 39 | l2 | 0.67 | 0/1946 | 0.84 | 0/2614 |
| 40 | L3 | 0.73 | 0/3146 | 0.82 | 1/4228 (0.0%) |
| 40 | l3 | 0.83 | 2/3146 (0.1%) | 0.90 | 2/4228 (0.0%) |
| 41 | L4 | 0.81 | 2/2800 (0.1%) | 0.91 | 3/3790 (0.1%) |
| 41 | l4 | 0.72 | 1/2800 (0.0%) | 0.87 | 0/3790 |
| 42 | L5 | 0.57 | 0/2425 | 0.71 | 0/3271 |
| 42 | l5 | 0.70 | 0/2408 | 0.82 | 4/3248 (0.1%) |
| 43 | L6 | 0.74 | 0/1260 | 0.79 | 0/1694 |
| 43 | l6 | 0.75 | 0/1269 | 0.82 | 1/1705 (0.1%) |
| 44 | L7 | 0.76 | 0/1821 | 0.88 | 2/2451 (0.1%) |
| 44 | l7 | 0.84 | 0/1828 | 0.88 | 4/2461 (0.2%) |
| 45 | L8 | 0.56 | 0/1836 | 0.69 | 0/2481 |
| 45 | l8 | 0.51 | 0/1795 | 0.64 | 0/2429 |
| 46 | L9 | 0.64 | 0/1539 | 0.77 | 0/2073 |
| 46 | l9 | 0.80 | 0/1539 | 0.84 | 0/2073 |
| 47 | M0 | 0.77 | 1/1741 (0.1%) | 0.83 | 1/2335 (0.0%) |
| 47 | m0 | 0.77 | 1/1758 (0.1%) | 0.83 | 0/2358 |
| 48 | M1 | 0.51 | 0/1374 | 0.70 | 0/1842 |
| 48 | m1 | 0.67 | 0/1374 | 0.85 | 2/1842 (0.1%) |
| 49 | M3 | 0.75 | 0/1568 | 0.84 | 1/2106 (0.0%) |
| 49 | m3 | 0.68 | 0/1573 | 0.80 | 0/2113 |
| 50 | M4 | 0.73 | 0/1068 | 0.76 | 0/1438 |
| 50 | m4 | 0.82 | 0/1074 | 0.82 | 1/1446 (0.1%) |
| 51 | M5 | 0.72 | 0/1757 | 0.84 | 0/2354 |
| 51 | m5 | 0.66 | 0/1757 | 0.80 | 2/2354 (0.1%) |
| 52 | M6 | 0.82 | 0/1585 | 0.85 | 1/2128 (0.0%) |
| 52 | m6 | 0.98 | 2/1585 (0.1%) | 0.96 | 2/2128 (0.1%) |
| 53 | M7 | 0.80 | 1/1443 (0.1%) | 0.84 | 2/1944 (0.1%) |
| 53 | m7 | 0.84 | 0/1250 | 0.84 | 0/1683 |
| 54 | M8 | 0.78 | 0/1465 | 0.91 | 1/1965 (0.1%) |
| 54 | m8 | 0.71 | 0/1465 | 0.94 | 5/1965 (0.3%) |
| 55 | M9 | 0.56 | 0/1538 | 0.66 | 0/2050 |
| 55 | m9 | 0.62 | 0/1538 | 0.72 | 0/2050 |
| 56 | N0 | 0.74 | 0/1481 | 0.84 | 3/1990 (0.2%) |
| 56 | n0 | 0.89 | 0/1481 | 0.89 | 0/1990 |
| 57 | N1 | 0.76 | 0/1300 | 0.78 | 0/1743 |
| 57 | n1 | 0.83 | 2/1300 (0.2%) | 0.82 | 1/1743 (0.1%) |
| 58 | N2 | 0.46 | 0/812 | 0.63 | 0/1099 |
| 58 | n2 | 0.50 | 0/794 | 0.67 | 0/1076 |
| 59 | N3 | 0.69 | 0/1018 | 0.83 | 1/1369 (0.1%) |
| 59 | n3 | 0.81 | 0/1018 | 0.87 | 0/1369 |
| 60 | N4 | 0.55 | 0/712 | 0.66 | 0/958 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 60 | n4 | 0.67 | 0/1052 | 0.79 | 0/1398 |
| 61 | N5 | 0.63 | 0/979 | 0.77 | 1/1321 (0.1%) |
| 61 | n5 | 0.67 | 0/974 | 0.79 | 0/1314 |
| 62 | N6 | 0.74 | 0/1004 | 0.87 | 1/1341 (0.1%) |
| 62 | n6 | 0.63 | 0/1004 | 0.79 | 0/1341 |
| 63 | N7 | 0.54 | 0/1118 | 0.70 | 0/1497 |
| 63 | n7 | 0.49 | 0/1118 | 0.65 | 0/1497 |
| 64 | N8 | 0.75 | 0/1204 | 0.90 | 0/1612 |
| 64 | n8 | 0.77 | 0/1204 | 0.87 | 0/1612 |
| 65 | N9 | 0.65 | 0/473 | 0.77 | 1/629 (0.2%) |
| 65 | n9 | 0.79 | 0/473 | 0.97 | 1/629 (0.2%) |
| 66 | O0 | 0.50 | 0/751 | 0.66 | 0/1008 |
| 66 | o0 | 0.52 | 0/775 | 0.69 | 0/1040 |
| 67 | O1 | 0.63 | 0/890 | 0.72 | 0/1196 |
| 67 | o1 | 0.72 | 0/897 | 0.84 | 0/1205 |
| 68 | O2 | 0.84 | 0/1041 | 0.90 | 1/1394 (0.1%) |
| 68 | o2 | 0.81 | 0/1041 | 0.90 | 2/1394 (0.1%) |
| 69 | O3 | 0.89 | 0/868 | 0.87 | 1/1168 (0.1%) |
| 69 | o3 | 0.90 | 0/868 | 0.90 | 0/1168 |
| 70 | O4 | 0.59 | 0/890 | 0.79 | 1/1189 (0.1%) |
| 70 | o4 | 0.56 | 0/890 | 0.76 | 0/1189 |
| 71 | O5 | 0.71 | 0/978 | 0.78 | 0/1301 |
| 71 | o5 | 0.56 | 0/974 | 0.68 | 0/1297 |
| 72 | O6 | 0.66 | 0/778 | 0.76 | 0/1034 |
| 72 | o6 | 0.55 | 0/777 | 0.73 | 0/1033 |
| 73 | O7 | 0.75 | 0/696 | 0.99 | 3/923 (0.3%) |
| 73 | o7 | 0.70 | 0/696 | 0.86 | 1/923 (0.1%) |
| 74 | O8 | 0.52 | 0/618 | 0.68 | 0/826 |
| 74 | o8 | 0.50 | 0/614 | 0.68 | 0/822 |
| 75 | O9 | 0.74 | 0/443 | 0.88 | 0/588 |
| 75 | o9 | 0.66 | 0/443 | 0.79 | 0/588 |
| 76 | Q0 | 0.69 | 0/423 | 0.82 | 0/562 |
| 76 | q0 | 0.94 | 1/423 (0.2%) | 0.92 | 0/562 |
| 77 | Q1 | 0.61 | 0/234 | 0.78 | 0/300 |
| 77 | q1 | 0.78 | 0/234 | 1.00 | 0/300 |
| 78 | Q2 | 0.88 | 1/860 (0.1%) | 0.90 | 0/1136 |
| 78 | q2 | 0.79 | 1/860 (0.1%) | 0.77 | 1/1136 (0.1%) |
| 79 | Q3 | 0.71 | 0/701 | 0.81 | 1/934 (0.1%) |
| 79 | q3 | 0.71 | 0/701 | 0.80 | 0/934 |
| 80 | e0 | 0.58 | 0/499 | 0.74 | 0/665 |
| 82 | p0 | 0.46 | 0/1092 | 0.61 | 0/1474 |
| All | All | 0.90 | 370/430074 (0.1%) | 1.30 | 4696/631364 (0.7%) |

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 |
|-----|-------|---------------------|---------------------|
| 6 | S4 | 0 | 1 |
| 7 | s5 | 0 | 1 |
| 9 | S7 | 0 | 2 |
| 9 | s7 | 0 | 1 |
| 10 | s8 | 0 | 1 |
| 11 | s9 | 0 | 1 |
| 16 | C4 | 0 | 2 |
| 18 | c6 | 0 | 1 |
| 19 | C7 | 0 | 1 |
| 25 | D3 | 0 | 1 |
| 27 | D5 | 0 | 1 |
| 28 | D6 | 0 | 1 |
| 33 | E1 | 0 | 1 |
| 39 | L2 | 0 | 1 |
| 39 | l2 | 0 | 1 |
| 40 | L3 | 0 | 1 |
| 43 | L6 | 0 | 1 |
| 43 | l6 | 0 | 1 |
| 44 | l7 | 0 | 1 |
| 45 | L8 | 0 | 1 |
| 46 | L9 | 0 | 1 |
| 48 | M1 | 0 | 1 |
| 52 | M6 | 0 | 1 |
| 52 | m6 | 0 | 1 |
| 54 | m8 | 0 | 1 |
| 56 | N0 | 0 | 1 |
| 56 | n0 | 0 | 1 |
| 59 | n3 | 0 | 1 |
| 64 | n8 | 0 | 1 |
| 65 | N9 | 0 | 2 |
| 67 | O1 | 0 | 1 |
| 72 | O6 | 0 | 1 |
| 81 | m2 | 0 | 1 |
| All | All | 0 | 36 |

