



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 02:43 AM EDT

PDB ID : 5ON6
Title : Crystal structure of haemanthamine bound to the 80S ribosome
Authors : Pellegrino, S.; Meyer, M.; Yusupova, G.; Yusupov, M.
Deposited on : 2017-08-03
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

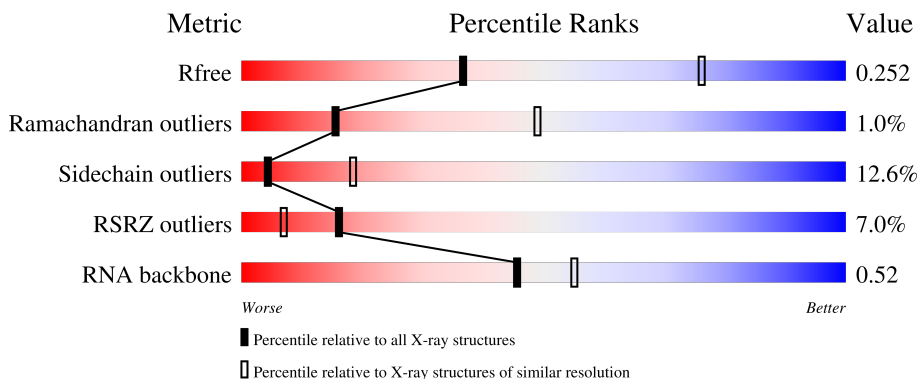
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 1094 (3.10-3.10) |
| Ramachandran outliers | 138981 | 1141 (3.10-3.10) |
| Sidechain outliers | 138945 | 1141 (3.10-3.10) |
| RSRZ outliers | 127900 | 1067 (3.10-3.10) |
| RNA backbone | 3102 | 1116 (3.40-2.80) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 1 | 3396 | |
| 1 | AR | 3396 | |
| 2 | 3 | 121 | |
| 2 | AS | 121 | |
| 3 | 4 | 158 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|-------------------------|
| 3 | AT | 158 | 4% 82% 18% |
| 4 | CD | 252 | % 90% 10% |
| 4 | j | 252 | 89% 11% |
| 5 | CE | 386 | 87% 13% |
| 5 | k | 386 | % 87% 13% |
| 6 | CF | 361 | 90% 10% |
| 6 | l | 361 | 89% 10% |
| 7 | CG | 296 | 4% 86% 14% |
| 7 | m | 296 | 6% 90% 10% |
| 8 | CH | 175 | 2% 78% 11% 11% |
| 8 | n | 175 | % 81% 7% 11% |
| 9 | CI | 222 | % 89% 10% |
| 9 | o | 222 | 2% 90% 9% |
| 10 | CJ | 233 | 14% 92% 8% |
| 10 | p | 233 | 6% 91% 9% |
| 11 | CK | 191 | 2% 85% 15% |
| 11 | q | 191 | 87% 13% |
| 12 | CL | 220 | 6% 84% 12% |
| 12 | r | 220 | % 82% 14% |
| 13 | CM | 169 | % 85% 15% |
| 13 | s | 169 | 2% 85% 14% |
| 14 | CN | 193 | 8% 83% 15% |
| 14 | t | 193 | 86% 13% |
| 15 | CO | 136 | % 88% 11% |
| 15 | u | 136 | 2% 85% 15% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 16 | CP | 203 | 92% 8% |
| 16 | v | 203 | 90% 10% |
| 17 | CQ | 197 | 2% 90% 9% |
| 17 | w | 197 | 88% 11% |
| 18 | CR | 183 | 16% 87% 13% |
| 18 | x | 183 | 11% 87% 12% |
| 19 | CS | 185 | 87% 13% |
| 19 | y | 185 | 89% 10% |
| 20 | CT | 188 | 5% 89% 11% |
| 20 | z | 188 | 4% 93% 7% |
| 21 | 0 | 172 | 85% 14% |
| 21 | CU | 172 | 85% 15% |
| 22 | 2 | 159 | 86% 14% |
| 22 | CV | 159 | 84% 16% |
| 23 | 5 | 100 | 12% 93% 7% |
| 23 | CW | 100 | 21% 89% 11% |
| 24 | CX | 136 | 92% 8% |
| 24 | IR | 136 | 3% 89% 11% |
| 25 | 6 | 1800 | 6% 77% 22% |
| 25 | A | 1800 | 7% 74% 24% |
| 26 | 7 | 98 | 30% 95% 5% |
| 26 | CY | 98 | 11% 88% 11% |
| 27 | 8 | 121 | 89% 11% |
| 27 | CZ | 121 | 3% 88% 12% |
| 28 | 9 | 126 | 5% 89% 11% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---------------------|
| 28 | DA | 126 | 6% 89% 11% |
| 29 | AA | 135 | 35% 90% 8% .. |
| 29 | DB | 135 | 12% 89% 10% . |
| 30 | AB | 148 | 91% 8% |
| 30 | DC | 148 | % 88% 11% . |
| 31 | AC | 58 | 88% 12% |
| 31 | DD | 58 | 86% 12% . |
| 32 | AD | 97 | 6% 89% 11% |
| 32 | DE | 97 | 95% 5% |
| 33 | AE | 109 | 2% 88% 12% |
| 33 | DF | 109 | 3% 83% 17% |
| 34 | AF | 127 | 2% 88% 12% |
| 34 | DG | 127 | 2% 90% 10% |
| 35 | AG | 106 | % 92% 8% |
| 35 | DH | 106 | % 93% 6% . |
| 36 | AH | 112 | 5% 90% 9% . |
| 36 | DI | 112 | % 91% 9% |
| 37 | AI | 119 | 5% 89% 10% . |
| 37 | DJ | 119 | 5% 83% 16% . |
| 38 | AJ | 99 | 3% 85% 15% |
| 38 | DK | 99 | 4% 90% 10% |
| 39 | AK | 87 | 3% 92% 8% |
| 39 | DL | 87 | 3% 87% 13% |
| 40 | AL | 77 | 3% 87% 13% |
| 40 | DM | 77 | 39% 91% 9% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 41 | AM | 50 | 86% 14% |
| 41 | DN | 50 | 92% 8% |
| 42 | AN | 52 | 10% 85% 15% |
| 42 | DO | 52 | 2% 90% 10% |
| 43 | AO | 25 | 88% 12% |
| 43 | DP | 25 | 84% 16% |
| 44 | AP | 105 | 9% 92% 8% |
| 44 | DQ | 105 | 91% 9% |
| 45 | AQ | 91 | 87% 13% |
| 45 | DR | 91 | 91% 9% |
| 46 | i | 272 | 7% 51% 7% 42% |
| 47 | m2 | 150 | 100% |
| 48 | sM | 104 | 6% 92% 7% |
| 49 | p0 | 311 | 17% 41% 5% 54% |
| 50 | B | 206 | 13% 88% 12% |
| 50 | s0 | 206 | 4% 86% 14% |
| 51 | C | 216 | 36% 88% 11% |
| 51 | s1 | 216 | 6% 86% 13% |
| 52 | D | 217 | % 88% 12% |
| 52 | s2 | 217 | % 84% 16% |
| 53 | E | 223 | 9% 89% 10% |
| 53 | s3 | 223 | 12% 90% 9% |
| 54 | F | 260 | 8% 90% 10% |
| 54 | s4 | 260 | 3% 91% 9% |
| 55 | G | 206 | 11% 89% 10% |

