



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:00 PM GMT

PDB ID : 4U55
Title : Crystal structure of Cryptopleurine bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-24
Resolution : 3.20 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : **FAILED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

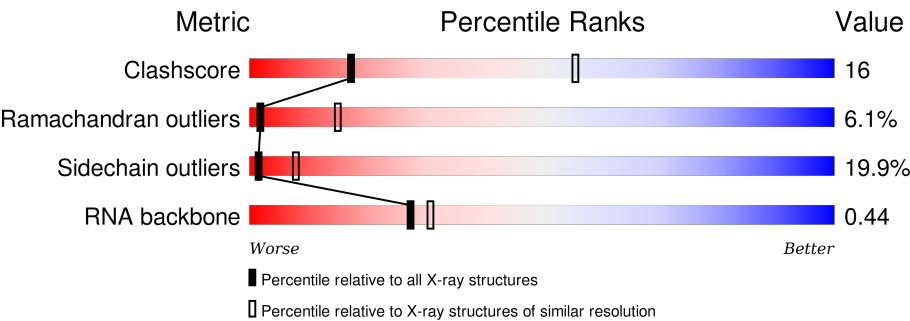
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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)) |
|-----------------------|-----------------------------|---|
| Clashscore | 102246 | 1024 (3.22-3.18) |
| Ramachandran outliers | 100387 | 1004 (3.22-3.18) |
| Sidechain outliers | 100360 | 1003 (3.22-3.18) |
| RNA backbone | 2183 | 1079 (3.70-2.70) |

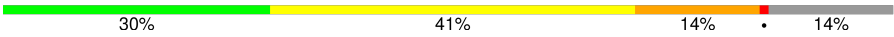





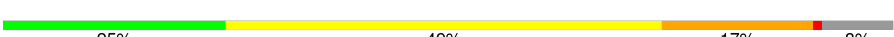

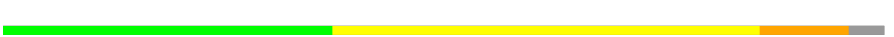

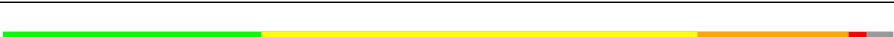


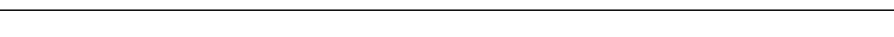
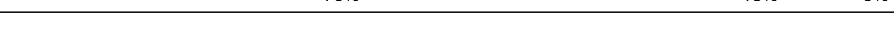
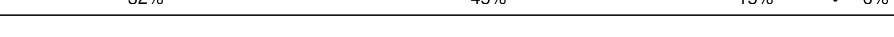

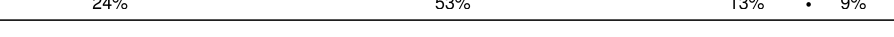

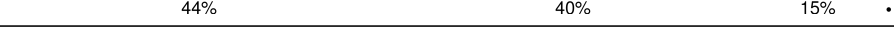

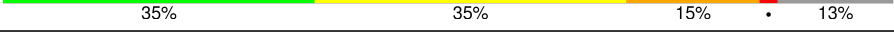



The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS failed to run properly.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | 2 | 1800 | <div><div></div><div>32%43%19%••</div></div> |
| 1 | 6 | 1800 | <div><div></div><div>34%44%19%•</div></div> |
| 2 | S0 | 251 | <div><div></div><div>25%43%14%•18%</div></div> |
| 2 | s0 | 251 | <div><div></div><div>62%18%•18%</div></div> |
| 3 | S1 | 254 | <div><div></div><div>15%49%18%•16%</div></div> |
| 3 | s1 | 254 | <div><div></div><div>66%18%•15%</div></div> |


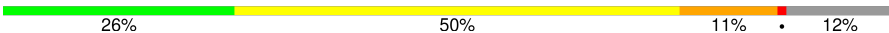



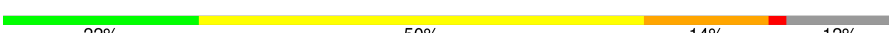





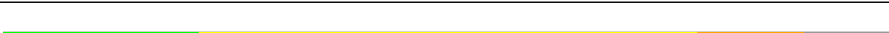












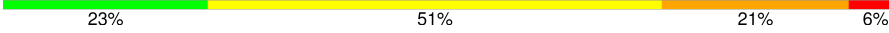
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 4 | S2 | 253 |  |
| 4 | s2 | 253 |  |
| 5 | S3 | 239 |  |
| 5 | s3 | 239 |  |
| 6 | S4 | 260 |  |
| 6 | s4 | 260 |  |
| 7 | S5 | 224 |  |
| 7 | s5 | 224 |  |
| 8 | S6 | 236 |  |
| 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 |  |



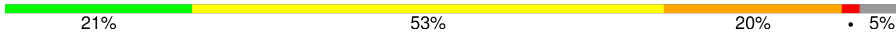

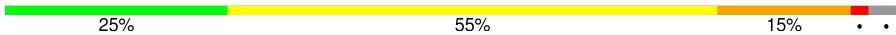

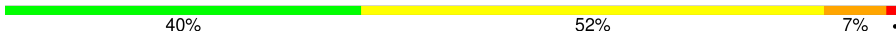
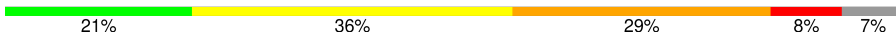

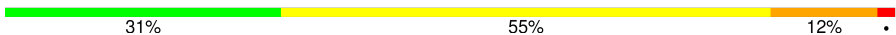



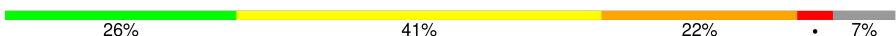
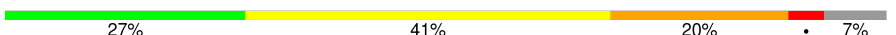

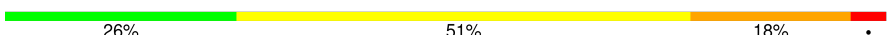
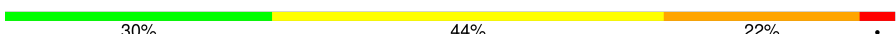







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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 16 | c4 | 136 |  |
| 17 | C5 | 141 |  |
| 17 | c5 | 141 |  |
| 18 | C6 | 142 |  |
| 18 | c6 | 142 |  |
| 19 | C7 | 136 |  |
| 19 | c7 | 136 |  |
| 20 | C8 | 145 |  |
| 20 | c8 | 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 |  |





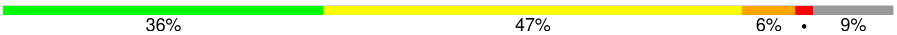

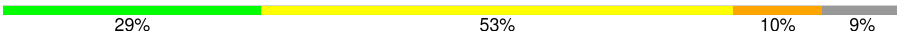

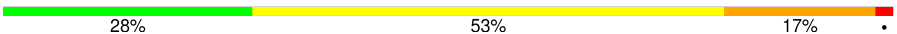

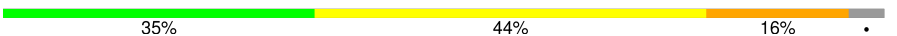

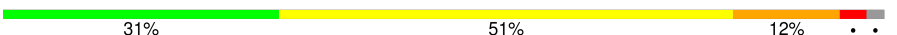












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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 29 | D7 | 81 |  |
| 29 | d7 | 81 |  |
| 30 | D8 | 66 |  |
| 30 | d8 | 66 |  |
| 31 | D9 | 55 |  |
| 31 | d9 | 55 |  |
| 32 | E0 | 60 |  |
| 33 | E1 | 76 |  |
| 33 | e1 | 76 |  |
| 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 |  |


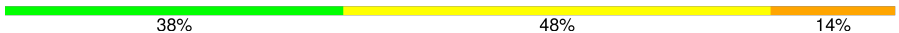



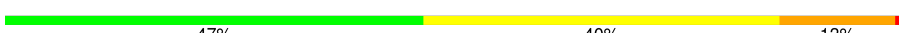





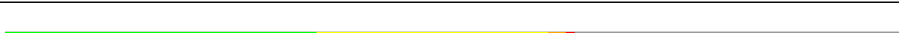






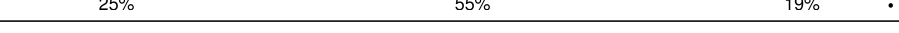






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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 42 | L5 | 296 |  |
| 42 | l5 | 296 |  |
| 43 | L6 | 175 |  |
| 43 | l6 | 175 |  |
| 44 | L7 | 243 |  |
| 44 | l7 | 243 |  |
| 45 | L8 | 255 |  |
| 45 | l8 | 255 |  |
| 46 | L9 | 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 |  |



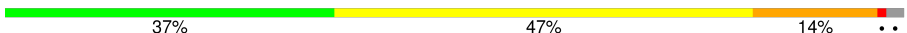



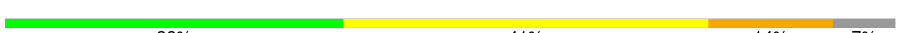


















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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 54 | m8 | 185 |  |
| 55 | M9 | 188 |  |
| 55 | m9 | 188 |  |
| 56 | N0 | 172 |  |
| 56 | n0 | 172 |  |
| 57 | N1 | 159 |  |
| 57 | n1 | 159 |  |
| 58 | N2 | 120 |  |
| 58 | n2 | 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 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 67 | O1 | 112 |  |
| 67 | o1 | 112 |  |
| 68 | O2 | 129 |  |
| 68 | o2 | 129 |  |
| 69 | O3 | 106 |  |
| 69 | o3 | 106 |  |
| 70 | O4 | 120 |  |
| 70 | o4 | 120 |  |
| 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 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 79 | q3 | 91 |  |
| 80 | e0 | 62 |  |
| 81 | p0 | 311 |  |
| 82 | m2 | 160 |  |
| 83 | p1 | 47 |  |
| 84 | p2 | 46 |  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 86 | OHX | 1 | 3954 | - | - | X | - |
| 86 | OHX | 1 | 3968 | - | - | X | - |
| 86 | OHX | 1 | 3973 | - | - | X | - |
| 86 | OHX | 1 | 4000 | - | - | X | - |
| 86 | OHX | 1 | 4025 | - | - | X | - |
| 86 | OHX | 1 | 4029 | - | - | X | - |
| 86 | OHX | 1 | 4041 | - | - | X | - |
| 86 | OHX | 1 | 4042 | - | - | X | - |
| 86 | OHX | 1 | 4053 | - | - | X | - |
| 86 | OHX | 1 | 4054 | - | - | X | - |
| 86 | OHX | 1 | 4079 | - | - | X | - |
| 86 | OHX | 1 | 4083 | - | - | X | - |
| 86 | OHX | 1 | 4145 | - | - | X | - |
| 86 | OHX | 1 | 4149 | - | - | X | - |
| 86 | OHX | 1 | 4154 | - | - | X | - |
| 86 | OHX | 1 | 4155 | - | - | X | - |
| 86 | OHX | 1 | 4162 | - | - | X | - |
| 86 | OHX | 1 | 4171 | - | - | X | - |
| 86 | OHX | 1 | 4196 | - | - | X | - |
| 86 | OHX | 2 | 2031 | - | - | X | - |
| 86 | OHX | 2 | 2044 | - | - | X | - |
| 86 | OHX | 2 | 2075 | - | - | X | - |
| 86 | OHX | 2 | 2089 | - | - | X | - |
| 86 | OHX | 2 | 2090 | - | - | X | - |
| 86 | OHX | 2 | 2098 | - | - | X | - |
| 86 | OHX | 2 | 2131 | - | - | X | - |
| 86 | OHX | 2 | 2145 | - | - | X | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 86 | OHX | 2 | 2161 | - | - | X | - |
| 86 | OHX | 5 | 3944 | - | - | X | - |
| 86 | OHX | 5 | 3964 | - | - | X | - |
| 86 | OHX | 5 | 3975 | - | - | X | - |
| 86 | OHX | 5 | 3980 | - | - | X | - |
| 86 | OHX | 5 | 4003 | - | - | X | - |
| 86 | OHX | 5 | 4004 | - | - | X | - |
| 86 | OHX | 5 | 4013 | - | - | X | - |
| 86 | OHX | 5 | 4022 | - | - | X | - |
| 86 | OHX | 5 | 4035 | - | - | X | - |
| 86 | OHX | 5 | 4037 | - | - | X | - |
| 86 | OHX | 5 | 4057 | - | - | X | - |
| 86 | OHX | 5 | 4068 | - | - | X | - |
| 86 | OHX | 5 | 4083 | - | - | X | - |
| 86 | OHX | 5 | 4093 | - | - | X | - |
| 86 | OHX | 5 | 4146 | - | - | X | - |
| 86 | OHX | 5 | 4191 | - | - | X | - |
| 86 | OHX | 5 | 4193 | - | - | X | - |
| 86 | OHX | 5 | 4200 | - | - | X | - |
| 86 | OHX | 5 | 4201 | - | - | X | - |
| 86 | OHX | 5 | 4202 | - | - | X | - |
| 86 | OHX | 5 | 4205 | - | - | X | - |
| 86 | OHX | 5 | 4219 | - | - | X | - |
| 86 | OHX | 5 | 4236 | - | - | X | - |
| 86 | OHX | 5 | 4240 | - | - | X | - |
| 86 | OHX | 5 | 4245 | - | - | X | - |
| 86 | OHX | 6 | 2060 | - | - | X | - |
| 86 | OHX | 6 | 2121 | - | - | X | - |
| 86 | OHX | 6 | 2147 | - | - | X | - |
| 86 | OHX | 6 | 2171 | - | - | X | - |
| 86 | OHX | 7 | 219 | - | - | X | - |
| 86 | OHX | 7 | 226 | - | - | X | - |
| 86 | OHX | 8 | 216 | - | - | X | - |
| 86 | OHX | 8 | 225 | - | - | X | - |
| 86 | OHX | 8 | 226 | - | - | X | - |
| 86 | OHX | C5 | 201 | - | - | X | - |
| 86 | OHX | O1 | 201 | - | - | X | - |
| 86 | OHX | O7 | 105 | - | - | X | - |

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 411206 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 | S | 0 | 0 | 0 |
| | | | 1481 | 951 | 265 | 265 | | | | |
| 9 | s7 | 186 | Total | C | N | O | S | 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 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| C5 | 137 | SER | ARG | conflict | UNP Q01855 |
| c5 | 137 | SER | ARG | conflict | UNP Q01855 |

- 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 | | | |
| 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 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 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 |
| | | | 679 | 402 | 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 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 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 | 13 | 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 | 14 | 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 | 15 | 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 | 16 | 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 | 17 | 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 | | | |
| 45 | 18 | 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 | 19 | 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 | S | 0 | 0 | 0 |
| | | | 1053 | 675 | 199 | 177 | 2 | | | |
| 50 | m4 | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1059 | 678 | 200 | 179 | 2 | | | |

- 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 | | | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 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 | | | |
| 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 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| O4 | 121 | LYS | - | expression tag | UNP P87262 |
| o4 | 121 | LYS | - | expression tag | UNP P87262 |

- 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 | | | |
| 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 60S acidic ribosomal protein P0.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 81 | p0 | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1076 | 686 | 192 | 195 | 3 | | | |

- Molecule 82 is a protein called Unknown protein chain m2.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 82 | m2 | 150 | Total | C | N | O | 0 | 0 | 0 |
| | | | 750 | 450 | 150 | 150 | | | |

- Molecule 83 is a protein called Unknown protein chain 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 chain 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 | 3 | Total | Mg | 0 | 0 |
| | | | 3 | 3 | | |
| 85 | m6 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 85 | n8 | 4 | Total | Mg | 0 | 0 |
| | | | 4 | 4 | | |
| 85 | q3 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 85 | o1 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 85 | N5 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 85 | 6 | 148 | Total | Mg | 0 | 0 |
| | | | 148 | 148 | | |
| 85 | sM | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 85 | O4 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 85 | m5 | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 85 | l3 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 85 | M1 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 85 | d6 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | 2 | 125 | Total 125 | Mg 125 | 0 | 0 |
| 85 | n0 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | L4 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | l7 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | M5 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | c9 | 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 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | M9 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | q0 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | SM | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | c8 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | M0 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 85 | c1 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | 5 | 505 | Total 505 | Mg 505 | 0 | 0 |
| 85 | L5 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | O7 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 85 | s6 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | Q2 | 1 | Total 1 | Mg 1 | 0 | 0 |

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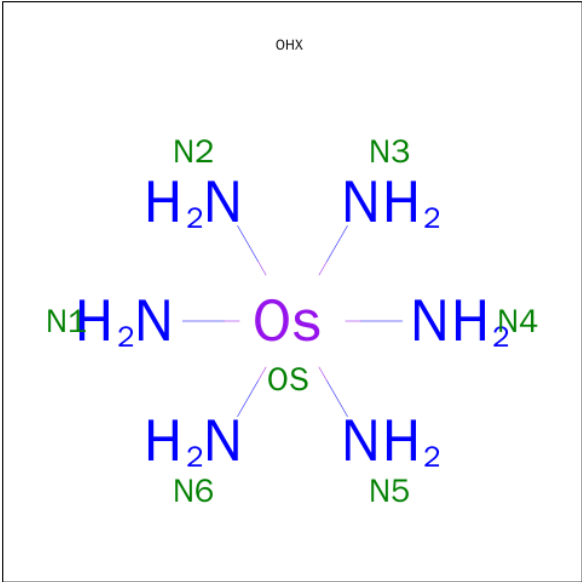
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 85 | d4 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | n9 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | 1 | 469 | Total 469 | Mg 469 | 0 | 0 |
| 85 | D0 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | S8 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | l2 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | O2 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | o7 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | o3 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | d3 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | M3 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 85 | N3 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | 4 | 21 | Total 21 | Mg 21 | 0 | 0 |
| 85 | n6 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | S4 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | L2 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | m1 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | l5 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | m7 | 5 | Total 5 | Mg 5 | 0 | 0 |
| 85 | M7 | 5 | Total 5 | Mg 5 | 0 | 0 |
| 85 | N8 | 5 | Total 5 | Mg 5 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 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 | 17 | Total 17 | Mg 17 | 0 | 0 |
| 85 | n3 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | q1 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | L3 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 85 | O5 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | N6 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | 8 | 14 | Total 14 | Mg 14 | 0 | 0 |
| 85 | l4 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | M6 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | N0 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | m0 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | 3 | 14 | Total 14 | Mg 14 | 0 | 0 |

- Molecule 86 is osmium (III) hexammine (three-letter code: OHX) (formula: H₁₂N₆Os).



| 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 | | |

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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 |
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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 | 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 |
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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 |
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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 |
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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 |
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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 |
| | | | 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 |
| | | | 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 | S8 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | C1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 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 | | |

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

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 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 | | |
| 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 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86 | L3 | 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 | M8 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | M9 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | N1 | 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 | 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 | O9 | 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 | | |

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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 |
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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 |
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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 |
| | | | 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 | s4 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | s8 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | s9 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 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 |
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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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| | | | 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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| | | | 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 | | |
| 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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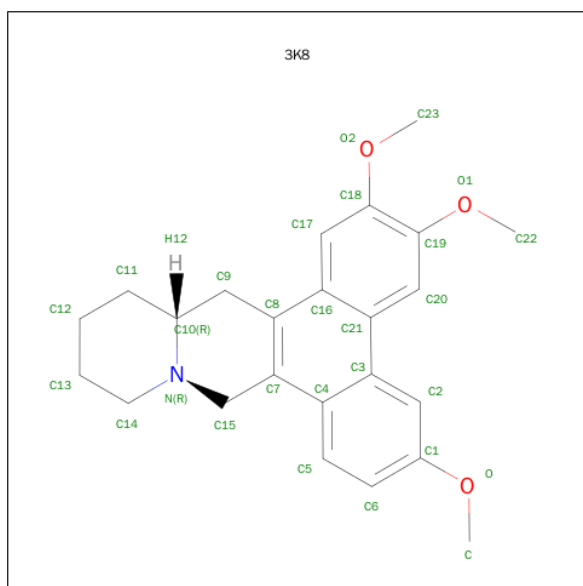
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|-----|-------|----------|-------|---|----|---------|---------|
| 86 | 8 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | 8 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | l3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | l3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | l3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | l4 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | l4 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | l5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | l5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | l5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | l9 | 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 | | |
| 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 | m9 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | n1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86 | n3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | n9 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | o3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | q2 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |

- Molecule 87 is (14aR)-2,3,6-trimethoxy-11,12,13,14,14a,15-hexahydro-9H-dibenzo[f,h]pyrido [1,2-b]isoquinoline (three-letter code: 3K8) (formula: C₂₄H₂₇NO₃).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 87 | 2 | 1 | Total | C | N | O | 0 | 0 |
| | | | 28 | 24 | 1 | 3 | | |
| 87 | 6 | 1 | Total | C | N | O | 0 | 0 |
| | | | 28 | 24 | 1 | 3 | | |

- Molecule 88 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 88 | q0 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 88 | D6 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 88 | Q2 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

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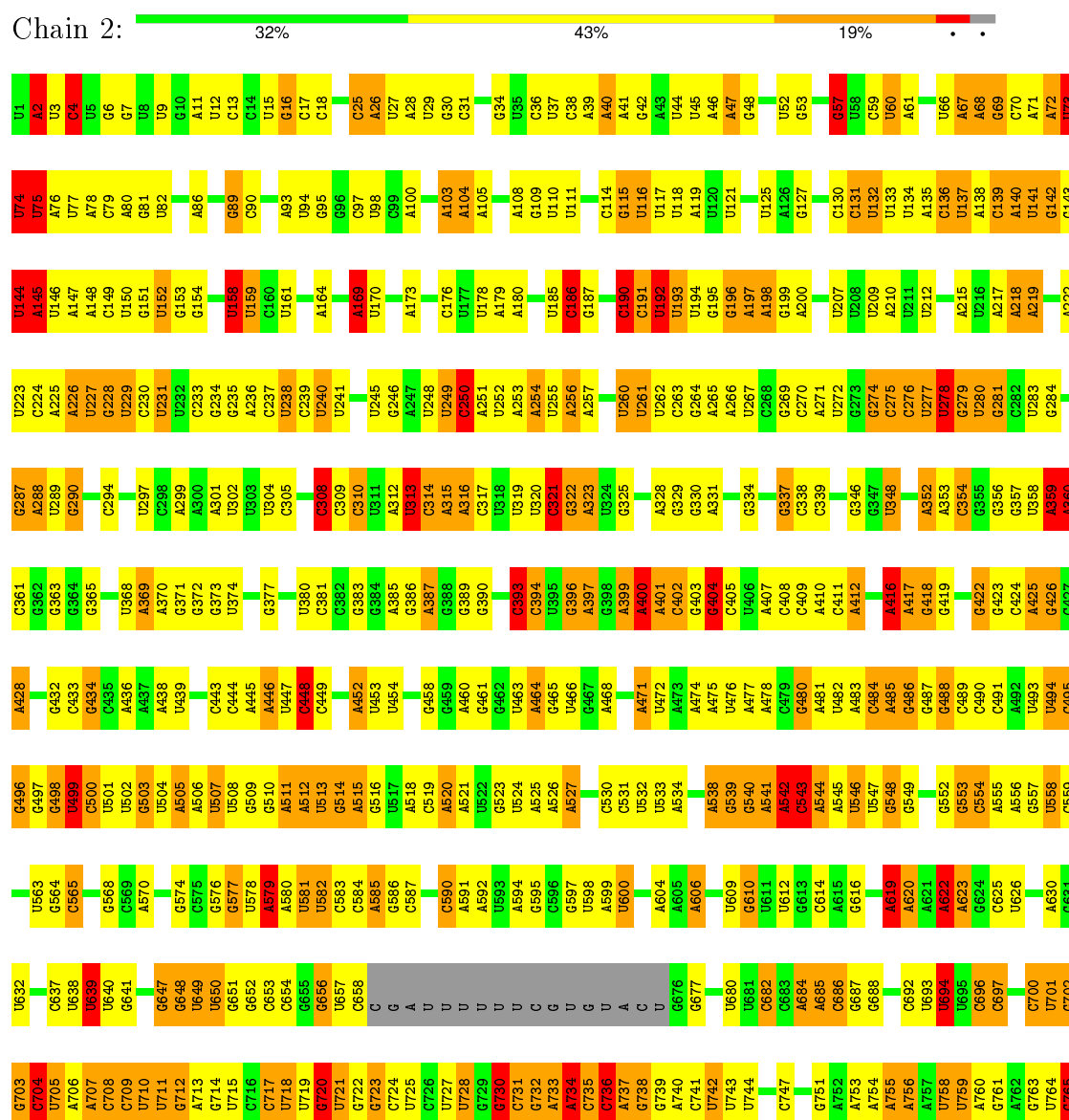
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 88 | e1 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 88 | Q3 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 88 | D9 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 88 | E1 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 88 | Q0 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 88 | d7 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 88 | q3 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 88 | d9 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 88 | D7 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 88 | d6 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 88 | o7 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 88 | O7 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 88 | q2 | 1 | Total 1 | Zn 1 | 0 | 0 |

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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



| | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|
| U1738 | A1671 | U1598 | G1531 | A1469 | G1330 | U1251 | A1183 | G1114 | C897 | U830 | U766 |
| C1739 | G1672 | C1599 | U1532 | A1470 | A1331 | U1252 | A1184 | U1115 | A1036 | U831 | U767 |
| A1740 | G1673 | A1600 | C1533 | A1471 | C1399 | U1253 | U1185 | A1116 | C1037 | U832 | C768 |
| | C1674 | G1601 | G1534 | C1472 | U1334 | U1254 | | | U1038 | U833 | |
| A1744 | C1675 | C1602 | U1535 | U1473 | U1335 | G1255 | A1189 | G1119 | A1039 | G901 | A770 |
| G1745 | U1676 | U1603 | G1536 | G1474 | | U1258 | C1190 | U1120 | G1040 | G902 | G838 |
| A1746 | C1677 | U1604 | C1537 | A1475 | C1338 | U1258 | U1191 | C1121 | G1041 | U839 | A771 |
| A1747 | A1678 | G1605 | C1538 | C1476 | G1405 | C1339 | C1192 | | G1042 | U840 | C773 |
| G1748 | C1679 | C1606 | G1539 | G1477 | U1340 | U1262 | A1193 | A1124 | A1043 | U841 | A774 |
| A1749 | G1680 | G1607 | G1540 | G1478 | U1401 | G1263 | U1194 | A1125 | | C842 | G775 |
| A1750 | A1681 | G1608 | G1541 | A1479 | C1342 | | C1195 | G1126 | G1046 | U843 | G776 |
| | U1682 | U1609 | G1542 | G1480 | U1343 | U1266 | U1196 | G1127 | | U911 | C777 |
| A1754 | C1683 | U1610 | A1543 | C1481 | A1344 | G1267 | C1197 | C1128 | U1052 | U844 | G778 |
| A1755 | U1684 | A1611 | U1544 | A1482 | A1345 | G1268 | U1198 | U1129 | G1053 | G845 | U779 |
| A1756 | G1685 | | A1545 | G1483 | A1346 | | G1199 | G1130 | G987 | A847 | A780 |
| C | | C1614 | G1546 | G1484 | U1413 | U1272 | U1201 | A1131 | U988 | U849 | U781 |
| G1760 | U | A1615 | | C1485 | A1348 | G1273 | G1201 | A1132 | U1067 | C849 | U782 |
| U1761 | U | G1616 | A1550 | G1486 | G1349 | C1274 | A1202 | A1133 | U1058 | U850 | G783 |
| A1765 | G | C1619 | G1553 | A1487 | U1350 | U1276 | A1203 | U1134 | U1059 | U851 | |
| A1766 | A | G1620 | U1554 | U1488 | G1351 | U1276 | C1134 | U1135 | A992 | C852 | |
| | G | U1621 | A1555 | C1489 | U1352 | G1277 | C1207 | A1061 | A993 | G853 | U921 |
| A1767 | A | G1622 | A1556 | U1491 | U1353 | | A1208 | A1138 | G994 | U854 | A788 |
| U1770 | A | C1623 | U1557 | A1492 | C1355 | G1281 | A1211 | A1139 | A995 | A855 | A789 |
| G | G | C1624 | U1558 | A1493 | U1356 | U1282 | G1212 | G1141 | U996 | A856 | U790 |
| G | G | C1625 | A1559 | C1494 | A1424 | U1283 | U1213 | A1142 | C1066 | C927 | A791 |
| G | G | A1560 | U1560 | C1495 | G1357 | C1284 | U1214 | A1143 | C1068 | G958 | U792 |
| U1773 | G | C1631 | U1561 | U1496 | A1427 | U1285 | C1359 | U1144 | A1001 | A930 | A793 |
| U1774 | G | A1562 | G1562 | U1497 | G1428 | U1286 | A1217 | U1145 | C1070 | U861 | U794 |
| U1775 | G | A1563 | C1563 | G1498 | G1429 | A1287 | G1218 | G1146 | U1071 | A862 | A796 |
| A1776 | C | A1564 | U1564 | A1499 | U1430 | U1288 | A1219 | A1147 | A993 | A863 | C797 |
| G | A | C1634 | C1565 | C1500 | C1431 | U1289 | C1220 | G1148 | U1005 | U864 | U798 |
| U1777 | A | C1637 | U1566 | G1501 | G1364 | U1290 | G1149 | G1074 | C1006 | A865 | A799 |
| C | C | C1638 | C1567 | | C1432 | G1291 | A1224 | G1150 | G1007 | G866 | U800 |
| A1780 | C | A1503 | A1506 | C1504 | G1365 | G1297 | U1225 | A1151 | U1080 | G867 | G801 |
| A1782 | C | C1536 | A1568 | A1505 | G1367 | | A1226 | A1152 | A1081 | C868 | G802 |
| C1783 | C | C1539 | A1569 | G1506 | G1435 | | U1227 | | U1089 | | |
| | A | G1642 | | A1506 | A1436 | U1300 | A1228 | G1155 | C1010 | | A807 |
| U1785 | U | U1643 | C1572 | U1507 | U1437 | U1301 | G1228 | C1156 | G1011 | G871 | U808 |
| U1786 | C | C1644 | A1573 | U1508 | U1370 | G1229 | G1229 | G1156 | U1012 | G872 | U808 |
| U1787 | C | G1645 | G1574 | C1509 | A1371 | U1302 | U1230 | A1157 | U1013 | U873 | A809 |
| U1788 | C | U1575 | G1575 | U1510 | U1372 | U1302 | U1231 | C1158 | U1015 | C874 | G810 |
| A | A | C1649 | U1578 | U1511 | | G1308 | U1232 | G1159 | C950 | G875 | G811 |
| G | G | U1650 | C1579 | G1512 | A1375 | C1309 | G1233 | A1160 | C1016 | G876 | A812 |
| A | A | A1651 | U1579 | | U1450 | U1310 | A1234 | C1161 | U1017 | | A813 |
| G | G | C1580 | C1580 | | C1451 | U1311 | C1235 | U1095 | U1018 | A881 | A814 |
| | C | G1654 | A1516 | A1516 | U1378 | U1311 | A1236 | A1163 | A1020 | G955 | G815 |
| G1717 | G1717 | A1555 | G1584 | U1517 | U1381 | U1314 | G1237 | G1164 | C1021 | C883 | G816 |
| G1718 | G1718 | U1556 | U1585 | C1518 | A1382 | U1315 | A1238 | G1165 | C1022 | A884 | A817 |
| A1719 | A1719 | U1557 | A1586 | U1519 | G1316 | U1316 | U1239 | A1166 | G1101 | G885 | C818 |
| U1720 | G1720 | G1558 | U1587 | G1520 | A1384 | G1317 | U1240 | G1167 | U1024 | U886 | G819 |
| | | A1559 | G1588 | G1521 | G1385 | C1318 | G1241 | U1168 | A1025 | A887 | U820 |
| | | C1560 | G1589 | U1522 | C1459 | G1386 | A1319 | G1169 | U1026 | U888 | U821 |
| G1726 | G1726 | U1561 | G1590 | G1523 | G1387 | U1320 | U1243 | U1106 | A1027 | U889 | U822 |
| A1728 | A1728 | C1562 | C1591 | A1524 | A1388 | A1321 | A1244 | G1172 | G1107 | C890 | G823 |
| | | A1563 | A1592 | A1525 | G1389 | A1322 | G1245 | C1173 | U1029 | A891 | G824 |
| A1731 | A1731 | C1564 | A1593 | A1526 | U1390 | C1323 | G1246 | C1174 | A1030 | A967 | U825 |
| U1732 | U1732 | U1665 | G1594 | C1527 | A1391 | G1324 | U1247 | U1175 | U1031 | U968 | U826 |
| C1733 | C1733 | U1666 | U1595 | U1528 | U1392 | G1324 | C1248 | G1176 | G1111 | C827 | U831 |
| | | A1667 | C1596 | C1529 | C1393 | G1329 | U1249 | U1172 | G1112 | G895 | U832 |
| | | | A1597 | A1530 | C1394 | G1329 | U1250 | U1173 | A1113 | U896 | A833 |


- Molecule 1: 18S ribosomal RNA

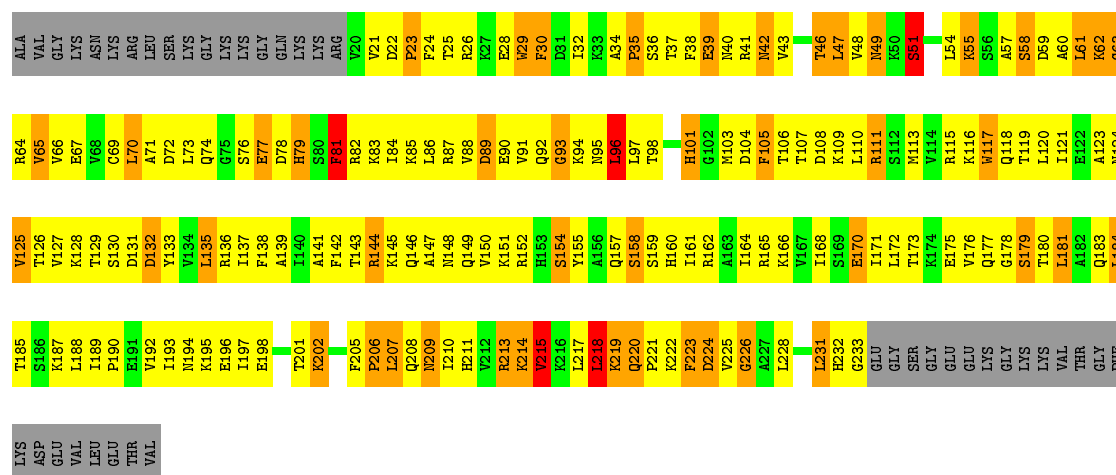
Chain 6:  34% 44% 19% .