The worst 5 of 370 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 78 | Q2 | 17 | CYS | CB-SG | 12.26 | 2.03 | 1.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 36 | 5 | 1152 | G | N9-C4 | -11.12 | 1.29 | 1.38 |
| 36 | 5 | 2726 | C | N3-C4 | -9.57 | 1.27 | 1.33 |
| 78 | q2 | 17 | CYS | CB-SG | 9.14 | 1.97 | 1.82 |
| 36 | 1 | 3181 | C | N3-C4 | -8.78 | 1.27 | 1.33 |

The worst 5 of 4696 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 36 | 5 | 1116 | G | O5'-P-OP1 | -18.97 | 87.94 | 110.70 |
| 36 | 5 | 1152 | G | C2-N3-C4 | -18.00 | 102.90 | 111.90 |
| 36 | 5 | 1152 | G | N3-C4-C5 | 17.23 | 137.22 | 128.60 |
| 36 | 5 | 1152 | G | N3-C4-N9 | -15.73 | 116.56 | 126.00 |
| 36 | 1 | 1495 | U | C5-C6-N1 | -15.66 | 114.87 | 122.70 |

There are no chirality outliers.

5 of 36 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 16 | C4 | 123 | SER | Peptide |
| 16 | C4 | 124 | ASP | Peptide |
| 6 | S4 | 167 | GLY | Peptide |
| 9 | S7 | 131 | PHE | Peptide |
| 9 | S7 | 30 | SER | 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%) | 139 (68%) | 40 (20%) | 25 (12%) | 0 | 1 |
| 2 | s0 | 204/251 (81%) | 148 (72%) | 37 (18%) | 19 (9%) | 0 | 4 |
| 3 | S1 | 212/254 (84%) | 147 (69%) | 38 (18%) | 27 (13%) | 0 | 1 |
| 3 | s1 | 214/254 (84%) | 164 (77%) | 34 (16%) | 16 (8%) | 1 | 7 |
| 4 | S2 | 215/253 (85%) | 177 (82%) | 26 (12%) | 12 (6%) | 2 | 11 |
| 4 | s2 | 215/253 (85%) | 171 (80%) | 27 (13%) | 17 (8%) | 1 | 6 |
| 5 | S3 | 221/239 (92%) | 176 (80%) | 32 (14%) | 13 (6%) | 1 | 10 |
| 5 | s3 | 221/239 (92%) | 172 (78%) | 30 (14%) | 19 (9%) | 1 | 5 |
| 6 | S4 | 258/260 (99%) | 205 (80%) | 39 (15%) | 14 (5%) | 2 | 12 |
| 6 | s4 | 258/260 (99%) | 206 (80%) | 34 (13%) | 18 (7%) | 1 | 7 |
| 7 | S5 | 204/224 (91%) | 149 (73%) | 38 (19%) | 17 (8%) | 1 | 5 |
| 7 | s5 | 204/224 (91%) | 145 (71%) | 44 (22%) | 15 (7%) | 1 | 7 |
| 8 | S6 | 224/236 (95%) | 194 (87%) | 20 (9%) | 10 (4%) | 2 | 15 |
| 8 | s6 | 216/236 (92%) | 184 (85%) | 20 (9%) | 12 (6%) | 2 | 11 |
| 9 | S7 | 182/189 (96%) | 132 (72%) | 33 (18%) | 17 (9%) | 0 | 4 |
| 9 | s7 | 184/189 (97%) | 142 (77%) | 23 (12%) | 19 (10%) | 0 | 3 |
| 10 | S8 | 184/200 (92%) | 150 (82%) | 23 (12%) | 11 (6%) | 1 | 10 |
| 10 | s8 | 184/200 (92%) | 155 (84%) | 21 (11%) | 8 (4%) | 2 | 16 |
| 11 | S9 | 183/196 (93%) | 146 (80%) | 24 (13%) | 13 (7%) | 1 | 7 |
| 11 | s9 | 183/196 (93%) | 144 (79%) | 25 (14%) | 14 (8%) | 1 | 6 |
| 12 | C0 | 94/105 (90%) | 68 (72%) | 17 (18%) | 9 (10%) | 0 | 4 |
| 12 | c0 | 92/105 (88%) | 60 (65%) | 16 (17%) | 16 (17%) | 0 | 1 |
| 13 | C1 | 153/155 (99%) | 118 (77%) | 22 (14%) | 13 (8%) | 1 | 5 |
| 13 | c1 | 144/155 (93%) | 112 (78%) | 25 (17%) | 7 (5%) | 2 | 14 |
| 14 | C2 | 122/142 (86%) | 70 (57%) | 28 (23%) | 24 (20%) | 0 | 0 |
| 14 | c2 | 122/142 (86%) | 68 (56%) | 36 (30%) | 18 (15%) | 0 | 1 |
| 15 | C3 | 148/150 (99%) | 120 (81%) | 16 (11%) | 12 (8%) | 1 | 6 |
| 15 | c3 | 148/150 (99%) | 112 (76%) | 23 (16%) | 13 (9%) | 1 | 5 |
| 16 | C4 | 125/136 (92%) | 92 (74%) | 22 (18%) | 11 (9%) | 1 | 5 |
| 16 | c4 | 126/136 (93%) | 94 (75%) | 22 (18%) | 10 (8%) | 1 | 6 |
| 17 | C5 | 122/141 (86%) | 89 (73%) | 24 (20%) | 9 (7%) | 1 | 7 |
| 17 | c5 | 133/141 (94%) | 87 (65%) | 28 (21%) | 18 (14%) | 0 | 1 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 18 | C6 | 139/142 (98%) | 108 (78%) | 18 (13%) | 13 (9%) | 0 | 4 |
| 18 | c6 | 140/142 (99%) | 111 (79%) | 19 (14%) | 10 (7%) | 1 | 7 |
| 19 | C7 | 116/136 (85%) | 86 (74%) | 19 (16%) | 11 (10%) | 0 | 4 |
| 19 | c7 | 113/136 (83%) | 84 (74%) | 21 (19%) | 8 (7%) | 1 | 7 |
| 20 | C8 | 143/145 (99%) | 110 (77%) | 22 (15%) | 11 (8%) | 1 | 6 |
| 20 | c8 | 143/145 (99%) | 112 (78%) | 21 (15%) | 10 (7%) | 1 | 7 |
| 21 | C9 | 141/143 (99%) | 114 (81%) | 20 (14%) | 7 (5%) | 2 | 14 |
| 21 | c9 | 141/143 (99%) | 109 (77%) | 27 (19%) | 5 (4%) | 3 | 21 |
| 22 | D0 | 105/120 (88%) | 87 (83%) | 13 (12%) | 5 (5%) | 2 | 14 |
| 22 | d0 | 108/120 (90%) | 83 (77%) | 13 (12%) | 12 (11%) | 0 | 2 |
| 23 | D1 | 85/87 (98%) | 54 (64%) | 21 (25%) | 10 (12%) | 0 | 2 |
| 23 | d1 | 85/87 (98%) | 66 (78%) | 12 (14%) | 7 (8%) | 1 | 5 |
| 24 | D2 | 127/129 (98%) | 103 (81%) | 20 (16%) | 4 (3%) | 4 | 23 |
| 24 | d2 | 127/129 (98%) | 111 (87%) | 14 (11%) | 2 (2%) | 9 | 36 |
| 25 | D3 | 142/144 (99%) | 107 (75%) | 22 (16%) | 13 (9%) | 1 | 4 |
| 25 | d3 | 142/144 (99%) | 120 (84%) | 16 (11%) | 6 (4%) | 3 | 17 |
| 26 | D4 | 132/134 (98%) | 107 (81%) | 20 (15%) | 5 (4%) | 3 | 19 |
| 26 | d4 | 132/134 (98%) | 101 (76%) | 22 (17%) | 9 (7%) | 1 | 8 |
| 27 | D5 | 68/107 (64%) | 39 (57%) | 18 (26%) | 11 (16%) | 0 | 1 |
| 27 | d5 | 67/107 (63%) | 51 (76%) | 13 (19%) | 3 (4%) | 2 | 15 |
| 28 | D6 | 95/97 (98%) | 55 (58%) | 21 (22%) | 19 (20%) | 0 | 0 |
| 28 | d6 | 95/97 (98%) | 72 (76%) | 14 (15%) | 9 (10%) | 0 | 4 |
| 29 | D7 | 79/81 (98%) | 58 (73%) | 16 (20%) | 5 (6%) | 1 | 9 |
| 29 | d7 | 79/81 (98%) | 64 (81%) | 10 (13%) | 5 (6%) | 1 | 9 |
| 30 | D8 | 61/66 (92%) | 45 (74%) | 11 (18%) | 5 (8%) | 1 | 5 |
| 30 | d8 | 61/66 (92%) | 40 (66%) | 15 (25%) | 6 (10%) | 0 | 3 |
| 31 | D9 | 51/55 (93%) | 43 (84%) | 6 (12%) | 2 (4%) | 3 | 18 |
| 31 | d9 | 51/55 (93%) | 41 (80%) | 4 (8%) | 6 (12%) | 0 | 2 |
| 32 | E0 | 58/60 (97%) | 48 (83%) | 7 (12%) | 3 (5%) | 2 | 13 |
| 33 | E1 | 69/76 (91%) | 31 (45%) | 22 (32%) | 16 (23%) | 0 | 0 |
| 33 | e1 | 74/76 (97%) | 35 (47%) | 18 (24%) | 21 (28%) | 0 | 0 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|----------|-------------|----|
| 34 | SR | 316/318 (99%) | 263 (83%) | 41 (13%) | 12 (4%) | 3 | 19 |
| 34 | sR | 316/318 (99%) | 269 (85%) | 37 (12%) | 10 (3%) | 4 | 22 |
| 35 | SM | 155/273 (57%) | 101 (65%) | 33 (21%) | 21 (14%) | 0 | 1 |
| 35 | sM | 98/273 (36%) | 56 (57%) | 29 (30%) | 13 (13%) | 0 | 1 |
| 39 | L2 | 250/253 (99%) | 208 (83%) | 30 (12%) | 12 (5%) | 2 | 14 |