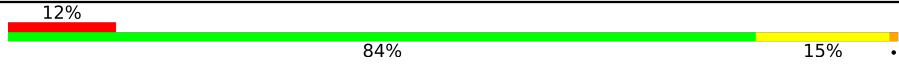

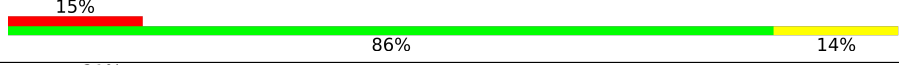
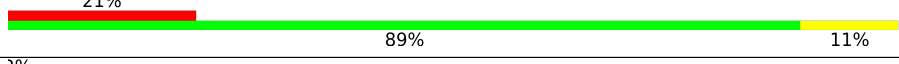
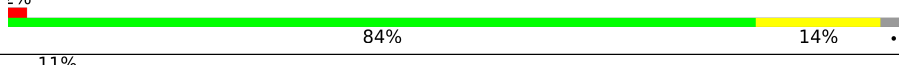
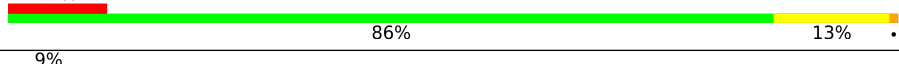
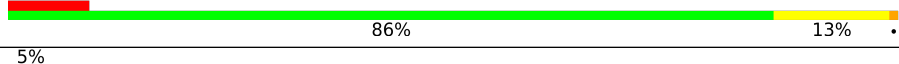

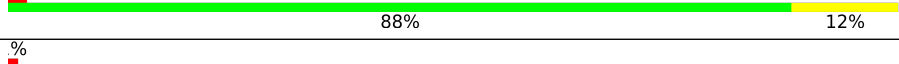
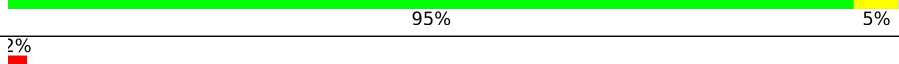


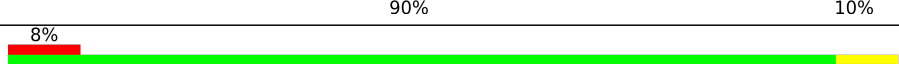
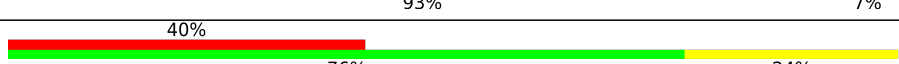
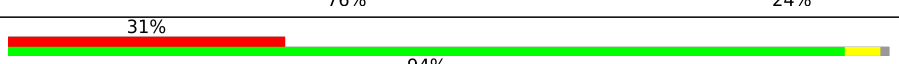
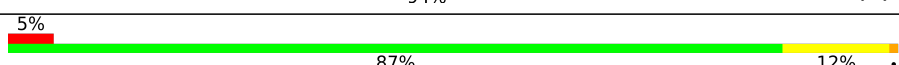
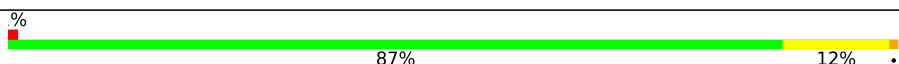
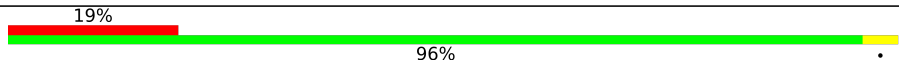
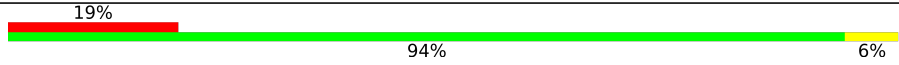


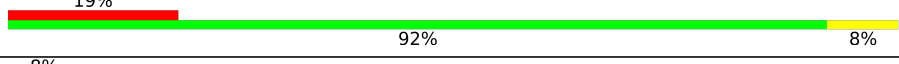
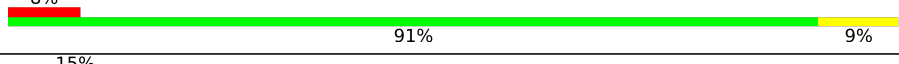


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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 55 | s5 | 206 | 17% 91% 9% |
| 56 | H | 226 | 17% 87% 13% |
| 56 | s6 | 226 | 12% 85% 11% . |
| 57 | I | 186 | 16% 87% 12% .. |
| 57 | s7 | 186 | 17% 87% 12% . |
| 58 | J | 199 | 5% 87% 6% . 6% |
| 58 | s8 | 199 | 7% 88% 6% . 6% |
| 59 | K | 185 | 18% 86% 12% . |
| 59 | s9 | 185 | 8% 84% 16% |
| 60 | L | 105 | 15% 82% 9% . 9% |
| 60 | c0 | 105 | 52% 78% 10% . 9% |
| 61 | M | 155 | 10% 92% 8% |
| 61 | c1 | 155 | 5% 84% 10% . 6% |
| 62 | N | 124 | 52% 81% 18% . |
| 62 | c2 | 124 | 70% 83% 15% . |
| 63 | O | 150 | 6% 89% 10% . |
| 63 | c3 | 150 | 3% 86% 12% . |
| 64 | P | 128 | 28% 90% 9% .. |
| 64 | c4 | 128 | 9% 89% 11% |
| 65 | Q | 141 | 5% 79% 8% . 12% |
| 65 | c5 | 141 | 11% 82% 12% . . |
| 66 | R | 142 | 18% 87% 12% .. |
| 66 | c6 | 142 | 11% 82% 18% |
| 67 | S | 125 | 11% 84% 11% . . |
| 67 | c7 | 125 | 5% 82% 11% 6% |