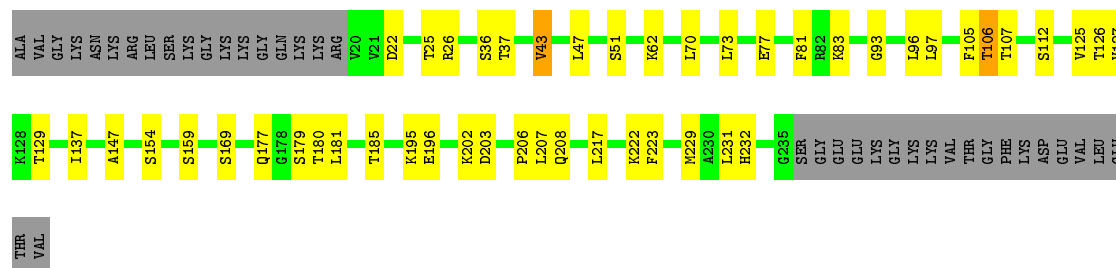
- Molecule 3: 40S ribosomal protein S1-A

Chain S1: 



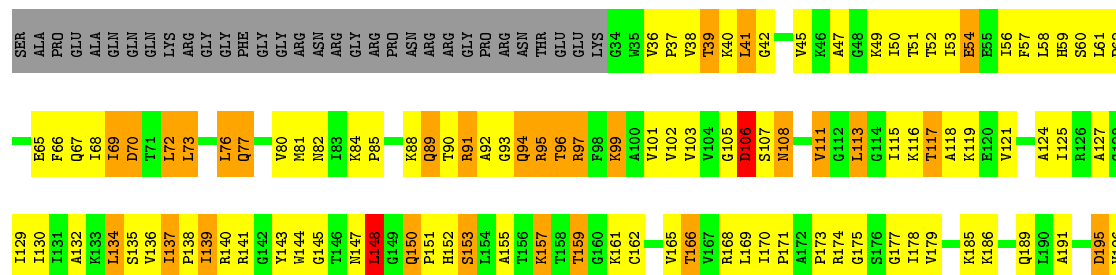
- Molecule 3: 40S ribosomal protein S1-A

Chain s1:



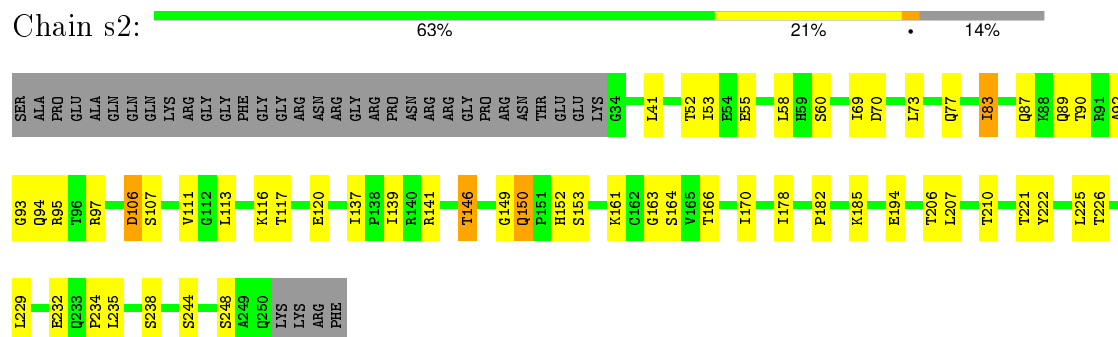
- Molecule 4: 40S ribosomal protein S2

Chain S2:

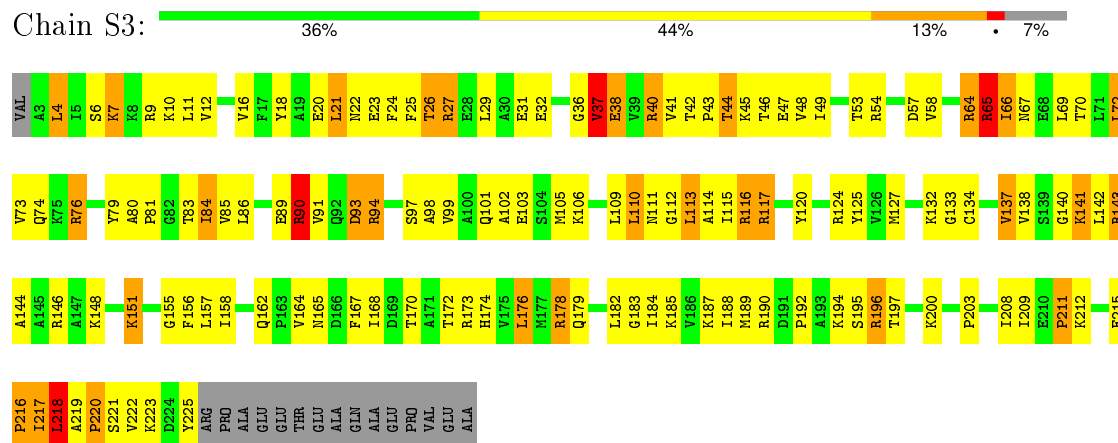




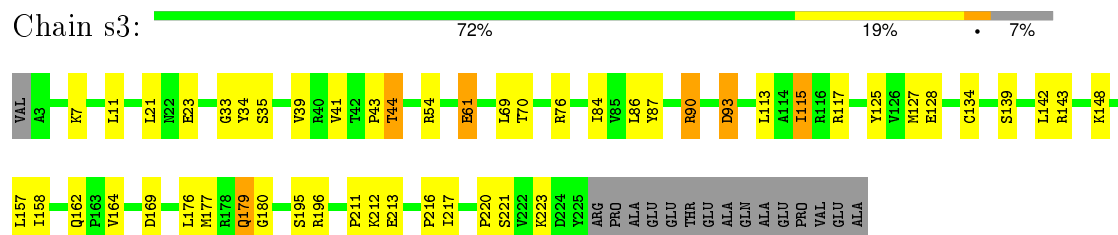
• Molecule 4: 40S ribosomal protein S2



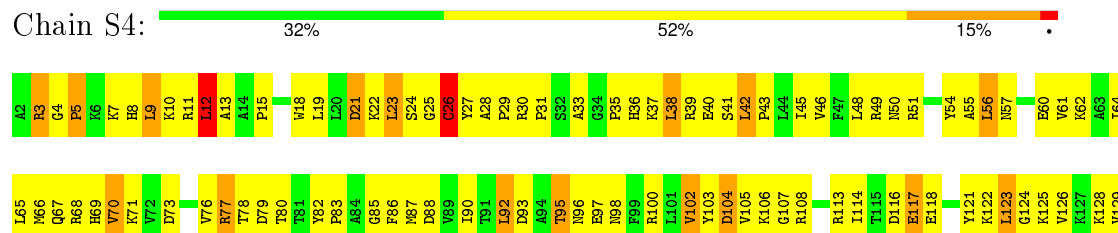
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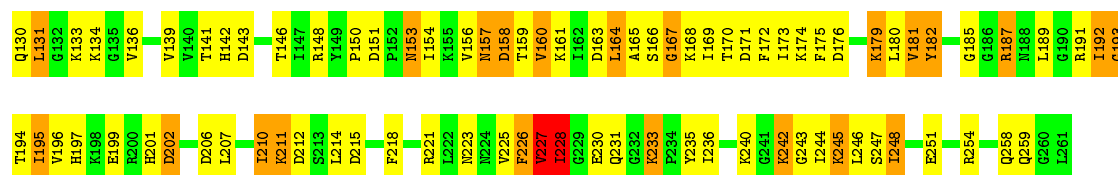


• Molecule 5: 40S ribosomal protein S3

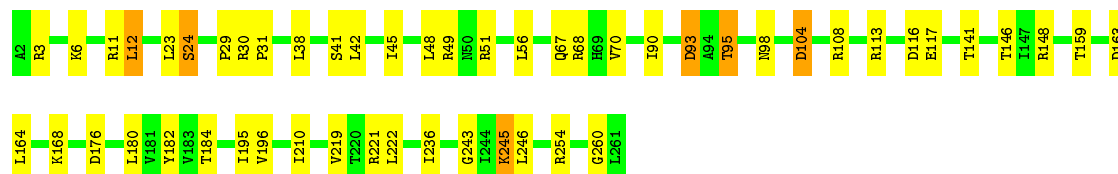
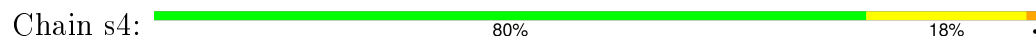


• Molecule 6: 40S ribosomal protein S4-A

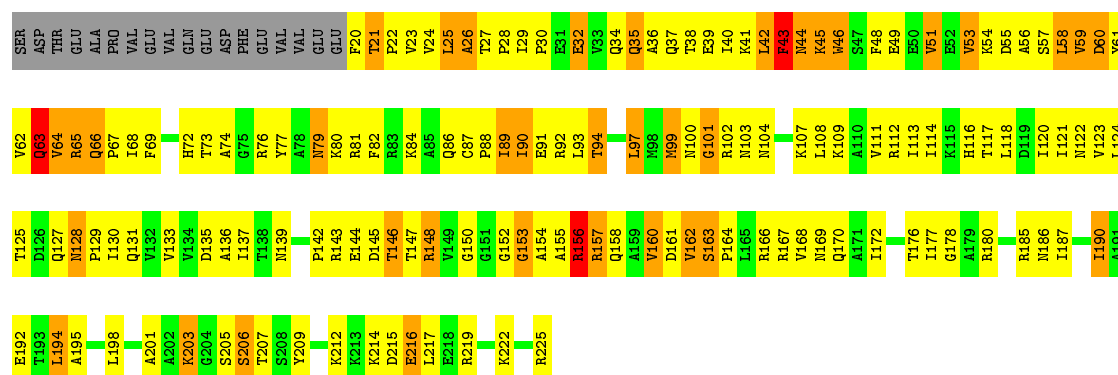




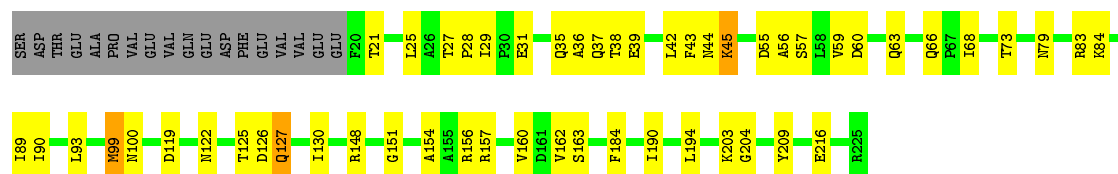
• Molecule 6: 40S ribosomal protein S4-A



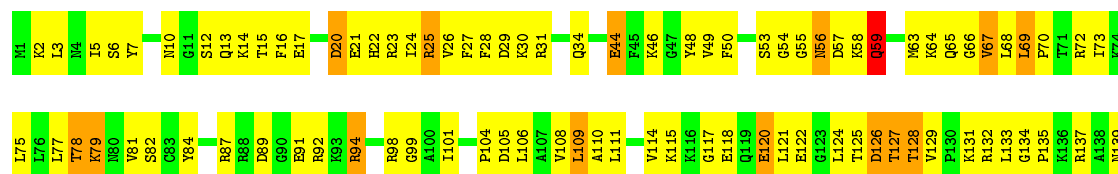
• Molecule 7: 40S ribosomal protein S5

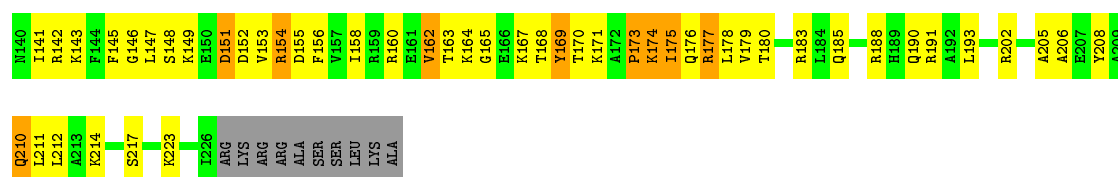


• Molecule 7: 40S ribosomal protein S5



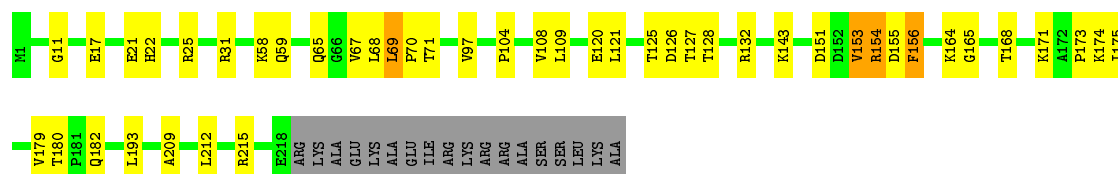
• Molecule 8: 40S ribosomal protein S6-A





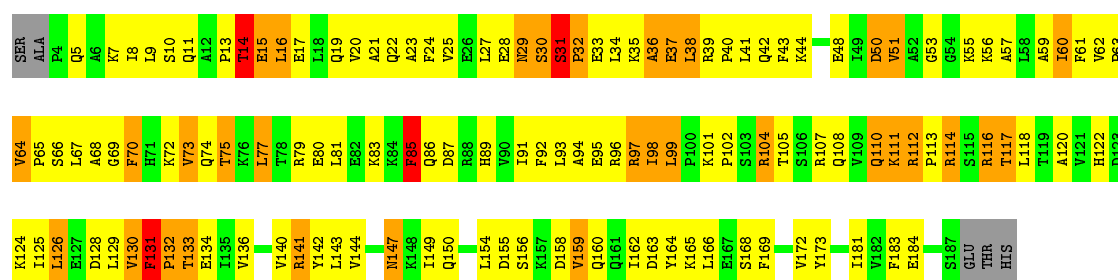
• Molecule 8: 40S ribosomal protein S6-A

Chain s6: 73% 17% 8%



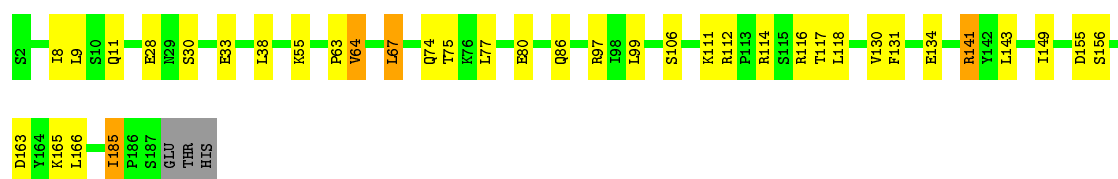
• Molecule 9: 40S ribosomal protein S7-A

Chain S7: 29% 49% 17%



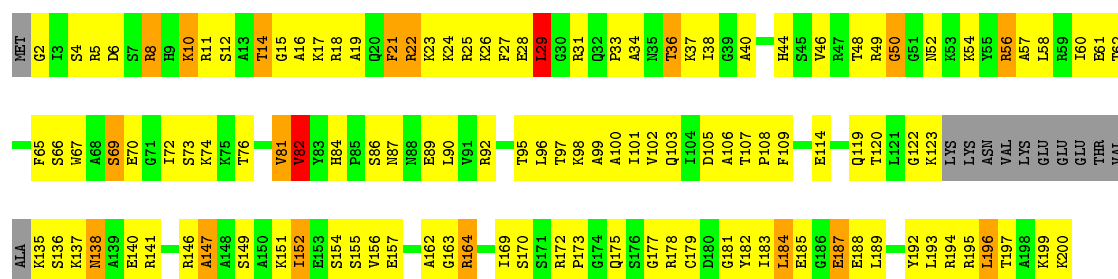
• Molecule 9: 40S ribosomal protein S7-A

Chain s7: 79% 17%

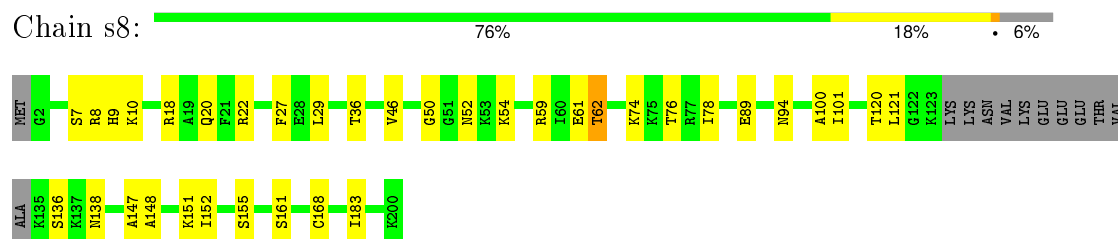


• Molecule 10: 40S ribosomal protein S8-A

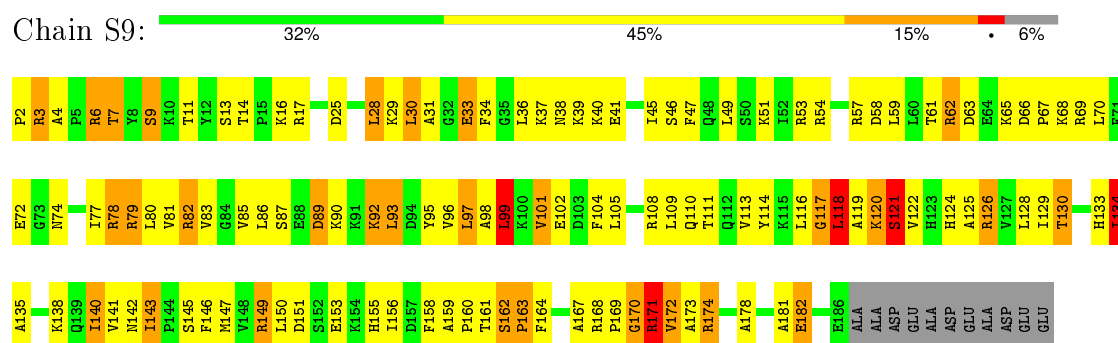
Chain S8: 34% 51% 9% 6%



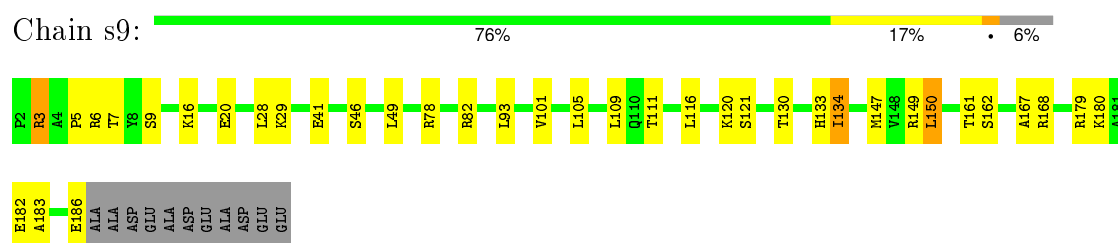
- Molecule 10: 40S ribosomal protein S8-A



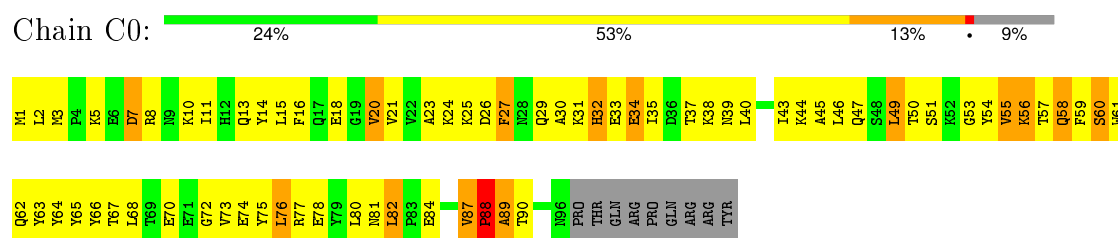
- Molecule 11: 40S ribosomal protein S9-A



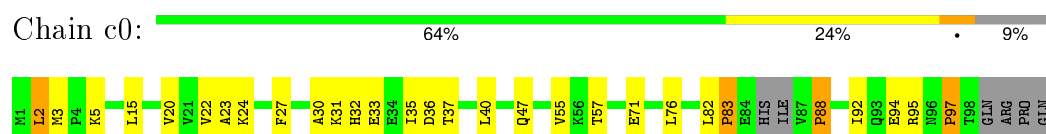
- Molecule 11: 40S ribosomal protein S9-A



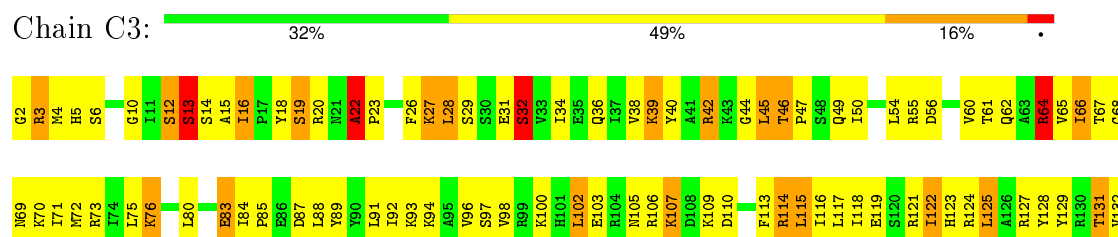
- Molecule 12: 40S ribosomal protein S10-A



- Molecule 12: 40S ribosomal protein S10-A



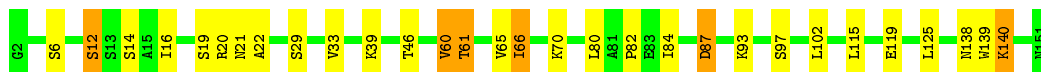
- Molecule 13: 40S ribosomal protein S11-A





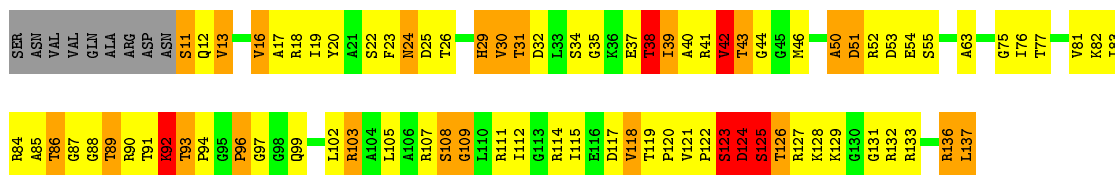
- Molecule 15: 40S ribosomal protein S13

Chain c3: 80% 16%



- Molecule 16: 40S ribosomal protein S14-A

Chain C4: 32% 40% 16% 7%



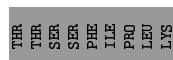
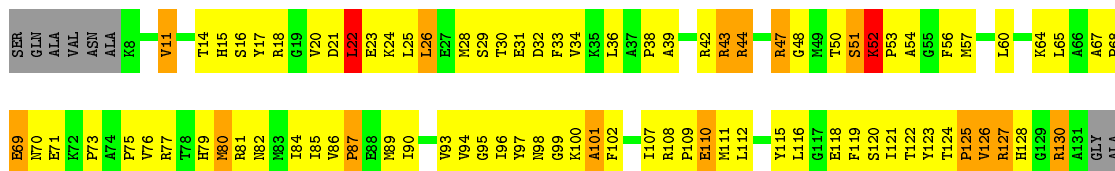
- Molecule 16: 40S ribosomal protein S14-A

Chain c4: 76% 15% 6%



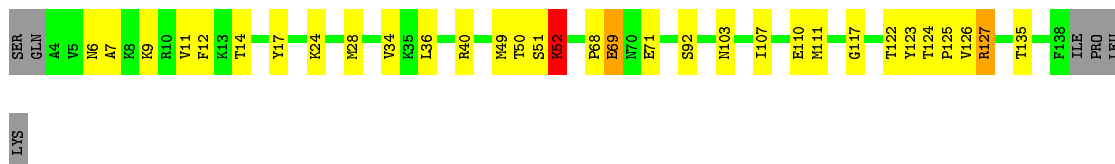
- Molecule 17: 40S ribosomal protein S15

Chain C5: 26% 50% 11% 12%

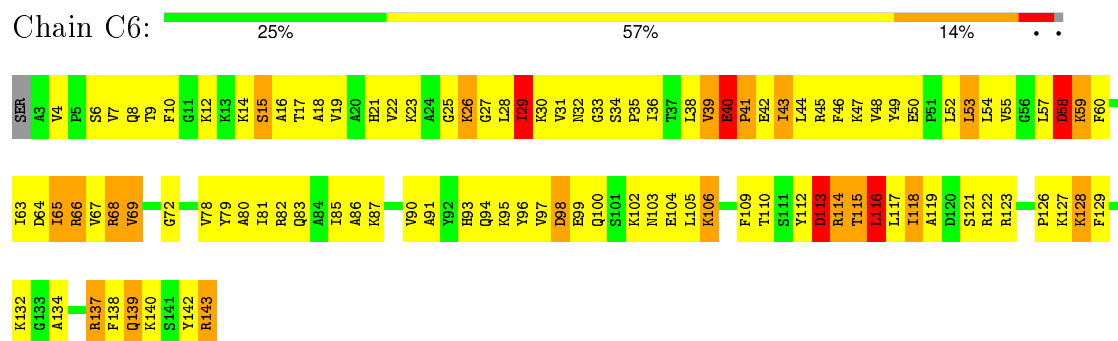


- Molecule 17: 40S ribosomal protein S15

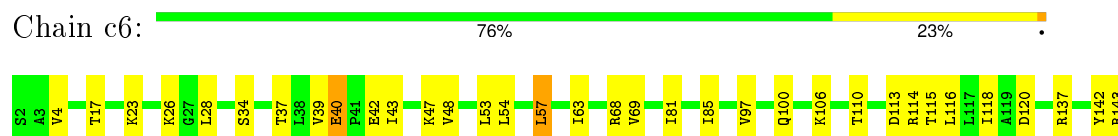
Chain c5: 73% 21% 6%



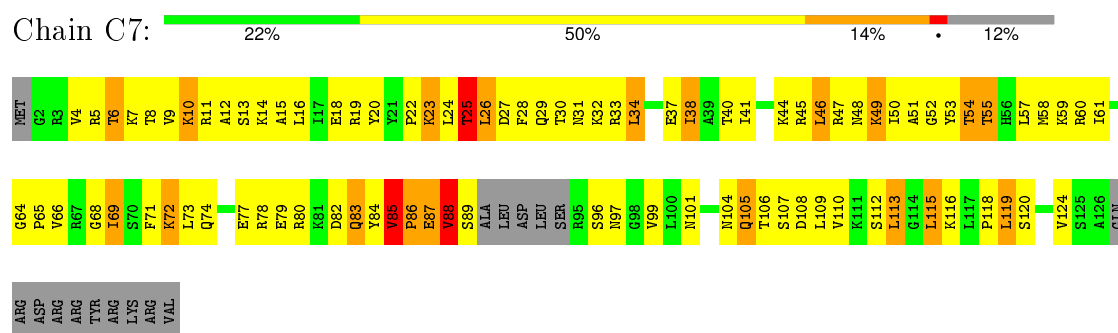
- Molecule 18: 40S ribosomal protein S16-A

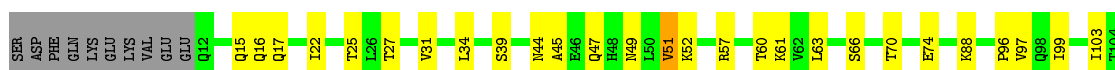


- Molecule 18: 40S ribosomal protein S16-A



- Molecule 19: 40S ribosomal protein S17-A

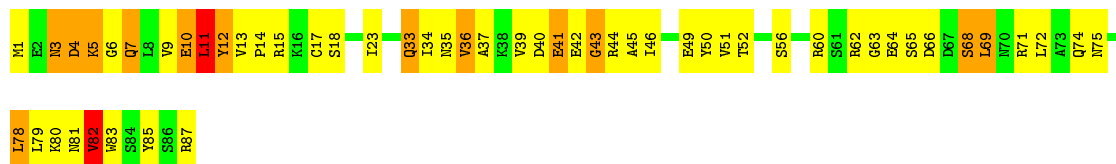






- Molecule 23: 40S ribosomal protein S21-A

Chain D1: 38% 45% 15%



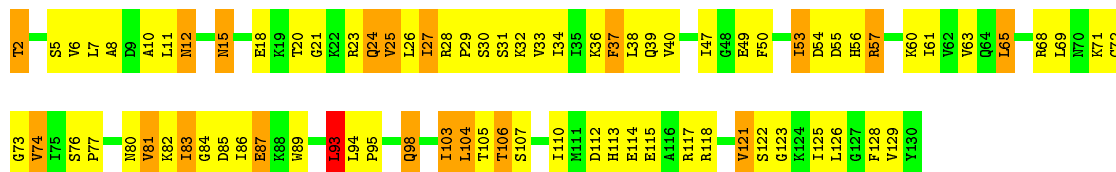
- Molecule 23: 40S ribosomal protein S21-A

Chain d1: 74% 23%



- Molecule 24: 40S ribosomal protein S22-A

Chain D2: 37% 47% 15%



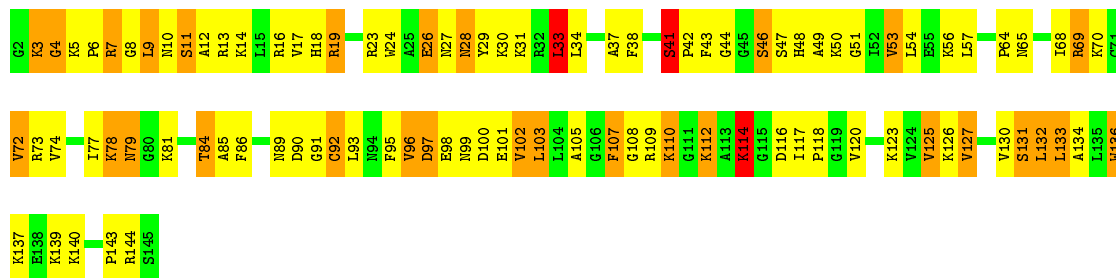
- Molecule 24: 40S ribosomal protein S22-A

Chain d2: 88% 11%



- Molecule 25: 40S ribosomal protein S23-A

Chain D3: 33% 45% 20%



- 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

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|--|--|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| P2 | K3 | K4 | R5 | A6 | S7 | J8 | G9 | R10 | N11 | K12 | K13 | G14 | R15 | | | K28 | S29 | I30 | P31 | K32 | D33 | K34 | K35 | I36 | K37 | R38 | K39 | A40 | I41 | R42 | N43 | I44 | V45 | E46 | A47 | A48 | A49 | V50 | R51 | D52 | L53 | | S57 | V58 | Y59 | P60 | E61 | Y62 | G63 | A64 | L64 | D65 |
|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|--|--|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|



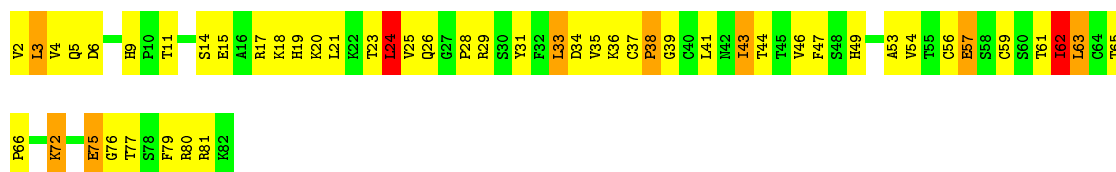
- Molecule 28: 40S ribosomal protein S26-B

Chain d6: 82% 16% .



- Molecule 29: 40S ribosomal protein S27-A

Chain D7: 37% 51% 10% .



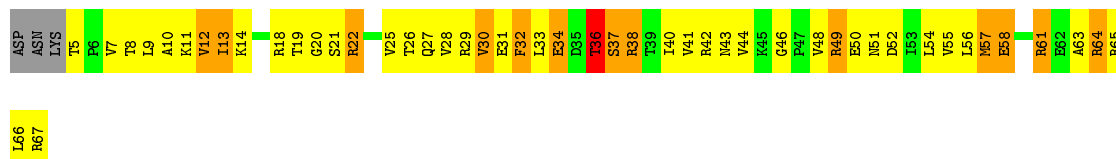
- Molecule 29: 40S ribosomal protein S27-A

Chain d7: 83% 16% .



- Molecule 30: 40S ribosomal protein S28-A

Chain D8: 21% 53% 20% 5% .



- Molecule 30: 40S ribosomal protein S28-A

Chain d8: 68% 26% 5% .



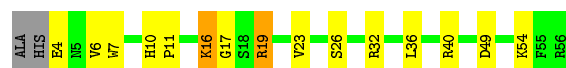
- Molecule 31: 40S ribosomal protein S29-A

Chain D9: 25% 55% 15% . .



- Molecule 31: 40S ribosomal protein S29-A

Chain d9: 

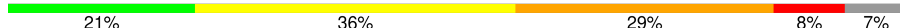


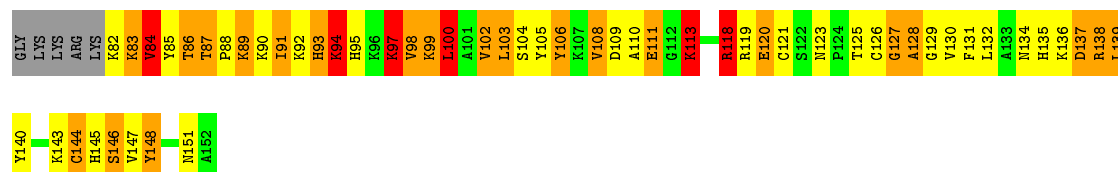
- Molecule 32: 40S ribosomal protein S30-A

Chain E0: 



- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1: 



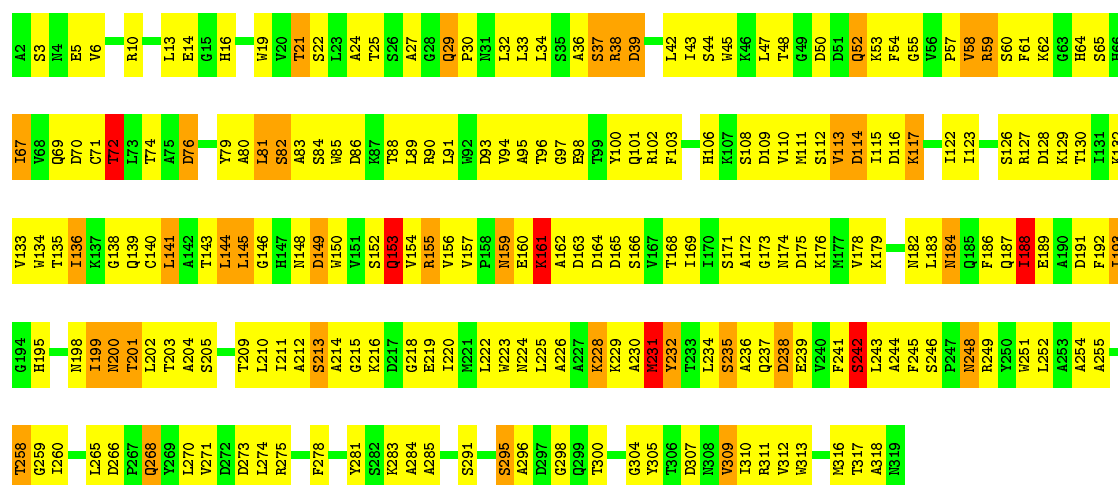
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1: 




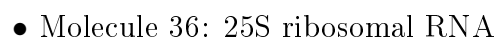
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR: 



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

Chain sR: 



| | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|------|------|------|------|------|---|------|------|------|------|
| U1265 | G1198 | A1136 | U1070 | G1001 | G875 | U811 | G575 | C614 | G548 | A | G412 | G345 | U276 | G206 |
| G1266 | C1199 | C1137 | U1071 | A1002 | A876 | G812 | G676 | U615 | A551 | A | U413 | C346 | G277 | U207 |
| U1267 | A1200 | U1138 | G1072 | A1003 | C877 | G813 | A677 | C618 | G552 | U | A418 | G347 | U278 | C208 |
| G1268 | G1201 | G1139 | U1073 | G940 | G878 | U814 | A744 | A619 | U553 | C | G419 | A348 | U279 | A209 |
| U1269 | A1202 | G1140 | U1074 | G1005 | U879 | G815 | U679 | U620 | U554 | U | G420 | U280 | G281 | U210 |
| A1270 | A1203 | G1141 | A1075 | G1006 | G880 | A816 | U681 | A623 | A584 | C | G421 | C350 | G282 | A211 |
| A1271 | A1204 | G1142 | U1076 | U1007 | C881 | A817 | C749 | U622 | U555 | G | A422 | A351 | G283 | |
| C1272 | U1207 | U1143 | U1078 | A1008 | A882 | C818 | U682 | A624 | U556 | C | A423 | A352 | G284 | G214 |
| U1273 | U1208 | A1144 | A1079 | A1009 | A883 | U819 | C753 | U625 | U557 | A | A424 | U354 | A285 | U217 |
| A1274 | G1209 | C1146 | A1080 | G1010 | A884 | A820 | U683 | G624 | U558 | U | G425 | A355 | U286 | G218 |
| U1278 | U1210 | G1147 | U1082 | U1015 | U885 | U821 | C757 | U626 | U559 | U | G426 | C356 | A219 | A219 |
| G1279 | U1211 | G1148 | U1083 | U1016 | G886 | G824 | A761 | U627 | C561 | C | U430 | A357 | A289 | G220 |
| C1280 | A1212 | G1149 | A1084 | C1016 | G887 | U825 | U762 | A628 | C562 | A | U431 | G358 | G290 | |
| G1281 | G1213 | A1150 | U1087 | G1017 | A888 | G826 | U689 | U629 | U563 | C | G432 | U359 | G291 | U223 |
| A1282 | U1214 | U1151 | U1088 | C1018 | U889 | A827 | U763 | A630 | U564 | U | A433 | G360 | U292 | G225 |
| C1283 | G1215 | A1152 | G1089 | G1019 | A890 | A828 | U764 | U631 | U565 | G | U434 | A361 | C226 | |
| G1284 | A1216 | G1153 | A1093 | G1020 | U891 | U829 | U765 | G632 | G566 | | U435 | A296 | G229 | |
| A1285 | C1217 | A1154 | U1094 | U1021 | C893 | A830 | U767 | C633 | G567 | | C436 | A297 | G230 | |
| U1286 | U1218 | C1155 | U1095 | A1022 | G894 | G831 | C768 | C634 | U568 | | U437 | A366 | G231 | |
| A1287 | A1219 | C1156 | U1096 | A1023 | A895 | G832 | U769 | G635 | A569 | | G438 | A367 | G232 | |
| G1288 | G1220 | G1157 | G1097 | U1024 | C896 | U833 | G770 | C636 | A498 | | A439 | G368 | G300 | |
| A1289 | U1221 | A1158 | A1098 | U1025 | U897 | U834 | A771 | C637 | A499 | | C440 | A369 | G301 | |
| C1290 | G1222 | G1159 | G1099 | G1026 | U898 | G835 | U772 | G638 | C500 | | U | U370 | G304 | G233 |
| A1291 | A1223 | C1160 | U1100 | A1030 | U899 | A836 | G773 | U639 | A501 | | G | U371 | U305 | A235 |
| G1292 | C1224 | G1161 | G1101 | U1031 | G900 | A837 | C774 | U640 | U502 | | U | A372 | | |
| U1293 | U1225 | A1162 | A1102 | U1032 | G901 | G838 | U775 | C641 | C503 | | U | A373 | U310 | G239 |
| G1294 | G1226 | G1163 | A1103 | U1033 | U905 | G839 | U776 | U642 | A504 | | U | A374 | C311 | U240 |
| A1295 | C1227 | A1164 | A1104 | U1034 | A906 | C840 | U778 | U643 | G505 | | U | A375 | C312 | G243 |
| G1296 | U1228 | G1165 | U1105 | G1035 | U906 | A841 | G779 | G644 | U506 | | U | A376 | U313 | |
| C1297 | A1229 | A1166 | A1106 | A1036 | G907 | G842 | A780 | A645 | U507 | | U | A377 | U314 | G244 |
| U1298 | G1230 | U1167 | G1107 | C1037 | U908 | A843 | G781 | A646 | U508 | | U | U381 | | |
| G1300 | G1231 | C1168 | C1108 | U1038 | G909 | G844 | U707 | A647 | A585 | | U | U382 | A317 | U245 |
| A1301 | A1232 | A1169 | U1109 | U1039 | G910 | U845 | G708 | C648 | C586 | | G | U383 | A318 | U246 |
| G1302 | G1233 | G1170 | U1110 | A1040 | G911 | A846 | U709 | A649 | U587 | | U | A384 | A319 | C247 |
| C1303 | U1234 | U1171 | U1111 | U1041 | C912 | A847 | A786 | C650 | G588 | | G | A385 | G320 | U248 |
| A1304 | A1235 | G1172 | A1112 | U1042 | G913 | A848 | A787 | G651 | A589 | | U | A386 | | U249 |
| U1305 | G1236 | G1173 | A1113 | C1043 | A913 | A849 | G788 | G652 | G590 | | C | | | U250 |
| G1306 | U1237 | C1174 | G1114 | U1044 | A914 | C849 | C789 | A653 | G591 | | C | A323 | A323 | G251 |
| U1307 | G1238 | U1175 | U1115 | U1045 | G915 | U850 | A789 | C654 | A592 | | U | A324 | A324 | U252 |
| A1308 | A1239 | G1176 | G1116 | A1046 | A916 | G854 | U790 | C655 | C593 | | C | A325 | A325 | A255 |
| G1309 | U1240 | G1177 | U1117 | U1047 | A917 | U855 | A791 | A656 | U594 | | U | A326 | A326 | G256 |
| U1310 | G1241 | A1178 | G1118 | C1048 | C918 | U856 | G792 | A657 | G595 | | G | A327 | A327 | |
| G1311 | A1242 | U1179 | U1119 | U1049 | U919 | G857 | G793 | U658 | | | U | A328 | A328 | C259 |
| C1312 | U1243 | A1180 | A1120 | U1050 | A920 | U858 | U794 | G659 | A598 | | C | A329 | A329 | U261 |
| G1313 | A1244 | U1181 | U1121 | U1051 | A921 | A859 | G795 | U660 | C599 | | U | A330 | A330 | G260 |
| U1314 | G1245 | A1182 | U1122 | U1052 | U922 | G860 | U796 | U661 | U601 | | C | A331 | A331 | U262 |
| C1315 | U1246 | C1183 | U1123 | A1053 | C923 | G861 | G797 | U662 | A399 | | U | A332 | A332 | G263 |
| U1316 | G1247 | A1184 | U1124 | U1054 | G924 | U862 | U798 | A663 | G400 | | U | A333 | A333 | G264 |
| A1317 | A1248 | G1185 | U1125 | U1055 | A925 | C863 | G800 | U664 | A603 | | U | A334 | A334 | |
| G1318 | U1249 | U1186 | U1126 | G1056 | A926 | C864 | A801 | A665 | G604 | | U | A402 | A402 | G267 |
| U1319 | C1250 | C1187 | G1127 | U1057 | C927 | U865 | C802 | G726 | U605 | | G | A403 | A403 | A268 |
| G1320 | G1251 | U1188 | U1128 | U1058 | C928 | U866 | C803 | G727 | G606 | | G | A404 | A404 | G269 |
| A1321 | U1252 | A1189 | A1129 | A1061 | A929 | G867 | C804 | G728 | A607 | | G | A405 | A405 | G270 |
| C1322 | G1253 | U1190 | U1130 | U1062 | U930 | C868 | C805 | G729 | A608 | | U | A406 | A406 | C271 |
| U1323 | A1254 | C1192 | A1131 | G1063 | C931 | G869 | A806 | C670 | G609 | | A | A407 | A407 | G272 |
| G1324 | U1255 | U1193 | G1132 | U1064 | U932 | G870 | A807 | U671 | G610 | | G | A408 | A408 | G273 |
| U1325 | G1256 | A1194 | U1133 | A1065 | A933 | U872 | C794 | A672 | A611 | | G | A409 | A409 | G274 |
| A1326 | U1257 | G1195 | A1134 | G1066 | U934 | U873 | G809 | U673 | U612 | | G | A410 | A410 | G275 |
| C1327 | G1258 | C1196 | U1135 | C1067 | U935 | U874 | A810 | A736 | G613 | | G | | | |
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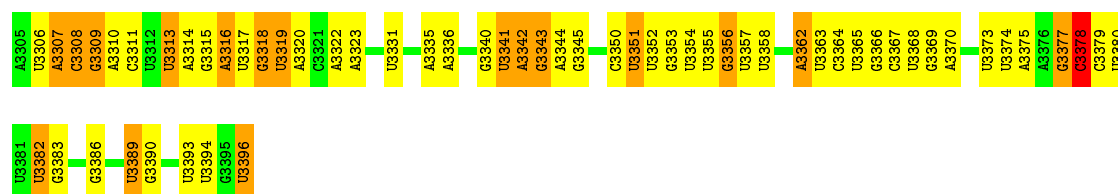
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| C2333 | U2268 | C2202 | C2136 | G | G | G1952 | A1874 | C1803 | G1731 | G1685 | A1588 | A1524 | A1454 | A1394 | U1329 |
| U2334 | U2269 | U2205 | U2137 | A | C | G1953 | G1875 | A1804 | A1731 | A1656 | A1589 | G1525 | U1455 | G1395 | A1330 |
| G2335 | G2272 | G2206 | A2138 | C | U | G1954 | U1876 | A1805 | U1732 | G1657 | G1590 | G1526 | G1456 | C1396 | U1331 |
| U2336 | G2273 | G2207 | A2139 | C | C | U1955 | U1877 | A1806 | G1733 | G1658 | G1591 | C1527 | U1457 | C1397 | A1332 |
| C2337 | U2274 | A2208 | U2140 | G | U | A | G1878 | G1807 | G1734 | U1659 | G1592 | G1528 | U1461 | U1398 | U1333 |
| C2338 | U2275 | U2209 | U2141 | U | G | G | A1879 | A1808 | G1735 | C1660 | A1593 | A1529 | G1466 | U1399 | U1334 |
| C2339 | G2276 | G2210 | A2142 | C | U | G | U1880 | A1809 | U1736 | G1661 | A1594 | U1530 | U1467 | C1400 | U1335 |
| U2340 | G2277 | G2211 | A2143 | C | U | G | A1881 | A1810 | U1740 | G1662 | U1595 | C1531 | A1401 | G1401 | U1336 |
| A2341 | G2278 | G2212 | A2144 | C | A | G | G1882 | A1811 | A1741 | C1663 | C1596 | C1532 | A1468 | C1402 | C1339 |
| U2342 | C2278 | U2213 | C2145 | U | G | G | A1883 | A1812 | U1742 | A1667 | G1598 | U1533 | C1469 | C1403 | U1340 |
| C2343 | A2279 | A2214 | A2146 | U | G | C | A1886 | A1813 | G1743 | G1668 | G1599 | A1534 | U1470 | G1404 | U1341 |
| U2344 | A2280 | C2214 | A2147 | C | C | C | U1887 | A1814 | G1744 | G1669 | G1599 | A1535 | U1471 | U1405 | U1342 |
| A2345 | A2281 | G2215 | U2148 | G | C | C | A1888 | A1815 | G1745 | C1670 | A1602 | G1536 | U1472 | A1406 | U1343 |
| C2346 | U2282 | G2216 | A2149 | U | G | C | A1891 | A1816 | U1746 | U1670 | A1603 | A1537 | G1473 | A1407 | U1344 |
| U2351 | G2283 | U2217 | G2150 | A | A | U | U1894 | A1817 | G1747 | G1674 | A1604 | A1538 | A1474 | A1408 | G1345 |
| A2352 | C2284 | G2218 | C2151 | C | C | U | A1895 | A1818 | U1748 | A1675 | A1546 | A1539 | A1475 | G1409 | G1346 |
| G2353 | C2285 | A2219 | A2152 | A | U | G | A1896 | A1819 | G1749 | A1676 | G1610 | U1547 | G1476 | U1347 | U1347 |
| C2354 | U2286 | G2220 | U2153 | A | A | G | G1897 | A1820 | A1750 | G1677 | A1612 | C1548 | U1484 | G1411 | U1348 |
| C2355 | C2287 | G2221 | U2154 | U | C | U | G1898 | A1821 | G1751 | U1680 | A1613 | G1543 | U1485 | G1412 | G1349 |
| U2356 | G2288 | A2222 | C2155 | U | U | C | A1899 | A1822 | A1752 | U1681 | C1608 | A1544 | G1486 | A1413 | A1350 |
| A2357 | U2289 | G2223 | C2156 | A | A | G | U1900 | A1823 | U1753 | U1682 | C1609 | A1545 | A1481 | G1414 | U1351 |
| C2358 | C2290 | U2224 | A2157 | C | C | G | A1901 | A1824 | G1754 | U1683 | G1611 | A1546 | A1482 | U1415 | A1352 |
| U2359 | G2291 | G2225 | A2158 | G | U | C | G1902 | A1825 | G1755 | U1684 | A1612 | G1547 | U1483 | G1416 | U1353 |
| C2360 | U2292 | U2226 | G2159 | G | U | C | U1903 | A1826 | U1756 | U1685 | A1613 | C1548 | U1484 | G1417 | G1354 |
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| U2362 | U2294 | U2228 | A2163 | U | G | C | U1905 | A1828 | U1758 | U1687 | C1615 | U1583 | G1487 | G1420 | U1356 |
| C2363 | U2295 | G2229 | A2164 | C | C | A | G1906 | A1829 | G1759 | U1688 | C1616 | U1584 | G1488 | C1421 | G1362 |
| U2364 | U2296 | A2230 | C2165 | C | C | U | C1907 | A1830 | G1760 | U1689 | C1617 | U1585 | A1489 | G1422 | A1363 |
| C2365 | G2297 | U2231 | A2166 | U | U | C | A1908 | A1831 | G1761 | C1690 | G1618 | C1556 | A1490 | C1423 | A1364 |
| U2366 | U2298 | G2232 | A2167 | G | U | G | U1909 | A1832 | U1762 | U1691 | A1619 | A1557 | A1491 | C1424 | U1365 |
| A2367 | C2299 | U2233 | A2168 | U | C | C | A1910 | A1833 | G1763 | U1692 | U1620 | A1558 | G1492 | U1425 | G1366 |
| C2368 | U2300 | G2234 | G2169 | U | U | G | U1911 | A1834 | U1764 | C1693 | A1621 | A1559 | G1493 | C1426 | A1366 |
| U2369 | G2301 | A2235 | G2170 | C | U | C | U1912 | A1835 | G1765 | U1694 | U1622 | G1560 | U1494 | U1427 | U1367 |
| C2370 | C2302 | U2236 | A2171 | G | G | U | U1913 | A1836 | G1766 | U1695 | G1623 | G1561 | A1495 | A1428 | U1368 |
| U2371 | U2303 | G2237 | G2172 | U | U | U | U1914 | A1837 | U1767 | A1696 | U1626 | C1562 | C1496 | G1429 | A1369 |
| C2372 | U2304 | U2238 | U2173 | A | C | C | U1915 | A1838 | U1768 | G1701 | U1627 | C1563 | C1497 | U1430 | G1370 |
| A2373 | U2305 | G2239 | U2174 | C | U | C | C1916 | A1839 | U1769 | U1702 | C1628 | U1564 | A1498 | G1431 | G1371 |
| U2374 | U2306 | U2240 | U2175 | A | A | U | C1917 | A1840 | U1770 | G1706 | U1629 | G1565 | G1500 | C1432 | C1372 |
| C2375 | A2241 | A2242 | U2176 | C | C | U | C1918 | A1841 | U1771 | C1707 | C1630 | U1566 | U1501 | A1433 | A1373 |
| U2376 | U2243 | U2243 | A2177 | C | C | U | G1919 | A1842 | U1772 | C1708 | C1631 | U1567 | C1502 | G1434 | G1374 |
| C2377 | A2244 | U2244 | C2178 | G | G | U | U1920 | A1843 | U1773 | A1707 | C1632 | U1568 | A1503 | G1435 | G1375 |
| U2378 | U2245 | G2245 | G2180 | C | C | U | G1921 | A1844 | U1774 | C1709 | A1633 | U1569 | A1504 | U1436 | C1376 |
| C2379 | G2246 | U2246 | A2181 | C | C | U | U1922 | A1845 | U1775 | C1710 | C1634 | U1570 | C1505 | G1437 | G1377 |
| U2380 | U2247 | G2247 | A2182 | U | U | A | A1923 | A1846 | U1776 | C1711 | G1635 | A1571 | C1506 | U1438 | U1378 |
| U2381 | C2248 | C2248 | U2183 | U | U | C | U1924 | A1847 | U1777 | G1712 | U1636 | U1572 | G1507 | G1379 | G1379 |
| U2382 | U2249 | G2249 | U2184 | C | C | U | A1925 | A1848 | U1778 | G1713 | A1637 | C1574 | C1508 | G1440 | G1380 |
| C2383 | U2250 | G2250 | G2185 | U | U | G | G1926 | A1849 | U1779 | U1716 | C1638 | A1575 | A1509 | U1442 | G1382 |
| A2384 | U2251 | U2251 | A2186 | A | A | U | U1927 | A1850 | U1780 | U1717 | U1639 | G1576 | G1510 | G1443 | U1383 |
| U2385 | G2252 | G2252 | U2187 | C | C | U | C1928 | A1851 | U1781 | U1718 | A1642 | C1578 | G1511 | U1444 | U1384 |
| C2386 | U2253 | U2253 | A2188 | U | U | C | U1929 | A1852 | U1782 | G1719 | A1643 | C1579 | G1512 | U1445 | C1385 |
| U2387 | U2254 | U2254 | U2189 | C | C | U | G1930 | A1853 | U1783 | U1720 | C1644 | A1580 | G1447 | A1446 | A1386 |
| C2388 | A2255 | G2255 | U2190 | G | G | U | U1931 | A1854 | U1784 | U1721 | C1645 | U1581 | U1448 | G1447 | G1387 |
| A2389 | U2256 | U2256 | U2191 | U | U | C | A1932 | A1855 | U1785 | U1722 | C1646 | C1582 | A1449 | U1388 | U1388 |
| U2390 | C2257 | G2257 | C2192 | C | C | U | G1933 | A1856 | U1786 | U1723 | G1650 | A1583 | G1519 | A1390 | A1390 |
| C2391 | U2258 | U2258 | U2193 | U | U | G | A1934 | A1857 | U1787 | U1724 | G1651 | U1584 | G1520 | G1450 | A1391 |
| U2392 | G2259 | U2259 | G2194 | C | C | U | G1935 | A1858 | U1788 | U1725 | G1652 | C1576 | U1521 | A1452 | G1392 |
| C2393 | U2260 | G2260 | C2195 | U | U | C | U1936 | A1859 | U1789 | U1726 | G1653 | G1577 | G1513 | U1453 | U1393 |
| U2394 | C2261 | U2261 | C2196 | C | C | U | G1937 | A1860 | U1790 | C1726 | U1654 | C1578 | G1514 | U1445 | A1394 |
| A2395 | U2262 | G2262 | C2197 | U | U | G | U1938 | A1861 | U1791 | U1727 | A1645 | C1579 | G1515 | U1446 | A1395 |
| C2396 | C2263 | U2263 | U2198 | C | C | U | G1939 | A1862 | U1792 | U1728 | C1646 | C1580 | G1516 | U1447 | G1396 |
| U2397 | U2264 | U2264 | U2199 | U | U | C | U1940 | A1863 | U1793 | U1729 | G1650 | A1584 | G1517 | U1448 | U1397 |
| C2398 | C2265 | G2265 | G2200 | G | G | U | G1941 | A1864 | U1794 | U1730 | G1651 | C1579 | G1518 | U1449 | A1398 |
| A2399 | U2266 | U2266 | G2201 | C | C | U | U1942 | A1865 | U1795 | U1731 | A1646 | C1580 | G1519 | A1450 | A1399 |
| U2400 | C2267 | G2267 | U2202 | U | U | A | C1943 | A1866 | U1796 | U1732 | C1647 | A1581 | G1520 | U1451 | U1399 |
| C2401 | U2268 | U2268 | C2203 | C | C | U | U1944 | A1867 | U1797 | U1733 | G1648 | C1582 | G1521 | A1452 | G1399 |
| U2402 | G2269 | U2269 | U2204 | U | U | C | A1945 | A1868 | U1798 | U1734 | G1649 | A1583 | U1522 | A1453 | U1400 |
| A2403 | U2270 | U2270 | U2205 | C | C | U | G1946 | A1869 | U1799 | U1735 | G1650 | A1584 | U1523 | A1454 | U1401 |
| U2404 | C2271 | G2271 | C2206 | U | U | C | U1947 | A1870 | U1800 | U1736 | G1651 | C1585 | U1524 | A1455 | U1402 |
| C2405 | U2272 | U2272 | U2207 | C | C | U | G1948 | A1871 | U1801 | U1737 | G1652 | A1586 | U1525 | A1456 | U1403 |
| U2406 | G2273 | U2273 | U2208 | U | U | A | U1949 | A1872 | U1802 | U1738 | G1653 | U1587 | U1526 | A1457 | U1404 |
| C2407 | A2274 | U2274 | U2209 | C | C | U | U1950 | A1873 | U1803 | U1739 | G1654 | A1588 | U1527 | A1458 | U1405 |
| U2408 | U2275 | G2275 | U2210 | U | U | C | U1951 | A1874 | U1804 | U1740 | G1655 | A1589 | U1528 | A1459 | U1406 |
| A2409 | C2276 | U2276 | U2211 | C | C | U | G1952 | A1875 | U1805 | U1741 | G1656 | A1590 | U1529 | A1460 | U1407 |
| U2410 | G2277 | U2277 | U2212 | U | U | C | U1953 | A1876 | U1806 | U1742 | G1657 | A1591 | U1530 | A1461 | U1408 |
| C2411 | A2278 | U2278 | U2213 | C | C | U | U1954 | A1877 | U1807 | U1743 | G1658 | A1592 | U1531 | A1462 | U1409 |
| U2412 | U2279 | U2279 | U2214 | U | U | C | U1955 | A1878 | U1808 | U1744 | G1659 | A1593 | U1532 | A1463 | U1410 |
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| C2415 | A2282 | G2282 | U2147 | U | G | C | A1883 | A1811 | U1747 | G1662 | U1596 | C1532 | A1466 | A1413 | A1350 |
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| A2417 | G2284 | U2284 | U2149 | C | C | U | U1888 | A1813 | G1749 | G1668 | G1598 | U1534 | A1468 | G1415 | A1352 |
| U2418 | C2285 | A2285 | U2150 | U | U | C | A1889 | A1814 | G1750 | G1669 | G1599 | A1535 | U1469 | G1416 | U1353 |
| C2419 | U2286 | G2286 | C2151 | C | C | U | A1891 | A1815 | U1751 | C1670 | A1602 | G1536 | U1470 | G1417 | U1354 |
| U2420 | G2287 | U2287 | U2152 | U | U | C | A1894 | A1816 | G1752 | U1680 | A1603 | A1537 | A1471 | A1418 | A1355 |
| A2421 | C2288 | A2288 | A2153 | A | A | G | U1894 | A1817 | U1753 | U1681 | C1604 | A1544 | A1472 | G1419 | U1356 |
| U2422 | U2289 | U2289 | U2154 | U | U | C | A1895 | A1818 | G1754 | U1682 | A1545 | A1544 | A1473 | G1420 | G1357 |
| C2423 | G2290 | G2 | | | | | | | | | | | | | |

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|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| A3342 | G3205 | C3076 | C3002 | A2940 | G2877 | A2813 | A2748 | U2683 | U2613 | C2539 | U2510 | G | A2401 |
| G3343 | C3206 | A3077 | G3003 | A2941 | G2878 | G2814 | G2749 | C2684 | G2614 | A2540 | A2511 | C | A2402 |
| G3344 | U3207 | U3078 | C3004 | G2942 | G2879 | G2815 | G2750 | G2687 | G2615 | U2541 | G | A2403 | |
| G3345 | G3208 | U3079 | A3005 | G2943 | U2880 | G2816 | G2751 | G2688 | U2542 | U2542 | U | A2404 | |
| U3346 | A3209 | G3080 | A3006 | G2944 | G2881 | G2817 | G2752 | U2689 | U2543 | C | C2405 | | |
| A3347 | G3212 | C3081 | U3007 | G2945 | U2882 | G2818 | G2753 | A2689 | G2618 | U2544 | G | C2406 | |
| G3348 | A3213 | C3082 | A3011 | A2946 | U2883 | A2819 | G2754 | G2690 | G2619 | C2545 | C | C2407 | |
| C3349 | U3214 | G3083 | A3012 | G2947 | C2884 | U2822 | C2755 | A2691 | G2620 | C2546 | U | U2408 | |
| C3350 | U3282 | C3084 | U3013 | G2948 | U2885 | U2823 | C2756 | A2692 | G2621 | A2547 | G | C2409 | |
| U3351 | G3283 | G3085 | U3014 | U2949 | U2886 | G2823 | C2757 | C2693 | C2622 | C2548 | U | U2410 | |
| U3352 | G3284 | A3086 | G3015 | G2950 | U2887 | G2824 | A2758 | A2694 | C2623 | C2549 | C | U2411 | |
| G3353 | G3285 | G3087 | A3016 | G2951 | U2888 | U2827 | C2759 | A2695 | G2624 | U2550 | A | G2412 | |
| G3354 | U3218 | A3088 | A3016 | G2952 | U2889 | G2828 | C2760 | A2696 | C2625 | U2551 | C | A2413 | |
| U3355 | G3219 | C3089 | U3019 | U2953 | A2890 | G2826 | G2761 | A2697 | C2552 | C2552 | U | G2414 | |
| G3356 | G3220 | C3090 | U3020 | U2954 | U2891 | U2829 | A2762 | G2698 | U2553 | C2553 | G | C2415 | |
| G3357 | C3221 | C3091 | A3021 | U2955 | U2892 | G2830 | U2763 | G2699 | A2554 | A2554 | A | U2416 | |
| U3358 | G3224 | C3092 | A3022 | A2956 | C2893 | G2831 | C2764 | G2700 | C2555 | A | U2417 | | |
| A3359 | A3225 | A3093 | U3023 | U2957 | G2894 | C2832 | C2765 | U2701 | C2556 | A | U2418 | | |
| C3360 | U3226 | U3094 | A3024 | U2958 | G2895 | A2833 | U2766 | A2702 | C2557 | U | C2419 | | |
| G3361 | A3227 | C3095 | A3024 | U2959 | A2896 | G2834 | U2767 | A2703 | U2558 | A | C2420 | | |
| A3362 | C3228 | C3096 | A3029 | C2960 | U2897 | U2835 | U2768 | A2704 | U2559 | C | U2421 | | |
| U3363 | G3229 | U3100 | G3030 | G2961 | U2898 | G2836 | U2769 | A2705 | C2560 | C | C2422 | | |
| A3364 | A3231 | G3101 | G3031 | U2965 | C2899 | A2837 | G2770 | G2706 | A2561 | A | U2423 | | |
| G3365 | G3232 | G3102 | A3032 | G2966 | C2899 | U2838 | U2771 | C2707 | A2562 | C | A2424 | | |
| C3366 | A3233 | A3103 | A3033 | G2967 | C2899 | G2839 | C2772 | C2708 | G2563 | U | G2425 | | |
| G3367 | G3234 | U3104 | C3034 | A2968 | U2900 | C2840 | C2773 | C2709 | G2564 | A | U2426 | | |
| U3368 | U3235 | U3105 | C3039 | U2969 | G2901 | U2841 | C2774 | C2710 | U2565 | C | U2427 | | |
| G3369 | G3236 | G3106 | A3040 | G2970 | U2902 | G2842 | U2775 | C2711 | C2566 | C | U2433 | | |
| A3370 | A3237 | G3107 | A3041 | A2971 | U2903 | U2843 | U2776 | U2712 | C2567 | U | U2434 | | |
| U3371 | C3238 | U3108 | U3042 | G2972 | G2903 | U2844 | U2777 | U2713 | C2568 | U | G2435 | | |
| G3372 | G3239 | A3109 | C3043 | U2973 | C2904 | U2845 | U2778 | G2714 | A2569 | A | U2436 | | |
| A3373 | U3240 | G3110 | C3044 | U2974 | G2905 | U2846 | A2779 | U2717 | U2570 | U2501 | U2501 | G2437 | |
| U3374 | G3241 | A3111 | G3045 | U2975 | C2912 | U2847 | U2780 | U2718 | C2572 | A2502 | A2443 | A2443 | |
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| A3377 | C3244 | C3114 | U3048 | U2978 | U2915 | U2853 | U2783 | U2723 | C2582 | U2510 | A | A2445 | |
| G3378 | U3245 | U3115 | A3049 | U2979 | G2916 | U2854 | G2784 | U2724 | C2582 | A2511 | G | A2445 | |
| U3379 | A3246 | G3116 | C3050 | U2980 | U2917 | U2855 | A2785 | U2725 | C2585 | A2514 | A | A2445 | |
| G3380 | G3247 | U3117 | U3051 | U2981 | G2918 | G2856 | A2790 | C2726 | G2586 | A2515 | G | A2445 | |
| C3381 | U3248 | C3118 | G3052 | U2982 | U2919 | U2857 | G2794 | U2727 | A2590 | A2519 | C | A2445 | |
| A3382 | A3249 | A3119 | G3053 | C2983 | U2920 | U2858 | U2795 | G2728 | A2591 | A2520 | G | A2445 | |
| G3383 | U3250 | G3120 | U3054 | C2984 | U2921 | U2859 | U2796 | U2729 | A2592 | U2521 | G | A2445 | |
| U3384 | G3251 | U3121 | U3055 | C2985 | U2922 | U2860 | C2797 | G2730 | C2593 | A2523 | A | A2445 | |
| G3385 | G3252 | A3122 | C3056 | U2986 | U2923 | U2861 | C2798 | U2731 | G2662 | A2601 | G | A2445 | |
| U3386 | G3253 | G3123 | U3057 | U2987 | C2924 | U2862 | U2799 | U2732 | G2663 | G2602 | A | A2445 | |
| A3387 | C3254 | U3124 | U3058 | U2988 | U2925 | U2863 | A2800 | G2733 | C2664 | U2603 | A | A2445 | |
| G3388 | U3255 | G3125 | G3059 | U2989 | C2926 | U2864 | G2801 | A2734 | U2665 | G2604 | A | A2445 | |
| U3389 | G3256 | U3126 | C3060 | G2990 | C2927 | U2865 | A2802 | U2735 | C2666 | G2605 | A | A2445 | |
| A3390 | U3257 | A3127 | G3061 | U2991 | C2928 | U2866 | A2803 | A2736 | U2667 | U2604 | U | A2445 | |
| G3391 | C3258 | U3128 | U3062 | U2992 | U2931 | U2867 | A2804 | C2737 | G2668 | C2531 | A | A2445 | |
| U3392 | G3259 | G3129 | U3063 | U2993 | U2932 | U2868 | U2795 | A2738 | G2606 | U2532 | A | A2445 | |
| A3393 | U3260 | A3130 | C3064 | A2994 | U2933 | U2869 | U2796 | A2739 | G2607 | U2533 | G | A2445 | |
| G3394 | G3261 | U3131 | U3065 | U2995 | U2934 | C2870 | U2807 | U2740 | G2608 | U2534 | U | A2445 | |
| U3395 | A3262 | G3132 | U3066 | U2996 | U2935 | G2871 | A2808 | A2743 | A2609 | A2535 | G | A2445 | |
| A3396 | G3263 | U3133 | U3067 | U2997 | U2936 | U2872 | C2809 | U2744 | G2610 | U2536 | G | A2445 | |
| G3397 | U3264 | C3134 | C3068 | U2998 | U2937 | U2873 | C2810 | G2745 | U2611 | U2537 | U | A2445 | |
| U3398 | C3265 | A3135 | U3069 | U2999 | U2938 | U2874 | A2811 | A2746 | U2612 | U2538 | A | A2445 | |
| A3399 | G3266 | U3136 | U3070 | U2999 | U2938 | U2875 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| G3400 | A3267 | G3136 | U3071 | U2999 | U2938 | U2876 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| U3401 | G3268 | U3137 | U3072 | U2999 | U2938 | U2877 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| G3402 | U3269 | A3138 | C3073 | U2999 | U2938 | U2878 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| A3403 | C3270 | G3139 | U3074 | U2999 | U2938 | U2879 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| U3404 | G3271 | U3140 | U3075 | U2999 | U2938 | U2880 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| G3405 | A3272 | C3141 | U3076 | U2999 | U2938 | U2881 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| U3406 | U3273 | G3142 | U3077 | U2999 | U2938 | U2882 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| A3407 | G3274 | A3143 | U3078 | U2999 | U2938 | U2883 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| G3408 | C3275 | U3144 | U3079 | U2999 | U2938 | U2884 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| U3409 | A3276 | G3145 | U3080 | U2999 | U2938 | U2885 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| G3410 | U3277 | A3146 | U3081 | U2999 | U2938 | U2886 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| A3411 | G3278 | U3147 | U3082 | U2999 | U2938 | U2887 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| U3412 | C3279 | G3148 | U3083 | U2999 | U2938 | U2888 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| G3413 | A3279 | A3149 | U3084 | U2999 | U2938 | U2889 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| U3414 | U3280 | U3150 | U3085 | U2999 | U2938 | U2890 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| G3415 | G3281 | G3151 | U3086 | U2999 | U2938 | U2891 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| A3416 | C3282 | A3152 | U3087 | U2999 | U2938 | U2892 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| U3417 | U3283 | U3153 | U3088 | U2999 | U2938 | U2893 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| G3418 | G3284 | C3154 | U3089 | U2999 | U2938 | U2894 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| U3419 | A3285 | U3155 | U3090 | U2999 | U2938 | U2895 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| G3420 | C3286 | G3156 | U3091 | U2999 | U2938 | U2896 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| U3421 | U3287 | U3157 | U3092 | U2999 | U2938 | U2897 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| G3422 | G3288 | G3158 | U3093 | U2999 | U2938 | U2898 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| A3423 | C3289 | U3159 | U3094 | U2999 | U2938 | U2899 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| U3424 | U3290 | U3160 | U3095 | U2999 | U2938 | U2900 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| G3425 | G3291 | C3161 | U3096 | U2999 | U2938 | U2901 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| U3426 | A3292 | G3162 | U3097 | U2999 | U2938 | U2902 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| G3427 | C3293 | A3163 | U3098 | U2999 | U2938 | U2903 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| U3428 | U3294 | C3164 | U3099 | U2999 | U2938 | U2904 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| A3429 | G3295 | A3165 | U3100 | U2999 | U2938 | U2905 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| U3430 | C3296 | U3166 | U3101 | U2999 | U2938 | U2906 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| G3431 | A3297 | A3167 | U3102 | U2999 | U2938 | U2907 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| U3432 | U3298 | G3168 | U3103 | U2999 | U2938 | U2908 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| G3433 | C3299 | A3169 | U3104 | U2999 | U2938 | U2909 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| A3434 | A3300 | U3170 | U3105 | U2999 | U2938 | U2910 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| U3435 | G3301 | U3171 | U3106 | U2999 | U2938 | U2911 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| G3436 | U3302 | G3172 | U3107 | U2999 | U2938 | U2912 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| U3437 | C3303 | A3173 | U3108 | U2999 | U2938 | U2913 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| A3438 | U3304 | G3174 | U3109 | U2999 | U2938 | U2914 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| G3439 | G3305 | A3175 | U3110 | U2999 | U2938 | U2915 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| U3440 | C3306 | G3176 | U3111 | U2999 | U2938 | U2916 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| G3441 | A3307 | U3177 | U3112 | U2999 | U2938 | U2917 | C2812 | A2747 | U2613 | U2539 | A | A2445 | |
| U3442 | | | | | | | | | | | | | |

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|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|-----|
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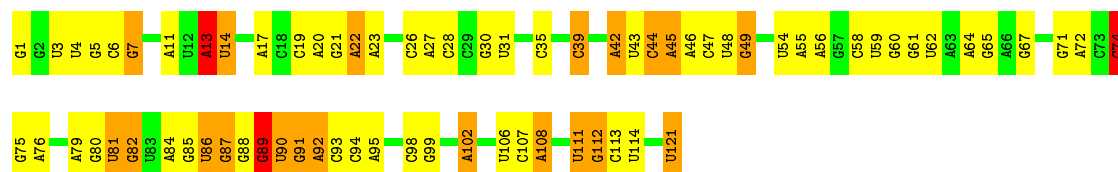
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PDB
PROTEIN DATA BANK

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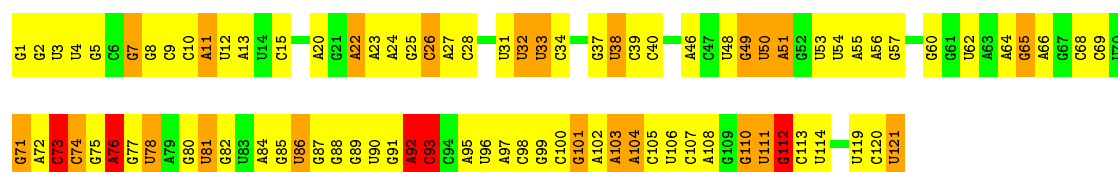
• Molecule 37: 5S ribosomal RNA

Chain 3: 40% 41% 17%



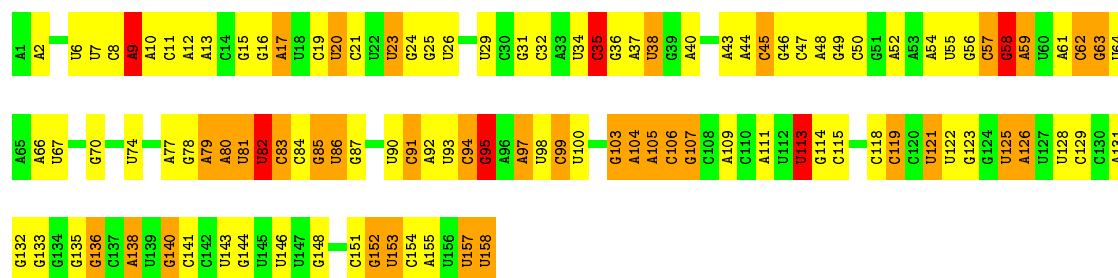
• Molecule 37: 5S ribosomal RNA

Chain 7: 26% 51% 18%



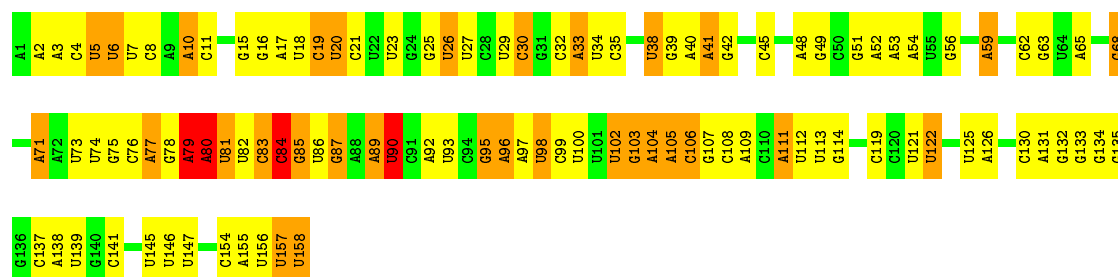
• Molecule 38: 5.8S ribosomal RNA

Chain 4: 30% 44% 22%

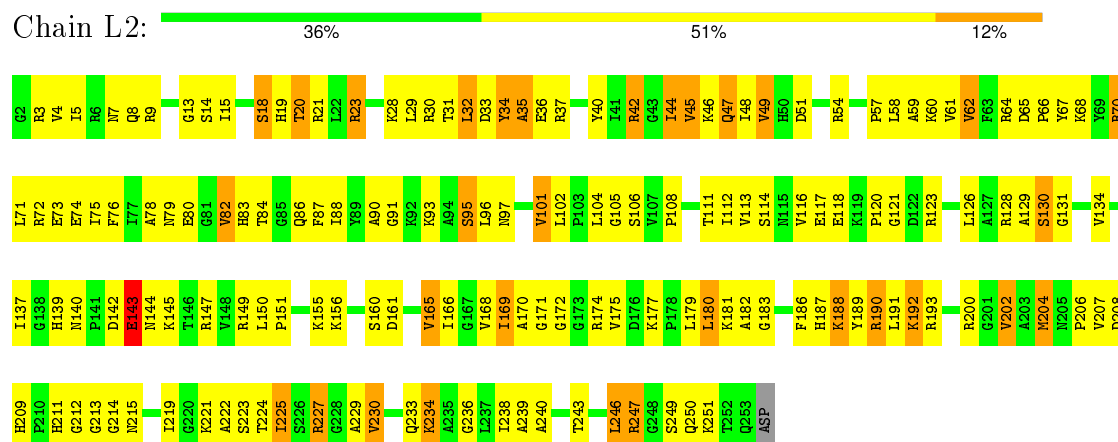


• Molecule 38: 5.8S ribosomal RNA

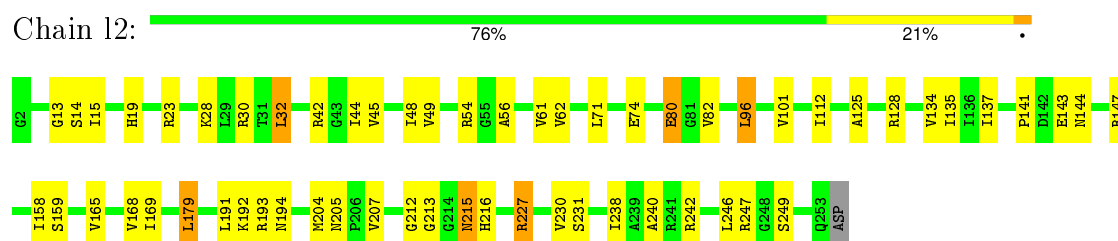
Chain 8: 34% 44% 20%



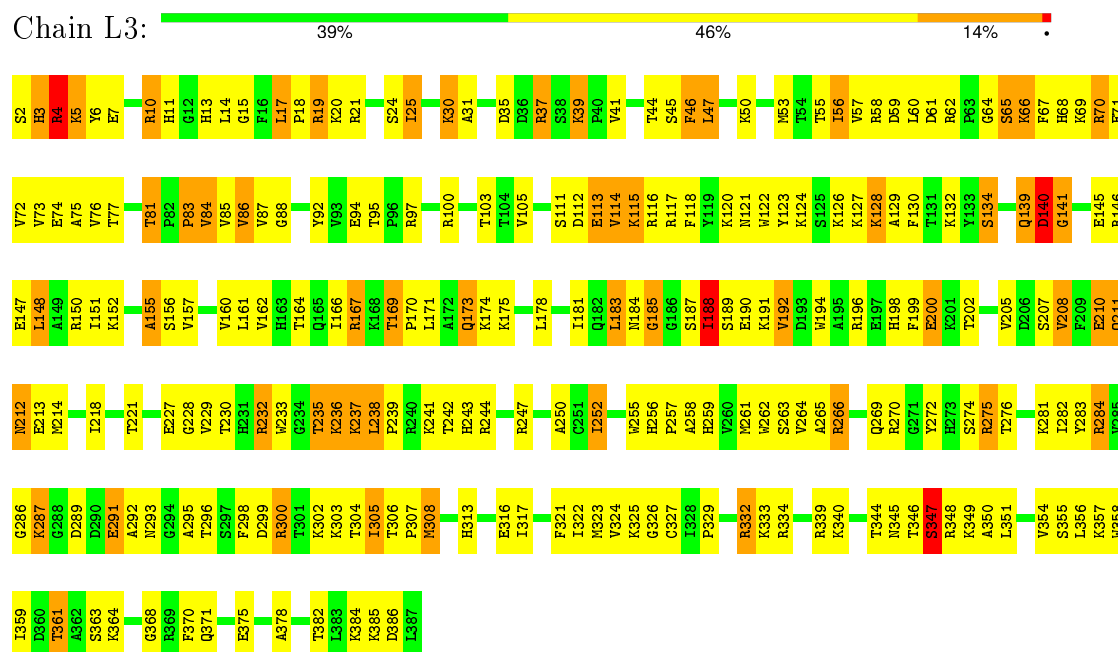
- Molecule 39: 60S ribosomal protein L2-A