| 39 | l2 | 250/253 (99%) | 206 (82%) | 26 (10%) | 18 (7%) | 1 | 7 |
| 40 | L3 | 384/386 (100%) | 319 (83%) | 46 (12%) | 19 (5%) | 2 | 14 |
| 40 | l3 | 384/386 (100%) | 331 (86%) | 40 (10%) | 13 (3%) | 3 | 22 |
| 41 | L4 | 359/361 (99%) | 289 (80%) | 42 (12%) | 28 (8%) | 1 | 6 |
| 41 | l4 | 359/361 (99%) | 290 (81%) | 44 (12%) | 25 (7%) | 1 | 7 |
| 42 | L5 | 294/296 (99%) | 235 (80%) | 42 (14%) | 17 (6%) | 1 | 11 |
| 42 | l5 | 292/296 (99%) | 244 (84%) | 36 (12%) | 12 (4%) | 3 | 17 |
| 43 | L6 | 152/175 (87%) | 126 (83%) | 21 (14%) | 5 (3%) | 4 | 22 |
| 43 | l6 | 153/175 (87%) | 129 (84%) | 21 (14%) | 3 (2%) | 7 | 32 |
| 44 | L7 | 220/243 (90%) | 175 (80%) | 35 (16%) | 10 (4%) | 2 | 15 |
| 44 | l7 | 221/243 (91%) | 179 (81%) | 34 (15%) | 8 (4%) | 3 | 20 |
| 45 | L8 | 231/255 (91%) | 176 (76%) | 42 (18%) | 13 (6%) | 2 | 11 |
| 45 | l8 | 229/255 (90%) | 179 (78%) | 32 (14%) | 18 (8%) | 1 | 6 |
| 46 | L9 | 189/191 (99%) | 159 (84%) | 23 (12%) | 7 (4%) | 3 | 20 |
| 46 | l9 | 189/191 (99%) | 159 (84%) | 24 (13%) | 6 (3%) | 4 | 22 |
| 47 | M0 | 207/220 (94%) | 165 (80%) | 27 (13%) | 15 (7%) | 1 | 7 |
| 47 | m0 | 209/220 (95%) | 155 (74%) | 39 (19%) | 15 (7%) | 1 | 7 |
| 48 | M1 | 167/173 (96%) | 120 (72%) | 27 (16%) | 20 (12%) | 0 | 2 |
| 48 | m1 | 167/173 (96%) | 134 (80%) | 22 (13%) | 11 (7%) | 1 | 8 |
| 49 | M3 | 191/198 (96%) | 151 (79%) | 29 (15%) | 11 (6%) | 1 | 11 |
| 49 | m3 | 192/198 (97%) | 159 (83%) | 17 (9%) | 16 (8%) | 1 | 5 |
| 50 | M4 | 134/137 (98%) | 108 (81%) | 17 (13%) | 9 (7%) | 1 | 8 |
| 50 | m4 | 135/137 (98%) | 113 (84%) | 18 (13%) | 4 (3%) | 4 | 24 |
| 51 | M5 | 201/203 (99%) | 176 (88%) | 20 (10%) | 5 (2%) | 5 | 27 |
| 51 | m5 | 201/203 (99%) | 167 (83%) | 26 (13%) | 8 (4%) | 3 | 18 |
| 52 | M6 | 195/198 (98%) | 172 (88%) | 18 (9%) | 5 (3%) | 5 | 27 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 52 | m6 | 195/198 (98%) | 164 (84%) | 22 (11%) | 9 (5%) | 2 | 15 |
| 53 | M7 | 181/183 (99%) | 139 (77%) | 32 (18%) | 10 (6%) | 2 | 11 |
| 53 | m7 | 153/183 (84%) | 134 (88%) | 17 (11%) | 2 (1%) | 12 | 40 |
| 54 | M8 | 183/185 (99%) | 154 (84%) | 24 (13%) | 5 (3%) | 5 | 26 |
| 54 | m8 | 183/185 (99%) | 151 (82%) | 27 (15%) | 5 (3%) | 5 | 26 |
| 55 | M9 | 186/188 (99%) | 157 (84%) | 25 (13%) | 4 (2%) | 6 | 30 |
| 55 | m9 | 186/188 (99%) | 154 (83%) | 28 (15%) | 4 (2%) | 6 | 30 |
| 56 | N0 | 170/172 (99%) | 151 (89%) | 13 (8%) | 6 (4%) | 3 | 21 |
| 56 | n0 | 170/172 (99%) | 157 (92%) | 11 (6%) | 2 (1%) | 13 | 42 |
| 57 | N1 | 157/159 (99%) | 134 (85%) | 16 (10%) | 7 (4%) | 2 | 15 |
| 57 | n1 | 157/159 (99%) | 128 (82%) | 23 (15%) | 6 (4%) | 3 | 19 |
| 58 | N2 | 98/120 (82%) | 74 (76%) | 16 (16%) | 8 (8%) | 1 | 5 |
| 58 | n2 | 96/120 (80%) | 79 (82%) | 11 (12%) | 6 (6%) | 1 | 9 |
| 59 | N3 | 134/136 (98%) | 119 (89%) | 12 (9%) | 3 (2%) | 6 | 30 |
| 59 | n3 | 134/136 (98%) | 124 (92%) | 9 (7%) | 1 (1%) | 22 | 54 |
| 60 | N4 | 96/155 (62%) | 69 (72%) | 19 (20%) | 8 (8%) | 1 | 5 |
| 60 | n4 | 133/155 (86%) | 108 (81%) | 14 (10%) | 11 (8%) | 1 | 5 |
| 61 | N5 | 119/141 (84%) | 107 (90%) | 11 (9%) | 1 (1%) | 19 | 51 |
| 61 | n5 | 118/141 (84%) | 92 (78%) | 17 (14%) | 9 (8%) | 1 | 6 |
| 62 | N6 | 124/126 (98%) | 107 (86%) | 13 (10%) | 4 (3%) | 4 | 22 |
| 62 | n6 | 124/126 (98%) | 109 (88%) | 11 (9%) | 4 (3%) | 4 | 22 |
| 63 | N7 | 133/135 (98%) | 105 (79%) | 20 (15%) | 8 (6%) | 1 | 10 |
| 63 | n7 | 133/135 (98%) | 99 (74%) | 24 (18%) | 10 (8%) | 1 | 7 |
| 64 | N8 | 146/148 (99%) | 112 (77%) | 25 (17%) | 9 (6%) | 1 | 10 |
| 64 | n8 | 146/148 (99%) | 114 (78%) | 24 (16%) | 8 (6%) | 2 | 11 |
| 65 | N9 | 56/58 (97%) | 48 (86%) | 7 (12%) | 1 (2%) | 8 | 35 |
| 65 | n9 | 56/58 (97%) | 36 (64%) | 14 (25%) | 6 (11%) | 0 | 3 |
| 66 | O0 | 95/104 (91%) | 81 (85%) | 12 (13%) | 2 (2%) | 7 | 31 |
| 66 | o0 | 98/104 (94%) | 90 (92%) | 7 (7%) | 1 (1%) | 15 | 46 |
| 67 | O1 | 107/112 (96%) | 92 (86%) | 8 (8%) | 7 (6%) | 1 | 9 |
| 67 | o1 | 107/112 (96%) | 83 (78%) | 12 (11%) | 12 (11%) | 0 | 2 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|------------|-----------|-------------|-----|
| 68 | O2 | 125/129 (97%) | 109 (87%) | 12 (10%) | 4 (3%) | 4 | 22 |
| 68 | o2 | 125/129 (97%) | 101 (81%) | 17 (14%) | 7 (6%) | 2 | 11 |
| 69 | O3 | 104/106 (98%) | 88 (85%) | 14 (14%) | 2 (2%) | 8 | 34 |
| 69 | o3 | 104/106 (98%) | 90 (86%) | 10 (10%) | 4 (4%) | 3 | 19 |
| 70 | O4 | 110/119 (92%) | 87 (79%) | 19 (17%) | 4 (4%) | 3 | 20 |
| 70 | o4 | 110/119 (92%) | 93 (84%) | 13 (12%) | 4 (4%) | 3 | 20 |
| 71 | O5 | 117/119 (98%) | 97 (83%) | 16 (14%) | 4 (3%) | 3 | 22 |
| 71 | o5 | 117/119 (98%) | 93 (80%) | 20 (17%) | 4 (3%) | 3 | 22 |
| 72 | O6 | 97/99 (98%) | 80 (82%) | 9 (9%) | 8 (8%) | 1 | 5 |
| 72 | o6 | 97/99 (98%) | 77 (79%) | 12 (12%) | 8 (8%) | 1 | 5 |
| 73 | O7 | 85/87 (98%) | 69 (81%) | 15 (18%) | 1 (1%) | 13 | 42 |
| 73 | o7 | 85/87 (98%) | 67 (79%) | 15 (18%) | 3 (4%) | 3 | 21 |
| 74 | O8 | 75/77 (97%) | 60 (80%) | 12 (16%) | 3 (4%) | 3 | 18 |
| 74 | o8 | 75/77 (97%) | 62 (83%) | 9 (12%) | 4 (5%) | 2 | 12 |
| 75 | O9 | 48/50 (96%) | 38 (79%) | 8 (17%) | 2 (4%) | 3 | 17 |
| 75 | o9 | 48/50 (96%) | 40 (83%) | 8 (17%) | 0 | 100 | 100 |
| 76 | Q0 | 50/52 (96%) | 45 (90%) | 3 (6%) | 2 (4%) | 3 | 18 |
| 76 | q0 | 50/52 (96%) | 43 (86%) | 5 (10%) | 2 (4%) | 3 | 18 |
| 77 | Q1 | 23/25 (92%) | 21 (91%) | 2 (9%) | 0 | 100 | 100 |
| 77 | q1 | 23/25 (92%) | 19 (83%) | 2 (9%) | 2 (9%) | 1 | 5 |
| 78 | Q2 | 103/105 (98%) | 72 (70%) | 23 (22%) | 8 (8%) | 1 | 6 |
| 78 | q2 | 103/105 (98%) | 93 (90%) | 8 (8%) | 2 (2%) | 8 | 34 |
| 79 | Q3 | 89/91 (98%) | 76 (85%) | 8 (9%) | 5 (6%) | 2 | 11 |
| 79 | q3 | 89/91 (98%) | 75 (84%) | 10 (11%) | 4 (4%) | 2 | 15 |
| 80 | e0 | 60/62 (97%) | 44 (73%) | 12 (20%) | 4 (7%) | 1 | 8 |
| 82 | p0 | 139/311 (45%) | 119 (86%) | 14 (10%) | 6 (4%) | 2 | 16 |
| All | All | 22333/24141 (92%) | 17773 (80%) | 3160 (14%) | 1400 (6%) | 1 | 9 |