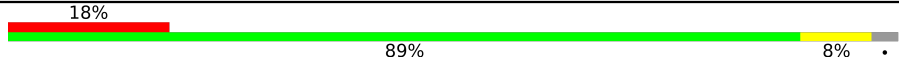
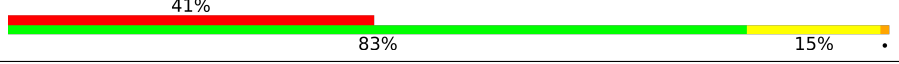
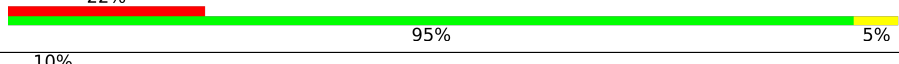
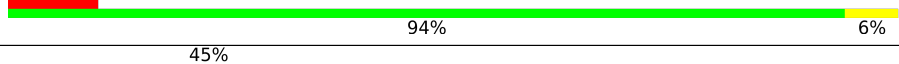

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 68 | T | 145 |  |
| 68 | c8 | 145 |  |
| 69 | U | 143 |  |
| 69 | c9 | 143 |  |
| 70 | V | 110 |  |
| 70 | d0 | 110 |  |
| 71 | W | 87 |  |
| 71 | d1 | 87 |  |
| 72 | X | 129 |  |
| 72 | d2 | 129 |  |
| 73 | Y | 144 |  |
| 73 | d3 | 144 |  |
| 74 | Z | 134 |  |
| 74 | d4 | 134 |  |
| 75 | a | 70 |  |
| 75 | d5 | 70 |  |
| 76 | b | 97 |  |
| 76 | d6 | 97 |  |
| 77 | c | 81 |  |
| 77 | d7 | 81 |  |
| 78 | d | 63 |  |
| 78 | d8 | 63 |  |
| 79 | d9 | 53 |  |
| 79 | e | 53 |  |
| 80 | e0 | 62 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 80 | f | 62 |  |
| 81 | g | 71 |  |
| 82 | h | 318 |  |
| 82 | sR | 318 |  |
| 83 | e1 | 51 |  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 84 | OHX | AR | 3737 | - | - | - | X |
| 85 | MG | 1 | 3744 | - | - | - | X |
| 85 | MG | 1 | 3800 | - | - | - | X |
| 85 | MG | 1 | 3801 | - | - | - | X |
| 85 | MG | 1 | 3820 | - | - | - | X |
| 85 | MG | 1 | 3930 | - | - | - | X |
| 85 | MG | 1 | 3941 | - | - | - | X |
| 85 | MG | 1 | 3965 | - | - | - | X |
| 85 | MG | 1 | 3983 | - | - | - | X |
| 85 | MG | 1 | 4001 | - | - | - | X |
| 85 | MG | 1 | 4012 | - | - | - | X |
| 85 | MG | 1 | 4023 | - | - | - | X |
| 85 | MG | 1 | 4053 | - | - | - | X |
| 85 | MG | 1 | 4092 | - | - | - | X |
| 85 | MG | 1 | 4101 | - | - | - | X |
| 85 | MG | 1 | 4104 | - | - | - | X |
| 85 | MG | 1 | 4129 | - | - | - | X |
| 85 | MG | 1 | 4152 | - | - | - | X |
| 85 | MG | 1 | 4158 | - | - | - | X |
| 85 | MG | 1 | 4190 | - | - | - | X |
| 85 | MG | 4 | 221 | - | - | - | X |
| 85 | MG | 4 | 229 | - | - | - | X |
| 85 | MG | 4 | 235 | - | - | - | X |
| 85 | MG | 6 | 2076 | - | - | - | X |
| 85 | MG | 6 | 2083 | - | - | - | X |
| 85 | MG | 6 | 2092 | - | - | - | X |
| 85 | MG | 6 | 2133 | - | - | - | X |
| 85 | MG | 6 | 2154 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 85 | MG | 6 | 2158 | - | - | - | X |
| 85 | MG | 6 | 2163 | - | - | - | X |
| 85 | MG | 6 | 2167 | - | - | - | X |
| 85 | MG | 6 | 2174 | - | - | - | X |
| 85 | MG | 6 | 2176 | - | - | - | X |
| 85 | MG | 6 | 2180 | - | - | - | X |
| 85 | MG | 6 | 2183 | - | - | - | X |
| 85 | MG | 6 | 2185 | - | - | - | X |
| 85 | MG | 6 | 2188 | - | - | - | X |
| 85 | MG | 6 | 2191 | - | - | - | X |
| 85 | MG | 6 | 2192 | - | - | - | X |
| 85 | MG | 6 | 2193 | - | - | - | X |
| 85 | MG | 6 | 2197 | - | - | - | X |
| 85 | MG | A | 2045 | - | - | - | X |
| 85 | MG | A | 2062 | - | - | - | X |
| 85 | MG | A | 2099 | - | - | - | X |
| 85 | MG | A | 2103 | - | - | - | X |
| 85 | MG | A | 2116 | - | - | - | X |
| 85 | MG | A | 2118 | - | - | - | X |
| 85 | MG | A | 2128 | - | - | - | X |
| 85 | MG | A | 2130 | - | - | - | X |
| 85 | MG | A | 2131 | - | - | - | X |
| 85 | MG | A | 2135 | - | - | - | X |
| 85 | MG | A | 2136 | - | - | - | X |
| 85 | MG | A | 2151 | - | - | - | X |
| 85 | MG | A | 2155 | - | - | - | X |
| 85 | MG | AR | 3803 | - | - | - | X |
| 85 | MG | AR | 3890 | - | - | - | X |
| 85 | MG | AR | 3971 | - | - | - | X |
| 85 | MG | AR | 3976 | - | - | - | X |
| 85 | MG | AR | 3998 | - | - | - | X |
| 85 | MG | AR | 4003 | - | - | - | X |
| 85 | MG | AR | 4005 | - | - | - | X |
| 85 | MG | AR | 4022 | - | - | - | X |
| 85 | MG | AR | 4024 | - | - | - | X |
| 85 | MG | AR | 4030 | - | - | - | X |
| 85 | MG | AR | 4034 | - | - | - | X |
| 85 | MG | AR | 4085 | - | - | - | X |
| 85 | MG | AR | 4097 | - | - | - | X |
| 85 | MG | AR | 4102 | - | - | - | X |
| 85 | MG | AR | 4110 | - | - | - | X |
| 85 | MG | AR | 4156 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|------------|-------------|--------------|------------|------------------|-----------------|----------------|-------------------------|
| 85 | MG | AR | 4174 | - | - | - | X |
| 85 | MG | AR | 4196 | - | - | - | X |
| 85 | MG | AR | 4255 | - | - | - | X |
| 85 | MG | AS | 228 | - | - | - | X |
| 85 | MG | CD | 302 | - | - | - | X |
| 85 | MG | V | 201 | - | - | - | X |
| 85 | MG | b | 101 | - | - | - | X |
| 85 | MG | l | 403 | - | - | - | X |
| 85 | MG | x | 206 | - | - | - | X |
| 87 | GOL | 6 | 2199 | - | - | - | X |
| 88 | ZN | d7 | 101 | - | - | - | X |