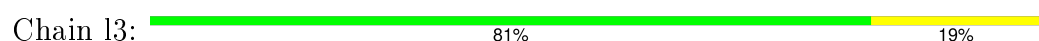
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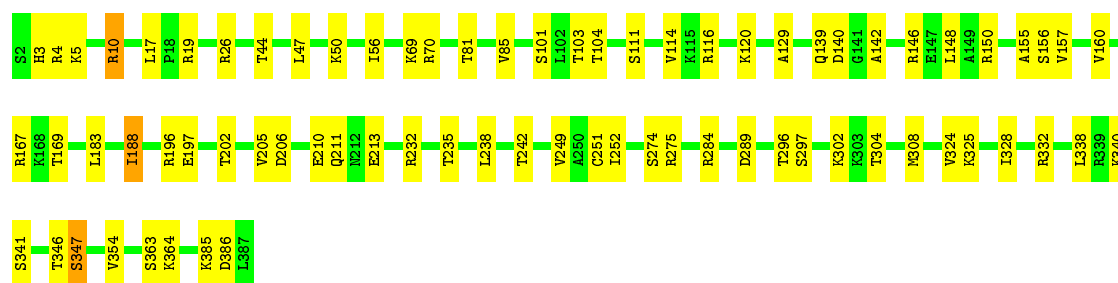


- Molecule 40: 60S ribosomal protein L3

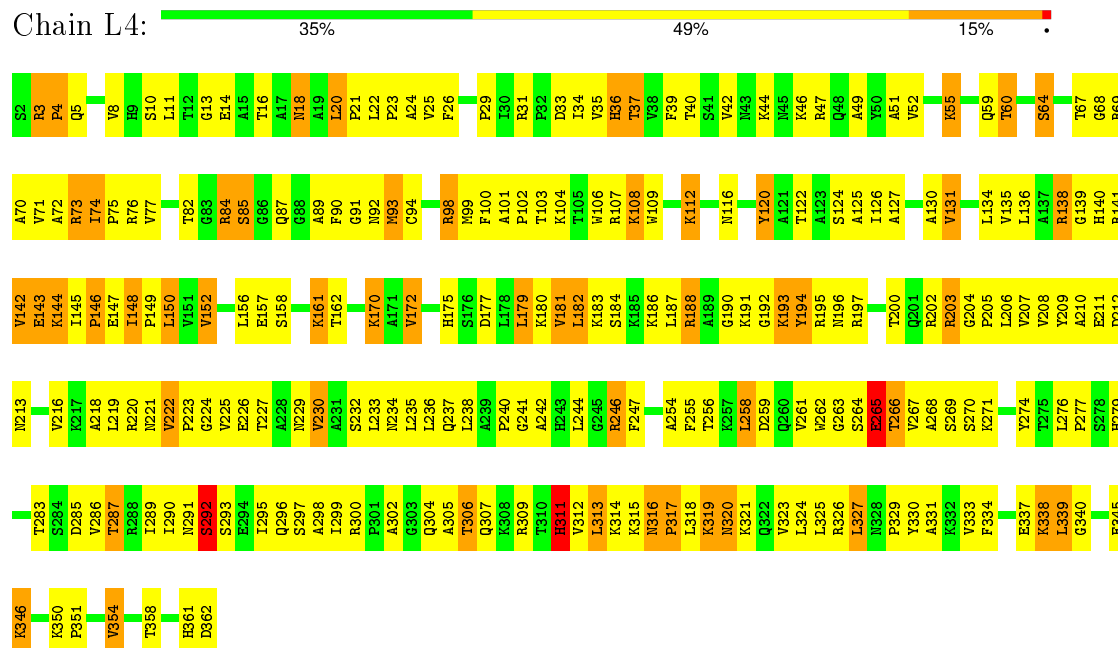


- Molecule 40: 60S ribosomal protein L3

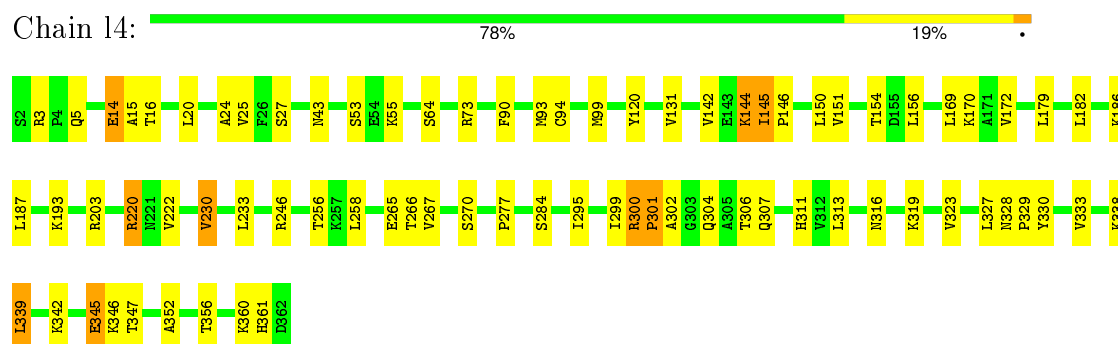




- Molecule 41: 60S ribosomal protein L4-A

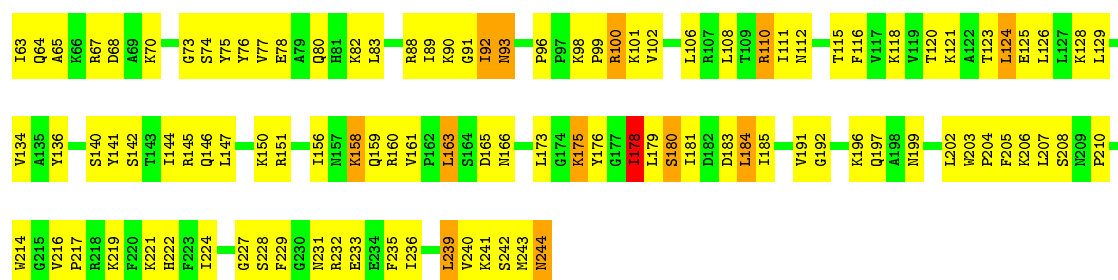


- Molecule 41: 60S ribosomal protein L4-A



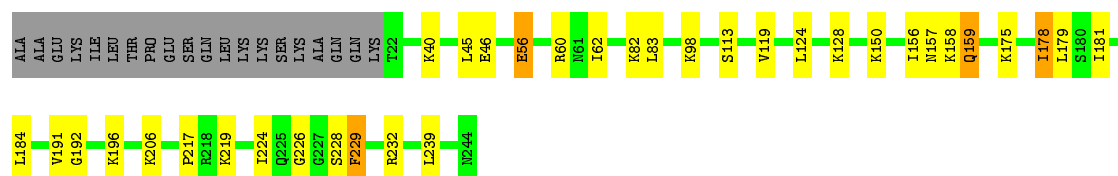
- Molecule 42: 60S ribosomal protein L5





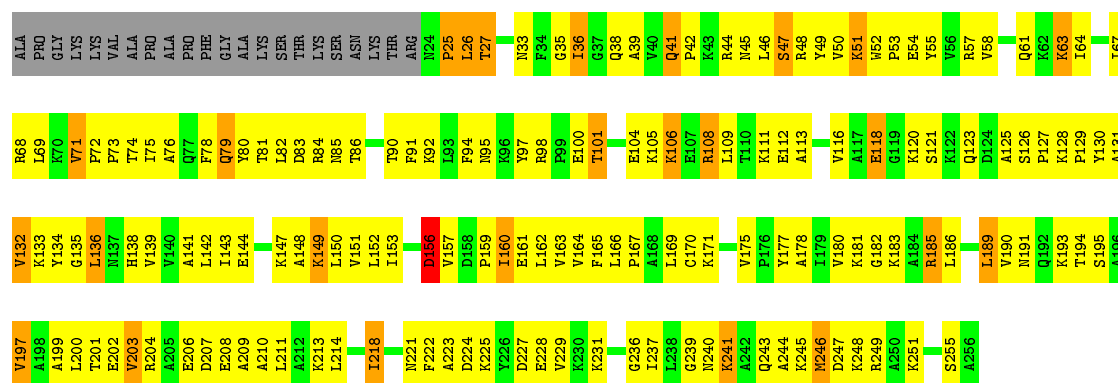
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Chain 17: 77% 13% 8%



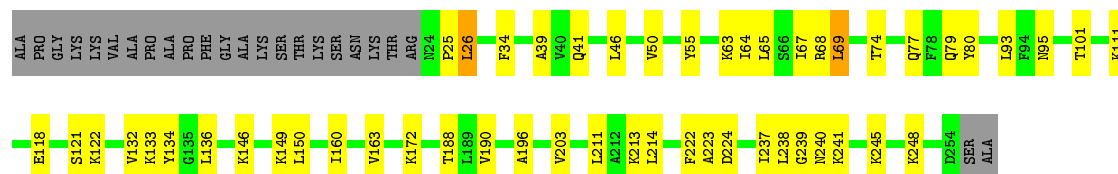
• Molecule 45: 60S ribosomal protein L8-A

Chain L8: 29% 53% 10% 9%



• Molecule 45: 60S ribosomal protein L8-A

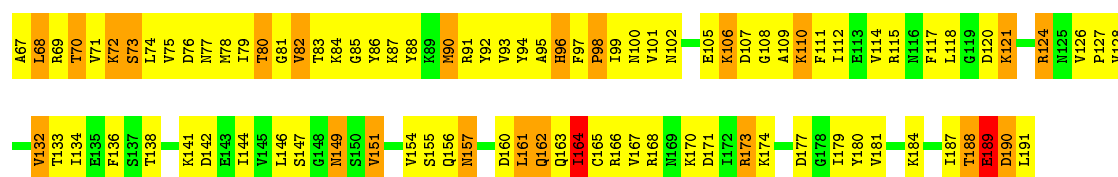
Chain l8: 70% 20% 9%



• Molecule 46: 60S ribosomal protein L9-A

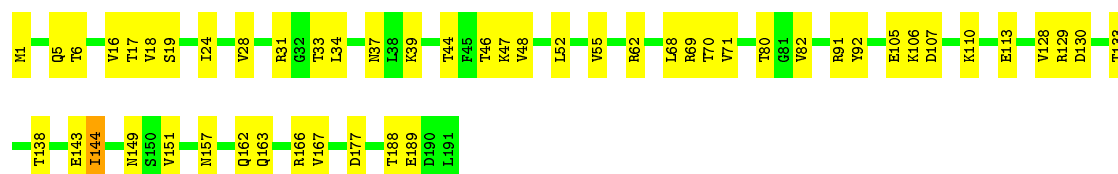
Chain L9: 28% 53% 17%





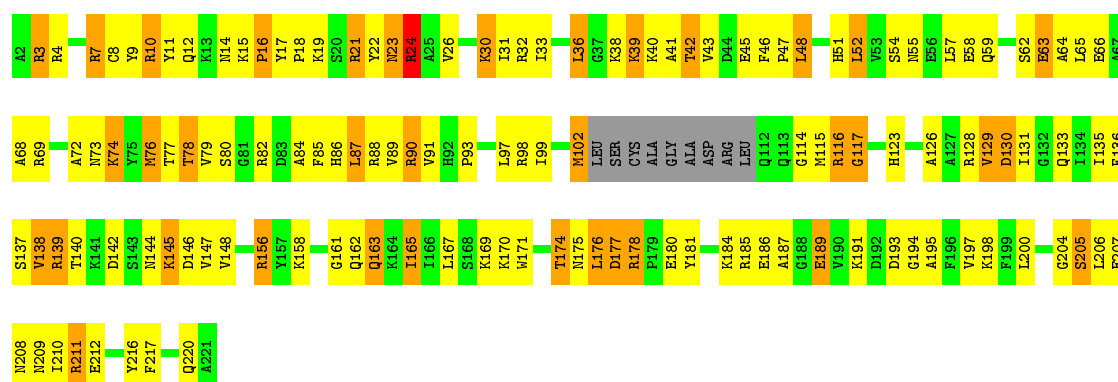
• Molecule 46: 60S ribosomal protein L9-A

Chain I9: 73% 26% .



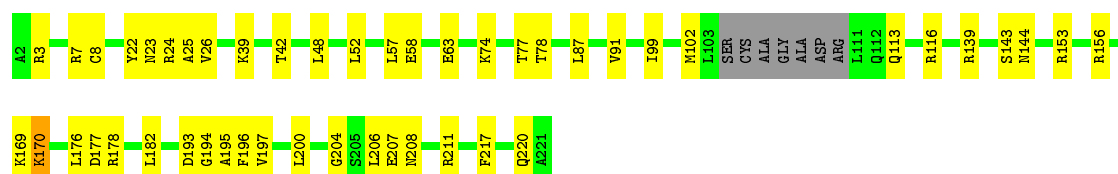
• Molecule 47: 60S ribosomal protein L10

Chain M0: 35% 44% 16% .



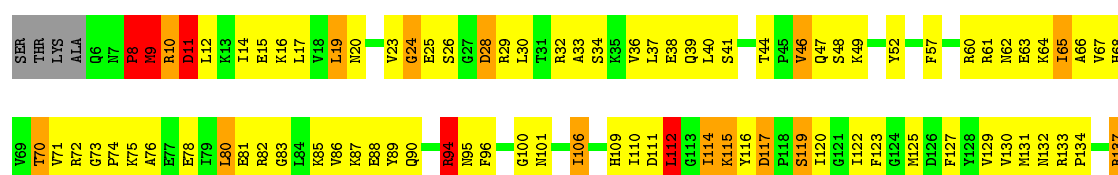
• Molecule 47: 60S ribosomal protein L10

Chain m0: 75% 21% .



• Molecule 48: 60S ribosomal protein L11-B

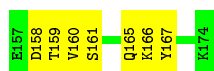
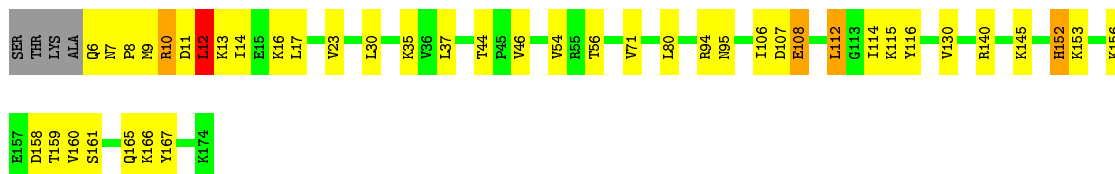
Chain M1: 31% 51% 12% . . .





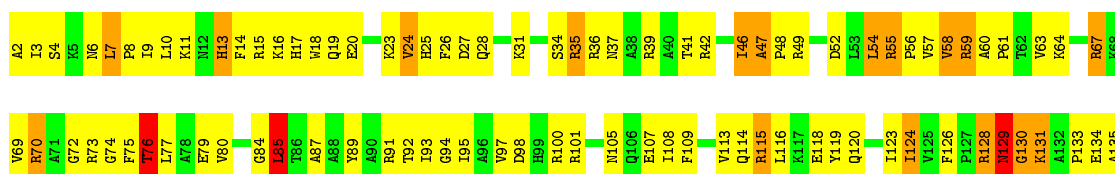
• Molecule 48: 60S ribosomal protein L11-B

Chain m1: 73% 22% ...



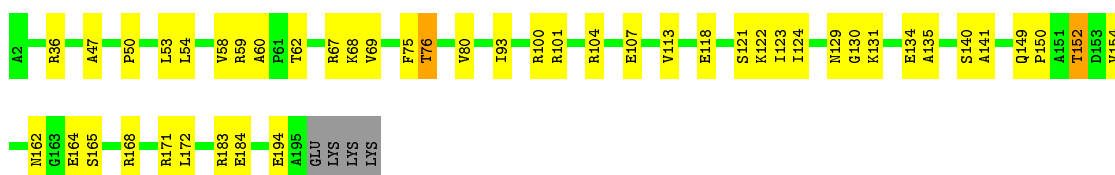
• Molecule 49: 60S ribosomal protein L13-A

Chain M3: 31% 51% 13% ..



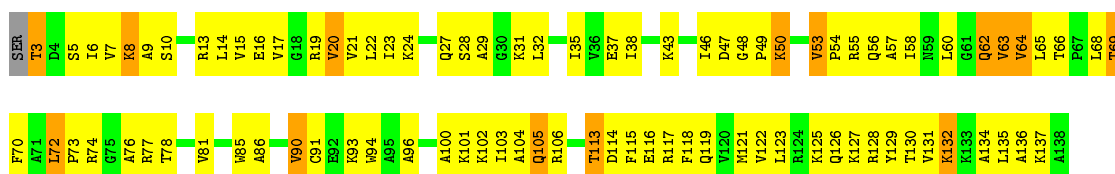
• Molecule 49: 60S ribosomal protein L13-A

Chain m3: 75% 22% ..



• Molecule 50: 60S ribosomal protein L14-A

Chain M4: 34% 55% 10% .



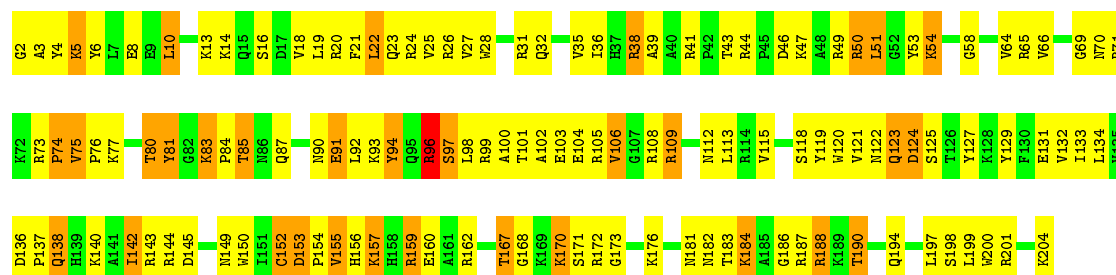
• Molecule 50: 60S ribosomal protein L14-A

Chain m4: 79% 20% .



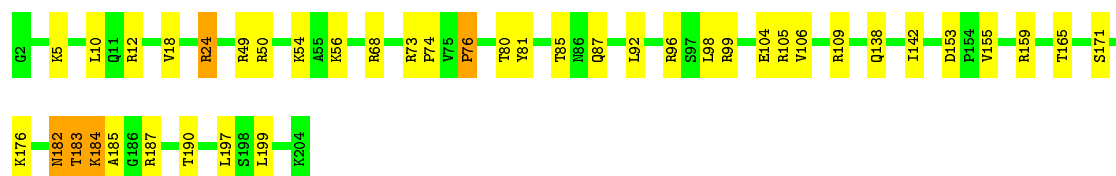
- Molecule 51: 60S ribosomal protein L15-A

Chain M5: 35% 48% 16%



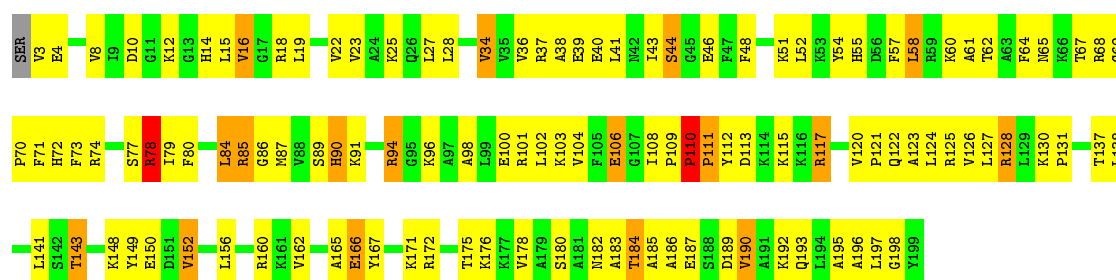
- Molecule 51: 60S ribosomal protein L15-A

Chain m5: 80% 18% .



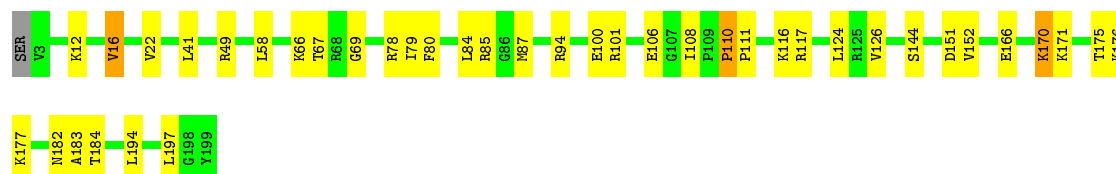
- Molecule 52: 60S ribosomal protein L16-A

Chain M6: 40% 50% 9% ..

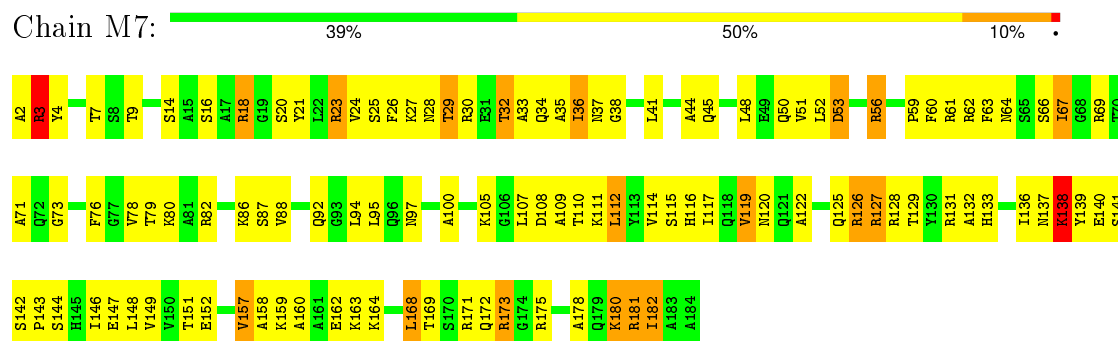


- Molecule 52: 60S ribosomal protein L16-A

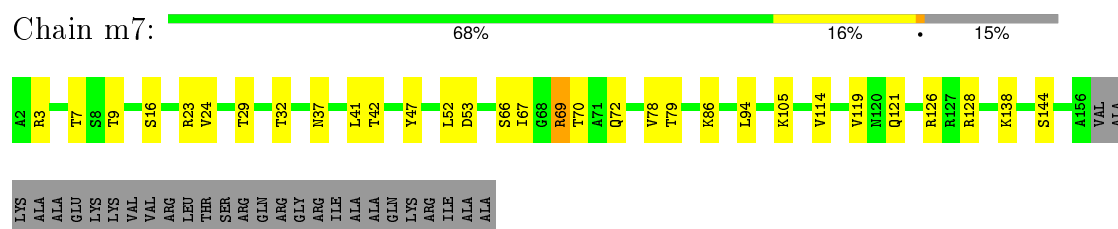
Chain m6: 79% 19% ..



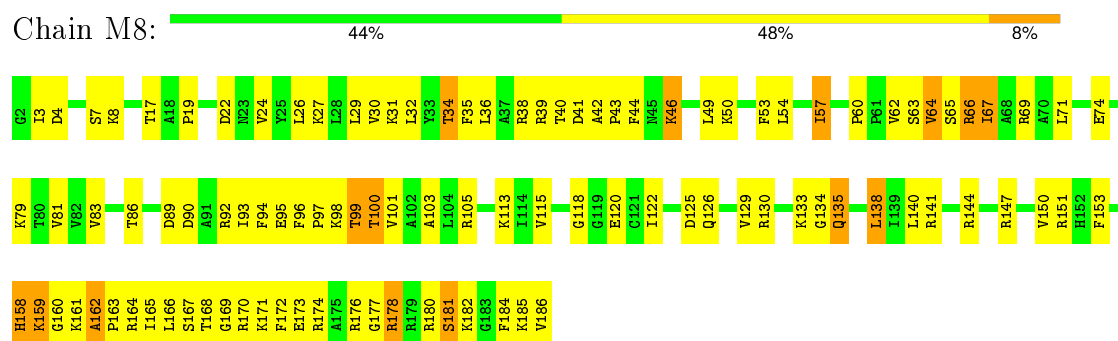
- Molecule 53: 60S ribosomal protein L17-A



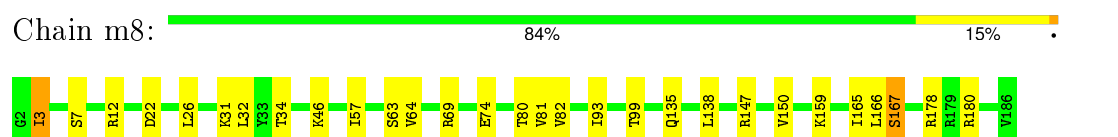
- Molecule 53: 60S ribosomal protein L17-A



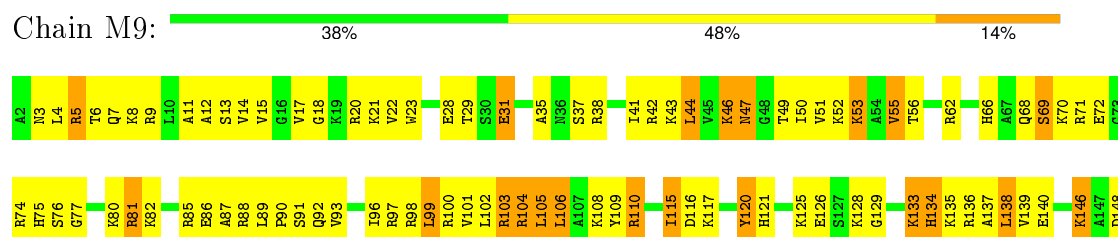
- Molecule 54: 60S ribosomal protein L18-A

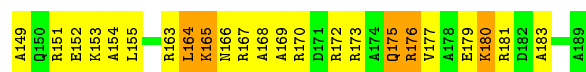


- Molecule 54: 60S ribosomal protein L18-A



- Molecule 55: 60S ribosomal protein L19-A





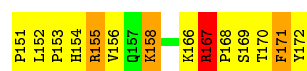
• Molecule 55: 60S ribosomal protein L19-A

Chain m9: 84% 15% .



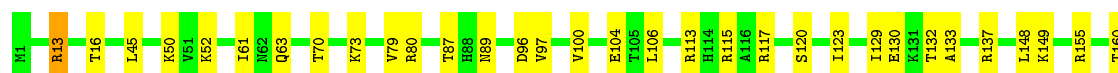
• Molecule 56: 60S ribosomal protein L20-A

Chain N0: 44% 41% 15% .



• Molecule 56: 60S ribosomal protein L20-A

Chain n0: 78% 21% .



• Molecule 57: 60S ribosomal protein L21-A

Chain N1: 47% 40% 13% .



• Molecule 57: 60S ribosomal protein L21-A

Chain n1: 82% 16% .



- Molecule 58: 60S ribosomal protein L22-A

Chain N2: 28% 43% 13% 17%

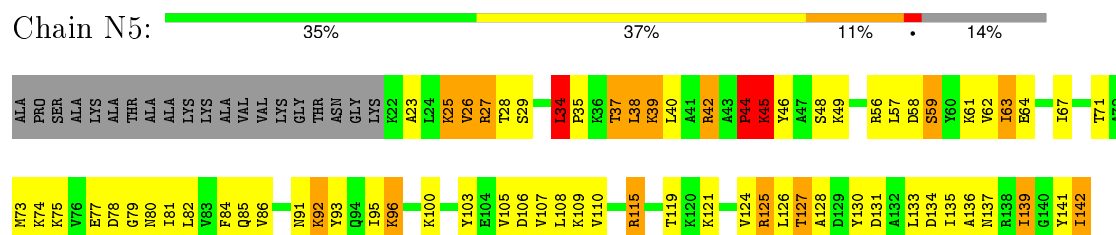


- Molecule 58: 60S ribosomal protein L22-A

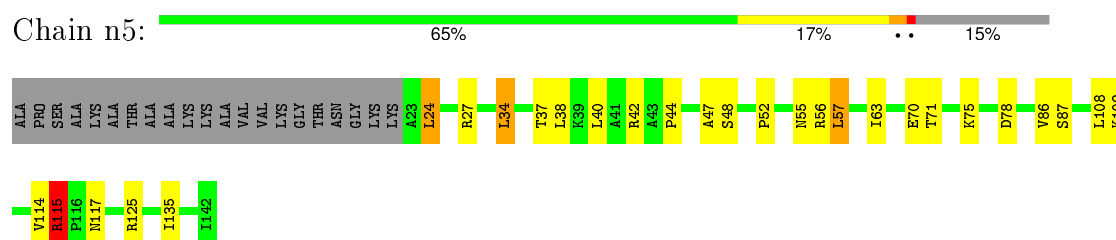
Chain n2: 65% 16% 18%



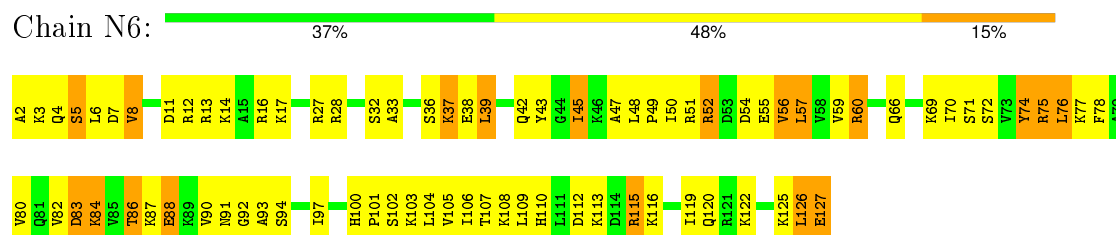
- Molecule 61: 60S ribosomal protein L25



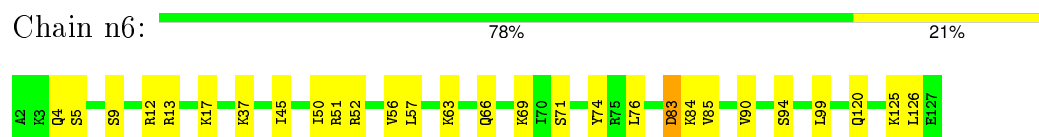
- Molecule 61: 60S ribosomal protein L25



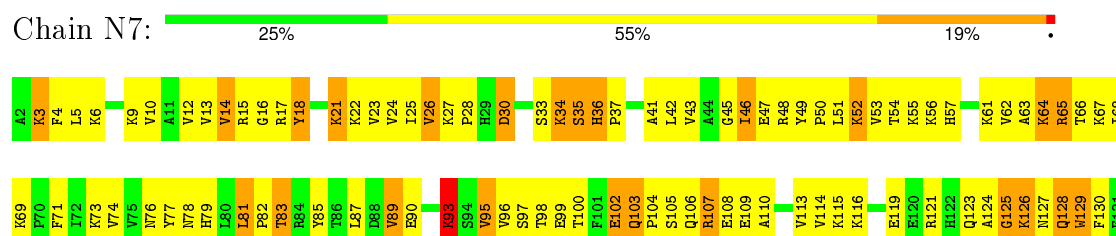
- Molecule 62: 60S ribosomal protein L26-A



- Molecule 62: 60S ribosomal protein L26-A

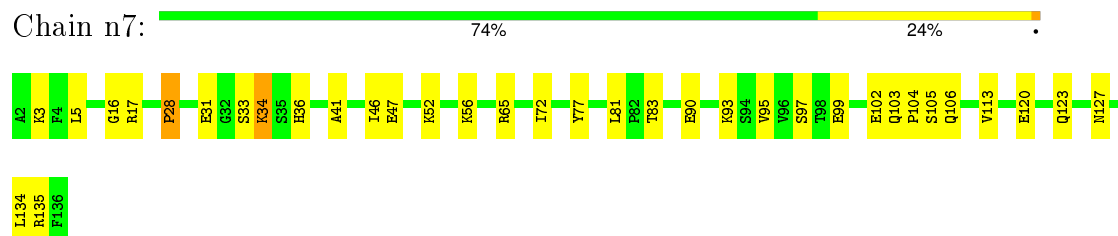


- Molecule 63: 60S ribosomal protein L27-A

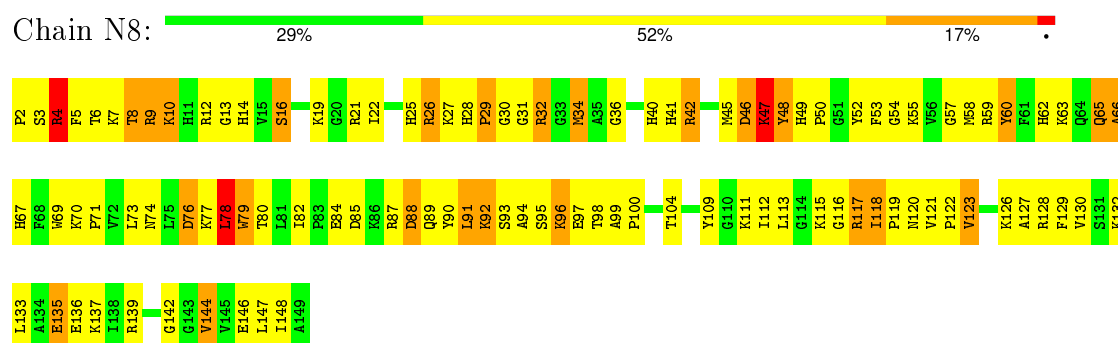


S132
K133
L134
R135
F136

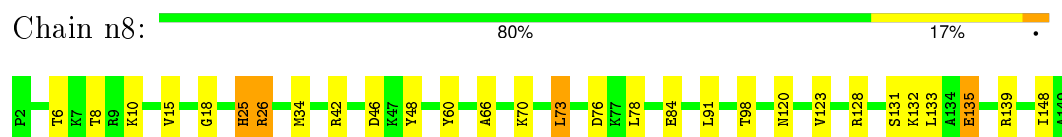
• Molecule 63: 60S ribosomal protein L27-A



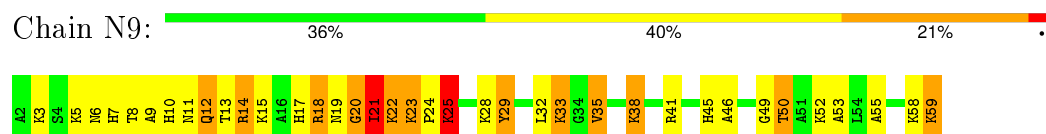
• Molecule 64: 60S ribosomal protein L28



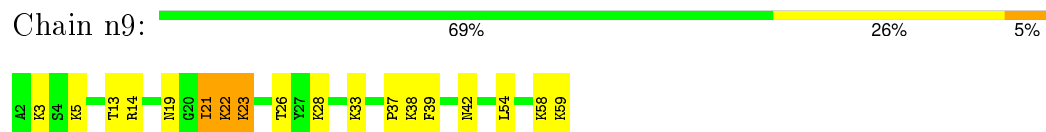
• Molecule 64: 60S ribosomal protein L28



• Molecule 65: 60S ribosomal protein L29

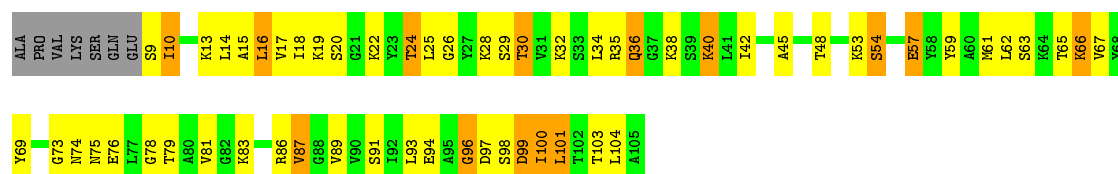


• Molecule 65: 60S ribosomal protein L29



• Molecule 66: 60S ribosomal protein L30





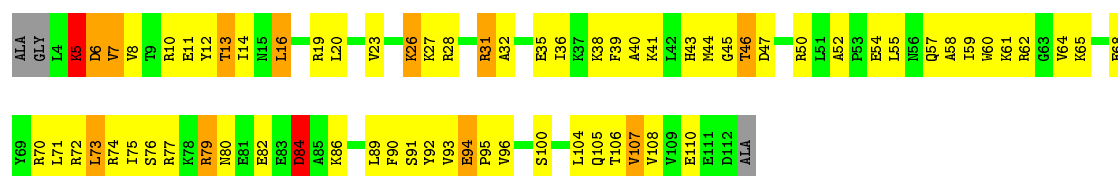
- Molecule 66: 60S ribosomal protein L30

Chain o0:



- Molecule 67: 60S ribosomal protein L31-A

Chain O1:



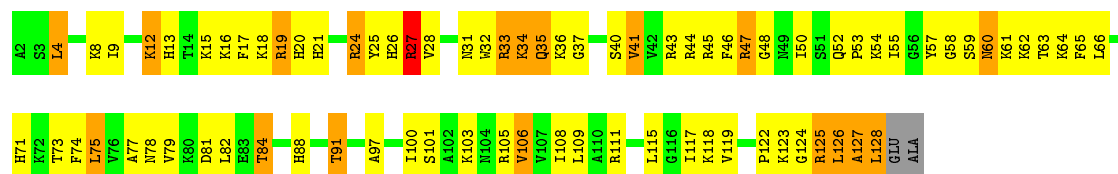
- Molecule 67: 60S ribosomal protein L31-A

Chain o1:



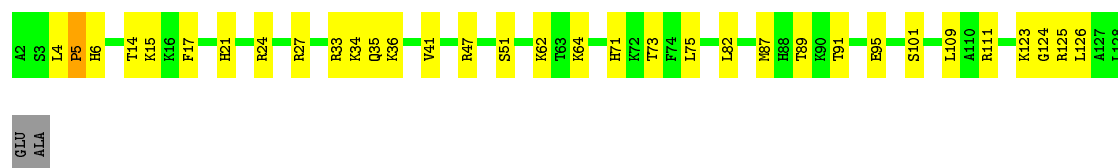
- Molecule 68: 60S ribosomal protein L32

Chain O2:

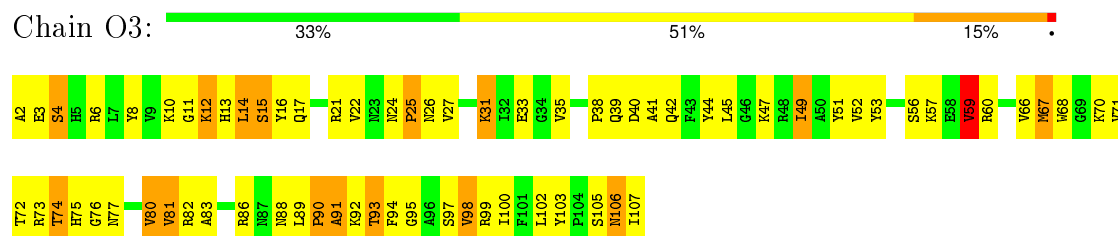


- Molecule 68: 60S ribosomal protein L32

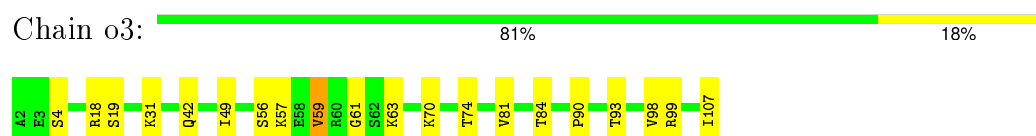
Chain o2:



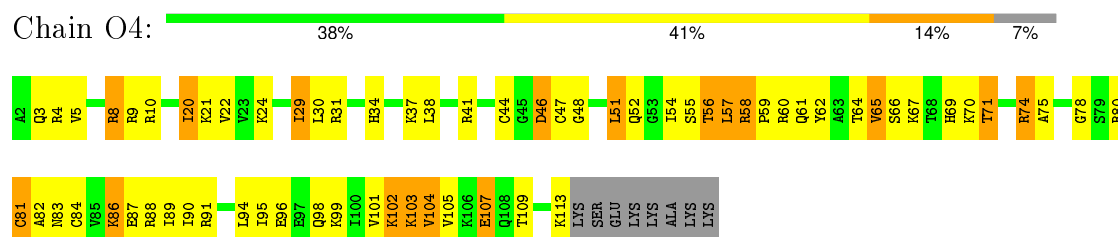
- Molecule 69: 60S ribosomal protein L33-A



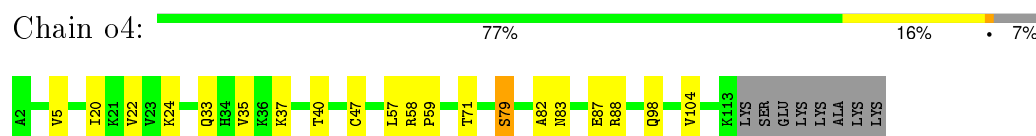
- Molecule 69: 60S ribosomal protein L33-A



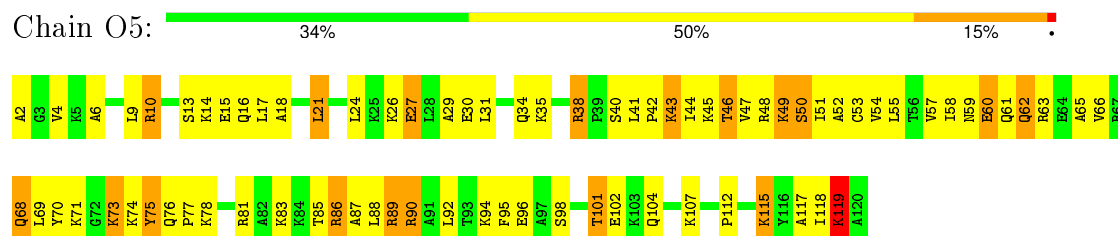
- Molecule 70: 60S ribosomal protein L34-A



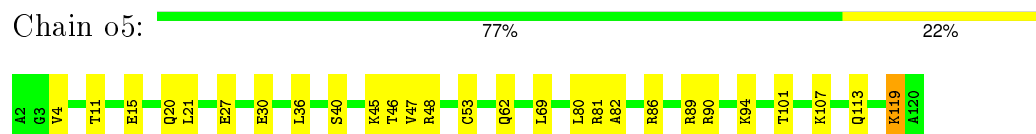
- Molecule 70: 60S ribosomal protein L34-A



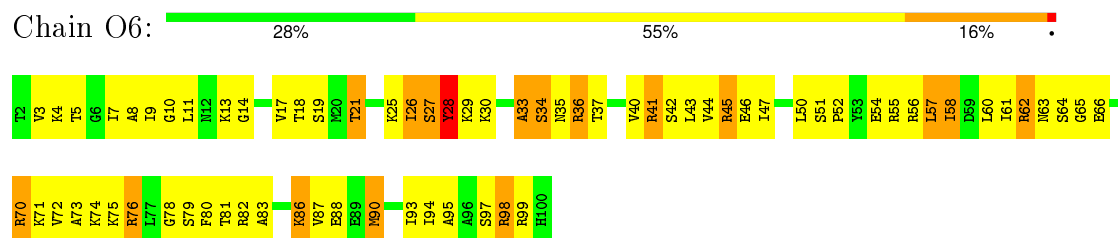
- Molecule 71: 60S ribosomal protein L35-A



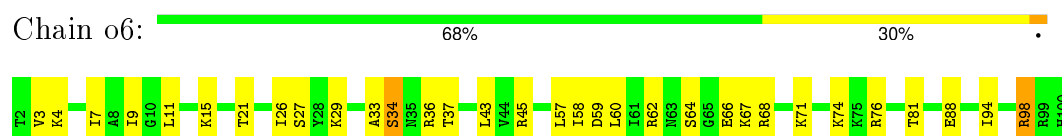
- Molecule 71: 60S ribosomal protein L35-A



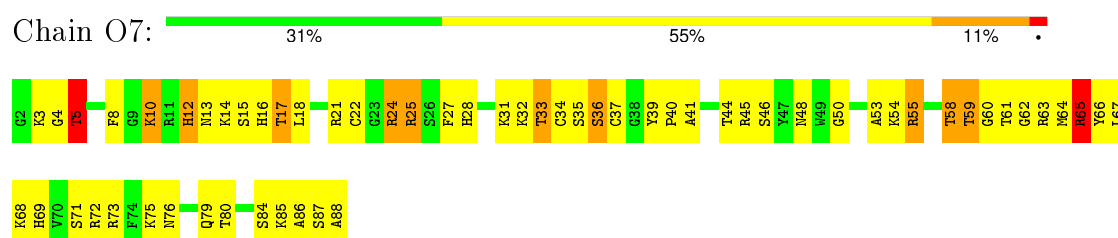
- Molecule 72: 60S ribosomal protein L36-A



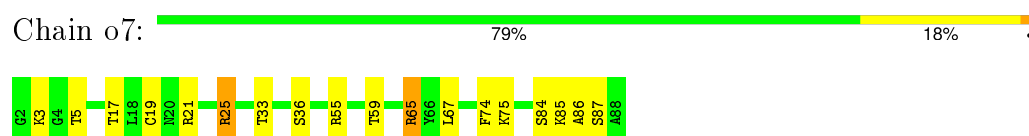
- Molecule 72: 60S ribosomal protein L36-A



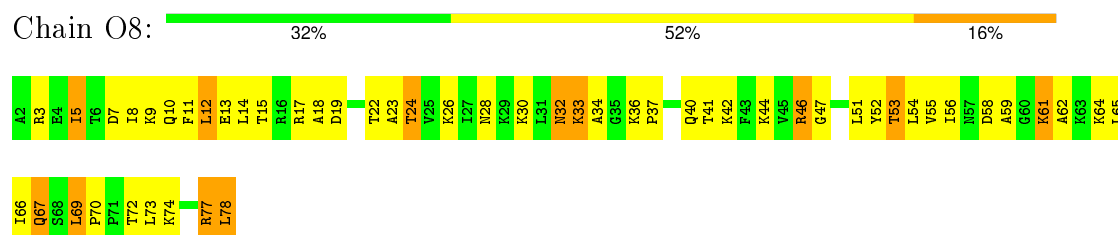
- Molecule 73: 60S ribosomal protein L37-A



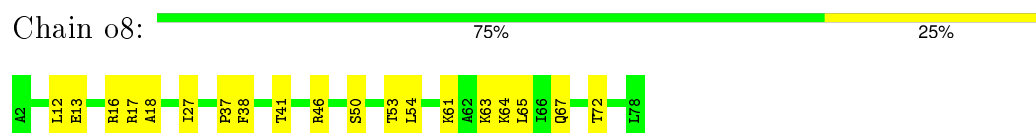
- Molecule 73: 60S ribosomal protein L37-A



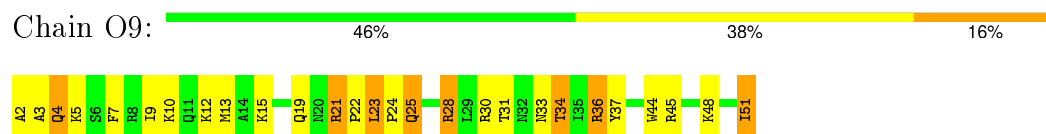
- Molecule 74: 60S ribosomal protein L38



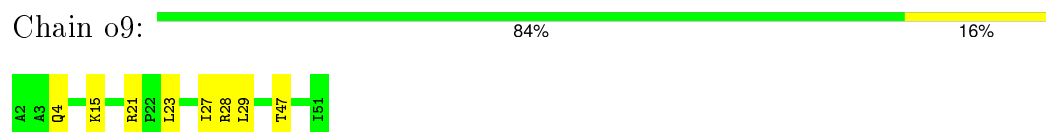
- Molecule 74: 60S ribosomal protein L38



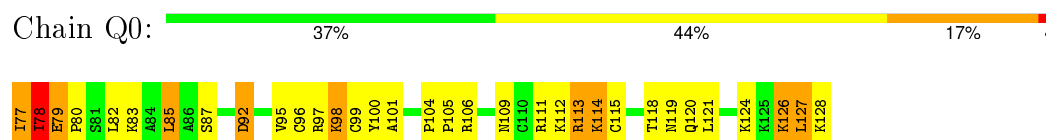
- Molecule 75: 60S ribosomal protein L39



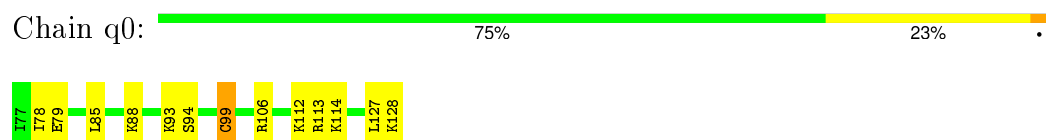
- Molecule 75: 60S ribosomal protein L39



- Molecule 76: Ubiquitin-60S ribosomal protein L40



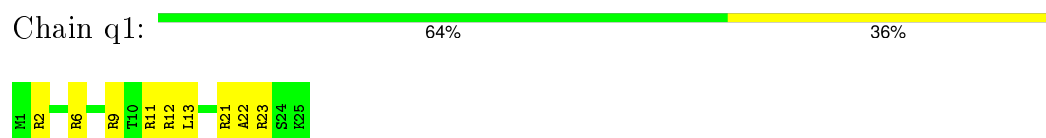
- Molecule 76: Ubiquitin-60S ribosomal protein L40



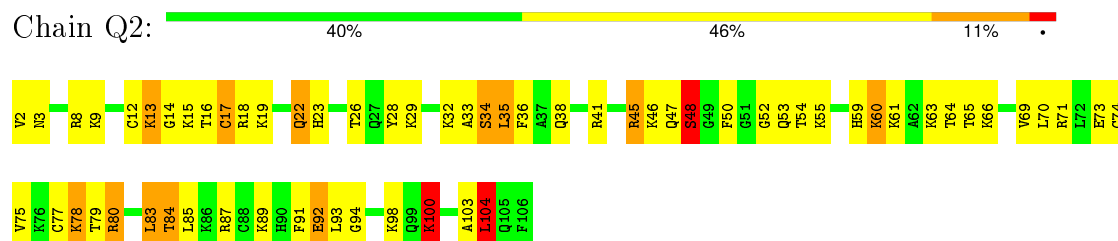
- Molecule 77: 60S ribosomal protein L41-A




- Molecule 77: 60S ribosomal protein L41-A



- Molecule 78: 60S ribosomal protein L42-A

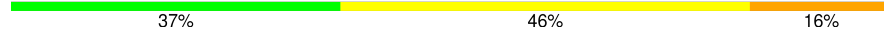


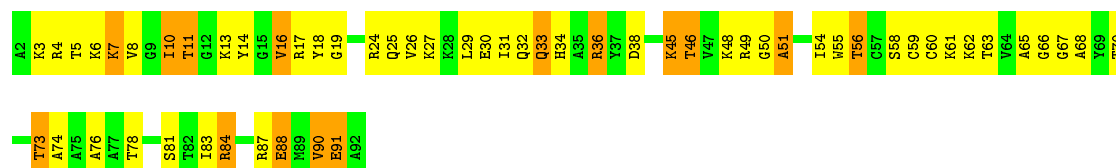
- Molecule 78: 60S ribosomal protein L42-A

Chain q2:  82% 16%




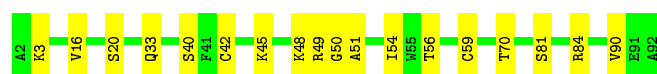
- Molecule 79: 60S ribosomal protein L43-A

Chain Q3:  37% 46% 16%



- Molecule 79: 60S ribosomal protein L43-A

Chain q3:  80% 20%




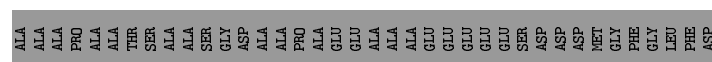
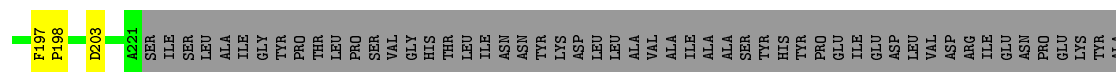
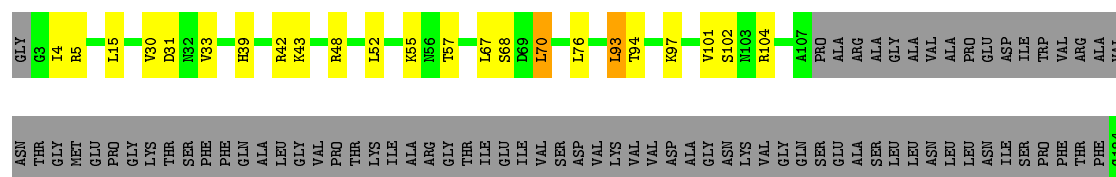
- Molecule 80: 40S ribosomal protein S30-A

Chain e0:  68% 29%



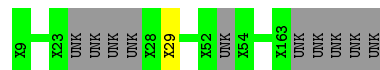
- Molecule 81: 60S acidic ribosomal protein P0

Chain p0:  38% 8% 54%



- Molecule 82: Unknown protein chain m2

Chain m2:  93% 6%



- Molecule 83: Unknown protein chain p1

Chain p1:  100%

There are no outlier residues recorded for this chain.

- Molecule 84: Unknown protein chain 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 will therefore be incomplete.

| Property | Value | Source |
|--|---|-----------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 435.15Å 287.07Å 303.24Å 90.00° 98.87° 90.00° | Depositor |
| Resolution (Å) | 99.87 – 3.20 | Depositor |
| % Data completeness (in resolution range) | 100.0 (99.87-3.20) | Depositor |
| R_{merge} | 0.37 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.28 (at 3.19Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: dev_1702) | Depositor |
| R, R_{free} | 0.194 , 0.246 | Depositor |
| Wilson B-factor (Å ²) | 88.0 | Xtriage |
| Anisotropy | 0.117 | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$ | Xtriage |
| Outliers | 1 of 1206031 reflections (0.000%) | Xtriage |
| Total number of atoms | 411206 | wwPDB-VP |
| Average B, all atoms (Å ²) | 76.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, OHX, ZN, 3K8

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 | 0.79 | 5/41698 (0.0%) | 1.34 | 378/64972 (0.6%) |
| 1 | 6 | 0.90 | 17/42765 (0.0%) | 1.39 | 452/66634 (0.7%) |
| 2 | S0 | 0.48 | 0/1617 | 0.67 | 0/2215 |
| 2 | s0 | 0.47 | 0/1623 | 0.71 | 0/2222 |
| 3 | S1 | 0.41 | 0/1735 | 0.68 | 2/2335 (0.1%) |
| 3 | s1 | 0.53 | 0/1748 | 0.70 | 0/2352 |
| 4 | S2 | 0.52 | 0/1665 | 0.65 | 0/2263 |
| 4 | s2 | 0.59 | 0/1665 | 0.74 | 0/2263 |
| 5 | S3 | 0.50 | 0/1759 | 0.69 | 0/2368 |
| 5 | s3 | 0.44 | 0/1759 | 0.59 | 0/2368 |
| 6 | S4 | 0.51 | 0/2109 | 0.74 | 1/2839 (0.0%) |
| 6 | s4 | 0.55 | 0/2109 | 0.78 | 0/2839 |
| 7 | S5 | 0.41 | 0/1629 | 0.62 | 0/2202 |
| 7 | s5 | 0.46 | 0/1629 | 0.66 | 0/2202 |
| 8 | S6 | 0.50 | 0/1823 | 0.67 | 0/2439 |
| 8 | s6 | 0.59 | 0/1779 | 0.73 | 0/2379 |
| 9 | S7 | 0.46 | 0/1506 | 0.69 | 0/2028 |
| 9 | s7 | 0.47 | 0/1516 | 0.70 | 1/2043 (0.0%) |
| 10 | S8 | 0.59 | 0/1514 | 0.78 | 1/2021 (0.0%) |
| 10 | s8 | 0.64 | 0/1514 | 0.70 | 0/2021 |
| 11 | S9 | 0.48 | 0/1519 | 0.69 | 0/2035 |
| 11 | s9 | 0.57 | 0/1519 | 0.76 | 2/2035 (0.1%) |
| 12 | C0 | 0.44 | 0/790 | 0.67 | 1/1069 (0.1%) |
| 12 | c0 | 0.38 | 0/777 | 0.67 | 3/1049 (0.3%) |
| 13 | C1 | 0.62 | 0/1240 | 0.76 | 0/1675 |
| 13 | c1 | 0.67 | 0/1194 | 0.77 | 0/1610 |
| 14 | C2 | 0.37 | 0/900 | 0.64 | 0/1224 |
| 14 | c2 | 0.29 | 0/900 | 0.56 | 0/1224 |
| 15 | C3 | 0.51 | 0/1215 | 0.70 | 2/1638 (0.1%) |
| 15 | c3 | 0.61 | 0/1215 | 0.69 | 0/1638 |
| 16 | C4 | 0.43 | 0/901 | 0.70 | 0/1217 |
| 16 | c4 | 0.56 | 0/960 | 0.75 | 0/1290 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | C5 | 0.48 | 0/998 | 0.69 | 0/1341 |
| 17 | c5 | 0.50 | 0/1060 | 0.69 | 0/1426 |
| 18 | C6 | 0.46 | 0/1125 | 0.71 | 2/1510 (0.1%) |
| 18 | c6 | 0.49 | 0/1131 | 0.70 | 0/1518 |
| 19 | C7 | 0.46 | 0/935 | 0.64 | 0/1254 |
| 19 | c7 | 0.51 | 0/914 | 0.70 | 0/1224 |
| 20 | C8 | 0.47 | 0/1211 | 0.65 | 1/1628 (0.1%) |
| 20 | c8 | 0.51 | 0/1211 | 0.73 | 2/1628 (0.1%) |
| 21 | C9 | 0.45 | 0/1130 | 0.66 | 0/1517 |
| 21 | c9 | 0.52 | 0/1130 | 0.68 | 0/1517 |
| 22 | D0 | 0.49 | 0/865 | 0.65 | 0/1169 |
| 22 | d0 | 0.47 | 0/892 | 0.65 | 0/1205 |
| 23 | D1 | 0.49 | 0/693 | 0.68 | 0/935 |
| 23 | d1 | 0.52 | 0/693 | 0.69 | 0/935 |
| 24 | D2 | 0.53 | 0/1038 | 0.74 | 2/1395 (0.1%) |
| 24 | d2 | 0.62 | 0/1038 | 0.78 | 1/1395 (0.1%) |
| 25 | D3 | 0.64 | 0/1139 | 0.80 | 2/1518 (0.1%) |
| 25 | d3 | 0.72 | 0/1139 | 0.85 | 2/1518 (0.1%) |
| 26 | D4 | 0.50 | 0/1087 | 0.64 | 0/1449 |
| 26 | d4 | 0.54 | 0/1087 | 0.73 | 0/1449 |
| 27 | D5 | 0.40 | 0/571 | 0.73 | 1/768 (0.1%) |
| 27 | d5 | 0.46 | 0/566 | 0.71 | 0/761 |
| 28 | D6 | 0.51 | 0/782 | 0.69 | 0/1047 |
| 28 | d6 | 0.56 | 0/782 | 0.69 | 0/1047 |
| 29 | D7 | 0.47 | 0/620 | 0.66 | 0/838 |
| 29 | d7 | 0.49 | 0/620 | 0.71 | 0/838 |
| 30 | D8 | 0.37 | 0/499 | 0.58 | 0/670 |
| 30 | d8 | 0.45 | 0/499 | 0.64 | 0/670 |
| 31 | D9 | 0.56 | 0/452 | 0.73 | 1/600 (0.2%) |
| 31 | d9 | 0.51 | 0/452 | 0.68 | 0/600 |
| 32 | E0 | 0.51 | 0/483 | 0.66 | 0/643 |
| 33 | E1 | 0.47 | 0/577 | 0.81 | 0/770 |
| 33 | e1 | 0.42 | 0/619 | 0.73 | 0/822 |
| 34 | SR | 0.41 | 0/2494 | 0.64 | 1/3393 (0.0%) |
| 34 | sR | 0.38 | 0/2495 | 0.57 | 0/3395 |
| 35 | SM | 0.54 | 0/1113 | 0.75 | 2/1502 (0.1%) |
| 35 | sM | 0.48 | 0/682 | 0.68 | 1/921 (0.1%) |
| 36 | 1 | 1.25 | 247/75394 (0.3%) | 1.73 | 2232/117545 (1.9%) |
| 36 | 5 | 1.26 | 266/75414 (0.4%) | 1.73 | 2109/117575 (1.8%) |
| 37 | 3 | 1.02 | 0/2883 | 1.46 | 30/4491 (0.7%) |
| 37 | 7 | 1.20 | 8/2883 (0.3%) | 1.73 | 86/4491 (1.9%) |
| 38 | 4 | 1.17 | 3/3746 (0.1%) | 1.69 | 85/5832 (1.5%) |
| 38 | 8 | 1.07 | 4/3746 (0.1%) | 1.54 | 64/5832 (1.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 39 | L2 | 0.81 | 0/1948 | 0.86 | 0/2617 |
| 39 | l2 | 0.72 | 0/1946 | 0.88 | 3/2614 (0.1%) |
| 40 | L3 | 0.80 | 1/3146 (0.0%) | 0.83 | 1/4228 (0.0%) |
| 40 | l3 | 0.90 | 1/3146 (0.0%) | 0.89 | 2/4228 (0.0%) |
| 41 | L4 | 0.86 | 0/2800 | 0.94 | 7/3790 (0.2%) |
| 41 | l4 | 0.82 | 1/2800 (0.0%) | 0.93 | 2/3790 (0.1%) |
| 42 | L5 | 0.58 | 0/2425 | 0.71 | 0/3271 |
| 42 | l5 | 0.74 | 1/2408 (0.0%) | 0.81 | 1/3248 (0.0%) |
| 43 | L6 | 0.82 | 0/1260 | 0.82 | 0/1694 |
| 43 | l6 | 0.84 | 0/1269 | 0.88 | 1/1705 (0.1%) |
| 44 | L7 | 0.85 | 0/1821 | 0.92 | 3/2451 (0.1%) |
| 44 | l7 | 0.95 | 1/1828 (0.1%) | 0.93 | 3/2461 (0.1%) |
| 45 | L8 | 0.60 | 0/1836 | 0.72 | 1/2481 (0.0%) |
| 45 | l8 | 0.54 | 0/1795 | 0.70 | 1/2429 (0.0%) |
| 46 | L9 | 0.73 | 0/1539 | 0.82 | 2/2073 (0.1%) |
| 46 | l9 | 0.84 | 0/1539 | 0.86 | 0/2073 |
| 47 | M0 | 0.78 | 1/1741 (0.1%) | 0.86 | 3/2335 (0.1%) |
| 47 | m0 | 0.80 | 1/1758 (0.1%) | 0.88 | 0/2358 |
| 48 | M1 | 0.53 | 0/1374 | 0.71 | 1/1842 (0.1%) |
| 48 | m1 | 0.69 | 0/1374 | 0.82 | 2/1842 (0.1%) |
| 49 | M3 | 0.81 | 0/1568 | 0.90 | 3/2106 (0.1%) |
| 49 | m3 | 0.73 | 0/1573 | 0.85 | 0/2113 |
| 50 | M4 | 0.84 | 0/1068 | 0.86 | 0/1438 |
| 50 | m4 | 0.92 | 0/1074 | 0.90 | 2/1446 (0.1%) |
| 51 | M5 | 0.83 | 1/1757 (0.1%) | 0.89 | 2/2354 (0.1%) |
| 51 | m5 | 0.72 | 0/1757 | 0.86 | 4/2354 (0.2%) |
| 52 | M6 | 0.96 | 2/1585 (0.1%) | 0.97 | 4/2128 (0.2%) |
| 52 | m6 | 1.04 | 2/1585 (0.1%) | 0.96 | 4/2128 (0.2%) |
| 53 | M7 | 0.84 | 1/1443 (0.1%) | 0.87 | 3/1944 (0.2%) |
| 53 | m7 | 0.97 | 1/1250 (0.1%) | 0.93 | 1/1683 (0.1%) |
| 54 | M8 | 0.84 | 0/1465 | 0.88 | 0/1965 |
| 54 | m8 | 0.78 | 0/1465 | 0.90 | 1/1965 (0.1%) |
| 55 | M9 | 0.61 | 0/1538 | 0.70 | 0/2050 |
| 55 | m9 | 0.65 | 0/1538 | 0.71 | 0/2050 |
| 56 | N0 | 0.86 | 0/1481 | 0.86 | 1/1990 (0.1%) |
| 56 | n0 | 0.93 | 0/1481 | 0.93 | 3/1990 (0.2%) |
| 57 | N1 | 0.84 | 0/1300 | 0.85 | 1/1743 (0.1%) |
| 57 | n1 | 0.93 | 3/1300 (0.2%) | 0.85 | 1/1743 (0.1%) |
| 58 | N2 | 0.44 | 0/812 | 0.62 | 0/1099 |
| 58 | n2 | 0.54 | 0/794 | 0.74 | 0/1076 |
| 59 | N3 | 0.79 | 0/1018 | 0.87 | 0/1369 |
| 59 | n3 | 0.90 | 0/1018 | 0.92 | 3/1369 (0.2%) |
| 60 | N4 | 0.64 | 0/712 | 0.74 | 0/958 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 60 | n4 | 0.69 | 0/1052 | 0.76 | 0/1398 |
| 61 | N5 | 0.69 | 0/979 | 0.83 | 1/1321 (0.1%) |
| 61 | n5 | 0.68 | 0/974 | 0.79 | 2/1314 (0.2%) |
| 62 | N6 | 0.77 | 0/1004 | 0.89 | 1/1341 (0.1%) |
| 62 | n6 | 0.71 | 0/1004 | 0.89 | 1/1341 (0.1%) |
| 63 | N7 | 0.59 | 0/1118 | 0.71 | 0/1497 |
| 63 | n7 | 0.53 | 0/1118 | 0.67 | 0/1497 |
| 64 | N8 | 0.83 | 1/1204 (0.1%) | 0.95 | 3/1612 (0.2%) |
| 64 | n8 | 0.78 | 0/1204 | 0.90 | 3/1612 (0.2%) |
| 65 | N9 | 0.74 | 0/473 | 0.88 | 1/629 (0.2%) |
| 65 | n9 | 0.85 | 0/473 | 1.01 | 1/629 (0.2%) |
| 66 | O0 | 0.55 | 0/751 | 0.68 | 0/1008 |
| 66 | o0 | 0.53 | 0/775 | 0.69 | 0/1040 |
| 67 | O1 | 0.70 | 0/890 | 0.78 | 1/1196 (0.1%) |
| 67 | o1 | 0.78 | 0/897 | 0.88 | 0/1205 |
| 68 | O2 | 0.90 | 0/1041 | 0.91 | 3/1394 (0.2%) |
| 68 | o2 | 0.89 | 0/1041 | 0.94 | 2/1394 (0.1%) |
| 69 | O3 | 0.97 | 0/868 | 0.91 | 0/1168 |
| 69 | o3 | 1.01 | 1/868 (0.1%) | 0.94 | 2/1168 (0.2%) |
| 70 | O4 | 0.68 | 0/890 | 0.83 | 1/1189 (0.1%) |
| 70 | o4 | 0.63 | 0/890 | 0.78 | 0/1189 |
| 71 | O5 | 0.78 | 0/978 | 0.85 | 0/1301 |
| 71 | o5 | 0.61 | 0/974 | 0.75 | 0/1297 |
| 72 | O6 | 0.67 | 0/778 | 0.86 | 0/1034 |
| 72 | o6 | 0.63 | 0/777 | 0.77 | 0/1033 |
| 73 | O7 | 0.90 | 0/696 | 1.01 | 3/923 (0.3%) |
| 73 | o7 | 0.75 | 0/696 | 0.86 | 2/923 (0.2%) |
| 74 | O8 | 0.59 | 0/618 | 0.70 | 0/826 |
| 74 | o8 | 0.50 | 0/614 | 0.69 | 0/822 |
| 75 | O9 | 0.81 | 0/443 | 0.93 | 0/588 |
| 75 | o9 | 0.74 | 0/443 | 0.91 | 0/588 |
| 76 | Q0 | 0.78 | 0/423 | 0.89 | 0/562 |
| 76 | q0 | 0.93 | 1/423 (0.2%) | 0.92 | 0/562 |
| 77 | Q1 | 0.65 | 0/234 | 0.82 | 0/300 |
| 77 | q1 | 0.81 | 0/234 | 1.10 | 1/300 (0.3%) |
| 78 | Q2 | 0.91 | 1/860 (0.1%) | 0.84 | 0/1136 |
| 78 | q2 | 0.89 | 2/860 (0.2%) | 0.82 | 0/1136 |
| 79 | Q3 | 0.80 | 0/701 | 0.83 | 0/934 |
| 79 | q3 | 0.80 | 0/701 | 0.85 | 1/934 (0.1%) |
| 80 | e0 | 0.57 | 0/499 | 0.74 | 0/665 |
| 81 | p0 | 0.46 | 0/1091 | 0.62 | 0/1472 |
| All | All | 0.96 | 573/430072 (0.1%) | 1.35 | 5562/631360 (0.9%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2 | s0 | 0 | 1 |
| 7 | S5 | 0 | 1 |
| 7 | s5 | 0 | 2 |
| 9 | S7 | 0 | 2 |
| 9 | s7 | 0 | 1 |
| 10 | S8 | 0 | 1 |
| 16 | C4 | 0 | 3 |
| 16 | c4 | 0 | 1 |
| 17 | c5 | 0 | 1 |
| 18 | C6 | 0 | 1 |
| 18 | c6 | 0 | 1 |
| 19 | C7 | 0 | 1 |
| 24 | d2 | 0 | 1 |
| 26 | d4 | 0 | 1 |
| 27 | D5 | 0 | 3 |
| 28 | D6 | 0 | 1 |
| 39 | L2 | 0 | 1 |
| 39 | l2 | 0 | 4 |
| 44 | l7 | 0 | 2 |
| 46 | L9 | 0 | 1 |
| 48 | M1 | 0 | 1 |
| 52 | M6 | 0 | 1 |
| 52 | m6 | 0 | 1 |
| 56 | N0 | 0 | 1 |
| 56 | n0 | 0 | 1 |
| 57 | N1 | 0 | 1 |
| 59 | n3 | 0 | 1 |
| 64 | N8 | 0 | 2 |
| 64 | n8 | 0 | 3 |
| 65 | N9 | 0 | 1 |
| 67 | O1 | 0 | 1 |
| 80 | e0 | 0 | 1 |
| 82 | m2 | 0 | 1 |
| All | All | 0 | 46 |

The worst 5 of 573 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 78 | q2 | 17 | CYS | CB-SG | 14.54 | 2.06 | 1.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 78 | Q2 | 17 | CYS | CB-SG | 14.44 | 2.06 | 1.82 |
| 36 | 5 | 1152 | G | N9-C4 | -12.25 | 1.28 | 1.38 |
| 36 | 5 | 2971 | A | N9-C4 | 9.75 | 1.43 | 1.37 |
| 36 | 5 | 1152 | G | N9-C8 | 9.62 | 1.44 | 1.37 |

The worst 5 of 5562 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 36 | 5 | 1152 | G | N3-C4-C5 | 28.50 | 142.85 | 128.60 |
| 36 | 5 | 1152 | G | N3-C4-N9 | -25.34 | 110.80 | 126.00 |
| 36 | 5 | 1152 | G | C2-N3-C4 | -23.17 | 100.31 | 111.90 |
| 36 | 5 | 424 | G | C5-C6-O6 | -17.79 | 117.92 | 128.60 |
| 36 | 5 | 1152 | G | C5-N7-C8 | -14.52 | 97.04 | 104.30 |

There are no chirality outliers.