5 of 1400 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | S0 | 4 | PRO |
| 2 | S0 | 39 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | S0 | 66 | ALA |
| 2 | S0 | 102 | PHE |
| 2 | S0 | 103 | THR |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%) | 135 (82%) | 29 (18%) | 2 | 8 |
| 2 | s0 | 165/209 (79%) | 131 (79%) | 34 (21%) | 1 | 4 |
| 3 | S1 | 191/223 (86%) | 149 (78%) | 42 (22%) | 1 | 3 |
| 3 | s1 | 192/223 (86%) | 156 (81%) | 36 (19%) | 1 | 6 |
| 4 | S2 | 176/204 (86%) | 134 (76%) | 42 (24%) | 0 | 2 |
| 4 | s2 | 176/204 (86%) | 128 (73%) | 48 (27%) | 0 | 1 |
| 5 | S3 | 182/194 (94%) | 141 (78%) | 41 (22%) | 1 | 3 |
| 5 | s3 | 182/194 (94%) | 144 (79%) | 38 (21%) | 1 | 4 |
| 6 | S4 | 221/221 (100%) | 177 (80%) | 44 (20%) | 1 | 5 |
| 6 | s4 | 221/221 (100%) | 183 (83%) | 38 (17%) | 2 | 9 |
| 7 | S5 | 173/190 (91%) | 143 (83%) | 30 (17%) | 2 | 8 |
| 7 | s5 | 173/190 (91%) | 144 (83%) | 29 (17%) | 2 | 9 |
| 8 | S6 | 188/201 (94%) | 154 (82%) | 34 (18%) | 1 | 7 |
| 8 | s6 | 187/201 (93%) | 153 (82%) | 34 (18%) | 1 | 7 |
| 9 | S7 | 165/169 (98%) | 135 (82%) | 30 (18%) | 1 | 7 |
| 9 | s7 | 165/169 (98%) | 130 (79%) | 35 (21%) | 1 | 4 |
| 10 | S8 | 150/161 (93%) | 117 (78%) | 33 (22%) | 1 | 3 |
| 10 | s8 | 150/161 (93%) | 124 (83%) | 26 (17%) | 2 | 8 |
| 11 | S9 | 158/165 (96%) | 120 (76%) | 38 (24%) | 0 | 2 |
| 11 | s9 | 158/165 (96%) | 120 (76%) | 38 (24%) | 0 | 2 |
| 12 | C0 | 77/98 (79%) | 66 (86%) | 11 (14%) | 3 | 15 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 12 | c0 | 73/98 (74%) | 63 (86%) | 10 (14%) | 3 | 16 |
| 13 | C1 | 129/136 (95%) | 109 (84%) | 20 (16%) | 2 | 12 |
| 13 | c1 | 129/136 (95%) | 104 (81%) | 25 (19%) | 1 | 5 |
| 14 | C2 | 88/118 (75%) | 67 (76%) | 21 (24%) | 0 | 2 |
| 14 | c2 | 88/118 (75%) | 71 (81%) | 17 (19%) | 1 | 6 |
| 15 | C3 | 127/127 (100%) | 104 (82%) | 23 (18%) | 1 | 7 |
| 15 | c3 | 127/127 (100%) | 93 (73%) | 34 (27%) | 0 | 1 |
| 16 | C4 | 81/104 (78%) | 61 (75%) | 20 (25%) | 0 | 2 |
| 16 | c4 | 97/104 (93%) | 69 (71%) | 28 (29%) | 0 | 1 |
| 17 | C5 | 101/117 (86%) | 83 (82%) | 18 (18%) | 2 | 8 |
| 17 | c5 | 103/117 (88%) | 90 (87%) | 13 (13%) | 4 | 19 |
| 18 | C6 | 117/118 (99%) | 92 (79%) | 25 (21%) | 1 | 4 |
| 18 | c6 | 118/118 (100%) | 91 (77%) | 27 (23%) | 1 | 3 |
| 19 | C7 | 94/124 (76%) | 70 (74%) | 24 (26%) | 0 | 2 |
| 19 | c7 | 92/124 (74%) | 74 (80%) | 18 (20%) | 1 | 5 |
| 20 | C8 | 128/128 (100%) | 102 (80%) | 26 (20%) | 1 | 5 |
| 20 | c8 | 128/128 (100%) | 99 (77%) | 29 (23%) | 1 | 3 |
| 21 | C9 | 115/115 (100%) | 93 (81%) | 22 (19%) | 1 | 6 |
| 21 | c9 | 115/115 (100%) | 91 (79%) | 24 (21%) | 1 | 4 |
| 22 | D0 | 100/113 (88%) | 81 (81%) | 19 (19%) | 1 | 6 |
| 22 | d0 | 103/113 (91%) | 76 (74%) | 27 (26%) | 0 | 2 |
| 23 | D1 | 74/74 (100%) | 56 (76%) | 18 (24%) | 0 | 2 |
| 23 | d1 | 74/74 (100%) | 53 (72%) | 21 (28%) | 0 | 1 |
| 24 | D2 | 110/110 (100%) | 92 (84%) | 18 (16%) | 2 | 10 |
| 24 | d2 | 110/110 (100%) | 96 (87%) | 14 (13%) | 4 | 19 |
| 25 | D3 | 119/119 (100%) | 100 (84%) | 19 (16%) | 2 | 11 |
| 25 | d3 | 119/119 (100%) | 94 (79%) | 25 (21%) | 1 | 4 |
| 26 | D4 | 112/112 (100%) | 92 (82%) | 20 (18%) | 2 | 8 |
| 26 | d4 | 112/112 (100%) | 91 (81%) | 21 (19%) | 1 | 6 |
| 27 | D5 | 61/88 (69%) | 42 (69%) | 19 (31%) | 0 | 1 |
| 27 | d5 | 61/88 (69%) | 53 (87%) | 8 (13%) | 4 | 17 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 28 | D6 | 83/83 (100%) | 60 (72%) | 23 (28%) | 0 | 1 |
| 28 | d6 | 83/83 (100%) | 62 (75%) | 21 (25%) | 0 | 2 |
| 29 | D7 | 70/70 (100%) | 58 (83%) | 12 (17%) | 2 | 9 |
| 29 | d7 | 70/70 (100%) | 62 (89%) | 8 (11%) | 5 | 22 |
| 30 | D8 | 56/59 (95%) | 44 (79%) | 12 (21%) | 1 | 4 |
| 30 | d8 | 56/59 (95%) | 46 (82%) | 10 (18%) | 2 | 8 |
| 31 | D9 | 47/48 (98%) | 41 (87%) | 6 (13%) | 4 | 18 |
| 31 | d9 | 47/48 (98%) | 35 (74%) | 12 (26%) | 0 | 2 |
| 32 | E0 | 51/51 (100%) | 42 (82%) | 9 (18%) | 2 | 8 |
| 33 | E1 | 62/66 (94%) | 41 (66%) | 21 (34%) | 0 | 1 |
| 33 | e1 | 66/66 (100%) | 50 (76%) | 16 (24%) | 0 | 2 |
| 34 | SR | 260/261 (100%) | 227 (87%) | 33 (13%) | 4 | 19 |
| 34 | sR | 260/261 (100%) | 221 (85%) | 39 (15%) | 3 | 13 |
| 35 | SM | 97/228 (42%) | 75 (77%) | 22 (23%) | 1 | 3 |
| 35 | sM | 54/228 (24%) | 42 (78%) | 12 (22%) | 1 | 3 |
| 39 | L2 | 193/195 (99%) | 155 (80%) | 38 (20%) | 1 | 5 |
| 39 | l2 | 192/195 (98%) | 150 (78%) | 42 (22%) | 1 | 3 |
| 40 | L3 | 321/322 (100%) | 250 (78%) | 71 (22%) | 1 | 3 |
| 40 | l3 | 320/322 (99%) | 250 (78%) | 70 (22%) | 1 | 3 |