2 Entry composition [i](#)

There are 88 unique types of molecules in this entry. The entry contains 410383 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 25S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| | | | Total | C | N | O | P | | | |
| 1 | 1 | 3149 | 67355 | 30086 | 12142 | 21978 | 3149 | 0 | 0 | 0 |
| 1 | AR | 3149 | 67355 | 30086 | 12142 | 21978 | 3149 | 0 | 0 | 0 |

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| | | | Total | C | N | O | P | | | |
| 2 | 3 | 121 | 2579 | 1152 | 461 | 845 | 121 | 0 | 0 | 0 |
| 2 | AS | 121 | 2579 | 1152 | 461 | 845 | 121 | 0 | 0 | 0 |

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|---------|-------|
| | | | Total | C | N | O | P | | | |
| 3 | 4 | 158 | 3353 | 1500 | 586 | 1109 | 158 | 0 | 0 | 0 |
| 3 | AT | 158 | 3353 | 1500 | 586 | 1109 | 158 | 0 | 0 | 0 |

- Molecule 4 is a protein called 60S ribosomal protein L2-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 4 | j | 252 | 1914 | 1191 | 388 | 334 | 1 | 0 | 0 | 0 |
| 4 | CD | 252 | 1914 | 1191 | 388 | 334 | 1 | 0 | 0 | 0 |

- Molecule 5 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5 | k | 386 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3075 | 1950 | 584 | 533 | 8 | | | |
| 5 | CE | 386 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3075 | 1950 | 584 | 533 | 8 | | | |

- Molecule 6 is a protein called 60S ribosomal protein L4-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 6 | l | 361 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2748 | 1729 | 522 | 494 | 3 | | | |
| 6 | CF | 361 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2748 | 1729 | 522 | 494 | 3 | | | |

- Molecule 7 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 7 | m | 296 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2375 | 1501 | 414 | 458 | 2 | | | |
| 7 | CG | 296 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2375 | 1501 | 414 | 458 | 2 | | | |

- Molecule 8 is a protein called 60S ribosomal protein L6-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | n | 156 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1239 | 800 | 222 | 216 | 1 | | | |
| 8 | CH | 156 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1239 | 800 | 222 | 216 | 1 | | | |

- Molecule 9 is a protein called 60S ribosomal protein L7-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 9 | o | 222 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1784 | 1151 | 324 | 308 | 1 | | | |
| 9 | CI | 222 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1784 | 1151 | 324 | 308 | 1 | | | |

- Molecule 10 is a protein called 60S ribosomal protein L8-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 10 | p | 233 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1804 | 1151 | 323 | 327 | 3 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 10 | CJ | 233 | 1804 | 1151 | 323 | 327 | 3 | 0 | 0 | 0 |

- Molecule 11 is a protein called 60S ribosomal protein L9-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 11 | q | 191 | 1518 | 963 | 274 | 277 | 4 | 0 | 0 | 0 |
| 11 | CK | 191 | 1518 | 963 | 274 | 277 | 4 | 0 | 0 | 0 |

- Molecule 12 is a protein called 60S ribosomal protein L10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 12 | r | 211 | 1705 | 1083 | 322 | 294 | 6 | 0 | 0 | 0 |
| 12 | CL | 211 | 1705 | 1083 | 322 | 294 | 6 | 0 | 0 | 0 |

- Molecule 13 is a protein called 60S ribosomal protein L11-B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 13 | s | 169 | 1353 | 847 | 253 | 249 | 4 | 0 | 0 | 0 |
| 13 | CM | 169 | 1353 | 847 | 253 | 249 | 4 | 0 | 0 | 0 |

- Molecule 14 is a protein called 60S ribosomal protein L13-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 14 | t | 193 | 1543 | 962 | 315 | 266 | 0 | 0 | 0 |
| 14 | CN | 193 | 1543 | 962 | 315 | 266 | 0 | 0 | 0 |

- Molecule 15 is a protein called 60S ribosomal protein L14-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 15 | u | 136 | 1053 | 675 | 199 | 177 | 2 | 0 | 0 | 0 |
| 15 | CO | 136 | 1053 | 675 | 199 | 177 | 2 | 0 | 0 | 0 |

- Molecule 16 is a protein called 60S ribosomal protein L15-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 16 | v | 203 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1720 | 1077 | 361 | 281 | 1 | | | |
| 16 | CP | 203 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1720 | 1077 | 361 | 281 | 1 | | | |

- Molecule 17 is a protein called 60S ribosomal protein L16-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 17 | w | 197 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1555 | 1003 | 289 | 262 | 1 | | | |
| 17 | CQ | 197 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1555 | 1003 | 289 | 262 | 1 | | | |

- Molecule 18 is a protein called 60S ribosomal protein L17-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 18 | x | 183 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1420 | 882 | 281 | 257 | | | |
| 18 | CR | 183 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1420 | 882 | 281 | 257 | | | |

- Molecule 19 is a protein called 60S ribosomal protein L18-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 19 | y | 185 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1441 | 908 | 290 | 241 | 2 | | | |
| 19 | CS | 185 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1441 | 908 | 290 | 241 | 2 | | | |

- Molecule 20 is a protein called 60S ribosomal protein L19-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 20 | z | 188 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1521 | 935 | 326 | 260 | | | |
| 20 | CT | 188 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1521 | 935 | 326 | 260 | | | |

- Molecule 21 is a protein called 60S ribosomal protein L20-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21 | 0 | 172 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1445 | 930 | 267 | 244 | 4 | | | |
| 21 | CU | 172 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1445 | 930 | 267 | 244 | 4 | | | |

- Molecule 22 is a protein called 60S ribosomal protein L21-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22 | 2 | 159 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1276 | 805 | 246 | 221 | 4 | | | |
| 22 | CV | 159 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1276 | 805 | 246 | 221 | 4 | | | |

- Molecule 23 is a protein called 60S ribosomal protein L22-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 23 | 5 | 100 | Total | C | N | O | 0 | 0 | 0 |
| | | | 796 | 516 | 131 | 149 | | | |
| 23 | CW | 100 | Total | C | N | O | 0 | 0 | 0 |
| | | | 796 | 516 | 131 | 149 | | | |

- Molecule 24 is a protein called 60S ribosomal protein L23-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24 | IR | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1003 | 628 | 189 | 179 | 7 | | | |
| 24 | CX | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1003 | 628 | 189 | 179 | 7 | | | |

- Molecule 25 is a RNA chain called 18S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 25 | 6 | 1783 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 37990 | 16984 | 6723 | 12500 | 1783 | | | |
| 25 | A | 1781 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 37948 | 16965 | 6715 | 12487 | 1781 | | | |

- Molecule 26 is a protein called 60S ribosomal protein L24-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26 | 7 | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 699 | 443 | 137 | 118 | 1 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 26 | CY | 98 | 699 | 443 | 137 | 118 | 1 | 0 | 0 | 0 |