5 of 46 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 16 | C4 | 38 | THR | Peptide |
| 7 | S5 | 44 | ASN | Peptide |
| 9 | S7 | 131 | PHE | Peptide |
| 9 | S7 | 31 | SER | Peptide |
| 10 | S8 | 147 | ALA | Peptide |

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 2 | 37283 | 0 | 18757 | 998 | 1 |
| 1 | 6 | 38238 | 0 | 19241 | 944 | 0 |
| 2 | S0 | 1577 | 0 | 1567 | 172 | 0 |
| 2 | s0 | 1583 | 0 | 1578 | 0 | 0 |
| 3 | S1 | 1709 | 0 | 1784 | 186 | 0 |
| 3 | s1 | 1722 | 0 | 1793 | 0 | 0 |
| 4 | S2 | 1635 | 0 | 1723 | 147 | 0 |
| 4 | s2 | 1635 | 0 | 1723 | 0 | 0 |
| 5 | S3 | 1734 | 0 | 1817 | 125 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5 | s3 | 1734 | 0 | 1817 | 0 | 0 |
| 6 | S4 | 2068 | 0 | 2154 | 170 | 0 |
| 6 | s4 | 2068 | 0 | 2154 | 0 | 0 |
| 7 | S5 | 1609 | 0 | 1675 | 156 | 0 |
| 7 | s5 | 1609 | 0 | 1675 | 0 | 0 |
| 8 | S6 | 1799 | 0 | 1878 | 146 | 0 |
| 8 | s6 | 1755 | 0 | 1846 | 0 | 0 |
| 9 | S7 | 1481 | 0 | 1572 | 125 | 0 |
| 9 | s7 | 1491 | 0 | 1578 | 0 | 0 |
| 10 | S8 | 1489 | 0 | 1525 | 123 | 0 |
| 10 | s8 | 1489 | 0 | 1525 | 0 | 0 |
| 11 | S9 | 1494 | 0 | 1573 | 144 | 0 |
| 11 | s9 | 1494 | 0 | 1573 | 0 | 0 |
| 12 | C0 | 773 | 0 | 729 | 73 | 0 |
| 12 | c0 | 762 | 0 | 699 | 0 | 0 |
| 13 | C1 | 1214 | 0 | 1259 | 85 | 0 |
| 13 | c1 | 1168 | 0 | 1231 | 0 | 0 |
| 14 | C2 | 892 | 0 | 891 | 54 | 0 |
| 14 | c2 | 892 | 0 | 891 | 0 | 0 |
| 15 | C3 | 1192 | 0 | 1255 | 118 | 0 |
| 15 | c3 | 1192 | 0 | 1255 | 0 | 0 |
| 16 | C4 | 891 | 0 | 883 | 112 | 0 |
| 16 | c4 | 949 | 0 | 985 | 0 | 0 |
| 17 | C5 | 977 | 0 | 1002 | 102 | 0 |
| 17 | c5 | 1039 | 0 | 1050 | 0 | 0 |
| 18 | C6 | 1105 | 0 | 1166 | 133 | 0 |
| 18 | c6 | 1111 | 0 | 1171 | 0 | 0 |
| 19 | C7 | 926 | 0 | 930 | 94 | 0 |
| 19 | c7 | 906 | 0 | 909 | 0 | 0 |
| 20 | C8 | 1192 | 0 | 1222 | 124 | 0 |
| 20 | c8 | 1192 | 0 | 1222 | 0 | 0 |
| 21 | C9 | 1112 | 0 | 1124 | 93 | 0 |
| 21 | c9 | 1112 | 0 | 1124 | 0 | 0 |
| 22 | D0 | 855 | 0 | 917 | 91 | 0 |
| 22 | d0 | 882 | 0 | 939 | 0 | 0 |
| 23 | D1 | 684 | 0 | 672 | 67 | 0 |
| 23 | d1 | 684 | 0 | 672 | 0 | 0 |
| 24 | D2 | 1021 | 0 | 1060 | 98 | 0 |
| 24 | d2 | 1021 | 0 | 1060 | 0 | 0 |
| 25 | D3 | 1121 | 0 | 1196 | 100 | 0 |
| 25 | d3 | 1121 | 0 | 1196 | 0 | 0 |
| 26 | D4 | 1073 | 0 | 1132 | 98 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 26 | d4 | 1073 | 0 | 1132 | 0 | 0 |
| 27 | D5 | 563 | 0 | 603 | 63 | 0 |
| 27 | d5 | 558 | 0 | 598 | 0 | 0 |
| 28 | D6 | 769 | 0 | 815 | 103 | 0 |
| 28 | d6 | 769 | 0 | 814 | 0 | 0 |
| 29 | D7 | 610 | 0 | 630 | 54 | 0 |
| 29 | d7 | 610 | 0 | 631 | 0 | 0 |
| 30 | D8 | 497 | 0 | 535 | 54 | 0 |
| 30 | d8 | 497 | 0 | 535 | 0 | 0 |
| 31 | D9 | 442 | 0 | 428 | 44 | 0 |
| 31 | d9 | 442 | 0 | 428 | 0 | 0 |
| 32 | E0 | 475 | 0 | 525 | 32 | 0 |
| 33 | E1 | 566 | 0 | 603 | 60 | 0 |
| 33 | e1 | 608 | 0 | 656 | 0 | 0 |
| 34 | SR | 2441 | 0 | 2397 | 197 | 0 |
| 34 | sR | 2442 | 0 | 2392 | 0 | 0 |
| 35 | SM | 1104 | 0 | 996 | 72 | 0 |
| 35 | sM | 679 | 0 | 603 | 0 | 0 |
| 36 | 1 | 67355 | 0 | 33839 | 1388 | 0 |
| 36 | 5 | 67376 | 0 | 33855 | 1332 | 1 |
| 37 | 3 | 2579 | 0 | 1304 | 63 | 0 |
| 37 | 7 | 2579 | 0 | 1304 | 49 | 0 |
| 38 | 4 | 3353 | 0 | 1695 | 68 | 0 |
| 38 | 8 | 3353 | 0 | 1695 | 67 | 0 |
| 39 | L2 | 1914 | 0 | 1981 | 157 | 0 |
| 39 | l2 | 1912 | 0 | 1976 | 0 | 0 |
| 40 | L3 | 3075 | 0 | 3142 | 280 | 0 |
| 40 | l3 | 3075 | 0 | 3142 | 0 | 0 |
| 41 | L4 | 2748 | 0 | 2859 | 253 | 0 |
| 41 | l4 | 2748 | 0 | 2859 | 0 | 0 |
| 42 | L5 | 2375 | 0 | 2325 | 211 | 0 |
| 42 | l5 | 2359 | 0 | 2311 | 0 | 0 |
| 43 | L6 | 1239 | 0 | 1326 | 90 | 0 |
| 43 | l6 | 1248 | 0 | 1339 | 0 | 0 |
| 44 | L7 | 1784 | 0 | 1862 | 150 | 0 |
| 44 | l7 | 1791 | 0 | 1869 | 0 | 0 |
| 45 | L8 | 1804 | 0 | 1877 | 152 | 0 |
| 45 | l8 | 1763 | 0 | 1819 | 0 | 0 |
| 46 | L9 | 1518 | 0 | 1587 | 144 | 0 |
| 46 | l9 | 1518 | 0 | 1587 | 0 | 0 |
| 47 | M0 | 1705 | 0 | 1735 | 141 | 0 |
| 47 | m0 | 1722 | 0 | 1755 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 48 | M1 | 1353 | 0 | 1383 | 110 | 0 |
| 48 | m1 | 1353 | 0 | 1383 | 0 | 0 |
| 49 | M3 | 1543 | 0 | 1608 | 158 | 0 |
| 49 | m3 | 1548 | 0 | 1613 | 0 | 0 |
| 50 | M4 | 1053 | 0 | 1149 | 94 | 0 |
| 50 | m4 | 1059 | 0 | 1154 | 0 | 0 |
| 51 | M5 | 1720 | 0 | 1779 | 143 | 0 |
| 51 | m5 | 1720 | 0 | 1779 | 0 | 0 |
| 52 | M6 | 1555 | 0 | 1659 | 127 | 0 |
| 52 | m6 | 1555 | 0 | 1659 | 0 | 0 |
| 53 | M7 | 1420 | 0 | 1437 | 112 | 0 |
| 53 | m7 | 1227 | 0 | 1236 | 0 | 0 |
| 54 | M8 | 1441 | 0 | 1543 | 107 | 0 |
| 54 | m8 | 1441 | 0 | 1543 | 0 | 0 |
| 55 | M9 | 1521 | 0 | 1617 | 121 | 0 |
| 55 | m9 | 1521 | 0 | 1617 | 0 | 0 |
| 56 | N0 | 1445 | 0 | 1487 | 108 | 0 |
| 56 | n0 | 1445 | 0 | 1487 | 0 | 0 |
| 57 | N1 | 1276 | 0 | 1323 | 108 | 0 |
| 57 | n1 | 1276 | 0 | 1323 | 0 | 0 |
| 58 | N2 | 796 | 0 | 812 | 55 | 0 |
| 58 | n2 | 778 | 0 | 791 | 0 | 0 |
| 59 | N3 | 1003 | 0 | 1048 | 90 | 0 |
| 59 | n3 | 1003 | 0 | 1048 | 0 | 0 |
| 60 | N4 | 699 | 0 | 640 | 26 | 0 |
| 60 | n4 | 1038 | 0 | 1071 | 0 | 0 |
| 61 | N5 | 964 | 0 | 1025 | 86 | 0 |
| 61 | n5 | 959 | 0 | 1023 | 0 | 0 |
| 62 | N6 | 993 | 0 | 1081 | 80 | 0 |
| 62 | n6 | 993 | 0 | 1081 | 0 | 0 |
| 63 | N7 | 1092 | 0 | 1155 | 92 | 0 |
| 63 | n7 | 1092 | 0 | 1155 | 0 | 0 |
| 64 | N8 | 1173 | 0 | 1215 | 137 | 0 |
| 64 | n8 | 1173 | 0 | 1215 | 0 | 0 |
| 65 | N9 | 462 | 0 | 491 | 41 | 0 |
| 65 | n9 | 462 | 0 | 491 | 0 | 0 |
| 66 | O0 | 743 | 0 | 797 | 59 | 0 |
| 66 | o0 | 767 | 0 | 816 | 0 | 0 |
| 67 | O1 | 876 | 0 | 912 | 63 | 0 |
| 67 | o1 | 883 | 0 | 918 | 0 | 0 |
| 68 | O2 | 1020 | 0 | 1090 | 85 | 0 |
| 68 | o2 | 1020 | 0 | 1090 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 69 | O3 | 850 | 0 | 880 | 66 | 0 |
| 69 | o3 | 850 | 0 | 880 | 0 | 0 |
| 70 | O4 | 880 | 0 | 945 | 69 | 0 |
| 70 | o4 | 880 | 0 | 945 | 0 | 0 |
| 71 | O5 | 969 | 0 | 1078 | 89 | 0 |
| 71 | o5 | 965 | 0 | 1067 | 0 | 0 |
| 72 | O6 | 771 | 0 | 849 | 74 | 0 |
| 72 | o6 | 770 | 0 | 846 | 0 | 0 |
| 73 | O7 | 681 | 0 | 682 | 60 | 0 |
| 73 | o7 | 681 | 0 | 683 | 0 | 0 |
| 74 | O8 | 612 | 0 | 682 | 46 | 0 |
| 74 | o8 | 608 | 0 | 671 | 0 | 0 |
| 75 | O9 | 436 | 0 | 475 | 49 | 0 |
| 75 | o9 | 436 | 0 | 475 | 0 | 0 |
| 76 | Q0 | 417 | 0 | 456 | 31 | 0 |
| 76 | q0 | 417 | 0 | 456 | 0 | 0 |
| 77 | Q1 | 233 | 0 | 284 | 29 | 0 |
| 77 | q1 | 233 | 0 | 284 | 0 | 0 |
| 78 | Q2 | 847 | 0 | 917 | 59 | 0 |
| 78 | q2 | 847 | 0 | 918 | 0 | 0 |
| 79 | Q3 | 694 | 0 | 734 | 58 | 0 |
| 79 | q3 | 694 | 0 | 734 | 0 | 0 |
| 80 | e0 | 491 | 0 | 542 | 0 | 0 |
| 81 | p0 | 1076 | 0 | 1040 | 0 | 0 |
| 82 | m2 | 750 | 0 | 170 | 0 | 0 |
| 83 | p1 | 235 | 0 | 52 | 0 | 0 |
| 84 | p2 | 230 | 0 | 51 | 0 | 0 |
| 85 | 1 | 469 | 0 | 0 | 0 | 0 |
| 85 | 2 | 125 | 0 | 0 | 0 | 0 |
| 85 | 3 | 14 | 0 | 0 | 0 | 0 |
| 85 | 4 | 21 | 0 | 0 | 0 | 0 |
| 85 | 5 | 505 | 0 | 0 | 0 | 0 |
| 85 | 6 | 148 | 0 | 0 | 0 | 0 |
| 85 | 7 | 17 | 0 | 0 | 0 | 0 |
| 85 | 8 | 14 | 0 | 0 | 0 | 0 |
| 85 | D0 | 1 | 0 | 0 | 0 | 0 |
| 85 | D3 | 1 | 0 | 0 | 0 | 0 |
| 85 | L2 | 1 | 0 | 0 | 0 | 0 |
| 85 | L3 | 3 | 0 | 0 | 0 | 0 |
| 85 | L4 | 1 | 0 | 0 | 0 | 0 |
| 85 | L5 | 2 | 0 | 0 | 0 | 0 |
| 85 | L7 | 3 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 85 | L8 | 1 | 0 | 0 | 0 | 0 |
| 85 | M0 | 3 | 0 | 0 | 0 | 0 |
| 85 | M1 | 1 | 0 | 0 | 0 | 0 |
| 85 | M3 | 3 | 0 | 0 | 0 | 0 |
| 85 | M5 | 1 | 0 | 0 | 0 | 0 |
| 85 | M6 | 1 | 0 | 0 | 0 | 0 |
| 85 | M7 | 5 | 0 | 0 | 0 | 0 |
| 85 | M9 | 1 | 0 | 0 | 0 | 0 |
| 85 | N0 | 1 | 0 | 0 | 0 | 0 |
| 85 | N3 | 2 | 0 | 0 | 0 | 0 |
| 85 | N5 | 1 | 0 | 0 | 0 | 0 |
| 85 | N6 | 2 | 0 | 0 | 0 | 0 |
| 85 | N8 | 5 | 0 | 0 | 0 | 0 |
| 85 | O2 | 1 | 0 | 0 | 0 | 0 |
| 85 | O4 | 1 | 0 | 0 | 0 | 0 |
| 85 | O5 | 1 | 0 | 0 | 0 | 0 |
| 85 | O7 | 3 | 0 | 0 | 0 | 0 |
| 85 | Q2 | 1 | 0 | 0 | 0 | 0 |
| 85 | S4 | 1 | 0 | 0 | 0 | 0 |
| 85 | S8 | 1 | 0 | 0 | 0 | 0 |
| 85 | SM | 1 | 0 | 0 | 0 | 0 |
| 85 | c1 | 1 | 0 | 0 | 0 | 0 |
| 85 | c7 | 1 | 0 | 0 | 0 | 0 |
| 85 | c8 | 1 | 0 | 0 | 0 | 0 |
| 85 | c9 | 1 | 0 | 0 | 0 | 0 |
| 85 | d3 | 1 | 0 | 0 | 0 | 0 |
| 85 | d4 | 1 | 0 | 0 | 0 | 0 |
| 85 | d6 | 1 | 0 | 0 | 0 | 0 |
| 85 | l2 | 1 | 0 | 0 | 0 | 0 |
| 85 | l3 | 1 | 0 | 0 | 0 | 0 |
| 85 | l4 | 1 | 0 | 0 | 0 | 0 |
| 85 | l5 | 2 | 0 | 0 | 0 | 0 |
| 85 | l7 | 1 | 0 | 0 | 0 | 0 |
| 85 | l9 | 1 | 0 | 0 | 0 | 0 |
| 85 | m0 | 1 | 0 | 0 | 0 | 0 |
| 85 | m1 | 1 | 0 | 0 | 0 | 0 |
| 85 | m5 | 2 | 0 | 0 | 0 | 0 |
| 85 | m6 | 1 | 0 | 0 | 0 | 0 |
| 85 | m7 | 5 | 0 | 0 | 0 | 0 |
| 85 | n0 | 2 | 0 | 0 | 0 | 0 |
| 85 | n3 | 2 | 0 | 0 | 0 | 0 |
| 85 | n6 | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 85 | n8 | 4 | 0 | 0 | 0 | 0 |
| 85 | n9 | 1 | 0 | 0 | 0 | 0 |
| 85 | o1 | 1 | 0 | 0 | 0 | 0 |
| 85 | o3 | 1 | 0 | 0 | 0 | 0 |
| 85 | o4 | 2 | 0 | 0 | 0 | 0 |
| 85 | o7 | 1 | 0 | 0 | 0 | 0 |
| 85 | q0 | 1 | 0 | 0 | 0 | 0 |
| 85 | q1 | 1 | 0 | 0 | 0 | 0 |
| 85 | q3 | 1 | 0 | 0 | 0 | 0 |
| 85 | s1 | 1 | 0 | 0 | 0 | 0 |
| 85 | s6 | 1 | 0 | 0 | 0 | 0 |
| 85 | s8 | 2 | 0 | 0 | 0 | 0 |
| 85 | sM | 2 | 0 | 0 | 0 | 0 |
| 86 | 1 | 2457 | 0 | 0 | 229 | 0 |
| 86 | 2 | 1092 | 0 | 0 | 109 | 0 |
| 86 | 3 | 77 | 0 | 0 | 5 | 0 |
| 86 | 4 | 98 | 0 | 0 | 7 | 0 |
| 86 | 5 | 2478 | 0 | 0 | 240 | 0 |
| 86 | 6 | 1106 | 0 | 0 | 107 | 0 |
| 86 | 7 | 77 | 0 | 0 | 10 | 0 |
| 86 | 8 | 119 | 0 | 0 | 18 | 0 |
| 86 | C1 | 7 | 0 | 0 | 0 | 0 |
| 86 | C3 | 7 | 0 | 0 | 1 | 0 |
| 86 | C5 | 7 | 0 | 0 | 5 | 0 |
| 86 | C8 | 7 | 0 | 0 | 0 | 0 |
| 86 | D9 | 7 | 0 | 0 | 1 | 0 |
| 86 | L3 | 21 | 0 | 0 | 2 | 0 |
| 86 | L4 | 7 | 0 | 0 | 0 | 0 |
| 86 | M0 | 7 | 0 | 0 | 1 | 0 |
| 86 | M5 | 7 | 0 | 0 | 1 | 0 |
| 86 | M7 | 14 | 0 | 0 | 2 | 0 |
| 86 | M8 | 7 | 0 | 0 | 0 | 0 |
| 86 | M9 | 7 | 0 | 0 | 0 | 0 |
| 86 | N1 | 7 | 0 | 0 | 2 | 0 |
| 86 | N9 | 7 | 0 | 0 | 0 | 0 |
| 86 | O1 | 7 | 0 | 0 | 6 | 0 |
| 86 | O2 | 7 | 0 | 0 | 0 | 0 |
| 86 | O3 | 7 | 0 | 0 | 1 | 0 |
| 86 | O7 | 14 | 0 | 0 | 6 | 0 |
| 86 | O9 | 7 | 0 | 0 | 1 | 0 |
| 86 | S8 | 7 | 0 | 0 | 0 | 0 |
| 86 | SR | 7 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 86 | c3 | 7 | 0 | 0 | 0 | 0 |
| 86 | c5 | 7 | 0 | 0 | 0 | 0 |
| 86 | c8 | 7 | 0 | 0 | 0 | 0 |
| 86 | d4 | 7 | 0 | 0 | 0 | 0 |
| 86 | d9 | 7 | 0 | 0 | 0 | 0 |
| 86 | l3 | 21 | 0 | 0 | 0 | 0 |
| 86 | l4 | 14 | 0 | 0 | 0 | 0 |
| 86 | l5 | 21 | 0 | 0 | 0 | 0 |
| 86 | l9 | 7 | 0 | 0 | 0 | 0 |
| 86 | m0 | 14 | 0 | 0 | 0 | 0 |
| 86 | m1 | 7 | 0 | 0 | 0 | 0 |
| 86 | m4 | 7 | 0 | 0 | 0 | 0 |
| 86 | m5 | 7 | 0 | 0 | 0 | 0 |
| 86 | m6 | 7 | 0 | 0 | 0 | 0 |
| 86 | m7 | 7 | 0 | 0 | 0 | 0 |
| 86 | m8 | 7 | 0 | 0 | 0 | 0 |
| 86 | m9 | 7 | 0 | 0 | 0 | 0 |
| 86 | n1 | 7 | 0 | 0 | 0 | 0 |
| 86 | n3 | 7 | 0 | 0 | 0 | 0 |
| 86 | n9 | 7 | 0 | 0 | 0 | 0 |
| 86 | o3 | 7 | 0 | 0 | 0 | 0 |
| 86 | q2 | 7 | 0 | 0 | 0 | 0 |
| 86 | s1 | 14 | 0 | 0 | 0 | 0 |
| 86 | s4 | 7 | 0 | 0 | 0 | 0 |
| 86 | s8 | 7 | 0 | 0 | 0 | 0 |
| 86 | s9 | 7 | 0 | 0 | 0 | 0 |
| 86 | sR | 7 | 0 | 0 | 0 | 0 |
| 87 | 2 | 28 | 0 | 27 | 4 | 0 |
| 87 | 6 | 28 | 0 | 27 | 1 | 0 |
| 88 | D6 | 1 | 0 | 0 | 0 | 0 |
| 88 | D7 | 1 | 0 | 0 | 0 | 0 |
| 88 | D9 | 1 | 0 | 0 | 0 | 0 |
| 88 | E1 | 1 | 0 | 0 | 0 | 0 |
| 88 | O7 | 1 | 0 | 0 | 0 | 0 |
| 88 | Q0 | 1 | 0 | 0 | 0 | 0 |
| 88 | Q2 | 1 | 0 | 0 | 0 | 0 |
| 88 | Q3 | 1 | 0 | 0 | 0 | 0 |
| 88 | d6 | 1 | 0 | 0 | 0 | 0 |
| 88 | d7 | 1 | 0 | 0 | 0 | 0 |
| 88 | d9 | 1 | 0 | 0 | 0 | 0 |
| 88 | e1 | 1 | 0 | 0 | 0 | 0 |
| 88 | o7 | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 88 | q0 | 1 | 0 | 0 | 0 | 0 |
| 88 | q2 | 1 | 0 | 0 | 0 | 0 |
| 88 | q3 | 1 | 0 | 0 | 0 | 0 |
| All | All | 411206 | 0 | 297328 | 11067 | 1 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 11067 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 78:Q2:17:CYS:CB | 78:Q2:17:CYS:SG | 2.06 | 1.43 |
| 40:L3:41:VAL:HA | 40:L3:185:GLY:HA3 | 1.44 | 1.07 |
| 36:5:3274:A:H3' | 36:5:3275:U:H5'' | 1.38 | 1.04 |
| 42:L5:111:GLN:HA | 42:L5:116:ASP:HB3 | 3.45 | 1.02 |
| 1:2:992:A:H2 | 1:2:1012:U:H3 | 1.09 | 1.01 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 1:2:1353:U:O2' | 36:5:3165:A:OP1[2_546] | 2.18 | 0.02 |

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%) | 148 (72%) | 39 (19%) | 17 (8%) | 1 | 7 |
| 2 | s0 | 204/251 (81%) | 148 (72%) | 32 (16%) | 24 (12%) | 0 | 3 |
| 3 | S1 | 212/254 (84%) | 149 (70%) | 34 (16%) | 29 (14%) | 0 | 1 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 3 | s1 | 214/254 (84%) | 178 (83%) | 23 (11%) | 13 (6%) | 2 | 15 |
| 4 | S2 | 215/253 (85%) | 178 (83%) | 26 (12%) | 11 (5%) | 2 | 20 |
| 4 | s2 | 215/253 (85%) | 169 (79%) | 30 (14%) | 16 (7%) | 1 | 9 |
| 5 | S3 | 221/239 (92%) | 173 (78%) | 28 (13%) | 20 (9%) | 1 | 5 |
| 5 | s3 | 221/239 (92%) | 176 (80%) | 29 (13%) | 16 (7%) | 1 | 10 |
| 6 | S4 | 258/260 (99%) | 203 (79%) | 38 (15%) | 17 (7%) | 1 | 12 |
| 6 | s4 | 258/260 (99%) | 209 (81%) | 29 (11%) | 20 (8%) | 1 | 8 |
| 7 | S5 | 204/224 (91%) | 155 (76%) | 28 (14%) | 21 (10%) | 1 | 4 |
| 7 | s5 | 204/224 (91%) | 156 (76%) | 26 (13%) | 22 (11%) | 0 | 3 |
| 8 | S6 | 224/236 (95%) | 191 (85%) | 22 (10%) | 11 (5%) | 3 | 22 |
| 8 | s6 | 216/236 (92%) | 179 (83%) | 22 (10%) | 15 (7%) | 1 | 10 |
| 9 | S7 | 182/189 (96%) | 137 (75%) | 25 (14%) | 20 (11%) | 0 | 3 |
| 9 | s7 | 184/189 (97%) | 140 (76%) | 28 (15%) | 16 (9%) | 1 | 5 |
| 10 | S8 | 184/200 (92%) | 154 (84%) | 21 (11%) | 9 (5%) | 3 | 22 |
| 10 | s8 | 184/200 (92%) | 161 (88%) | 12 (6%) | 11 (6%) | 2 | 16 |
| 11 | S9 | 183/196 (93%) | 147 (80%) | 24 (13%) | 12 (7%) | 1 | 12 |
| 11 | s9 | 183/196 (93%) | 149 (81%) | 26 (14%) | 8 (4%) | 3 | 24 |
| 12 | C0 | 94/105 (90%) | 70 (74%) | 18 (19%) | 6 (6%) | 2 | 13 |
| 12 | c0 | 92/105 (88%) | 66 (72%) | 11 (12%) | 15 (16%) | 0 | 1 |
| 13 | C1 | 153/155 (99%) | 118 (77%) | 17 (11%) | 18 (12%) | 0 | 3 |
| 13 | c1 | 144/155 (93%) | 114 (79%) | 24 (17%) | 6 (4%) | 3 | 26 |
| 14 | C2 | 122/142 (86%) | 75 (62%) | 21 (17%) | 26 (21%) | 0 | 0 |
| 14 | c2 | 122/142 (86%) | 71 (58%) | 31 (25%) | 20 (16%) | 0 | 1 |
| 15 | C3 | 148/150 (99%) | 123 (83%) | 12 (8%) | 13 (9%) | 1 | 5 |
| 15 | c3 | 148/150 (99%) | 115 (78%) | 22 (15%) | 11 (7%) | 1 | 9 |
| 16 | C4 | 125/136 (92%) | 95 (76%) | 15 (12%) | 15 (12%) | 0 | 2 |
| 16 | c4 | 126/136 (93%) | 104 (82%) | 16 (13%) | 6 (5%) | 3 | 22 |
| 17 | C5 | 122/141 (86%) | 81 (66%) | 28 (23%) | 13 (11%) | 0 | 3 |
| 17 | c5 | 133/141 (94%) | 90 (68%) | 26 (20%) | 17 (13%) | 0 | 2 |
| 18 | C6 | 139/142 (98%) | 109 (78%) | 20 (14%) | 10 (7%) | 1 | 10 |
| 18 | c6 | 140/142 (99%) | 112 (80%) | 16 (11%) | 12 (9%) | 1 | 6 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 19 | C7 | 116/136 (85%) | 82 (71%) | 25 (22%) | 9 (8%) | 1 | 8 |
| 19 | c7 | 113/136 (83%) | 87 (77%) | 14 (12%) | 12 (11%) | 0 | 3 |
| 20 | C8 | 143/145 (99%) | 115 (80%) | 15 (10%) | 13 (9%) | 1 | 5 |
| 20 | c8 | 143/145 (99%) | 117 (82%) | 20 (14%) | 6 (4%) | 3 | 26 |
| 21 | C9 | 141/143 (99%) | 115 (82%) | 20 (14%) | 6 (4%) | 3 | 25 |
| 21 | c9 | 141/143 (99%) | 115 (82%) | 22 (16%) | 4 (3%) | 6 | 37 |
| 22 | D0 | 105/120 (88%) | 82 (78%) | 20 (19%) | 3 (3%) | 6 | 36 |
| 22 | d0 | 108/120 (90%) | 84 (78%) | 14 (13%) | 10 (9%) | 1 | 5 |
| 23 | D1 | 85/87 (98%) | 64 (75%) | 15 (18%) | 6 (7%) | 1 | 10 |
| 23 | d1 | 85/87 (98%) | 70 (82%) | 8 (9%) | 7 (8%) | 1 | 7 |
| 24 | D2 | 127/129 (98%) | 105 (83%) | 20 (16%) | 2 (2%) | 12 | 54 |
| 24 | d2 | 127/129 (98%) | 113 (89%) | 13 (10%) | 1 (1%) | 24 | 69 |
| 25 | D3 | 142/144 (99%) | 115 (81%) | 14 (10%) | 13 (9%) | 1 | 5 |
| 25 | d3 | 142/144 (99%) | 123 (87%) | 13 (9%) | 6 (4%) | 3 | 26 |
| 26 | D4 | 132/134 (98%) | 107 (81%) | 19 (14%) | 6 (4%) | 3 | 24 |
| 26 | d4 | 132/134 (98%) | 100 (76%) | 21 (16%) | 11 (8%) | 1 | 7 |
| 27 | D5 | 68/107 (64%) | 45 (66%) | 13 (19%) | 10 (15%) | 0 | 1 |
| 27 | d5 | 67/107 (63%) | 52 (78%) | 12 (18%) | 3 (4%) | 3 | 24 |
| 28 | D6 | 95/97 (98%) | 61 (64%) | 17 (18%) | 17 (18%) | 0 | 0 |
| 28 | d6 | 95/97 (98%) | 71 (75%) | 16 (17%) | 8 (8%) | 1 | 6 |
| 29 | D7 | 79/81 (98%) | 62 (78%) | 11 (14%) | 6 (8%) | 1 | 9 |
| 29 | d7 | 79/81 (98%) | 59 (75%) | 15 (19%) | 5 (6%) | 2 | 13 |
| 30 | D8 | 61/66 (92%) | 45 (74%) | 11 (18%) | 5 (8%) | 1 | 7 |
| 30 | d8 | 61/66 (92%) | 46 (75%) | 10 (16%) | 5 (8%) | 1 | 7 |
| 31 | D9 | 51/55 (93%) | 41 (80%) | 7 (14%) | 3 (6%) | 2 | 16 |
| 31 | d9 | 51/55 (93%) | 37 (72%) | 8 (16%) | 6 (12%) | 0 | 3 |
| 32 | E0 | 58/60 (97%) | 42 (72%) | 12 (21%) | 4 (7%) | 1 | 10 |
| 33 | E1 | 69/76 (91%) | 34 (49%) | 11 (16%) | 24 (35%) | 0 | 0 |
| 33 | e1 | 74/76 (97%) | 34 (46%) | 22 (30%) | 18 (24%) | 0 | 0 |
| 34 | SR | 316/318 (99%) | 238 (75%) | 56 (18%) | 22 (7%) | 1 | 10 |
| 34 | sR | 316/318 (99%) | 261 (83%) | 39 (12%) | 16 (5%) | 2 | 20 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|----------|-------------|----|
| 35 | SM | 155/273 (57%) | 109 (70%) | 26 (17%) | 20 (13%) | 0 | 2 |
| 35 | sM | 98/273 (36%) | 61 (62%) | 23 (24%) | 14 (14%) | 0 | 1 |
| 39 | L2 | 250/253 (99%) | 218 (87%) | 22 (9%) | 10 (4%) | 4 | 27 |
| 39 | l2 | 250/253 (99%) | 209 (84%) | 26 (10%) | 15 (6%) | 2 | 16 |
| 40 | L3 | 384/386 (100%) | 333 (87%) | 34 (9%) | 17 (4%) | 3 | 24 |
| 40 | l3 | 384/386 (100%) | 339 (88%) | 32 (8%) | 13 (3%) | 5 | 31 |
| 41 | L4 | 359/361 (99%) | 302 (84%) | 40 (11%) | 17 (5%) | 3 | 22 |
| 41 | l4 | 359/361 (99%) | 293 (82%) | 40 (11%) | 26 (7%) | 1 | 10 |
| 42 | L5 | 294/296 (99%) | 239 (81%) | 34 (12%) | 21 (7%) | 1 | 10 |
| 42 | l5 | 292/296 (99%) | 252 (86%) | 32 (11%) | 8 (3%) | 6 | 39 |
| 43 | L6 | 152/175 (87%) | 134 (88%) | 16 (10%) | 2 (1%) | 15 | 59 |
| 43 | l6 | 153/175 (87%) | 127 (83%) | 23 (15%) | 3 (2%) | 9 | 48 |
| 44 | L7 | 220/243 (90%) | 195 (89%) | 19 (9%) | 6 (3%) | 6 | 39 |
| 44 | l7 | 221/243 (91%) | 193 (87%) | 23 (10%) | 5 (2%) | 8 | 44 |
| 45 | L8 | 231/255 (91%) | 188 (81%) | 36 (16%) | 7 (3%) | 5 | 35 |
| 45 | l8 | 229/255 (90%) | 181 (79%) | 31 (14%) | 17 (7%) | 1 | 9 |
| 46 | L9 | 189/191 (99%) | 156 (82%) | 25 (13%) | 8 (4%) | 3 | 26 |
| 46 | l9 | 189/191 (99%) | 162 (86%) | 23 (12%) | 4 (2%) | 9 | 46 |
| 47 | M0 | 207/220 (94%) | 172 (83%) | 21 (10%) | 14 (7%) | 1 | 11 |
| 47 | m0 | 209/220 (95%) | 165 (79%) | 30 (14%) | 14 (7%) | 1 | 12 |
| 48 | M1 | 167/173 (96%) | 127 (76%) | 24 (14%) | 16 (10%) | 1 | 5 |
| 48 | m1 | 167/173 (96%) | 142 (85%) | 10 (6%) | 15 (9%) | 1 | 5 |
| 49 | M3 | 191/198 (96%) | 156 (82%) | 23 (12%) | 12 (6%) | 2 | 13 |
| 49 | m3 | 192/198 (97%) | 149 (78%) | 25 (13%) | 18 (9%) | 1 | 5 |
| 50 | M4 | 134/137 (98%) | 115 (86%) | 12 (9%) | 7 (5%) | 2 | 19 |
| 50 | m4 | 135/137 (98%) | 120 (89%) | 13 (10%) | 2 (2%) | 13 | 55 |
| 51 | M5 | 201/203 (99%) | 179 (89%) | 17 (8%) | 5 (2%) | 7 | 41 |
| 51 | m5 | 201/203 (99%) | 175 (87%) | 17 (8%) | 9 (4%) | 3 | 24 |
| 52 | M6 | 195/198 (98%) | 176 (90%) | 14 (7%) | 5 (3%) | 7 | 40 |
| 52 | m6 | 195/198 (98%) | 170 (87%) | 18 (9%) | 7 (4%) | 4 | 30 |
| 53 | M7 | 181/183 (99%) | 150 (83%) | 22 (12%) | 9 (5%) | 3 | 21 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 53 | m7 | 153/183 (84%) | 136 (89%) | 12 (8%) | 5 (3%) | 5 | 32 |
| 54 | M8 | 183/185 (99%) | 157 (86%) | 20 (11%) | 6 (3%) | 5 | 32 |
| 54 | m8 | 183/185 (99%) | 158 (86%) | 23 (13%) | 2 (1%) | 17 | 62 |
| 55 | M9 | 186/188 (99%) | 158 (85%) | 23 (12%) | 5 (3%) | 6 | 39 |
| 55 | m9 | 186/188 (99%) | 165 (89%) | 20 (11%) | 1 (0%) | 34 | 78 |
| 56 | N0 | 170/172 (99%) | 150 (88%) | 17 (10%) | 3 (2%) | 11 | 51 |
| 56 | n0 | 170/172 (99%) | 154 (91%) | 15 (9%) | 1 (1%) | 30 | 75 |
| 57 | N1 | 157/159 (99%) | 132 (84%) | 19 (12%) | 6 (4%) | 4 | 28 |
| 57 | n1 | 157/159 (99%) | 143 (91%) | 13 (8%) | 1 (1%) | 30 | 75 |
| 58 | N2 | 98/120 (82%) | 77 (79%) | 17 (17%) | 4 (4%) | 3 | 27 |
| 58 | n2 | 96/120 (80%) | 76 (79%) | 14 (15%) | 6 (6%) | 2 | 13 |
| 59 | N3 | 134/136 (98%) | 120 (90%) | 12 (9%) | 2 (2%) | 13 | 55 |
| 59 | n3 | 134/136 (98%) | 122 (91%) | 9 (7%) | 3 (2%) | 8 | 45 |
| 60 | N4 | 96/155 (62%) | 69 (72%) | 17 (18%) | 10 (10%) | 1 | 4 |
| 60 | n4 | 133/155 (86%) | 106 (80%) | 17 (13%) | 10 (8%) | 1 | 9 |
| 61 | N5 | 119/141 (84%) | 103 (87%) | 10 (8%) | 6 (5%) | 3 | 21 |
| 61 | n5 | 118/141 (84%) | 94 (80%) | 15 (13%) | 9 (8%) | 1 | 9 |
| 62 | N6 | 124/126 (98%) | 110 (89%) | 11 (9%) | 3 (2%) | 7 | 43 |
| 62 | n6 | 124/126 (98%) | 112 (90%) | 7 (6%) | 5 (4%) | 4 | 27 |
| 63 | N7 | 133/135 (98%) | 108 (81%) | 12 (9%) | 13 (10%) | 1 | 4 |
| 63 | n7 | 133/135 (98%) | 101 (76%) | 21 (16%) | 11 (8%) | 1 | 7 |
| 64 | N8 | 146/148 (99%) | 120 (82%) | 19 (13%) | 7 (5%) | 3 | 22 |
| 64 | n8 | 146/148 (99%) | 117 (80%) | 21 (14%) | 8 (6%) | 2 | 18 |
| 65 | N9 | 56/58 (97%) | 47 (84%) | 5 (9%) | 4 (7%) | 1 | 10 |
| 65 | n9 | 56/58 (97%) | 37 (66%) | 13 (23%) | 6 (11%) | 0 | 3 |
| 66 | O0 | 95/104 (91%) | 86 (90%) | 8 (8%) | 1 (1%) | 17 | 62 |
| 66 | o0 | 98/104 (94%) | 88 (90%) | 9 (9%) | 1 (1%) | 19 | 65 |
| 67 | O1 | 107/112 (96%) | 96 (90%) | 5 (5%) | 6 (6%) | 2 | 18 |
| 67 | o1 | 107/112 (96%) | 84 (78%) | 15 (14%) | 8 (8%) | 1 | 9 |
| 68 | O2 | 125/129 (97%) | 106 (85%) | 14 (11%) | 5 (4%) | 4 | 27 |
| 68 | o2 | 125/129 (97%) | 105 (84%) | 15 (12%) | 5 (4%) | 4 | 27 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|------------|-----------|-------------|-----|
| 69 | O3 | 104/106 (98%) | 94 (90%) | 6 (6%) | 4 (4%) | 4 | 28 |
| 69 | o3 | 104/106 (98%) | 94 (90%) | 7 (7%) | 3 (3%) | 6 | 36 |
| 70 | O4 | 110/120 (92%) | 90 (82%) | 19 (17%) | 1 (1%) | 21 | 67 |
| 70 | o4 | 110/120 (92%) | 97 (88%) | 10 (9%) | 3 (3%) | 6 | 39 |
| 71 | O5 | 117/119 (98%) | 104 (89%) | 10 (8%) | 3 (3%) | 7 | 40 |
| 71 | o5 | 117/119 (98%) | 100 (86%) | 14 (12%) | 3 (3%) | 7 | 40 |
| 72 | O6 | 97/99 (98%) | 72 (74%) | 17 (18%) | 8 (8%) | 1 | 7 |
| 72 | o6 | 97/99 (98%) | 81 (84%) | 11 (11%) | 5 (5%) | 2 | 19 |
| 73 | O7 | 85/87 (98%) | 72 (85%) | 12 (14%) | 1 (1%) | 16 | 60 |
| 73 | o7 | 85/87 (98%) | 68 (80%) | 12 (14%) | 5 (6%) | 2 | 16 |
| 74 | O8 | 75/77 (97%) | 61 (81%) | 12 (16%) | 2 (3%) | 6 | 39 |
| 74 | o8 | 75/77 (97%) | 64 (85%) | 8 (11%) | 3 (4%) | 4 | 27 |
| 75 | O9 | 48/50 (96%) | 42 (88%) | 5 (10%) | 1 (2%) | 9 | 46 |
| 75 | o9 | 48/50 (96%) | 40 (83%) | 8 (17%) | 0 | 100 | 100 |
| 76 | Q0 | 50/52 (96%) | 44 (88%) | 4 (8%) | 2 (4%) | 4 | 27 |
| 76 | q0 | 50/52 (96%) | 49 (98%) | 0 | 1 (2%) | 9 | 48 |
| 77 | Q1 | 23/25 (92%) | 22 (96%) | 1 (4%) | 0 | 100 | 100 |
| 77 | q1 | 23/25 (92%) | 20 (87%) | 2 (9%) | 1 (4%) | 3 | 25 |
| 78 | Q2 | 103/105 (98%) | 76 (74%) | 19 (18%) | 8 (8%) | 1 | 8 |
| 78 | q2 | 103/105 (98%) | 86 (84%) | 14 (14%) | 3 (3%) | 6 | 36 |
| 79 | Q3 | 89/91 (98%) | 76 (85%) | 10 (11%) | 3 (3%) | 5 | 31 |
| 79 | q3 | 89/91 (98%) | 81 (91%) | 7 (8%) | 1 (1%) | 17 | 62 |
| 80 | e0 | 60/62 (97%) | 44 (73%) | 8 (13%) | 8 (13%) | 0 | 1 |
| 81 | p0 | 139/311 (45%) | 110 (79%) | 21 (15%) | 8 (6%) | 2 | 17 |
| All | All | 22333/24143 (92%) | 18176 (81%) | 2788 (12%) | 1369 (6%) | 2 | 15 |