| 41 | L4 | 288/288 (100%) | 224 (78%) | 64 (22%) | 1 | 3 |
| 41 | l4 | 288/288 (100%) | 222 (77%) | 66 (23%) | 1 | 3 |
| 42 | L5 | 244/244 (100%) | 199 (82%) | 45 (18%) | 1 | 7 |
| 42 | l5 | 243/244 (100%) | 190 (78%) | 53 (22%) | 1 | 4 |
| 43 | L6 | 134/152 (88%) | 115 (86%) | 19 (14%) | 3 | 15 |
| 43 | l6 | 135/152 (89%) | 114 (84%) | 21 (16%) | 2 | 12 |
| 44 | L7 | 186/204 (91%) | 162 (87%) | 24 (13%) | 4 | 18 |
| 44 | l7 | 187/204 (92%) | 158 (84%) | 29 (16%) | 2 | 12 |
| 45 | L8 | 187/207 (90%) | 145 (78%) | 42 (22%) | 1 | 3 |
| 45 | l8 | 177/207 (86%) | 143 (81%) | 34 (19%) | 1 | 6 |
| 46 | L9 | 171/171 (100%) | 136 (80%) | 35 (20%) | 1 | 4 |
| 46 | l9 | 171/171 (100%) | 127 (74%) | 44 (26%) | 0 | 2 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 47 | M0 | 177/186 (95%) | 143 (81%) | 34 (19%) | 1 | 6 |
| 47 | m0 | 179/186 (96%) | 146 (82%) | 33 (18%) | 1 | 7 |
| 48 | M1 | 147/150 (98%) | 116 (79%) | 31 (21%) | 1 | 4 |
| 48 | m1 | 147/150 (98%) | 110 (75%) | 37 (25%) | 0 | 2 |
| 49 | M3 | 154/158 (98%) | 130 (84%) | 24 (16%) | 2 | 12 |
| 49 | m3 | 154/158 (98%) | 123 (80%) | 31 (20%) | 1 | 5 |
| 50 | M4 | 107/108 (99%) | 88 (82%) | 19 (18%) | 2 | 8 |
| 50 | m4 | 108/108 (100%) | 89 (82%) | 19 (18%) | 2 | 8 |
| 51 | M5 | 175/175 (100%) | 142 (81%) | 33 (19%) | 1 | 6 |
| 51 | m5 | 175/175 (100%) | 142 (81%) | 33 (19%) | 1 | 6 |
| 52 | M6 | 160/161 (99%) | 133 (83%) | 27 (17%) | 2 | 9 |
| 52 | m6 | 160/161 (99%) | 126 (79%) | 34 (21%) | 1 | 4 |
| 53 | M7 | 140/145 (97%) | 110 (79%) | 30 (21%) | 1 | 4 |
| 53 | m7 | 125/145 (86%) | 100 (80%) | 25 (20%) | 1 | 5 |
| 54 | M8 | 150/150 (100%) | 132 (88%) | 18 (12%) | 5 | 20 |
| 54 | m8 | 150/150 (100%) | 120 (80%) | 30 (20%) | 1 | 5 |
| 55 | M9 | 153/153 (100%) | 125 (82%) | 28 (18%) | 1 | 7 |
| 55 | m9 | 153/153 (100%) | 126 (82%) | 27 (18%) | 2 | 8 |
| 56 | N0 | 156/156 (100%) | 125 (80%) | 31 (20%) | 1 | 5 |
| 56 | n0 | 156/156 (100%) | 120 (77%) | 36 (23%) | 1 | 3 |
| 57 | N1 | 136/136 (100%) | 109 (80%) | 27 (20%) | 1 | 5 |
| 57 | n1 | 136/136 (100%) | 104 (76%) | 32 (24%) | 1 | 3 |
| 58 | N2 | 87/106 (82%) | 77 (88%) | 10 (12%) | 5 | 22 |
| 58 | n2 | 85/106 (80%) | 69 (81%) | 16 (19%) | 1 | 6 |
| 59 | N3 | 104/104 (100%) | 84 (81%) | 20 (19%) | 1 | 6 |
| 59 | n3 | 104/104 (100%) | 90 (86%) | 14 (14%) | 4 | 16 |
| 60 | N4 | 57/129 (44%) | 51 (90%) | 6 (10%) | 7 | 25 |
| 60 | n4 | 100/129 (78%) | 83 (83%) | 17 (17%) | 2 | 9 |
| 61 | N5 | 104/117 (89%) | 81 (78%) | 23 (22%) | 1 | 3 |
| 61 | n5 | 104/117 (89%) | 82 (79%) | 22 (21%) | 1 | 4 |
| 62 | N6 | 109/109 (100%) | 83 (76%) | 26 (24%) | 0 | 2 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 62 | n6 | 109/109 (100%) | 85 (78%) | 24 (22%) | 1 | 3 |
| 63 | N7 | 115/115 (100%) | 89 (77%) | 26 (23%) | 1 | 3 |
| 63 | n7 | 115/115 (100%) | 90 (78%) | 25 (22%) | 1 | 4 |
| 64 | N8 | 118/118 (100%) | 96 (81%) | 22 (19%) | 1 | 7 |
| 64 | n8 | 118/118 (100%) | 94 (80%) | 24 (20%) | 1 | 5 |
| 65 | N9 | 46/46 (100%) | 37 (80%) | 9 (20%) | 1 | 5 |
| 65 | n9 | 46/46 (100%) | 35 (76%) | 11 (24%) | 0 | 2 |
| 66 | O0 | 81/87 (93%) | 61 (75%) | 20 (25%) | 0 | 2 |
| 66 | o0 | 84/87 (97%) | 67 (80%) | 17 (20%) | 1 | 5 |
| 67 | O1 | 92/96 (96%) | 73 (79%) | 19 (21%) | 1 | 4 |
| 67 | o1 | 94/96 (98%) | 70 (74%) | 24 (26%) | 0 | 2 |
| 68 | O2 | 109/110 (99%) | 86 (79%) | 23 (21%) | 1 | 4 |
| 68 | o2 | 109/110 (99%) | 85 (78%) | 24 (22%) | 1 | 3 |
| 69 | O3 | 90/90 (100%) | 74 (82%) | 16 (18%) | 2 | 8 |
| 69 | o3 | 90/90 (100%) | 70 (78%) | 20 (22%) | 1 | 3 |
| 70 | O4 | 95/101 (94%) | 74 (78%) | 21 (22%) | 1 | 3 |
| 70 | o4 | 95/101 (94%) | 73 (77%) | 22 (23%) | 1 | 3 |
| 71 | O5 | 104/104 (100%) | 84 (81%) | 20 (19%) | 1 | 6 |
| 71 | o5 | 103/104 (99%) | 80 (78%) | 23 (22%) | 1 | 3 |
| 72 | O6 | 81/81 (100%) | 64 (79%) | 17 (21%) | 1 | 4 |
| 72 | o6 | 80/81 (99%) | 58 (72%) | 22 (28%) | 0 | 1 |
| 73 | O7 | 70/70 (100%) | 55 (79%) | 15 (21%) | 1 | 4 |
| 73 | o7 | 70/70 (100%) | 57 (81%) | 13 (19%) | 1 | 7 |
| 74 | O8 | 68/68 (100%) | 50 (74%) | 18 (26%) | 0 | 1 |
| 74 | o8 | 67/68 (98%) | 51 (76%) | 16 (24%) | 0 | 2 |
| 75 | O9 | 45/45 (100%) | 38 (84%) | 7 (16%) | 2 | 12 |
| 75 | o9 | 45/45 (100%) | 37 (82%) | 8 (18%) | 2 | 8 |
| 76 | Q0 | 47/47 (100%) | 40 (85%) | 7 (15%) | 3 | 13 |
| 76 | q0 | 47/47 (100%) | 33 (70%) | 14 (30%) | 0 | 1 |
| 77 | Q1 | 23/23 (100%) | 16 (70%) | 7 (30%) | 0 | 1 |
| 77 | q1 | 23/23 (100%) | 15 (65%) | 8 (35%) | 0 | 1 |