- Molecule 27 is a protein called 60S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 27 | 8 | 121 | 964 | 620 | 169 | 173 | 2 | 0 | 0 | 0 |
| 27 | CZ | 121 | 964 | 620 | 169 | 173 | 2 | 0 | 0 | 0 |

- Molecule 28 is a protein called 60S ribosomal protein L26-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|---|
| | | | Total | C | N | O | | | | |
| 28 | 9 | 126 | 993 | 625 | 192 | 176 | | 0 | 0 | 0 |
| 28 | DA | 126 | 993 | 625 | 192 | 176 | | 0 | 0 | 0 |

- Molecule 29 is a protein called 60S ribosomal protein L27-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|---|
| | | | Total | C | N | O | | | | |
| 29 | AA | 135 | 1092 | 710 | 202 | 180 | | 0 | 0 | 0 |
| 29 | DB | 135 | 1092 | 710 | 202 | 180 | | 0 | 0 | 0 |

- Molecule 30 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 30 | AB | 148 | 1173 | 749 | 231 | 190 | 3 | 0 | 0 | 0 |
| 30 | DC | 148 | 1173 | 749 | 231 | 190 | 3 | 0 | 0 | 0 |

- Molecule 31 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|---|
| | | | Total | C | N | O | | | | |
| 31 | AC | 58 | 462 | 289 | 100 | 73 | | 0 | 0 | 0 |
| 31 | DD | 58 | 462 | 289 | 100 | 73 | | 0 | 0 | 0 |

- Molecule 32 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32 | AD | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 743 | 479 | 124 | 139 | 1 | | | |
| 32 | DE | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 743 | 479 | 124 | 139 | 1 | | | |

- Molecule 33 is a protein called 60S ribosomal protein L31-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33 | AE | 109 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 876 | 556 | 167 | 152 | 1 | | | |
| 33 | DF | 109 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 876 | 556 | 167 | 152 | 1 | | | |

- Molecule 34 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34 | AF | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1020 | 647 | 205 | 167 | 1 | | | |
| 34 | DG | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1020 | 647 | 205 | 167 | 1 | | | |

- Molecule 35 is a protein called 60S ribosomal protein L33-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35 | AG | 106 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 850 | 540 | 165 | 144 | 1 | | | |
| 35 | DH | 106 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 850 | 540 | 165 | 144 | 1 | | | |

- Molecule 36 is a protein called 60S ribosomal protein L34-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36 | AH | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 880 | 545 | 179 | 152 | 4 | | | |
| 36 | DI | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 880 | 545 | 179 | 152 | 4 | | | |

- Molecule 37 is a protein called 60S ribosomal protein L35-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37 | AI | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 969 | 615 | 186 | 167 | 1 | | | |
| 37 | DJ | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 969 | 615 | 186 | 167 | 1 | | | |

- Molecule 38 is a protein called 60S ribosomal protein L36-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38 | AJ | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 771 | 481 | 156 | 132 | 2 | | | |
| 38 | DK | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 771 | 481 | 156 | 132 | 2 | | | |

- Molecule 39 is a protein called 60S ribosomal protein L37-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39 | AK | 87 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 681 | 414 | 148 | 114 | 5 | | | |
| 39 | DL | 87 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 681 | 414 | 148 | 114 | 5 | | | |

- Molecule 40 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 40 | AL | 77 | Total | C | N | O | 0 | 0 | 0 |
| | | | 612 | 391 | 115 | 106 | | | |
| 40 | DM | 77 | Total | C | N | O | 0 | 0 | 0 |
| | | | 612 | 391 | 115 | 106 | | | |

- Molecule 41 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 41 | AM | 50 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 436 | 272 | 97 | 65 | 2 | | | |
| 41 | DN | 50 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 436 | 272 | 97 | 65 | 2 | | | |

- Molecule 42 is a protein called Ubiquitin-60S ribosomal protein L40.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 42 | AN | 52 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 417 | 259 | 86 | 67 | 5 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 42 | DO | 52 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 417 | 259 | 86 | 67 | 5 | | | |

- Molecule 43 is a protein called 60S ribosomal protein L41-B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 43 | AO | 25 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 233 | 142 | 63 | 27 | 1 | | | |
| 43 | DP | 25 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 233 | 142 | 63 | 27 | 1 | | | |

- Molecule 44 is a protein called 60S ribosomal protein L42-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44 | AP | 105 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 847 | 534 | 170 | 138 | 5 | | | |
| 44 | DQ | 105 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 847 | 534 | 170 | 138 | 5 | | | |

- Molecule 45 is a protein called 60S ribosomal protein L43-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45 | AQ | 91 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 694 | 429 | 138 | 121 | 6 | | | |
| 45 | DR | 91 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 694 | 429 | 138 | 121 | 6 | | | |

- Molecule 46 is a protein called Suppressor protein STM1.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 46 | i | 159 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1104 | 652 | 221 | 231 | | | |

- Molecule 47 is a protein called 60S ribosomal protein L12.

| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|---------|---------|-------|---|
| 47 | m2 | 150 | Total | C | N | O | 0 | 0 | 0 |
| | | | 750 | 450 | 150 | 150 | | | |

- Molecule 48 is a protein called Suppressor protein STM1,Suppressor protein STM1.

| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|---------|---------|-------|---|
| | | | Total | C | N | | | | O |
| 48 | sM | 104 | 680 | 403 | 140 | 137 | 0 | 0 | 0 |

- Molecule 49 is a protein called 60S acidic ribosomal protein P0.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 49 | p0 | 143 | 1076 | 686 | 192 | 195 | 3 | 0 | 0 | 0 |

- Molecule 50 is a protein called 40S ribosomal protein S0-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 50 | B | 206 | 1577 | 1014 | 278 | 283 | 2 | 0 | 0 | 0 |
| 50 | s0 | 206 | 1583 | 1017 | 281 | 283 | 2 | 0 | 0 | 0 |

- Molecule 51 is a protein called 40S ribosomal protein S1-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 51 | C | 214 | 1709 | 1084 | 310 | 311 | 4 | 0 | 0 | 0 |
| 51 | s1 | 216 | 1722 | 1091 | 312 | 315 | 4 | 0 | 0 | 0 |

- Molecule 52 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 52 | D | 217 | 1635 | 1047 | 289 | 297 | 2 | 0 | 0 | 0 |
| 52 | s2 | 217 | 1635 | 1047 | 289 | 297 | 2 | 0 | 0 | 0 |

- Molecule 53 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 53 | E | 223 | 1734 | 1101 | 313 | 314 | 6 | 0 | 0 | 0 |
| 53 | s3 | 223 | 1734 | 1101 | 313 | 314 | 6 | 0 | 0 | 0 |