5 of 1369 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | S0 | 4 | PRO |
| 2 | S0 | 39 | ASN |
| 2 | S0 | 66 | ALA |
| 2 | S0 | 139 | VAL |
| 2 | S0 | 158 | VAL |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 | 11 |
| 2 | s0 | 165/209 (79%) | 134 (81%) | 31 (19%) | 2 | 10 |
| 3 | S1 | 191/223 (86%) | 154 (81%) | 37 (19%) | 2 | 9 |
| 3 | s1 | 192/223 (86%) | 155 (81%) | 37 (19%) | 2 | 9 |
| 4 | S2 | 176/204 (86%) | 138 (78%) | 38 (22%) | 1 | 6 |
| 4 | s2 | 176/204 (86%) | 131 (74%) | 45 (26%) | 0 | 2 |
| 5 | S3 | 182/194 (94%) | 145 (80%) | 37 (20%) | 1 | 7 |
| 5 | s3 | 182/194 (94%) | 141 (78%) | 41 (22%) | 1 | 5 |
| 6 | S4 | 221/221 (100%) | 170 (77%) | 51 (23%) | 1 | 4 |
| 6 | s4 | 221/221 (100%) | 183 (83%) | 38 (17%) | 2 | 12 |
| 7 | S5 | 173/190 (91%) | 137 (79%) | 36 (21%) | 1 | 7 |
| 7 | s5 | 173/190 (91%) | 141 (82%) | 32 (18%) | 2 | 10 |
| 8 | S6 | 188/201 (94%) | 154 (82%) | 34 (18%) | 2 | 11 |
| 8 | s6 | 187/201 (93%) | 153 (82%) | 34 (18%) | 2 | 10 |
| 9 | S7 | 165/169 (98%) | 136 (82%) | 29 (18%) | 2 | 11 |
| 9 | s7 | 165/169 (98%) | 142 (86%) | 23 (14%) | 4 | 20 |
| 10 | S8 | 150/161 (93%) | 129 (86%) | 21 (14%) | 4 | 20 |
| 10 | s8 | 150/161 (93%) | 124 (83%) | 26 (17%) | 2 | 12 |
| 11 | S9 | 158/165 (96%) | 121 (77%) | 37 (23%) | 1 | 4 |
| 11 | s9 | 158/165 (96%) | 128 (81%) | 30 (19%) | 2 | 10 |
| 12 | C0 | 77/98 (79%) | 66 (86%) | 11 (14%) | 4 | 19 |
| 12 | c0 | 73/98 (74%) | 58 (80%) | 15 (20%) | 1 | 7 |
| 13 | C1 | 129/136 (95%) | 111 (86%) | 18 (14%) | 4 | 20 |
| 13 | c1 | 129/136 (95%) | 99 (77%) | 30 (23%) | 1 | 4 |
| 14 | C2 | 88/118 (75%) | 69 (78%) | 19 (22%) | 1 | 6 |
| 14 | c2 | 88/118 (75%) | 62 (70%) | 26 (30%) | 0 | 1 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 15 | C3 | 127/127 (100%) | 101 (80%) | 26 (20%) | 1 | 7 |
| 15 | c3 | 127/127 (100%) | 102 (80%) | 25 (20%) | 1 | 8 |
| 16 | C4 | 81/104 (78%) | 58 (72%) | 23 (28%) | 0 | 1 |
| 16 | c4 | 97/104 (93%) | 77 (79%) | 20 (21%) | 1 | 7 |
| 17 | C5 | 101/117 (86%) | 87 (86%) | 14 (14%) | 4 | 20 |
| 17 | c5 | 103/117 (88%) | 85 (82%) | 18 (18%) | 2 | 12 |
| 18 | C6 | 117/118 (99%) | 92 (79%) | 25 (21%) | 1 | 6 |
| 18 | c6 | 118/118 (100%) | 95 (80%) | 23 (20%) | 2 | 9 |
| 19 | C7 | 94/124 (76%) | 73 (78%) | 21 (22%) | 1 | 5 |
| 19 | c7 | 92/124 (74%) | 73 (79%) | 19 (21%) | 1 | 7 |
| 20 | C8 | 128/128 (100%) | 97 (76%) | 31 (24%) | 1 | 3 |
| 20 | c8 | 128/128 (100%) | 98 (77%) | 30 (23%) | 1 | 4 |
| 21 | C9 | 115/115 (100%) | 87 (76%) | 28 (24%) | 1 | 3 |
| 21 | c9 | 115/115 (100%) | 97 (84%) | 18 (16%) | 3 | 15 |
| 22 | D0 | 100/113 (88%) | 80 (80%) | 20 (20%) | 1 | 8 |
| 22 | d0 | 103/113 (91%) | 77 (75%) | 26 (25%) | 1 | 2 |
| 23 | D1 | 74/74 (100%) | 58 (78%) | 16 (22%) | 1 | 6 |
| 23 | d1 | 74/74 (100%) | 55 (74%) | 19 (26%) | 0 | 2 |
| 24 | D2 | 110/110 (100%) | 89 (81%) | 21 (19%) | 2 | 10 |
| 24 | d2 | 110/110 (100%) | 95 (86%) | 15 (14%) | 5 | 22 |
| 25 | D3 | 119/119 (100%) | 95 (80%) | 24 (20%) | 1 | 7 |
| 25 | d3 | 119/119 (100%) | 97 (82%) | 22 (18%) | 2 | 10 |
| 26 | D4 | 112/112 (100%) | 95 (85%) | 17 (15%) | 3 | 17 |
| 26 | d4 | 112/112 (100%) | 94 (84%) | 18 (16%) | 3 | 14 |
| 27 | D5 | 61/88 (69%) | 49 (80%) | 12 (20%) | 1 | 8 |
| 27 | d5 | 61/88 (69%) | 51 (84%) | 10 (16%) | 3 | 13 |
| 28 | D6 | 83/83 (100%) | 65 (78%) | 18 (22%) | 1 | 6 |
| 28 | d6 | 83/83 (100%) | 73 (88%) | 10 (12%) | 6 | 28 |
| 29 | D7 | 70/70 (100%) | 59 (84%) | 11 (16%) | 3 | 15 |
| 29 | d7 | 70/70 (100%) | 60 (86%) | 10 (14%) | 4 | 19 |
| 30 | D8 | 56/59 (95%) | 41 (73%) | 15 (27%) | 0 | 2 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 30 | d8 | 56/59 (95%) | 42 (75%) | 14 (25%) | 1 | 2 |
| 31 | D9 | 47/48 (98%) | 38 (81%) | 9 (19%) | 2 | 10 |
| 31 | d9 | 47/48 (98%) | 36 (77%) | 11 (23%) | 1 | 4 |
| 32 | E0 | 51/51 (100%) | 43 (84%) | 8 (16%) | 3 | 15 |
| 33 | E1 | 62/66 (94%) | 47 (76%) | 15 (24%) | 1 | 3 |
| 33 | e1 | 66/66 (100%) | 47 (71%) | 19 (29%) | 0 | 1 |
| 34 | SR | 260/261 (100%) | 213 (82%) | 47 (18%) | 2 | 11 |
| 34 | sR | 260/261 (100%) | 232 (89%) | 28 (11%) | 8 | 33 |
| 35 | SM | 97/228 (42%) | 69 (71%) | 28 (29%) | 0 | 1 |
| 35 | sM | 54/228 (24%) | 40 (74%) | 14 (26%) | 0 | 2 |
| 39 | L2 | 193/195 (99%) | 153 (79%) | 40 (21%) | 1 | 7 |
| 39 | l2 | 192/195 (98%) | 149 (78%) | 43 (22%) | 1 | 5 |
| 40 | L3 | 320/322 (99%) | 251 (78%) | 69 (22%) | 1 | 6 |
| 40 | l3 | 320/322 (99%) | 258 (81%) | 62 (19%) | 2 | 9 |
| 41 | L4 | 288/288 (100%) | 225 (78%) | 63 (22%) | 1 | 6 |
| 41 | l4 | 288/288 (100%) | 230 (80%) | 58 (20%) | 1 | 7 |
| 42 | L5 | 244/244 (100%) | 197 (81%) | 47 (19%) | 2 | 9 |
| 42 | l5 | 243/244 (100%) | 191 (79%) | 52 (21%) | 1 | 6 |
| 43 | L6 | 134/152 (88%) | 118 (88%) | 16 (12%) | 6 | 28 |
| 43 | l6 | 135/152 (89%) | 112 (83%) | 23 (17%) | 2 | 12 |
| 44 | L7 | 186/204 (91%) | 165 (89%) | 21 (11%) | 7 | 31 |
| 44 | l7 | 187/204 (92%) | 158 (84%) | 29 (16%) | 3 | 15 |
| 45 | L8 | 187/207 (90%) | 151 (81%) | 36 (19%) | 2 | 9 |
| 45 | l8 | 177/207 (86%) | 141 (80%) | 36 (20%) | 1 | 7 |
| 46 | L9 | 171/171 (100%) | 137 (80%) | 34 (20%) | 1 | 8 |
| 46 | l9 | 171/171 (100%) | 123 (72%) | 48 (28%) | 0 | 1 |
| 47 | M0 | 177/186 (95%) | 139 (78%) | 38 (22%) | 1 | 6 |
| 47 | m0 | 179/186 (96%) | 145 (81%) | 34 (19%) | 2 | 10 |
| 48 | M1 | 147/150 (98%) | 123 (84%) | 24 (16%) | 3 | 14 |
| 48 | m1 | 147/150 (98%) | 115 (78%) | 32 (22%) | 1 | 6 |
| 49 | M3 | 154/158 (98%) | 123 (80%) | 31 (20%) | 1 | 7 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 49 | m3 | 154/158 (98%) | 124 (80%) | 30 (20%) | 2 | 9 |
| 50 | M4 | 107/108 (99%) | 87 (81%) | 20 (19%) | 2 | 10 |
| 50 | m4 | 108/108 (100%) | 81 (75%) | 27 (25%) | 1 | 2 |
| 51 | M5 | 175/175 (100%) | 143 (82%) | 32 (18%) | 2 | 10 |
| 51 | m5 | 175/175 (100%) | 142 (81%) | 33 (19%) | 2 | 10 |
| 52 | M6 | 160/161 (99%) | 141 (88%) | 19 (12%) | 6 | 28 |
| 52 | m6 | 160/161 (99%) | 130 (81%) | 30 (19%) | 2 | 10 |
| 53 | M7 | 140/145 (97%) | 107 (76%) | 33 (24%) | 1 | 4 |
| 53 | m7 | 125/145 (86%) | 100 (80%) | 25 (20%) | 1 | 8 |
| 54 | M8 | 150/150 (100%) | 126 (84%) | 24 (16%) | 3 | 14 |
| 54 | m8 | 150/150 (100%) | 122 (81%) | 28 (19%) | 2 | 10 |
| 55 | M9 | 153/153 (100%) | 121 (79%) | 32 (21%) | 1 | 7 |
| 55 | m9 | 153/153 (100%) | 123 (80%) | 30 (20%) | 1 | 9 |
| 56 | N0 | 156/156 (100%) | 127 (81%) | 29 (19%) | 2 | 10 |
| 56 | n0 | 156/156 (100%) | 122 (78%) | 34 (22%) | 1 | 6 |
| 57 | N1 | 136/136 (100%) | 111 (82%) | 25 (18%) | 2 | 10 |
| 57 | n1 | 136/136 (100%) | 108 (79%) | 28 (21%) | 1 | 7 |
| 58 | N2 | 87/106 (82%) | 70 (80%) | 17 (20%) | 2 | 9 |
| 58 | n2 | 85/106 (80%) | 70 (82%) | 15 (18%) | 2 | 11 |
| 59 | N3 | 104/104 (100%) | 87 (84%) | 17 (16%) | 3 | 14 |
| 59 | n3 | 104/104 (100%) | 89 (86%) | 15 (14%) | 4 | 19 |
| 60 | N4 | 57/129 (44%) | 51 (90%) | 6 (10%) | 8 | 35 |
| 60 | n4 | 100/129 (78%) | 82 (82%) | 18 (18%) | 2 | 11 |
| 61 | N5 | 104/117 (89%) | 84 (81%) | 20 (19%) | 2 | 10 |
| 61 | n5 | 104/117 (89%) | 82 (79%) | 22 (21%) | 1 | 7 |
| 62 | N6 | 109/109 (100%) | 85 (78%) | 24 (22%) | 1 | 6 |
| 62 | n6 | 109/109 (100%) | 86 (79%) | 23 (21%) | 1 | 7 |
| 63 | N7 | 115/115 (100%) | 93 (81%) | 22 (19%) | 2 | 10 |
| 63 | n7 | 115/115 (100%) | 89 (77%) | 26 (23%) | 1 | 5 |
| 64 | N8 | 118/118 (100%) | 95 (80%) | 23 (20%) | 2 | 9 |
| 64 | n8 | 118/118 (100%) | 99 (84%) | 19 (16%) | 3 | 14 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 65 | N9 | 46/46 (100%) | 33 (72%) | 13 (28%) | 0 | 1 |
| 65 | n9 | 46/46 (100%) | 32 (70%) | 14 (30%) | 0 | 1 |
| 66 | O0 | 81/87 (93%) | 64 (79%) | 17 (21%) | 1 | 7 |
| 66 | o0 | 84/87 (97%) | 67 (80%) | 17 (20%) | 1 | 7 |
| 67 | O1 | 92/96 (96%) | 74 (80%) | 18 (20%) | 1 | 9 |
| 67 | o1 | 94/96 (98%) | 68 (72%) | 26 (28%) | 0 | 1 |
| 68 | O2 | 109/110 (99%) | 88 (81%) | 21 (19%) | 2 | 9 |
| 68 | o2 | 109/110 (99%) | 81 (74%) | 28 (26%) | 0 | 2 |
| 69 | O3 | 90/90 (100%) | 75 (83%) | 15 (17%) | 3 | 13 |
| 69 | o3 | 90/90 (100%) | 75 (83%) | 15 (17%) | 3 | 13 |
| 70 | O4 | 95/102 (93%) | 74 (78%) | 21 (22%) | 1 | 5 |
| 70 | o4 | 95/102 (93%) | 77 (81%) | 18 (19%) | 2 | 10 |
| 71 | O5 | 104/104 (100%) | 81 (78%) | 23 (22%) | 1 | 5 |
| 71 | o5 | 103/104 (99%) | 78 (76%) | 25 (24%) | 1 | 3 |
| 72 | O6 | 81/81 (100%) | 59 (73%) | 22 (27%) | 0 | 2 |
| 72 | o6 | 80/81 (99%) | 51 (64%) | 29 (36%) | 0 | 0 |
| 73 | O7 | 70/70 (100%) | 52 (74%) | 18 (26%) | 0 | 2 |
| 73 | o7 | 70/70 (100%) | 57 (81%) | 13 (19%) | 2 | 10 |
| 74 | O8 | 68/68 (100%) | 52 (76%) | 16 (24%) | 1 | 4 |
| 74 | o8 | 67/68 (98%) | 51 (76%) | 16 (24%) | 1 | 3 |
| 75 | O9 | 45/45 (100%) | 38 (84%) | 7 (16%) | 3 | 15 |
| 75 | o9 | 45/45 (100%) | 37 (82%) | 8 (18%) | 2 | 11 |
| 76 | Q0 | 47/47 (100%) | 36 (77%) | 11 (23%) | 1 | 4 |
| 76 | q0 | 47/47 (100%) | 35 (74%) | 12 (26%) | 1 | 2 |
| 77 | Q1 | 23/23 (100%) | 18 (78%) | 5 (22%) | 1 | 6 |
| 77 | q1 | 23/23 (100%) | 16 (70%) | 7 (30%) | 0 | 1 |
| 78 | Q2 | 90/90 (100%) | 69 (77%) | 21 (23%) | 1 | 4 |
| 78 | q2 | 90/90 (100%) | 74 (82%) | 16 (18%) | 2 | 11 |
| 79 | Q3 | 71/71 (100%) | 55 (78%) | 16 (22%) | 1 | 5 |
| 79 | q3 | 71/71 (100%) | 55 (78%) | 16 (22%) | 1 | 5 |
| 80 | e0 | 53/53 (100%) | 40 (76%) | 13 (24%) | 1 | 3 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|-------------------|-------------|------------|--------------------|
| 81 | p0 | 105/253 (42%) | 85 (81%) | 20 (19%) | 2 10 |
| All | All | 18728/20241 (92%) | 15006 (80%) | 3722 (20%) | 1 8 |

5 of 3722 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 70 | O4 | 71 | THR |
| 8 | s6 | 175 | ILE |
| 64 | n8 | 135 | GLU |
| 72 | O6 | 81 | THR |
| 3 | s1 | 185 | THR |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | M7 | 179 | GLN |
| 70 | O4 | 3 | GLN |
| 62 | n6 | 4 | GLN |
| 62 | N6 | 120 | GLN |
| 75 | O9 | 50 | ASN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------------|-------------------|-----------------|
| 1 | 2 | 1747/1800 (97%) | 509 (29%) | 56 (3%) |
| 1 | 6 | 1793/1800 (99%) | 472 (26%) | 48 (2%) |
| 36 | 1 | 3145/3396 (92%) | 704 (22%) | 78 (2%) |
| 36 | 5 | 3145/3396 (92%) | 688 (21%) | 76 (2%) |
| 37 | 3 | 120/121 (99%) | 17 (14%) | 2 (1%) |
| 37 | 7 | 120/121 (99%) | 24 (20%) | 2 (1%) |
| 38 | 4 | 157/158 (99%) | 36 (22%) | 5 (3%) |
| 38 | 8 | 157/158 (99%) | 38 (24%) | 2 (1%) |
| All | All | 10384/10950 (94%) | 2488 (23%) | 269 (2%) |

5 of 2488 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 2 | 2 | A |
| 1 | 2 | 4 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 2 | 25 | C |
| 1 | 2 | 26 | A |
| 1 | 2 | 27 | U |

5 of 269 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 36 | 1 | 3056 | U |
| 1 | 6 | 217 | A |
| 36 | 5 | 2772 | C |
| 36 | 1 | 3218 | A |
| 38 | 4 | 59 | A |

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2559 ligands modelled in this entry, 1426 are monoatomic - leaving 1133 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 | 1 | 3861 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3862 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3863 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3864 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3865 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3866 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 1 | 3867 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3868 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3869 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3870 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3871 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3872 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3873 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3874 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3875 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3876 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3877 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3878 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3879 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3880 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3881 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3882 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3883 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3884 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3885 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3886 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3887 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3888 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3889 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3890 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3891 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3892 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3893 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3894 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3895 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3896 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3897 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3898 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3899 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3900 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3901 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3902 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3903 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3904 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3905 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3906 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3907 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3908 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3909 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 1 | 3910 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3911 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3912 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3913 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3914 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3915 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3916 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3917 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3918 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3919 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3920 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3921 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3922 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3923 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3924 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3925 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3926 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3927 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3928 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3929 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3930 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3931 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3932 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3933 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3934 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3935 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3936 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3937 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3938 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3939 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3940 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3941 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3942 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3943 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3944 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3945 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3946 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3947 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3948 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3949 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3950 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3951 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3952 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 1 | 3953 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3954 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3955 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3956 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3957 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3958 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3959 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3960 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3961 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3962 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3963 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3964 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3965 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3966 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3967 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3968 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3969 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3970 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3971 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3972 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3973 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3974 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3975 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3976 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3977 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3978 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3979 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3980 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3981 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3982 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3983 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3984 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3985 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3986 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3987 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3988 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3989 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3990 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3991 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3992 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3993 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3994 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3995 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 1 | 3996 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3997 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3998 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 3999 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4000 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4001 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4002 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4003 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4004 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4005 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4006 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4007 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4008 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4009 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4010 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4011 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4012 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4013 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4014 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4015 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4016 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4017 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4018 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4019 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4020 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4021 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4022 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4023 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4024 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4025 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4026 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4027 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4028 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4029 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4030 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4031 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4032 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4033 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4034 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4035 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4036 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4037 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4038 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 1 | 4039 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4040 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4041 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4042 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4043 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4044 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4045 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4046 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4047 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4048 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4049 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4050 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4051 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4052 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4053 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4054 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4055 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4056 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4057 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4058 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4059 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4060 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4061 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4062 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4063 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4064 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4065 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4066 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4067 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4068 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4069 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4070 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4071 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4072 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4073 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4074 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4075 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4076 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4077 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4078 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4079 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4080 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4081 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 1 | 4082 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4083 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4084 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4085 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4086 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4087 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4088 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4089 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4090 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4091 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4092 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4093 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4094 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4095 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4096 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4097 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4098 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4099 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4100 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4101 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4102 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4103 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4104 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4105 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4106 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4107 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4108 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4109 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4110 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4111 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4112 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4113 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4114 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4115 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4116 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4117 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4118 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4119 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4120 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4121 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4122 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4123 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4124 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 1 | 4125 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4126 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4127 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4128 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4129 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4130 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4131 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4132 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4133 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4134 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4135 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4136 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4137 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4138 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4139 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4140 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4141 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4142 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4143 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4144 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4145 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4146 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4147 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4148 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4149 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4150 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4151 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4152 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4153 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4154 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4155 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4156 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4157 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4158 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4159 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4160 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4161 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4162 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4163 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4164 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4165 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4166 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4167 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 1 | 4168 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4169 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4170 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4171 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4172 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4173 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4174 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4175 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4176 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4177 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4178 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4179 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4180 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4181 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4182 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4183 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4184 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4185 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4186 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4187 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4188 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4189 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4190 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4191 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4192 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4193 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4194 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4195 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4196 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4197 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4198 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4199 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4200 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4202 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4203 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4204 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4205 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4206 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4207 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4208 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4209 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 1 | 4210 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 1 | 4211 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2023 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2024 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2025 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2026 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2027 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2028 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2029 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2030 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2031 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2032 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2033 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2034 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2035 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2036 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2037 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2038 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2039 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2040 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2041 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2042 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2043 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2044 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2045 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2046 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2047 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2048 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2049 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2050 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2051 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2052 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2053 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2054 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2055 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2056 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2057 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2058 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2059 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2060 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2061 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2062 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2063 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2064 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 2 | 2065 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2066 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2067 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2068 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2069 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2070 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2071 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2072 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2073 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2074 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2075 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2076 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2077 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2078 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2079 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2080 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2081 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2082 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2083 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2084 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2085 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2086 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2087 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2088 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2089 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2090 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2091 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2092 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2093 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2094 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2095 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2096 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2097 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2098 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2099 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2100 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2101 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2102 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2103 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2104 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2105 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2106 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2107 | - | 0,6,6 | 0.00 | - | 0,15,15 | 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 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2109 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2110 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2111 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2112 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2113 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2114 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2115 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2116 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2117 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2118 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2119 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2120 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2121 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2122 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2123 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2124 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2125 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2126 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2127 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2128 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2129 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2130 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2131 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2132 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2133 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2134 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2135 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2136 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2137 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2138 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2139 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2140 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2141 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2142 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2143 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2144 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2145 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2146 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2147 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2148 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2149 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2150 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 2 | 2151 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2152 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2153 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2154 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2155 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2156 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2157 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2158 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2159 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2160 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2161 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2162 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2163 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2164 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2165 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2166 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2167 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2168 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2169 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2170 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2171 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2172 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2173 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2174 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2175 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2176 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2177 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 2 | 2178 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 87 | 3K8 | 2 | 2179 | - | 32,32,32 | 0.74 | 1 (3%) | 45,47,47 | 0.82 | 1 (2%) |
| 86 | OHX | 3 | 215 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 3 | 216 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 3 | 217 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 3 | 218 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 3 | 219 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 3 | 220 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 3 | 221 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 3 | 222 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 3 | 223 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 3 | 224 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 3 | 225 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 4 | 222 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 4 | 223 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 4 | 224 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 4 | 225 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 4 | 226 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 4 | 227 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 4 | 228 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 4 | 229 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 4 | 230 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 4 | 231 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 4 | 232 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 4 | 233 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 4 | 234 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 4 | 235 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3901 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3902 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3903 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3904 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3905 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3906 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3907 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3908 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3909 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3910 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3911 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3912 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3913 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3914 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3915 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3916 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3917 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3918 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3919 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3920 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3921 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3922 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3923 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3924 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3925 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3926 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3927 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3928 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3929 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3930 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3931 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3932 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 5 | 3933 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3934 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3935 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3936 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3937 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3938 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3939 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3940 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3941 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3942 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3943 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3944 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3945 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3946 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3947 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3948 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3949 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3950 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3951 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3952 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3953 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3954 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3955 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3956 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3957 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3958 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3959 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3960 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3961 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3962 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3963 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3964 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3965 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3966 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3967 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3968 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3969 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3970 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3971 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3972 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3973 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3974 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3975 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 5 | 3976 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3977 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3978 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3979 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3980 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3981 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3982 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3983 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3984 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3985 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3986 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3987 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3988 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3989 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3990 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3991 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3992 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3993 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3994 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3995 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3996 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3997 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3998 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 3999 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4000 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4001 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4002 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4003 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4004 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4005 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4006 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4007 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4008 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4009 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4010 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4011 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4012 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4013 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4014 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4015 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4016 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4017 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4018 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 5 | 4019 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4020 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4021 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4022 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4023 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4024 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4025 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4026 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4027 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4028 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4029 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4030 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4031 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4032 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4033 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4034 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4035 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4036 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4037 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4038 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4039 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4040 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4041 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4042 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4043 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4044 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4045 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4046 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4047 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4048 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4049 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4050 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4051 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4052 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4053 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4054 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4055 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4056 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4057 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4058 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4059 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4060 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4061 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 5 | 4062 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4063 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4064 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4065 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4066 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4067 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4068 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4069 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4070 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4071 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4072 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4073 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4074 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4075 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4076 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4077 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4078 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4079 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4080 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4081 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4082 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4083 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4084 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4085 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4086 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4087 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4088 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4089 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4090 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4091 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4092 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4093 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4094 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4095 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4096 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4097 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4098 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4099 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4100 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4101 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4102 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4103 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4104 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 5 | 4105 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4106 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4107 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4108 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4109 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4110 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4111 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4112 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4113 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4114 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4115 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4116 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4117 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4118 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4119 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4120 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4121 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4122 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4123 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4124 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4125 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4126 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4127 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4128 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4129 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4130 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4131 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4132 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4133 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4134 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4135 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4136 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4137 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4138 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4139 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4140 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4141 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4142 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4143 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4144 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4145 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4146 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4147 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 5 | 4148 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4149 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4150 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4151 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4152 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4153 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4154 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4155 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4156 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4157 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4158 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4159 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4160 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4161 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4162 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4163 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4164 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4165 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4166 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4167 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4168 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4169 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4170 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4171 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4172 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4173 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4174 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4175 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4176 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4177 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4178 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4179 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4180 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4181 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4182 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4183 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4184 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4185 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4186 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4187 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4188 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4189 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4190 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 5 | 4191 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4192 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4193 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4194 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4195 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4196 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4197 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4198 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4199 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4200 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4202 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4203 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4204 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4205 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4206 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4207 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4208 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4209 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4210 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4211 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4212 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4213 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4214 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4215 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4216 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4217 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4218 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4219 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4220 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4221 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4222 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4223 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4224 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4225 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4226 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4227 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4228 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4229 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4230 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4231 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4232 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4233 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 5 | 4234 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4235 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4236 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4237 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4238 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4239 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4240 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4241 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4242 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4243 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4244 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4245 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4246 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4247 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4248 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4249 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4250 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4251 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4252 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4253 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 5 | 4254 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2047 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2048 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2049 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2050 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2051 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2052 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2053 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2054 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2055 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2056 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2057 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2058 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2059 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2060 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2061 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2062 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2063 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2064 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2065 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2066 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2067 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2068 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 6 | 2069 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2070 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2071 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2072 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2073 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2074 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2075 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2076 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2077 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2078 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2079 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2080 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2081 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2082 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2083 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2084 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2085 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2086 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2087 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2088 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2089 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2090 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2091 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2092 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2093 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2094 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2095 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2096 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2097 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2098 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2099 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2100 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2101 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2102 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2103 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2104 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2105 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2106 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2107 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2108 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2109 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2110 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2111 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 6 | 2112 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2113 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2114 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2115 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2116 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2117 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2118 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2119 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2120 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2121 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2122 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2123 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2124 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2125 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2126 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2127 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2128 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2129 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2130 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2131 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2132 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2133 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2134 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2135 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2136 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2137 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2138 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2139 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2140 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2141 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2142 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2143 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2144 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2145 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2146 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2147 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2148 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2149 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2150 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2151 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2152 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2153 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2154 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 6 | 2155 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2156 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2157 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2158 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2159 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2160 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2161 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2162 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2163 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2164 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2165 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2166 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2167 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2168 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2169 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2170 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2171 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2172 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2173 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2174 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2175 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2176 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2177 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2178 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2179 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2180 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2181 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2182 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2183 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2184 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2185 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2186 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2187 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2188 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2189 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2190 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2191 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2192 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2193 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2194 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2195 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2196 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2197 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | 6 | 2198 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2199 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2200 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2202 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2203 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 6 | 2204 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 87 | 3K8 | 6 | 2205 | - | 32,32,32 | 0.54 | 0 | 45,47,47 | 0.70 | 1 (2%) |
| 86 | OHX | 7 | 217 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 7 | 218 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 7 | 219 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 7 | 220 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 7 | 221 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 7 | 222 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 7 | 223 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 7 | 224 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 7 | 225 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 7 | 226 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 7 | 227 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 8 | 215 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 8 | 216 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 8 | 217 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 8 | 218 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 8 | 219 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 8 | 220 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 8 | 221 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 8 | 222 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 8 | 223 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 8 | 224 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 8 | 225 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 8 | 226 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 8 | 227 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 8 | 228 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 8 | 229 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 8 | 230 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | 8 | 231 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | C1 | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | C3 | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | C5 | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | C8 | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | D9 | 102 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | L3 | 404 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | L3 | 405 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | L3 | 406 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | L4 | 402 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | M0 | 304 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | M5 | 302 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | M7 | 206 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | M7 | 207 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | M8 | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | M9 | 202 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | N1 | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | N9 | 101 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | O1 | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | O2 | 202 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | O3 | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | O7 | 105 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | O7 | 106 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | O9 | 101 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | S8 | 302 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | SR | 401 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | c3 | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | c5 | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | c8 | 202 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | d4 | 202 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | d9 | 102 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | l3 | 402 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | l3 | 403 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | l3 | 404 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | l4 | 402 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | l4 | 403 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | l5 | 303 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | l5 | 304 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | l5 | 305 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | l9 | 202 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | m0 | 302 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | m0 | 303 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | m1 | 202 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | m4 | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | m5 | 303 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | m6 | 202 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | m7 | 206 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | m8 | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | m9 | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | n1 | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | n3 | 203 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | n9 | 102 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | o3 | 202 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | q2 | 502 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | s1 | 302 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | s1 | 303 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | s4 | 301 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | s8 | 303 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | s9 | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | OHX | sR | 401 | - | 0,6,6 | 0.00 | - | 0,15,15 | 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 |
|-----|------|-------|------|------|---------|----------|---------|
| 86 | OHX | 1 | 3861 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3862 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3863 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3864 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3865 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3866 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3867 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3868 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3869 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3870 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3871 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3872 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3873 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3874 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3875 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3876 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3877 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3878 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3879 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3880 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3881 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3882 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3883 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3884 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3885 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3886 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3887 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 86 | OHX | 1 | 3888 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3889 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3890 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3891 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3892 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3893 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3894 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3895 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3896 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3897 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3898 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3899 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3900 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3901 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3902 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3903 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3904 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3905 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3906 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3907 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3908 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3909 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3910 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3911 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3912 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3913 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3914 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3915 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3916 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3917 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3918 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3919 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3920 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3921 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3922 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3923 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3924 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3925 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3926 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3927 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3928 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3929 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 86 | OHX | 1 | 3930 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3931 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3932 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3933 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3934 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3935 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3936 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3937 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3938 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3939 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3940 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3941 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3942 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3943 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3944 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3945 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3946 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3947 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3948 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3949 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3950 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3951 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3952 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3953 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3954 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3955 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3956 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3957 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3958 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3959 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3960 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3961 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3962 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3963 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3964 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3965 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3966 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3967 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3968 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3969 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3970 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3971 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 86 | OHX | 1 | 3972 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3973 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3974 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3975 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3976 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3977 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3978 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3979 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3980 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3981 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3982 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3983 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3984 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3985 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3986 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3987 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3988 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3989 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3990 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3991 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3992 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3993 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3994 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3995 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3996 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3997 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3998 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 3999 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4000 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4002 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4003 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4004 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4005 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4006 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4007 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4008 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4009 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4010 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4011 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4012 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4013 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 86 | OHX | 1 | 4014 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4015 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4016 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4017 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4018 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4019 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4020 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4021 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4022 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4023 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4024 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4025 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4026 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4027 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4028 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4029 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4030 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4031 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4032 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4033 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4034 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4035 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4036 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4037 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4038 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4039 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4040 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4041 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4042 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4043 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4044 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4045 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4046 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4047 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4048 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4049 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4050 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4051 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4052 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4053 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4054 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4055 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 86 | OHX | 1 | 4056 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4057 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4058 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4059 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4060 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4061 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4062 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4063 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4064 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4065 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4066 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4067 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4068 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4069 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4070 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4071 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4072 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4073 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4074 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4075 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4076 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4077 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4078 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4079 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4080 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4081 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4082 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4083 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4084 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4085 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4086 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4087 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4088 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4089 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4090 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4091 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4092 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4093 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4094 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4095 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4096 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4097 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 86 | OHX | 1 | 4098 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4099 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4100 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4101 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4102 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4103 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4104 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4105 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4106 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4107 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4108 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4109 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4110 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4111 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4112 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4113 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4114 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4115 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4116 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4117 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4118 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4119 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4120 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4121 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4122 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4123 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4124 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4125 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4126 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4127 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4128 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4129 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4130 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4131 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4132 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4133 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4134 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4135 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4136 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4137 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4138 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4139 | - | - | 0/0/0/0 | 0/0/0/0 |

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Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 86 | OHX | 1 | 4140 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4141 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4142 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4143 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4144 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4145 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4146 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4147 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4148 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4149 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4150 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4151 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4152 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4153 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4154 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4155 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4156 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4157 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4158 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4159 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4160 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4161 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4162 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4163 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4164 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4165 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4166 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4167 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4168 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4169 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4170 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4171 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4172 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4173 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4174 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4175 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4176 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4177 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4178 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4179 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4180 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4181 | - | - | 0/0/0/0 | 0/0/0/0 |