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Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|------------|-------------|---|
| 78 | Q2 | 90/90 (100%) | 68 (76%) | 22 (24%) | 0 | 2 |
| 78 | q2 | 90/90 (100%) | 73 (81%) | 17 (19%) | 1 | 6 |
| 79 | Q3 | 71/71 (100%) | 58 (82%) | 13 (18%) | 1 | 7 |
| 79 | q3 | 71/71 (100%) | 55 (78%) | 16 (22%) | 1 | 3 |
| 80 | e0 | 53/53 (100%) | 38 (72%) | 15 (28%) | 0 | 1 |
| 82 | p0 | 105/253 (42%) | 84 (80%) | 21 (20%) | 1 | 5 |
| All | All | 18729/20239 (92%) | 14954 (80%) | 3775 (20%) | 1 | 5 |

5 of 3775 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 71 | O5 | 21 | LEU |
| 9 | s7 | 129 | LEU |
| 64 | n8 | 65 | GLN |
| 74 | O8 | 3 | ARG |
| 4 | s2 | 90 | THR |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 61 | N5 | 111 | ASN |
| 11 | s9 | 124 | HIS |
| 57 | n1 | 122 | GLN |
| 65 | N9 | 48 | HIS |
| 79 | Q3 | 33 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------------|-------------------|-----------------|
| 1 | 2 | 1747/1800 (97%) | 511 (29%) | 56 (3%) |
| 1 | 6 | 1793/1800 (99%) | 498 (27%) | 50 (2%) |
| 36 | 1 | 3145/3396 (92%) | 747 (23%) | 83 (2%) |
| 36 | 5 | 3145/3396 (92%) | 744 (23%) | 85 (2%) |
| 37 | 3 | 120/121 (99%) | 19 (15%) | 3 (2%) |
| 37 | 7 | 120/121 (99%) | 23 (19%) | 3 (2%) |
| 38 | 4 | 157/158 (99%) | 45 (28%) | 4 (2%) |
| 38 | 8 | 157/158 (99%) | 41 (26%) | 2 (1%) |
| All | All | 10384/10950 (94%) | 2628 (25%) | 286 (2%) |

5 of 2628 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 2 | 2 | A |
| 1 | 2 | 4 | C |
| 1 | 2 | 20 | G |
| 1 | 2 | 21 | U |
| 1 | 2 | 25 | C |

5 of 286 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 36 | 1 | 3218 | A |
| 1 | 6 | 542 | A |
| 36 | 5 | 2887 | A |
| 36 | 1 | 3319 | U |
| 38 | 4 | 125 | U |