- Molecule 54 is a protein called 40S ribosomal protein S4-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 54 | F | 260 | Total 2068 | C 1316 | N 389 | O 360 | S 3 | 0 | 0 | 0 |
| 54 | s4 | 260 | Total 2068 | C 1316 | N 389 | O 360 | S 3 | 0 | 0 | 0 |

- Molecule 55 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 55 | G | 206 | Total 1609 | C 1007 | N 300 | O 299 | S 3 | 0 | 0 | 0 |
| 55 | s5 | 206 | Total 1609 | C 1007 | N 300 | O 299 | S 3 | 0 | 0 | 0 |

- Molecule 56 is a protein called 40S ribosomal protein S6-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 56 | H | 226 | Total 1799 | C 1129 | N 346 | O 321 | S 3 | 0 | 0 | 0 |
| 56 | s6 | 218 | Total 1755 | C 1102 | N 337 | O 313 | S 3 | 0 | 0 | 0 |

- Molecule 57 is a protein called 40S ribosomal protein S7-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 57 | I | 184 | Total 1481 | C 951 | N 265 | O 265 | 0 | 0 | 0 |
| 57 | s7 | 186 | Total 1491 | C 957 | N 267 | O 267 | 0 | 0 | 0 |

- Molecule 58 is a protein called 40S ribosomal protein S8-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 58 | J | 188 | Total 1489 | C 925 | N 298 | O 264 | S 2 | 0 | 0 | 0 |
| 58 | s8 | 188 | Total 1489 | C 925 | N 298 | O 264 | S 2 | 0 | 0 | 0 |

- Molecule 59 is a protein called 40S ribosomal protein S9-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 59 | K | 185 | Total 1494 | C 943 | N 289 | O 261 | S 1 | 0 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 59 | s9 | 185 | 1494 | 943 | 289 | 261 | 1 | 0 | 0 | 0 |

- Molecule 60 is a protein called 40S ribosomal protein S10-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 60 | L | 96 | 772 | 499 | 126 | 145 | 2 | 0 | 0 | 0 |
| 60 | c0 | 96 | 760 | 489 | 125 | 144 | 2 | 0 | 0 | 0 |

- Molecule 61 is a protein called 40S ribosomal protein S11-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 61 | M | 155 | 1213 | 774 | 230 | 206 | 3 | 0 | 0 | 0 |
| 61 | c1 | 146 | 1168 | 747 | 221 | 197 | 3 | 0 | 0 | 0 |

- Molecule 62 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 62 | N | 124 | 890 | 560 | 156 | 172 | 2 | 0 | 0 | 0 |
| 62 | c2 | 124 | 890 | 560 | 156 | 172 | 2 | 0 | 0 | 0 |

- Molecule 63 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 63 | O | 150 | 1192 | 759 | 224 | 207 | 2 | 0 | 0 | 0 |
| 63 | c3 | 150 | 1192 | 759 | 224 | 207 | 2 | 0 | 0 | 0 |

- Molecule 64 is a protein called 40S ribosomal protein S14-B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 64 | P | 127 | 891 | 545 | 182 | 163 | 1 | 0 | 0 | 0 |
| 64 | c4 | 128 | 949 | 582 | 188 | 176 | 3 | 0 | 0 | 0 |

- Molecule 65 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 65 | Q | 124 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 977 | 622 | 182 | 166 | 7 | | | |
| 65 | c5 | 135 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1039 | 658 | 196 | 178 | 7 | | | |

- Molecule 66 is a protein called 40S ribosomal protein S16-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 66 | R | 141 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1105 | 708 | 203 | 194 | | | |
| 66 | c6 | 142 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1111 | 711 | 204 | 196 | | | |

- Molecule 67 is a protein called 40S ribosomal protein S17-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 67 | S | 120 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 926 | 577 | 177 | 170 | 2 | | | |
| 67 | c7 | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 906 | 563 | 174 | 167 | 2 | | | |

- Molecule 68 is a protein called 40S ribosomal protein S18-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 68 | T | 145 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1192 | 743 | 237 | 210 | 2 | | | |
| 68 | c8 | 145 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1192 | 743 | 237 | 210 | 2 | | | |

- Molecule 69 is a protein called 40S ribosomal protein S19-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 69 | U | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1112 | 694 | 208 | 208 | 2 | | | |
| 69 | c9 | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1112 | 694 | 208 | 208 | 2 | | | |

- Molecule 70 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 70 | V | 107 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 855 | 539 | 156 | 159 | 1 | | | |
| 70 | d0 | 110 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 882 | 554 | 161 | 166 | 1 | | | |

- Molecule 71 is a protein called 40S ribosomal protein S21-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 71 | W | 87 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 684 | 420 | 125 | 137 | 2 | | | |
| 71 | d1 | 87 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 684 | 420 | 125 | 137 | 2 | | | |

- Molecule 72 is a protein called 40S ribosomal protein S22-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 72 | X | 129 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1021 | 650 | 188 | 180 | 3 | | | |
| 72 | d2 | 129 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1021 | 650 | 188 | 180 | 3 | | | |

- Molecule 73 is a protein called 40S ribosomal protein S23-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 73 | Y | 144 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1121 | 708 | 220 | 191 | 2 | | | |
| 73 | d3 | 144 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1121 | 708 | 220 | 191 | 2 | | | |

- Molecule 74 is a protein called 40S ribosomal protein S24-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 74 | Z | 134 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1073 | 676 | 208 | 189 | | | |
| 74 | d4 | 134 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1073 | 676 | 208 | 189 | | | |

- Molecule 75 is a protein called 40S ribosomal protein S25-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 75 | a | 70 | Total | C | N | O | 0 | 0 | 0 |
| | | | 563 | 360 | 104 | 99 | | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 75 | d5 | 69 | Total | C | N | O | 0 | 0 | 0 |
| | | | 558 | 357 | 103 | 98 | | | |

- Molecule 76 is a protein called 40S ribosomal protein S26-B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 76 | b | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 769 | 475 | 160 | 129 | 5 | | | |
| 76 | d6 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 769 | 475 | 160 | 129 | 5 | | | |

- Molecule 77 is a protein called 40S ribosomal protein S27-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 77 | c | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 610 | 382 | 110 | 113 | 5 | | | |
| 77 | d7 | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 610 | 382 | 110 | 113 | 5 | | | |

- Molecule 78 is a protein called 40S ribosomal protein S28-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 78 | d | 63 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 497 | 306 | 99 | 91 | 1 | | | |
| 78 | d8 | 63 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 497 | 306 | 99 | 91 | 1 | | | |