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Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 86 | OHX | 1 | 4182 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4183 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4184 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4185 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4186 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4187 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4188 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4189 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4190 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4191 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4192 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4193 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4194 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4195 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4196 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4197 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4198 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4199 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4200 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4202 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4203 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4204 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4205 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4206 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4207 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4208 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4209 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4210 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 1 | 4211 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2023 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2024 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2025 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2026 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2027 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2028 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2029 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2030 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2031 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2032 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2033 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2034 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 86 | OHX | 2 | 2035 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2036 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2037 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2038 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2039 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2040 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2041 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2042 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2043 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2044 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2045 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2046 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2047 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2048 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2049 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2050 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2051 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2052 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2053 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2054 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2055 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2056 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2057 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2058 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2059 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2060 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2061 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2062 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2063 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2064 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2065 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2066 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2067 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2068 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2069 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2070 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2071 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2072 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2073 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2074 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2075 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2076 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 86 | OHX | 2 | 2077 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2078 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2079 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2080 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2081 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2082 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2083 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2084 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2085 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2086 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2087 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2088 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2089 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2090 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2091 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2092 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2093 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2094 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2095 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2096 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2097 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2098 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2099 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2100 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2101 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2102 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2103 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2104 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2105 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2106 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2107 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2108 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2109 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2110 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2111 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2112 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2113 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2114 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2115 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2116 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2117 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2118 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 86 | OHX | 2 | 2119 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2120 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2121 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2122 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2123 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2124 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2125 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2126 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2127 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2128 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2129 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2130 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2131 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2132 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2133 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2134 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2135 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2136 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2137 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2138 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2139 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2140 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2141 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2142 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2143 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2144 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2145 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2146 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2147 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2148 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2149 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2150 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2151 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2152 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2153 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2154 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2155 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2156 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2157 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2158 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2159 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2160 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 86 | OHX | 2 | 2161 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2162 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2163 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2164 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2165 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2166 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2167 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2168 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2169 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2170 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2171 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2172 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2173 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2174 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2175 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2176 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2177 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 2 | 2178 | - | - | 0/0/0/0 | 0/0/0/0 |
| 87 | 3K8 | 2 | 2179 | - | - | 0/6/25/25 | 0/5/5/5 |
| 86 | OHX | 3 | 215 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 3 | 216 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 3 | 217 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 3 | 218 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 3 | 219 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 3 | 220 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 3 | 221 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 3 | 222 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 3 | 223 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 3 | 224 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 3 | 225 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 4 | 222 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 4 | 223 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 4 | 224 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 4 | 225 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 4 | 226 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 4 | 227 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 4 | 228 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 4 | 229 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 4 | 230 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 4 | 231 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 4 | 232 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 4 | 233 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 86 | OHX | 4 | 234 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 4 | 235 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3901 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3902 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3903 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3904 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3905 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3906 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3907 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3908 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3909 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3910 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3911 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3912 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3913 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3914 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3915 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3916 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3917 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3918 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3919 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3920 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3921 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3922 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3923 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3924 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3925 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3926 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3927 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3928 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3929 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3930 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3931 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3932 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3933 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3934 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3935 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3936 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3937 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3938 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3939 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3940 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 86 | OHX | 5 | 3941 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3942 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3943 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3944 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3945 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3946 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3947 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3948 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3949 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3950 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3951 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3952 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3953 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3954 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3955 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3956 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3957 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3958 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3959 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3960 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3961 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3962 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3963 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3964 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3965 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3966 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3967 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3968 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3969 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3970 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3971 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3972 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3973 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3974 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3975 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3976 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3977 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3978 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3979 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3980 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3981 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3982 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 86 | OHX | 5 | 3983 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3984 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3985 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3986 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3987 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3988 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3989 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3990 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3991 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3992 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3993 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3994 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3995 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3996 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3997 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3998 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 3999 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4000 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4002 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4003 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4004 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4005 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4006 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4007 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4008 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4009 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4010 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4011 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4012 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4013 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4014 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4015 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4016 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4017 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4018 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4019 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4020 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4021 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4022 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4023 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4024 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 86 | OHX | 5 | 4025 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4026 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4027 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4028 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4029 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4030 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4031 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4032 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4033 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4034 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4035 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4036 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4037 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4038 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4039 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4040 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4041 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4042 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4043 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4044 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4045 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4046 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4047 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4048 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4049 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4050 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4051 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4052 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4053 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4054 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4055 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4056 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4057 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4058 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4059 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4060 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4061 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4062 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4063 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4064 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4065 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4066 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 86 | OHX | 5 | 4067 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4068 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4069 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4070 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4071 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4072 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4073 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4074 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4075 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4076 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4077 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4078 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4079 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4080 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4081 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4082 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4083 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4084 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4085 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4086 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4087 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4088 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4089 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4090 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4091 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4092 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4093 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4094 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4095 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4096 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4097 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4098 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4099 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4100 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4101 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4102 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4103 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4104 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4105 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4106 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4107 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4108 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 86 | OHX | 5 | 4109 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4110 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4111 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4112 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4113 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4114 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4115 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4116 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4117 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4118 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4119 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4120 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4121 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4122 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4123 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4124 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4125 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4126 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4127 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4128 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4129 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4130 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4131 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4132 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4133 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4134 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4135 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4136 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4137 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4138 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4139 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4140 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4141 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4142 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4143 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4144 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4145 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4146 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4147 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4148 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4149 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4150 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 86 | OHX | 5 | 4151 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4152 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4153 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4154 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4155 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4156 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4157 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4158 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4159 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4160 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4161 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4162 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4163 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4164 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4165 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4166 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4167 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4168 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4169 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4170 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4171 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4172 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4173 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4174 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4175 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4176 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4177 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4178 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4179 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4180 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4181 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4182 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4183 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4184 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4185 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4186 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4187 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4188 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4189 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4190 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4191 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4192 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 86 | OHX | 5 | 4193 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4194 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4195 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4196 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4197 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4198 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4199 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4200 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4202 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4203 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4204 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4205 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4206 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4207 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4208 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4209 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4210 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4211 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4212 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4213 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4214 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4215 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4216 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4217 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4218 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4219 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4220 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4221 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4222 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4223 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4224 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4225 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4226 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4227 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4228 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4229 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4230 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4231 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4232 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4233 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4234 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 86 | OHX | 5 | 4235 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4236 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4237 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4238 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4239 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4240 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4241 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4242 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4243 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4244 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4245 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4246 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4247 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4248 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4249 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4250 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4251 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4252 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4253 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 5 | 4254 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2047 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2048 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2049 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2050 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2051 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2052 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2053 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2054 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2055 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2056 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2057 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2058 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2059 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2060 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2061 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2062 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2063 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2064 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2065 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2066 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2067 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2068 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 86 | OHX | 6 | 2069 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2070 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2071 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2072 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2073 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2074 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2075 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2076 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2077 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2078 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2079 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2080 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2081 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2082 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2083 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2084 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2085 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2086 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2087 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2088 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2089 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2090 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2091 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2092 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2093 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2094 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2095 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2096 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2097 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2098 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2099 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2100 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2101 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2102 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2103 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2104 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2105 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2106 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2107 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2108 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2109 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2110 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 86 | OHX | 6 | 2111 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2112 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2113 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2114 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2115 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2116 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2117 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2118 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2119 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2120 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2121 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2122 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2123 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2124 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2125 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2126 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2127 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2128 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2129 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2130 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2131 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2132 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2133 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2134 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2135 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2136 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2137 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2138 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2139 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2140 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2141 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2142 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2143 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2144 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2145 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2146 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2147 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2148 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2149 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2150 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2151 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2152 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 86 | OHX | 6 | 2153 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2154 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2155 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2156 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2157 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2158 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2159 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2160 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2161 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2162 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2163 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2164 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2165 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2166 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2167 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2168 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2169 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2170 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2171 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2172 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2173 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2174 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2175 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2176 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2177 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2178 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2179 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2180 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2181 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2182 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2183 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2184 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2185 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2186 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2187 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2188 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2189 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2190 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2191 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2192 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2193 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2194 | - | - | 0/0/0/0 | 0/0/0/0 |

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Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 86 | OHX | 6 | 2195 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2196 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2197 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2198 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2199 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2200 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2202 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2203 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 6 | 2204 | - | - | 0/0/0/0 | 0/0/0/0 |
| 87 | 3K8 | 6 | 2205 | - | - | 0/6/25/25 | 0/5/5/5 |
| 86 | OHX | 7 | 217 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 7 | 218 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 7 | 219 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 7 | 220 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 7 | 221 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 7 | 222 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 7 | 223 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 7 | 224 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 7 | 225 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 7 | 226 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 7 | 227 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 8 | 215 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 8 | 216 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 8 | 217 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 8 | 218 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 8 | 219 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 8 | 220 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 8 | 221 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 8 | 222 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 8 | 223 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 8 | 224 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 8 | 225 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 8 | 226 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 8 | 227 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 8 | 228 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 8 | 229 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 8 | 230 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | 8 | 231 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | C1 | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | C3 | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | C5 | 201 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|---------|
| 86 | OHX | C8 | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | D9 | 102 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | L3 | 404 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | L3 | 405 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | L3 | 406 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | L4 | 402 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | M0 | 304 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | M5 | 302 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | M7 | 206 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | M7 | 207 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | M8 | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | M9 | 202 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | N1 | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | N9 | 101 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | O1 | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | O2 | 202 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | O3 | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | O7 | 105 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | O7 | 106 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | O9 | 101 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | S8 | 302 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | SR | 401 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | c3 | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | c5 | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | c8 | 202 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | d4 | 202 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | d9 | 102 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | l3 | 402 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | l3 | 403 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | l3 | 404 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | l4 | 402 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | l4 | 403 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | l5 | 303 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | l5 | 304 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | l5 | 305 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | l9 | 202 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | m0 | 302 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | m0 | 303 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | m1 | 202 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | m4 | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | m5 | 303 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | m6 | 202 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|---------|
| 86 | OHX | m7 | 206 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | m8 | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | m9 | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | n1 | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | n3 | 203 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | n9 | 102 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | o3 | 202 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | q2 | 502 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | s1 | 302 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | s1 | 303 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | s4 | 301 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | s8 | 303 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | s9 | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | OHX | sR | 401 | - | - | 0/0/0/0 | 0/0/0/0 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 87 | 2 | 2179 | 3K8 | C8-C7 | 3.18 | 1.42 | 1.37 |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 87 | 2 | 2179 | 3K8 | C15-C7-C4 | -3.29 | 116.14 | 120.52 |
| 87 | 6 | 2205 | 3K8 | C20-C19-C18 | -2.13 | 117.97 | 120.11 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

485 monomers are involved in 748 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 86 | 1 | 3862 | OHX | 1 | 0 |
| 86 | 1 | 3863 | OHX | 1 | 0 |
| 86 | 1 | 3865 | OHX | 1 | 0 |
| 86 | 1 | 3869 | OHX | 1 | 0 |
| 86 | 1 | 3871 | OHX | 1 | 0 |
| 86 | 1 | 3873 | OHX | 2 | 0 |
| 86 | 1 | 3875 | OHX | 1 | 0 |
| 86 | 1 | 3876 | OHX | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 86 | 1 | 3877 | OHX | 1 | 0 |
| 86 | 1 | 3878 | OHX | 3 | 0 |
| 86 | 1 | 3879 | OHX | 1 | 0 |
| 86 | 1 | 3880 | OHX | 2 | 0 |
| 86 | 1 | 3881 | OHX | 1 | 0 |
| 86 | 1 | 3883 | OHX | 1 | 0 |
| 86 | 1 | 3884 | OHX | 1 | 0 |
| 86 | 1 | 3885 | OHX | 1 | 0 |
| 86 | 1 | 3887 | OHX | 1 | 0 |
| 86 | 1 | 3889 | OHX | 1 | 0 |
| 86 | 1 | 3897 | OHX | 1 | 0 |
| 86 | 1 | 3902 | OHX | 1 | 0 |
| 86 | 1 | 3908 | OHX | 1 | 0 |
| 86 | 1 | 3921 | OHX | 1 | 0 |
| 86 | 1 | 3923 | OHX | 2 | 0 |
| 86 | 1 | 3927 | OHX | 2 | 0 |
| 86 | 1 | 3929 | OHX | 2 | 0 |
| 86 | 1 | 3930 | OHX | 1 | 0 |
| 86 | 1 | 3936 | OHX | 1 | 0 |
| 86 | 1 | 3942 | OHX | 1 | 0 |
| 86 | 1 | 3943 | OHX | 1 | 0 |
| 86 | 1 | 3944 | OHX | 1 | 0 |
| 86 | 1 | 3947 | OHX | 1 | 0 |
| 86 | 1 | 3950 | OHX | 1 | 0 |
| 86 | 1 | 3953 | OHX | 2 | 0 |
| 86 | 1 | 3954 | OHX | 4 | 0 |
| 86 | 1 | 3956 | OHX | 3 | 0 |
| 86 | 1 | 3959 | OHX | 1 | 0 |
| 86 | 1 | 3961 | OHX | 1 | 0 |
| 86 | 1 | 3962 | OHX | 1 | 0 |
| 86 | 1 | 3964 | OHX | 1 | 0 |
| 86 | 1 | 3968 | OHX | 7 | 0 |
| 86 | 1 | 3969 | OHX | 1 | 0 |
| 86 | 1 | 3971 | OHX | 2 | 0 |
| 86 | 1 | 3972 | OHX | 1 | 0 |
| 86 | 1 | 3973 | OHX | 4 | 0 |
| 86 | 1 | 3974 | OHX | 2 | 0 |
| 86 | 1 | 3975 | OHX | 1 | 0 |
| 86 | 1 | 3978 | OHX | 1 | 0 |
| 86 | 1 | 3979 | OHX | 1 | 0 |
| 86 | 1 | 3980 | OHX | 2 | 0 |
| 86 | 1 | 3981 | OHX | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 86 | 1 | 3986 | OHX | 1 | 0 |
| 86 | 1 | 3988 | OHX | 2 | 0 |
| 86 | 1 | 3992 | OHX | 1 | 0 |
| 86 | 1 | 3994 | OHX | 1 | 0 |
| 86 | 1 | 3996 | OHX | 1 | 0 |
| 86 | 1 | 3998 | OHX | 1 | 0 |
| 86 | 1 | 3999 | OHX | 1 | 0 |
| 86 | 1 | 4000 | OHX | 8 | 0 |
| 86 | 1 | 4003 | OHX | 2 | 0 |
| 86 | 1 | 4005 | OHX | 1 | 0 |
| 86 | 1 | 4007 | OHX | 1 | 0 |
| 86 | 1 | 4010 | OHX | 2 | 0 |
| 86 | 1 | 4012 | OHX | 1 | 0 |
| 86 | 1 | 4014 | OHX | 1 | 0 |
| 86 | 1 | 4016 | OHX | 1 | 0 |
| 86 | 1 | 4018 | OHX | 1 | 0 |
| 86 | 1 | 4020 | OHX | 1 | 0 |
| 86 | 1 | 4024 | OHX | 1 | 0 |
| 86 | 1 | 4025 | OHX | 6 | 0 |
| 86 | 1 | 4027 | OHX | 1 | 0 |
| 86 | 1 | 4029 | OHX | 5 | 0 |
| 86 | 1 | 4030 | OHX | 1 | 0 |
| 86 | 1 | 4031 | OHX | 1 | 0 |
| 86 | 1 | 4035 | OHX | 2 | 0 |
| 86 | 1 | 4036 | OHX | 2 | 0 |
| 86 | 1 | 4037 | OHX | 1 | 0 |
| 86 | 1 | 4038 | OHX | 1 | 0 |
| 86 | 1 | 4041 | OHX | 4 | 0 |
| 86 | 1 | 4042 | OHX | 7 | 0 |
| 86 | 1 | 4043 | OHX | 1 | 0 |
| 86 | 1 | 4045 | OHX | 2 | 0 |
| 86 | 1 | 4053 | OHX | 6 | 0 |
| 86 | 1 | 4054 | OHX | 5 | 0 |
| 86 | 1 | 4055 | OHX | 2 | 0 |
| 86 | 1 | 4057 | OHX | 1 | 0 |
| 86 | 1 | 4060 | OHX | 2 | 0 |
| 86 | 1 | 4061 | OHX | 1 | 0 |
| 86 | 1 | 4062 | OHX | 1 | 0 |
| 86 | 1 | 4064 | OHX | 1 | 0 |
| 86 | 1 | 4065 | OHX | 1 | 0 |
| 86 | 1 | 4066 | OHX | 1 | 0 |
| 86 | 1 | 4072 | OHX | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 86 | 1 | 4074 | OHX | 1 | 0 |
| 86 | 1 | 4079 | OHX | 5 | 0 |
| 86 | 1 | 4081 | OHX | 1 | 0 |
| 86 | 1 | 4083 | OHX | 5 | 0 |
| 86 | 1 | 4084 | OHX | 2 | 0 |
| 86 | 1 | 4087 | OHX | 2 | 0 |
| 86 | 1 | 4089 | OHX | 1 | 0 |
| 86 | 1 | 4094 | OHX | 1 | 0 |
| 86 | 1 | 4095 | OHX | 1 | 0 |
| 86 | 1 | 4097 | OHX | 2 | 0 |
| 86 | 1 | 4098 | OHX | 1 | 0 |
| 86 | 1 | 4099 | OHX | 1 | 0 |
| 86 | 1 | 4106 | OHX | 1 | 0 |
| 86 | 1 | 4109 | OHX | 1 | 0 |
| 86 | 1 | 4113 | OHX | 1 | 0 |
| 86 | 1 | 4117 | OHX | 1 | 0 |
| 86 | 1 | 4119 | OHX | 1 | 0 |
| 86 | 1 | 4121 | OHX | 2 | 0 |
| 86 | 1 | 4124 | OHX | 1 | 0 |
| 86 | 1 | 4127 | OHX | 1 | 0 |
| 86 | 1 | 4134 | OHX | 1 | 0 |
| 86 | 1 | 4137 | OHX | 1 | 0 |
| 86 | 1 | 4138 | OHX | 3 | 0 |
| 86 | 1 | 4139 | OHX | 3 | 0 |
| 86 | 1 | 4140 | OHX | 1 | 0 |
| 86 | 1 | 4142 | OHX | 3 | 0 |
| 86 | 1 | 4145 | OHX | 7 | 0 |
| 86 | 1 | 4146 | OHX | 1 | 0 |
| 86 | 1 | 4148 | OHX | 1 | 0 |
| 86 | 1 | 4149 | OHX | 5 | 0 |
| 86 | 1 | 4153 | OHX | 3 | 0 |
| 86 | 1 | 4154 | OHX | 4 | 0 |
| 86 | 1 | 4155 | OHX | 6 | 0 |
| 86 | 1 | 4157 | OHX | 1 | 0 |
| 86 | 1 | 4158 | OHX | 1 | 0 |
| 86 | 1 | 4162 | OHX | 5 | 0 |
| 86 | 1 | 4163 | OHX | 2 | 0 |
| 86 | 1 | 4164 | OHX | 1 | 0 |
| 86 | 1 | 4165 | OHX | 1 | 0 |
| 86 | 1 | 4166 | OHX | 2 | 0 |
| 86 | 1 | 4167 | OHX | 1 | 0 |
| 86 | 1 | 4171 | OHX | 10 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 86 | 1 | 4173 | OHX | 1 | 0 |
| 86 | 1 | 4174 | OHX | 1 | 0 |
| 86 | 1 | 4179 | OHX | 1 | 0 |
| 86 | 1 | 4180 | OHX | 3 | 0 |
| 86 | 1 | 4182 | OHX | 1 | 0 |
| 86 | 1 | 4183 | OHX | 1 | 0 |
| 86 | 1 | 4187 | OHX | 1 | 0 |
| 86 | 1 | 4193 | OHX | 1 | 0 |
| 86 | 1 | 4194 | OHX | 1 | 0 |
| 86 | 1 | 4196 | OHX | 6 | 0 |
| 86 | 1 | 4197 | OHX | 1 | 0 |
| 86 | 1 | 4201 | OHX | 3 | 0 |
| 86 | 1 | 4202 | OHX | 1 | 0 |
| 86 | 1 | 4204 | OHX | 1 | 0 |
| 86 | 2 | 2023 | OHX | 1 | 0 |
| 86 | 2 | 2024 | OHX | 1 | 0 |
| 86 | 2 | 2026 | OHX | 2 | 0 |
| 86 | 2 | 2031 | OHX | 7 | 0 |
| 86 | 2 | 2033 | OHX | 1 | 0 |
| 86 | 2 | 2034 | OHX | 1 | 0 |
| 86 | 2 | 2035 | OHX | 1 | 0 |
| 86 | 2 | 2036 | OHX | 2 | 0 |
| 86 | 2 | 2038 | OHX | 1 | 0 |
| 86 | 2 | 2039 | OHX | 2 | 0 |
| 86 | 2 | 2042 | OHX | 1 | 0 |
| 86 | 2 | 2044 | OHX | 7 | 0 |
| 86 | 2 | 2045 | OHX | 1 | 0 |
| 86 | 2 | 2046 | OHX | 1 | 0 |
| 86 | 2 | 2047 | OHX | 1 | 0 |
| 86 | 2 | 2048 | OHX | 1 | 0 |
| 86 | 2 | 2051 | OHX | 1 | 0 |
| 86 | 2 | 2052 | OHX | 1 | 0 |
| 86 | 2 | 2054 | OHX | 2 | 0 |
| 86 | 2 | 2058 | OHX | 1 | 0 |
| 86 | 2 | 2062 | OHX | 1 | 0 |
| 86 | 2 | 2064 | OHX | 1 | 0 |
| 86 | 2 | 2065 | OHX | 1 | 0 |
| 86 | 2 | 2070 | OHX | 2 | 0 |
| 86 | 2 | 2073 | OHX | 1 | 0 |
| 86 | 2 | 2074 | OHX | 2 | 0 |
| 86 | 2 | 2075 | OHX | 6 | 0 |
| 86 | 2 | 2076 | OHX | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 86 | 2 | 2078 | OHX | 1 | 0 |
| 86 | 2 | 2082 | OHX | 2 | 0 |
| 86 | 2 | 2083 | OHX | 2 | 0 |
| 86 | 2 | 2084 | OHX | 1 | 0 |
| 86 | 2 | 2085 | OHX | 2 | 0 |
| 86 | 2 | 2086 | OHX | 1 | 0 |
| 86 | 2 | 2089 | OHX | 5 | 0 |
| 86 | 2 | 2090 | OHX | 5 | 0 |
| 86 | 2 | 2091 | OHX | 1 | 0 |
| 86 | 2 | 2092 | OHX | 1 | 0 |
| 86 | 2 | 2093 | OHX | 2 | 0 |
| 86 | 2 | 2095 | OHX | 2 | 0 |
| 86 | 2 | 2096 | OHX | 2 | 0 |
| 86 | 2 | 2098 | OHX | 7 | 0 |
| 86 | 2 | 2103 | OHX | 1 | 0 |
| 86 | 2 | 2104 | OHX | 1 | 0 |
| 86 | 2 | 2105 | OHX | 1 | 0 |
| 86 | 2 | 2107 | OHX | 1 | 0 |
| 86 | 2 | 2108 | OHX | 2 | 0 |
| 86 | 2 | 2109 | OHX | 1 | 0 |
| 86 | 2 | 2110 | OHX | 3 | 0 |
| 86 | 2 | 2114 | OHX | 1 | 0 |
| 86 | 2 | 2120 | OHX | 1 | 0 |
| 86 | 2 | 2125 | OHX | 1 | 0 |
| 86 | 2 | 2127 | OHX | 1 | 0 |
| 86 | 2 | 2129 | OHX | 1 | 0 |
| 86 | 2 | 2130 | OHX | 1 | 0 |
| 86 | 2 | 2131 | OHX | 7 | 0 |
| 86 | 2 | 2132 | OHX | 1 | 0 |
| 86 | 2 | 2134 | OHX | 1 | 0 |
| 86 | 2 | 2136 | OHX | 1 | 0 |
| 86 | 2 | 2138 | OHX | 1 | 0 |
| 86 | 2 | 2141 | OHX | 1 | 0 |
| 86 | 2 | 2144 | OHX | 1 | 0 |
| 86 | 2 | 2145 | OHX | 7 | 0 |
| 86 | 2 | 2148 | OHX | 1 | 0 |
| 86 | 2 | 2154 | OHX | 1 | 0 |
| 86 | 2 | 2156 | OHX | 1 | 0 |
| 86 | 2 | 2158 | OHX | 1 | 0 |
| 86 | 2 | 2159 | OHX | 1 | 0 |
| 86 | 2 | 2161 | OHX | 6 | 0 |
| 86 | 2 | 2167 | OHX | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 86 | 2 | 2168 | OHX | 1 | 0 |
| 86 | 2 | 2171 | OHX | 1 | 0 |
| 87 | 2 | 2179 | 3K8 | 4 | 0 |
| 86 | 3 | 216 | OHX | 1 | 0 |
| 86 | 3 | 218 | OHX | 1 | 0 |
| 86 | 3 | 220 | OHX | 1 | 0 |
| 86 | 3 | 221 | OHX | 1 | 0 |
| 86 | 3 | 225 | OHX | 2 | 0 |
| 86 | 4 | 222 | OHX | 1 | 0 |
| 86 | 4 | 224 | OHX | 1 | 0 |
| 86 | 4 | 225 | OHX | 1 | 0 |
| 86 | 4 | 227 | OHX | 1 | 0 |
| 86 | 4 | 228 | OHX | 1 | 0 |
| 86 | 4 | 231 | OHX | 2 | 0 |
| 86 | 5 | 3901 | OHX | 2 | 0 |
| 86 | 5 | 3903 | OHX | 1 | 0 |
| 86 | 5 | 3907 | OHX | 1 | 0 |
| 86 | 5 | 3909 | OHX | 3 | 0 |
| 86 | 5 | 3912 | OHX | 1 | 0 |
| 86 | 5 | 3914 | OHX | 2 | 0 |
| 86 | 5 | 3917 | OHX | 1 | 0 |
| 86 | 5 | 3918 | OHX | 2 | 0 |
| 86 | 5 | 3921 | OHX | 2 | 0 |
| 86 | 5 | 3926 | OHX | 1 | 0 |
| 86 | 5 | 3927 | OHX | 1 | 0 |
| 86 | 5 | 3938 | OHX | 1 | 0 |
| 86 | 5 | 3944 | OHX | 7 | 0 |
| 86 | 5 | 3947 | OHX | 1 | 0 |
| 86 | 5 | 3950 | OHX | 1 | 0 |
| 86 | 5 | 3955 | OHX | 1 | 0 |
| 86 | 5 | 3956 | OHX | 1 | 0 |
| 86 | 5 | 3958 | OHX | 1 | 0 |
| 86 | 5 | 3959 | OHX | 2 | 0 |
| 86 | 5 | 3960 | OHX | 1 | 0 |
| 86 | 5 | 3961 | OHX | 1 | 0 |
| 86 | 5 | 3962 | OHX | 1 | 0 |
| 86 | 5 | 3964 | OHX | 4 | 0 |
| 86 | 5 | 3971 | OHX | 1 | 0 |
| 86 | 5 | 3974 | OHX | 2 | 0 |
| 86 | 5 | 3975 | OHX | 6 | 0 |
| 86 | 5 | 3978 | OHX | 1 | 0 |
| 86 | 5 | 3980 | OHX | 9 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 86 | 5 | 3984 | OHX | 1 | 0 |
| 86 | 5 | 3986 | OHX | 1 | 0 |
| 86 | 5 | 3989 | OHX | 1 | 0 |
| 86 | 5 | 3991 | OHX | 1 | 0 |
| 86 | 5 | 3993 | OHX | 3 | 0 |
| 86 | 5 | 3998 | OHX | 1 | 0 |
| 86 | 5 | 4003 | OHX | 6 | 0 |
| 86 | 5 | 4004 | OHX | 4 | 0 |
| 86 | 5 | 4005 | OHX | 1 | 0 |
| 86 | 5 | 4007 | OHX | 1 | 0 |
| 86 | 5 | 4009 | OHX | 2 | 0 |
| 86 | 5 | 4010 | OHX | 1 | 0 |
| 86 | 5 | 4011 | OHX | 1 | 0 |
| 86 | 5 | 4013 | OHX | 6 | 0 |
| 86 | 5 | 4015 | OHX | 1 | 0 |
| 86 | 5 | 4016 | OHX | 1 | 0 |
| 86 | 5 | 4017 | OHX | 1 | 0 |
| 86 | 5 | 4019 | OHX | 1 | 0 |
| 86 | 5 | 4021 | OHX | 2 | 0 |
| 86 | 5 | 4022 | OHX | 6 | 0 |
| 86 | 5 | 4025 | OHX | 3 | 0 |
| 86 | 5 | 4026 | OHX | 2 | 0 |
| 86 | 5 | 4028 | OHX | 1 | 0 |
| 86 | 5 | 4029 | OHX | 1 | 0 |
| 86 | 5 | 4030 | OHX | 1 | 0 |
| 86 | 5 | 4031 | OHX | 1 | 0 |
| 86 | 5 | 4032 | OHX | 1 | 0 |
| 86 | 5 | 4033 | OHX | 1 | 0 |
| 86 | 5 | 4035 | OHX | 5 | 0 |
| 86 | 5 | 4036 | OHX | 3 | 0 |
| 86 | 5 | 4037 | OHX | 5 | 0 |
| 86 | 5 | 4041 | OHX | 2 | 0 |
| 86 | 5 | 4048 | OHX | 1 | 0 |
| 86 | 5 | 4051 | OHX | 1 | 0 |
| 86 | 5 | 4052 | OHX | 1 | 0 |
| 86 | 5 | 4053 | OHX | 1 | 0 |
| 86 | 5 | 4056 | OHX | 1 | 0 |
| 86 | 5 | 4057 | OHX | 6 | 0 |
| 86 | 5 | 4068 | OHX | 7 | 0 |
| 86 | 5 | 4069 | OHX | 1 | 0 |
| 86 | 5 | 4070 | OHX | 1 | 0 |
| 86 | 5 | 4074 | OHX | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 86 | 5 | 4075 | OHX | 1 | 0 |
| 86 | 5 | 4076 | OHX | 1 | 0 |
| 86 | 5 | 4077 | OHX | 1 | 0 |
| 86 | 5 | 4083 | OHX | 5 | 0 |
| 86 | 5 | 4090 | OHX | 2 | 0 |
| 86 | 5 | 4091 | OHX | 1 | 0 |
| 86 | 5 | 4093 | OHX | 6 | 0 |
| 86 | 5 | 4094 | OHX | 1 | 0 |
| 86 | 5 | 4095 | OHX | 1 | 0 |
| 86 | 5 | 4096 | OHX | 2 | 0 |
| 86 | 5 | 4099 | OHX | 1 | 0 |
| 86 | 5 | 4100 | OHX | 2 | 0 |
| 86 | 5 | 4102 | OHX | 1 | 0 |
| 86 | 5 | 4104 | OHX | 1 | 0 |
| 86 | 5 | 4105 | OHX | 2 | 0 |
| 86 | 5 | 4108 | OHX | 1 | 0 |
| 86 | 5 | 4110 | OHX | 1 | 0 |
| 86 | 5 | 4114 | OHX | 1 | 0 |
| 86 | 5 | 4120 | OHX | 1 | 0 |
| 86 | 5 | 4121 | OHX | 2 | 0 |
| 86 | 5 | 4122 | OHX | 1 | 0 |
| 86 | 5 | 4123 | OHX | 1 | 0 |
| 86 | 5 | 4129 | OHX | 1 | 0 |
| 86 | 5 | 4130 | OHX | 1 | 0 |
| 86 | 5 | 4131 | OHX | 2 | 0 |
| 86 | 5 | 4133 | OHX | 1 | 0 |
| 86 | 5 | 4134 | OHX | 1 | 0 |
| 86 | 5 | 4140 | OHX | 1 | 0 |
| 86 | 5 | 4141 | OHX | 1 | 0 |
| 86 | 5 | 4144 | OHX | 1 | 0 |
| 86 | 5 | 4146 | OHX | 6 | 0 |
| 86 | 5 | 4147 | OHX | 1 | 0 |
| 86 | 5 | 4148 | OHX | 2 | 0 |
| 86 | 5 | 4149 | OHX | 1 | 0 |
| 86 | 5 | 4155 | OHX | 1 | 0 |
| 86 | 5 | 4157 | OHX | 1 | 0 |
| 86 | 5 | 4161 | OHX | 2 | 0 |
| 86 | 5 | 4163 | OHX | 1 | 0 |
| 86 | 5 | 4164 | OHX | 1 | 0 |
| 86 | 5 | 4170 | OHX | 1 | 0 |
| 86 | 5 | 4174 | OHX | 1 | 0 |
| 86 | 5 | 4179 | OHX | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 86 | 5 | 4182 | OHX | 1 | 0 |
| 86 | 5 | 4183 | OHX | 1 | 0 |
| 86 | 5 | 4186 | OHX | 1 | 0 |
| 86 | 5 | 4187 | OHX | 1 | 0 |
| 86 | 5 | 4189 | OHX | 1 | 0 |
| 86 | 5 | 4191 | OHX | 6 | 0 |
| 86 | 5 | 4192 | OHX | 1 | 0 |
| 86 | 5 | 4193 | OHX | 6 | 0 |
| 86 | 5 | 4194 | OHX | 1 | 0 |
| 86 | 5 | 4195 | OHX | 1 | 0 |
| 86 | 5 | 4197 | OHX | 1 | 0 |
| 86 | 5 | 4199 | OHX | 2 | 0 |
| 86 | 5 | 4200 | OHX | 11 | 0 |
| 86 | 5 | 4201 | OHX | 7 | 0 |
| 86 | 5 | 4202 | OHX | 7 | 0 |
| 86 | 5 | 4203 | OHX | 3 | 0 |
| 86 | 5 | 4205 | OHX | 5 | 0 |
| 86 | 5 | 4213 | OHX | 1 | 0 |
| 86 | 5 | 4219 | OHX | 8 | 0 |
| 86 | 5 | 4221 | OHX | 1 | 0 |
| 86 | 5 | 4223 | OHX | 1 | 0 |
| 86 | 5 | 4225 | OHX | 1 | 0 |
| 86 | 5 | 4226 | OHX | 1 | 0 |
| 86 | 5 | 4228 | OHX | 1 | 0 |
| 86 | 5 | 4230 | OHX | 1 | 0 |
| 86 | 5 | 4231 | OHX | 1 | 0 |
| 86 | 5 | 4236 | OHX | 6 | 0 |
| 86 | 5 | 4239 | OHX | 1 | 0 |
| 86 | 5 | 4240 | OHX | 5 | 0 |
| 86 | 5 | 4241 | OHX | 1 | 0 |
| 86 | 5 | 4242 | OHX | 1 | 0 |
| 86 | 5 | 4245 | OHX | 7 | 0 |
| 86 | 5 | 4249 | OHX | 1 | 0 |
| 86 | 5 | 4250 | OHX | 1 | 0 |
| 86 | 5 | 4251 | OHX | 2 | 0 |
| 86 | 6 | 2048 | OHX | 1 | 0 |
| 86 | 6 | 2050 | OHX | 2 | 0 |
| 86 | 6 | 2055 | OHX | 1 | 0 |
| 86 | 6 | 2056 | OHX | 1 | 0 |
| 86 | 6 | 2058 | OHX | 1 | 0 |
| 86 | 6 | 2060 | OHX | 7 | 0 |
| 86 | 6 | 2062 | OHX | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 86 | 6 | 2063 | OHX | 1 | 0 |
| 86 | 6 | 2066 | OHX | 1 | 0 |
| 86 | 6 | 2067 | OHX | 2 | 0 |
| 86 | 6 | 2069 | OHX | 1 | 0 |
| 86 | 6 | 2071 | OHX | 1 | 0 |
| 86 | 6 | 2072 | OHX | 2 | 0 |
| 86 | 6 | 2075 | OHX | 1 | 0 |
| 86 | 6 | 2076 | OHX | 1 | 0 |
| 86 | 6 | 2078 | OHX | 1 | 0 |
| 86 | 6 | 2084 | OHX | 1 | 0 |
| 86 | 6 | 2087 | OHX | 1 | 0 |
| 86 | 6 | 2089 | OHX | 1 | 0 |
| 86 | 6 | 2092 | OHX | 1 | 0 |
| 86 | 6 | 2093 | OHX | 1 | 0 |
| 86 | 6 | 2094 | OHX | 1 | 0 |
| 86 | 6 | 2096 | OHX | 1 | 0 |
| 86 | 6 | 2097 | OHX | 1 | 0 |
| 86 | 6 | 2101 | OHX | 3 | 0 |
| 86 | 6 | 2103 | OHX | 1 | 0 |
| 86 | 6 | 2104 | OHX | 1 | 0 |
| 86 | 6 | 2106 | OHX | 1 | 0 |
| 86 | 6 | 2108 | OHX | 2 | 0 |
| 86 | 6 | 2109 | OHX | 1 | 0 |
| 86 | 6 | 2110 | OHX | 1 | 0 |
| 86 | 6 | 2112 | OHX | 1 | 0 |
| 86 | 6 | 2113 | OHX | 1 | 0 |
| 86 | 6 | 2115 | OHX | 1 | 0 |
| 86 | 6 | 2118 | OHX | 1 | 0 |
| 86 | 6 | 2120 | OHX | 1 | 0 |
| 86 | 6 | 2121 | OHX | 8 | 0 |
| 86 | 6 | 2122 | OHX | 1 | 0 |
| 86 | 6 | 2123 | OHX | 1 | 0 |
| 86 | 6 | 2124 | OHX | 2 | 0 |
| 86 | 6 | 2125 | OHX | 1 | 0 |
| 86 | 6 | 2126 | OHX | 3 | 0 |
| 86 | 6 | 2127 | OHX | 2 | 0 |
| 86 | 6 | 2129 | OHX | 1 | 0 |
| 86 | 6 | 2131 | OHX | 2 | 0 |
| 86 | 6 | 2137 | OHX | 1 | 0 |
| 86 | 6 | 2138 | OHX | 2 | 0 |
| 86 | 6 | 2139 | OHX | 1 | 0 |
| 86 | 6 | 2144 | OHX | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 86 | 6 | 2146 | OHX | 1 | 0 |
| 86 | 6 | 2147 | OHX | 7 | 0 |
| 86 | 6 | 2149 | OHX | 1 | 0 |
| 86 | 6 | 2150 | OHX | 2 | 0 |
| 86 | 6 | 2151 | OHX | 1 | 0 |
| 86 | 6 | 2154 | OHX | 2 | 0 |
| 86 | 6 | 2159 | OHX | 1 | 0 |
| 86 | 6 | 2160 | OHX | 1 | 0 |
| 86 | 6 | 2162 | OHX | 1 | 0 |
| 86 | 6 | 2165 | OHX | 1 | 0 |
| 86 | 6 | 2168 | OHX | 1 | 0 |
| 86 | 6 | 2171 | OHX | 8 | 0 |
| 86 | 6 | 2175 | OHX | 1 | 0 |
| 86 | 6 | 2176 | OHX | 1 | 0 |
| 86 | 6 | 2178 | OHX | 1 | 0 |
| 86 | 6 | 2179 | OHX | 1 | 0 |
| 86 | 6 | 2182 | OHX | 1 | 0 |
| 86 | 6 | 2183 | OHX | 1 | 0 |
| 86 | 6 | 2186 | OHX | 1 | 0 |
| 86 | 6 | 2188 | OHX | 1 | 0 |
| 86 | 6 | 2189 | OHX | 3 | 0 |
| 86 | 6 | 2190 | OHX | 1 | 0 |
| 86 | 6 | 2192 | OHX | 1 | 0 |
| 86 | 6 | 2195 | OHX | 1 | 0 |
| 86 | 6 | 2196 | OHX | 1 | 0 |
| 86 | 6 | 2201 | OHX | 1 | 0 |
| 86 | 6 | 2202 | OHX | 1 | 0 |
| 86 | 6 | 2204 | OHX | 1 | 0 |
| 87 | 6 | 2205 | 3K8 | 1 | 0 |
| 86 | 7 | 219 | OHX | 7 | 0 |
| 86 | 7 | 220 | OHX | 2 | 0 |
| 86 | 7 | 222 | OHX | 1 | 0 |
| 86 | 7 | 226 | OHX | 6 | 0 |
| 86 | 8 | 215 | OHX | 1 | 0 |
| 86 | 8 | 216 | OHX | 7 | 0 |
| 86 | 8 | 217 | OHX | 1 | 0 |
| 86 | 8 | 218 | OHX | 1 | 0 |
| 86 | 8 | 220 | OHX | 1 | 0 |
| 86 | 8 | 223 | OHX | 1 | 0 |
| 86 | 8 | 225 | OHX | 6 | 0 |
| 86 | 8 | 226 | OHX | 4 | 0 |
| 86 | 8 | 230 | OHX | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 86 | C3 | 201 | OHX | 1 | 0 |
| 86 | C5 | 201 | OHX | 5 | 0 |
| 86 | D9 | 102 | OHX | 1 | 0 |
| 86 | L3 | 404 | OHX | 1 | 0 |
| 86 | L3 | 405 | OHX | 1 | 0 |
| 86 | M0 | 304 | OHX | 1 | 0 |
| 86 | M5 | 302 | OHX | 1 | 0 |
| 86 | M7 | 206 | OHX | 1 | 0 |
| 86 | M7 | 207 | OHX | 1 | 0 |
| 86 | N1 | 201 | OHX | 2 | 0 |
| 86 | O1 | 201 | OHX | 6 | 0 |
| 86 | O3 | 201 | OHX | 1 | 0 |
| 86 | O7 | 105 | OHX | 5 | 0 |
| 86 | O7 | 106 | OHX | 1 | 0 |
| 86 | O9 | 101 | OHX | 1 | 0 |

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 will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.