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 2554 ligands modelled in this entry, 1422 are monoatomic - leaving 1132 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 | 2 | 2039 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2189 | 1 | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2128 | - | 0,6,6 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 5 | 4219 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4104 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2090 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | M9 | 203 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2174 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2114 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2138 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4147 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4192 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3938 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4190 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4184 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 3 | 215 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2161 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4080 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4049 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3964 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2122 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4000 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4048 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 4 | 229 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4105 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2083 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4137 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4092 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4169 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3969 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4167 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2130 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 3 | 222 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3913 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2186 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2088 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4185 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3996 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | n3 | 204 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4054 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3994 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4051 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | l5 | 304 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | O9 | 101 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 7 | 218 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4139 | - | 0,6,6 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 5 | 3904 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4110 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3866 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | M0 | 304 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3991 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4035 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3906 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4035 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2175 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3937 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4195 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4206 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2048 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2082 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4016 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2111 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2053 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4127 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2116 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4028 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4000 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4208 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3986 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 8 | 225 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4176 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4094 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4038 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4064 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2051 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3912 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4178 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4093 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 7 | 224 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2071 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4209 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4065 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2033 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2168 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4003 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 3 | 219 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 4 | 224 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2086 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3966 | - | 0,6,6 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 6 | 2196 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2124 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4058 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2171 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4194 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2143 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4211 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4049 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4171 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4088 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3963 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2173 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2155 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4026 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2161 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4082 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4171 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4186 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4132 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4189 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2053 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2115 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2139 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4239 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2089 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2101 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2191 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3940 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3974 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4069 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | L4 | 403 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4090 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3893 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4165 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3899 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3901 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4099 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3936 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3984 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4073 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3990 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4135 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3899 | - | 0,6,6 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 3 | 221 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4218 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2184 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4240 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2075 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4030 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | O3 | 202 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4229 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2069 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 14 | 403 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 7 | 219 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2128 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3930 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3954 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2137 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4012 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3948 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | m6 | 203 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2032 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3874 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2056 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2105 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3982 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2136 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2097 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4070 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2026 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3887 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4106 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2096 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4072 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2156 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3872 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4086 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3952 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3965 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4006 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2066 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2119 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4095 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4008 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2097 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3984 | - | 0,6,6 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 1 | 4157 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4132 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2046 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4071 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4233 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3891 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3881 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | D3 | 202 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4115 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4040 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4131 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4117 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4241 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3992 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4036 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4125 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2084 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4183 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4164 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4004 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | m7 | 206 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2146 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4223 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3943 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2170 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4066 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3998 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2078 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4120 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3987 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4215 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4103 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4102 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4189 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4090 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2145 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2112 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2176 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4196 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3963 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4200 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2051 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2063 | - | 0,6,6 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 2 | 2141 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3882 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3924 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2165 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3912 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3929 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4099 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3983 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4060 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3934 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2102 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2044 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2041 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | O6 | 201 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2119 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4007 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2117 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4165 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 15 | 307 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2087 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3961 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4206 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3905 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 13 | 404 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4010 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4039 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3927 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4077 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4230 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3922 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3875 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3976 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4093 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2111 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3907 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 7 | 225 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4200 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4084 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2046 | - | 0,6,6 | 0.00 | - | - | | |
| 88 | 3J6 | 5 | 4246 | 85 | 21,24,24 | 1.17 | 1 (4%) | 25,42,42 | 1.19 | 2 (8%) |
| 86 | OHX | 1 | 4154 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 4 | 225 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2140 | - | 0,6,6 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 1 | 4046 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 3 | 218 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2080 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4225 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4052 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 7 | 223 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3895 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3900 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2040 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4007 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2134 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4094 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2131 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4222 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2090 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3957 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4145 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4204 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4182 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3992 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2147 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4092 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3919 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4166 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3955 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4163 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2160 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2049 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3871 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2098 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2203 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4113 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3894 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2150 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3870 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4100 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2166 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4042 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 4 | 236 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3985 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4086 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2060 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2193 | - | 0,6,6 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 5 | 4009 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4245 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3937 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3939 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4012 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 4 | 232 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2105 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3890 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2120 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2145 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 7 | 220 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4102 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4042 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4052 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4076 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3896 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2080 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4158 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | o7 | 502 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4144 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3998 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2167 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3982 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2190 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4010 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2113 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2065 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3971 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4198 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4169 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3950 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2087 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3972 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 4 | 231 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2159 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4047 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2056 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4205 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3967 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2148 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3975 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3959 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | c5 | 201 | - | 0,6,6 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 2 | 2096 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3917 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3909 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2065 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2064 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4156 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | SR | 401 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3958 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2151 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4170 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2094 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4083 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4109 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4063 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4126 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4107 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4021 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3909 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4024 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2129 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3928 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3995 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2045 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2178 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4124 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4031 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4129 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3903 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2104 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3880 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | O1 | 201 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4167 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2120 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2118 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4179 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4037 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2086 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2126 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4030 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4112 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4051 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3914 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2079 | - | 0,6,6 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 5 | 4159 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2073 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4085 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4168 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4157 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3942 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2081 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2127 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4110 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4138 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3956 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2076 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4061 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4117 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4145 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4023 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2154 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4014 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4152 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3978 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4055 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2059 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 8 | 217 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3897 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4214 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4068 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2136 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3980 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2091 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4040 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2085 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3934 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2182 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2146 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | M7 | 206 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 7 | 222 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3966 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4203 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2109 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4202 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4059 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3979 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | n3 | 203 | - | 0,6,6 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 6 | 2169 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2083 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4067 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4130 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4184 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4208 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4027 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3995 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4142 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2168 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2109 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2185 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 8 | 231 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4025 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2067 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 7 | 226 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2175 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4187 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2172 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2049 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3956 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2076 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3878 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4180 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4050 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | o3 | 203 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3969 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4211 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2201 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4172 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2113 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3978 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3972 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2180 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4153 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2054 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4142 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | c3 | 201 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4057 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | d9 | 102 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4065 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3974 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4123 | - | 0,6,6 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 2 | 2025 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2125 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2104 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3893 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3902 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4199 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3915 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3997 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4121 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4063 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4226 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4074 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2036 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 15 | 306 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2094 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4091 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2038 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2093 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4150 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4224 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4096 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2043 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4014 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4129 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3913 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4005 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3957 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3945 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4136 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | m8 | 201 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2154 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3908 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2204 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4207 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2082 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4101 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3990 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | o7 | 503 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4158 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4153 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | m1 | 202 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4156 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2159 | - | 0,6,6 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 1 | 4089 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4083 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3908 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3983 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4088 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 3 | 225 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 3 | 226 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3947 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2070 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4133 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4108 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2027 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4064 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3941 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | M7 | 205 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4174 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3910 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2134 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2181 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3987 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | s1 | 302 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3962 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4150 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4128 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4079 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4161 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3976 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3979 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3916 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4146 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4109 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2158 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 4 | 228 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2194 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3961 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2164 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2052 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2177 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2066 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2142 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4191 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4244 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4062 | - | 0,6,6 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 5 | 3921 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2130 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3902 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4021 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3938 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3928 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2078 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4148 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2054 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4201 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2165 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3925 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4017 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4100 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2155 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2172 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2112 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2173 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3950 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2074 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4198 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2162 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4203 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4201 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2064 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2144 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4077 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3947 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4085 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2085 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | S8 | 302 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4016 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3898 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4155 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4013 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3897 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2170 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4160 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2031 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2131 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2110 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3905 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4152 | - | 0,6,6 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 5 | 3973 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4036 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3926 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4128 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | d4 | 201 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | s8 | 303 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2069 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4137 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4026 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4168 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | l5 | 305 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4031 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | m4 | 201 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2030 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3911 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4041 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3933 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4003 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | O7 | 103 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3933 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2024 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4149 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 8 | 223 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4024 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4025 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3922 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4140 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2061 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4231 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2163 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4022 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4217 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3907 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2166 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4055 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4182 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2197 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4062 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2057 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2061 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2103 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4044 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4131 | - | 0,6,6 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 6 | 2106 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4087 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4134 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2163 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2118 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3944 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4113 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3975 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2093 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4046 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4087 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4108 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3906 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2048 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4056 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4053 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4001 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4210 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4066 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3941 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3973 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4075 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4078 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2116 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4179 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4133 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4236 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4001 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4111 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2153 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4143 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2144 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3923 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2124 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4089 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4111 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2081 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4190 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3999 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4196 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4204 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2135 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2195 | - | 0,6,6 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 1 | 3929 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4191 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4116 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 8 | 230 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4019 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3919 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4205 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2199 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | D9 | 102 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2057 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4043 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | C3 | 202 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4166 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4004 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3989 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3918 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | L3 | 404 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4161 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2063 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2125 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4045 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2042 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4125 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2095 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2164 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | S6 | 301 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4212 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4181 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3989 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 8 | 218 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4034 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 8 | 222 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4018 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3962 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4154 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2107 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2108 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 4 | 234 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 8 | 220 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3993 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4175 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2077 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4119 | - | 0,6,6 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 5 | 3948 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 8 | 229 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4114 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2079 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2099 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2149 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2095 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4181 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3894 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | M5 | 303 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3883 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4043 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4227 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4095 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3927 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2152 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2132 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4078 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4059 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4180 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 4 | 223 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3930 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4033 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2052 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4101 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 8 | 228 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2152 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4091 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2123 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3877 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4202 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4121 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2068 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 4 | 226 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3945 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2029 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2028 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4053 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3952 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2102 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3970 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 4 | 221 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3968 | - | 0,6,6 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 1 | 3981 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3915 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4207 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3965 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 3 | 216 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3942 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4220 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4041 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4143 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4097 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4106 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3939 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4074 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4103 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4177 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4071 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 8 | 219 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2123 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | C8 | 201 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2058 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2148 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4172 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4209 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2084 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2047 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4122 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4033 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | m0 | 302 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4149 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3867 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4104 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3968 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3993 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2151 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4076 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4193 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4216 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2070 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2035 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2058 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4175 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4194 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4124 | - | 0,6,6 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 2 | 2108 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4188 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 8 | 224 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4070 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2073 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3885 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4114 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4011 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2133 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4029 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2101 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2037 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4058 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4192 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2156 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3924 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4047 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2074 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4032 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4019 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4148 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3918 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2140 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 19 | 202 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2062 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3904 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4126 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4160 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4127 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4020 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3954 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4073 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2192 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4155 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2100 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4221 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | L3 | 405 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4237 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4015 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2034 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3916 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4140 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3964 | - | 0,6,6 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | sR | 401 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4097 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2160 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4151 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4193 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3994 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4118 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4195 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4116 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | c8 | 203 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 14 | 402 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4188 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3946 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2121 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3901 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2187 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4080 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3999 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4163 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2072 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3921 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2142 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4017 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2075 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2177 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3955 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2055 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4082 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3971 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4060 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3896 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4056 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2174 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2092 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4081 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4015 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2150 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3926 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3931 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4037 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2110 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3940 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4122 | - | 0,6,6 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 2 | 2059 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 3 | 223 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3986 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3931 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2167 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4028 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3988 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3996 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3910 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2117 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4115 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4213 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2050 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2200 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2089 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4096 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4002 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2139 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3936 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4020 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2135 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4061 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2137 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4141 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3960 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | m5 | 303 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3932 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2100 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3959 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2122 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2023 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4210 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4136 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3900 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3892 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4162 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3951 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4123 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4243 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2129 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3903 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2126 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4075 | - | 0,6,6 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 1 | 3873 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3988 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2141 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3869 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2092 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3949 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4187 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2153 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2202 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2114 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2127 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4173 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3944 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4023 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4178 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2121 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4011 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4038 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4039 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4139 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2133 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | n9 | 102 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2176 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4174 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3898 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4048 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4212 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3953 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3977 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4199 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2068 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4018 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2132 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4164 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 4 | 235 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2179 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2158 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2157 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 4 | 227 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4009 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4069 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4045 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4147 | - | 0,6,6 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | m0 | 303 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | s1 | 303 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2198 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4079 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4134 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2178 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3991 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3935 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4027 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4146 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 8 | 227 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4050 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2067 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2183 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4176 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2103 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4183 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3943 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2157 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2138 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3868 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4044 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4197 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2098 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 4 | 222 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3960 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4054 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | o2 | 201 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4119 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4013 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3970 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4098 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2188 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3985 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3911 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3925 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3920 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3923 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2047 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 8 | 221 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 8 | 226 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3884 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4170 | - | 0,6,6 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 2 | 2077 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4068 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4185 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3967 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2169 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 8 | 216 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4186 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4002 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | Q2 | 502 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2179 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4232 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3932 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4238 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2162 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4098 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 3 | 217 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3949 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4057 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 3 | 224 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2115 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3935 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2149 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2091 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4067 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4072 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4022 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | q2 | 502 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4130 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | N9 | 101 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4162 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3876 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2171 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2050 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4029 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2088 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2106 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2107 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4197 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4107 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3914 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4034 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3895 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3953 | - | 0,6,6 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 1 | 4120 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4105 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4173 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 4 | 233 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2099 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3980 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | C5 | 201 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3997 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3879 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4228 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2060 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4008 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4151 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3886 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3889 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4118 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4242 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2071 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2147 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4235 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4177 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4084 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3981 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4159 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4081 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | l3 | 405 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4234 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 4 | 230 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3946 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4005 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4006 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3977 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4032 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3917 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4135 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2045 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2062 | - | 0,6,6 | 0.00 | - | - | | |
| 88 | 3J6 | 1 | 4213 | 85 | 21,24,24 | 2.31 | 3 (14%) | 25,42,42 | 1.98 | 6 (24%) |
| 86 | OHX | 2 | 2143 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 7 | 221 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 7 | 227 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3920 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3958 | - | 0,6,6 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 5 | 4112 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 3951 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 2 | 2055 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 3 | 220 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 5 | 4138 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 3888 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 6 | 2072 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | n6 | 203 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4144 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | O4 | 201 | - | 0,6,6 | 0.00 | - | - | | |
| 86 | OHX | 1 | 4141 | - | 0,6,6 | 0.00 | - | - | | |