- Molecule 79 is a protein called 40S ribosomal protein S29-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 79 | e | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 442 | 274 | 92 | 72 | 4 | | | |
| 79 | d9 | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 442 | 274 | 92 | 72 | 4 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 80 | f | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 475 | 299 | 98 | 77 | 1 | | | |
| 80 | e0 | 62 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 491 | 309 | 101 | 80 | 1 | | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|---------|
| 84 | 1 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 1 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 1 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 1 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 1 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 1 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 1 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 1 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 1 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 1 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 1 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 1 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 1 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 1 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 1 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 1 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 1 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 1 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 1 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 1 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 1 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|------------|--------------|-----------------|--------------|---|----|----------------|----------------|
| 84 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 1 | 1 | | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | k | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | l | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | r | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | v | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | x | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | x | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | y | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | z | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|---------|
| | | | Total | N | Os | | |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|---------|
| | | | Total | N | Os | | |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
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| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
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| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
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| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|---------|
| | | | Total | N | Os | | |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|---------|
| | | | Total | N | Os | | |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
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| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | 6 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | 6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AC | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AG | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AH | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AK | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AM | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AP | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|------------|--------------|-----------------|--------------|---|----|----------------|----------------|
| | | | Total | N | Os | | |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|------------|--------------|-----------------|--------------|---|----|----------------|----------------|
| 84 | AR | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | AR | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | AR | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | AR | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | AR | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | AR | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | AR | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | AR | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | AR | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | AR | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | AR | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | AR | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | AR | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | AR | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | AR | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | AR | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | AR | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AS | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AS | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | AS | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AS | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AS | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AS | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AS | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AS | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AS | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AS | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AS | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AT | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AT | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AT | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AT | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AT | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AT | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AT | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AT | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AT | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AT | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AT | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AT | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AT | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | AT | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AT | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AT | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AT | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AT | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | CE | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | CE | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | CF | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | CF | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | CG | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | CG | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | CK | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | CL | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | CM | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | CP | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | CV | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | CX | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | CX | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | DD | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | DH | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | DQ | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|------------|--------------|-----------------|--------------|---|----|----------------|----------------|
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | Total | N | Os | | |
| | | | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|---------|
| | | | Total | N | Os | | |
| 84 | A | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | A | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | A | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | A | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | A | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | A | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | A | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | A | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | A | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | A | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | A | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | A | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | A | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | A | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | A | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | A | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | A | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | A | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | A | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 84 | A | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 84 | A | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | A | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | A | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | A | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | A | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | A | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | A | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | A | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | A | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | A | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | A | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | A | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | A | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | A | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | A | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | J | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | K | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | M | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | O | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 84 | Q | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | T | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | e | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | h | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | s8 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | c1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | c3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | c4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | c5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | c8 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | d9 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| | | | Total | Mg | | |
| 85 | 1 | 498 | 498 | 498 | 0 | 0 |
| 85 | 3 | 13 | 13 | 13 | 0 | 0 |
| 85 | 4 | 25 | 25 | 25 | 0 | 0 |
| 85 | j | 2 | 2 | 2 | 0 | 0 |
| 85 | k | 3 | 3 | 3 | 0 | 0 |
| 85 | l | 3 | 3 | 3 | 0 | 0 |
| 85 | n | 1 | 1 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|---------------------|---------|---------|
| 85 | o | 2 | Total Mg 2 2 | 0 | 0 |
| 85 | r | 1 | Total Mg 1 1 | 0 | 0 |
| 85 | s | 1 | Total Mg 1 1 | 0 | 0 |
| 85 | t | 3 | Total Mg 3 3 | 0 | 0 |
| 85 | v | 3 | Total Mg 3 3 | 0 | 0 |
| 85 | w | 2 | Total Mg 2 2 | 0 | 0 |
| 85 | x | 7 | Total Mg 7 7 | 0 | 0 |
| 85 | z | 1 | Total Mg 1 1 | 0 | 0 |
| 85 | lR | 1 | Total Mg 1 1 | 0 | 0 |
| 85 | 6 | 146 | Total Mg 146 146 | 0 | 0 |
| 85 | AB | 7 | Total Mg 7 7 | 0 | 0 |
| 85 | AF | 2 | Total Mg 2 2 | 0 | 0 |
| 85 | AG | 1 | Total Mg 1 1 | 0 | 0 |
| 85 | AH | 1 | Total Mg 1 1 | 0 | 0 |
| 85 | AK | 1 | Total Mg 1 1 | 0 | 0 |
| 85 | AP | 1 | Total Mg 1 1 | 0 | 0 |
| 85 | AR | 515 | Total Mg 515 515 | 0 | 0 |
| 85 | AS | 20 | Total Mg 20 20 | 0 | 0 |
| 85 | AT | 14 | Total Mg 14 14 | 0 | 0 |
| 85 | CD | 2 | Total Mg 2 2 | 0 | 0 |
| 85 | CE | 5 | Total Mg 5 5 | 0 | 0 |

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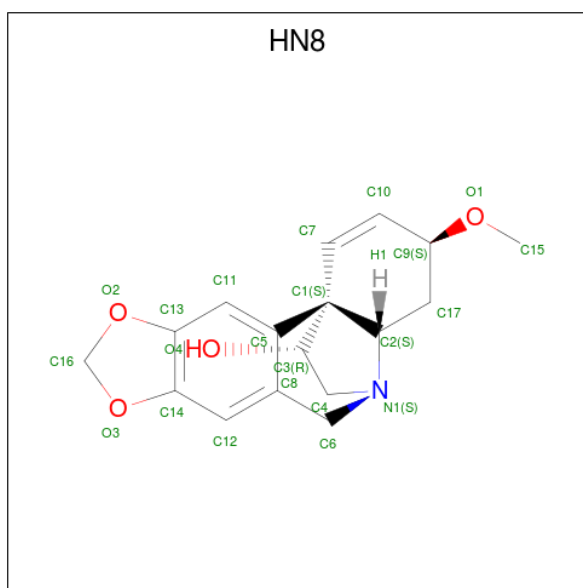
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 85 | CF | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | CG | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | CI | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | CJ | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | CK | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | CL | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | CM | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | CO | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | CP | 4 | Total 4 | Mg 4 | 0 | 0 |
| 85 | CQ | 4 | Total 4 | Mg 4 | 0 | 0 |
| 85 | CR | 5 | Total 5 | Mg 5 | 0 | 0 |
| 85 | CU | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | CX | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | DA | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | DC | 4 | Total 4 | Mg 4 | 0 | 0 |
| 85 | DE | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | DH | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | DI | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | DL | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | DO | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | DQ | 2 | Total 2 | Mg 2 | 0 | 0 |