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 | 3J6 | 1 | 4213 | 85 | - | 0/3/68/68 | 0/5/4/4 |
| 88 | 3J6 | 5 | 4246 | 85 | - | 3/3/68/68 | 0/5/4/4 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 88 | 1 | 4213 | 3J6 | C4-C3 | 7.70 | 1.66 | 1.54 |
| 88 | 1 | 4213 | 3J6 | O2-C11 | 6.28 | 1.55 | 1.44 |
| 88 | 1 | 4213 | 3J6 | C11-C7 | -2.53 | 1.49 | 1.56 |
| 88 | 5 | 4246 | 3J6 | C4-C3 | 2.33 | 1.58 | 1.54 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 88 | 1 | 4213 | 3J6 | O2-C12-C11 | 5.21 | 64.68 | 59.35 |
| 88 | 1 | 4213 | 3J6 | C11-C7-C4 | -4.60 | 103.63 | 106.74 |
| 88 | 1 | 4213 | 3J6 | O2-C11-C7 | -3.21 | 113.91 | 117.98 |
| 88 | 1 | 4213 | 3J6 | O3-C3-C4 | 3.06 | 116.13 | 112.50 |
| 88 | 1 | 4213 | 3J6 | C12-O2-C11 | -2.81 | 57.23 | 60.91 |

There are no chirality outliers.

All (3) torsion outliers are listed below:

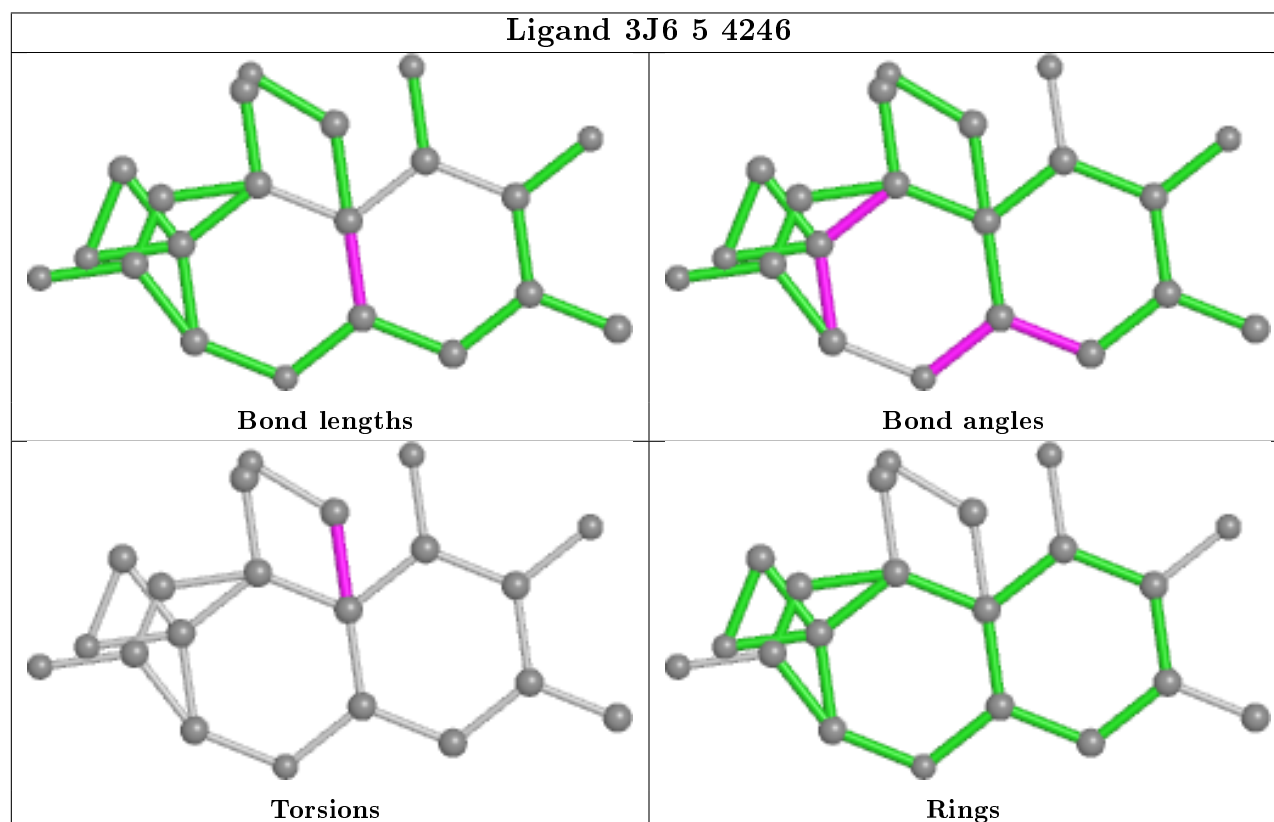
| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|--------------|
| 88 | 5 | 4246 | 3J6 | O5-C14-C4-C5 |
| 88 | 5 | 4246 | 3J6 | O5-C14-C4-C7 |
| 88 | 5 | 4246 | 3J6 | O5-C14-C4-C3 |

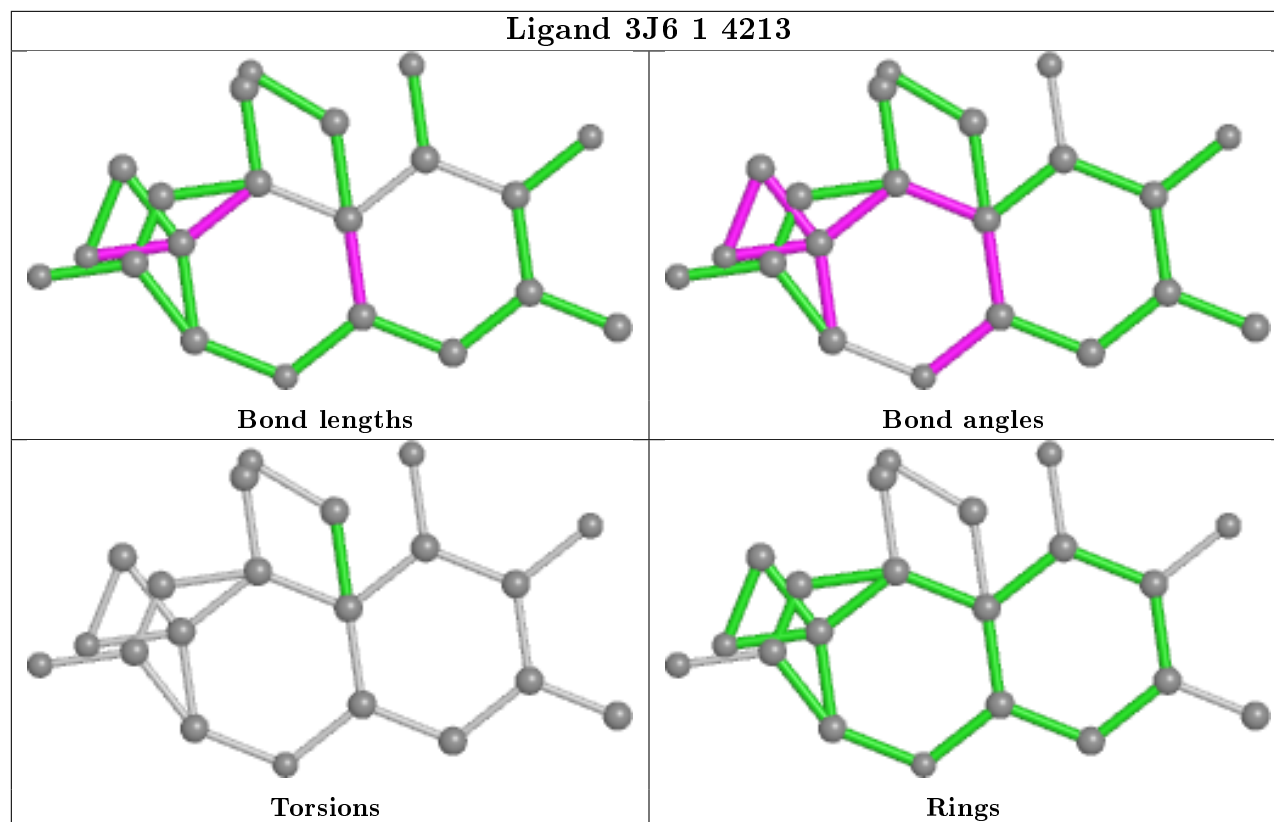
There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 86 | S6 | 301 | OHX | 0 | 1 |

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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