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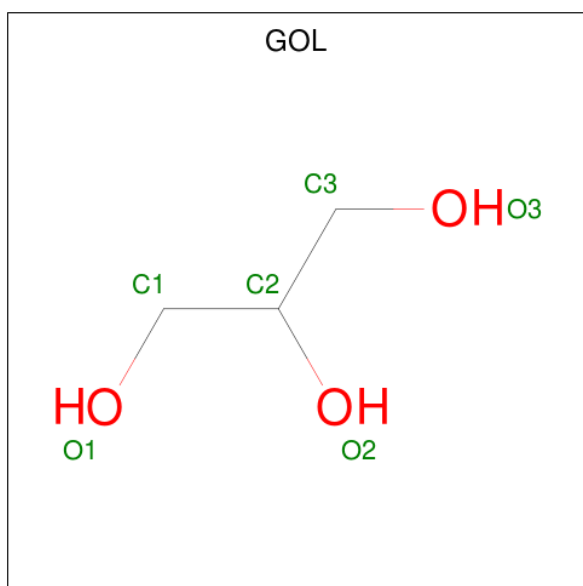
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|---------------------|---------|---------|
| 85 | sM | 2 | Total Mg 2 2 | 0 | 0 |
| 85 | A | 116 | Total Mg 116 116 | 0 | 0 |
| 85 | D | 1 | Total Mg 1 1 | 0 | 0 |
| 85 | F | 1 | Total Mg 1 1 | 0 | 0 |
| 85 | H | 1 | Total Mg 1 1 | 0 | 0 |
| 85 | T | 1 | Total Mg 1 1 | 0 | 0 |
| 85 | U | 1 | Total Mg 1 1 | 0 | 0 |
| 85 | V | 1 | Total Mg 1 1 | 0 | 0 |
| 85 | Y | 1 | Total Mg 1 1 | 0 | 0 |
| 85 | b | 1 | Total Mg 1 1 | 0 | 0 |
| 85 | s4 | 1 | Total Mg 1 1 | 0 | 0 |
| 85 | s6 | 1 | Total Mg 1 1 | 0 | 0 |
| 85 | s8 | 1 | Total Mg 1 1 | 0 | 0 |
| 85 | c1 | 1 | Total Mg 1 1 | 0 | 0 |
| 85 | c6 | 1 | Total Mg 1 1 | 0 | 0 |
| 85 | c8 | 1 | Total Mg 1 1 | 0 | 0 |
| 85 | c9 | 1 | Total Mg 1 1 | 0 | 0 |
| 85 | d3 | 2 | Total Mg 2 2 | 0 | 0 |
| 85 | d4 | 1 | Total Mg 1 1 | 0 | 0 |
| 85 | d5 | 1 | Total Mg 1 1 | 0 | 0 |
| 85 | d6 | 2 | Total Mg 2 2 | 0 | 0 |

- Molecule 86 is Haemanthamine (three-letter code: HN8) (formula: $C_{17}H_{19}NO_4$).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 86 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 22 | 17 | 1 | 4 | | |
| 86 | AR | 1 | Total | C | N | O | 0 | 0 |
| | | | 22 | 17 | 1 | 4 | | |

- Molecule 87 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 87 | v | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 87 | 6 | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 87 | AR | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 87 | AR | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 87 | A | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |

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

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 88 | AK | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 88 | AN | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 88 | AP | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 88 | AQ | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 88 | DL | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 88 | DO | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 88 | DQ | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 88 | DR | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 88 | b | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 88 | c | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 88 | e | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 88 | g | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 88 | d6 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 88 | d7 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 88 | d9 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

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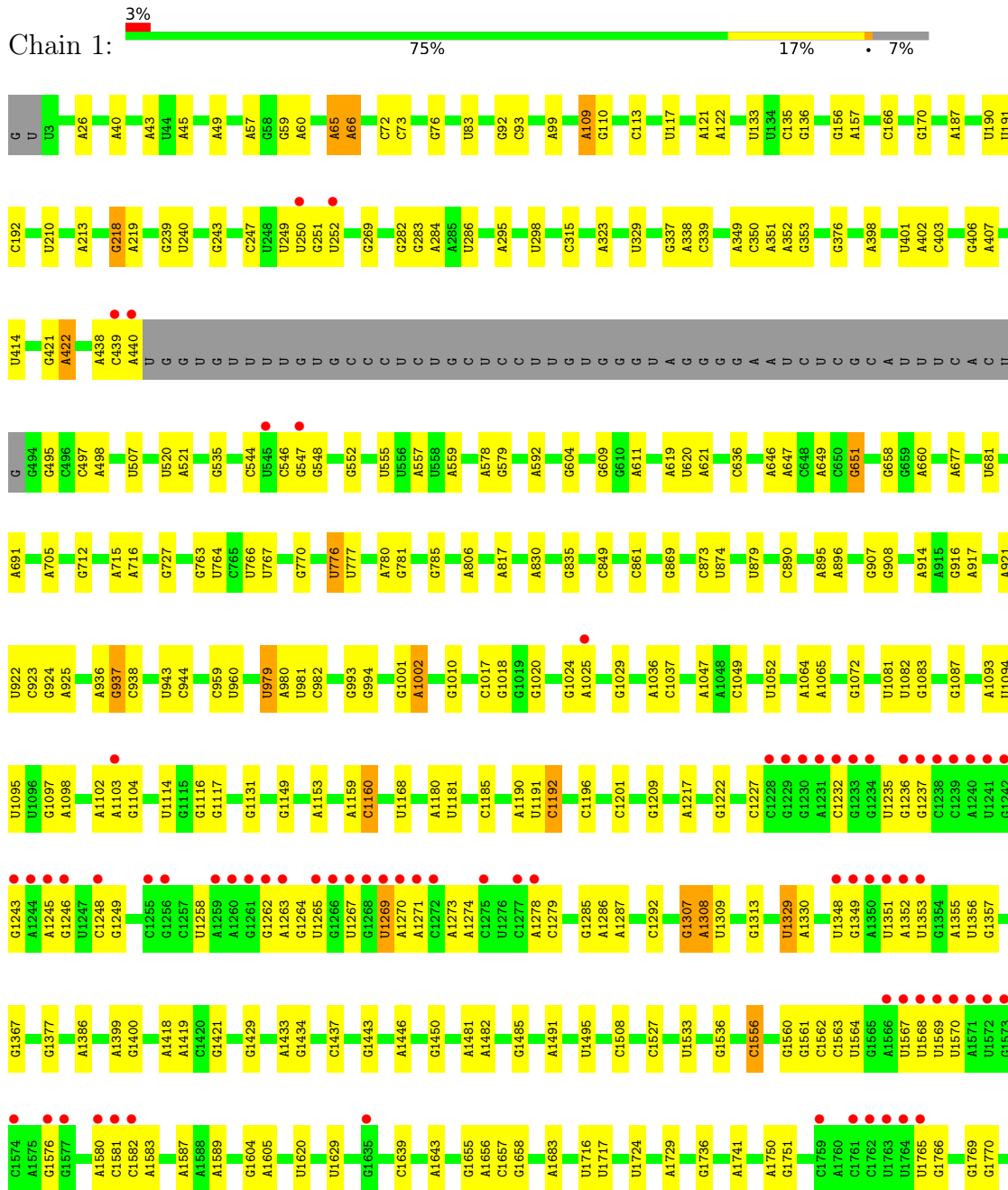
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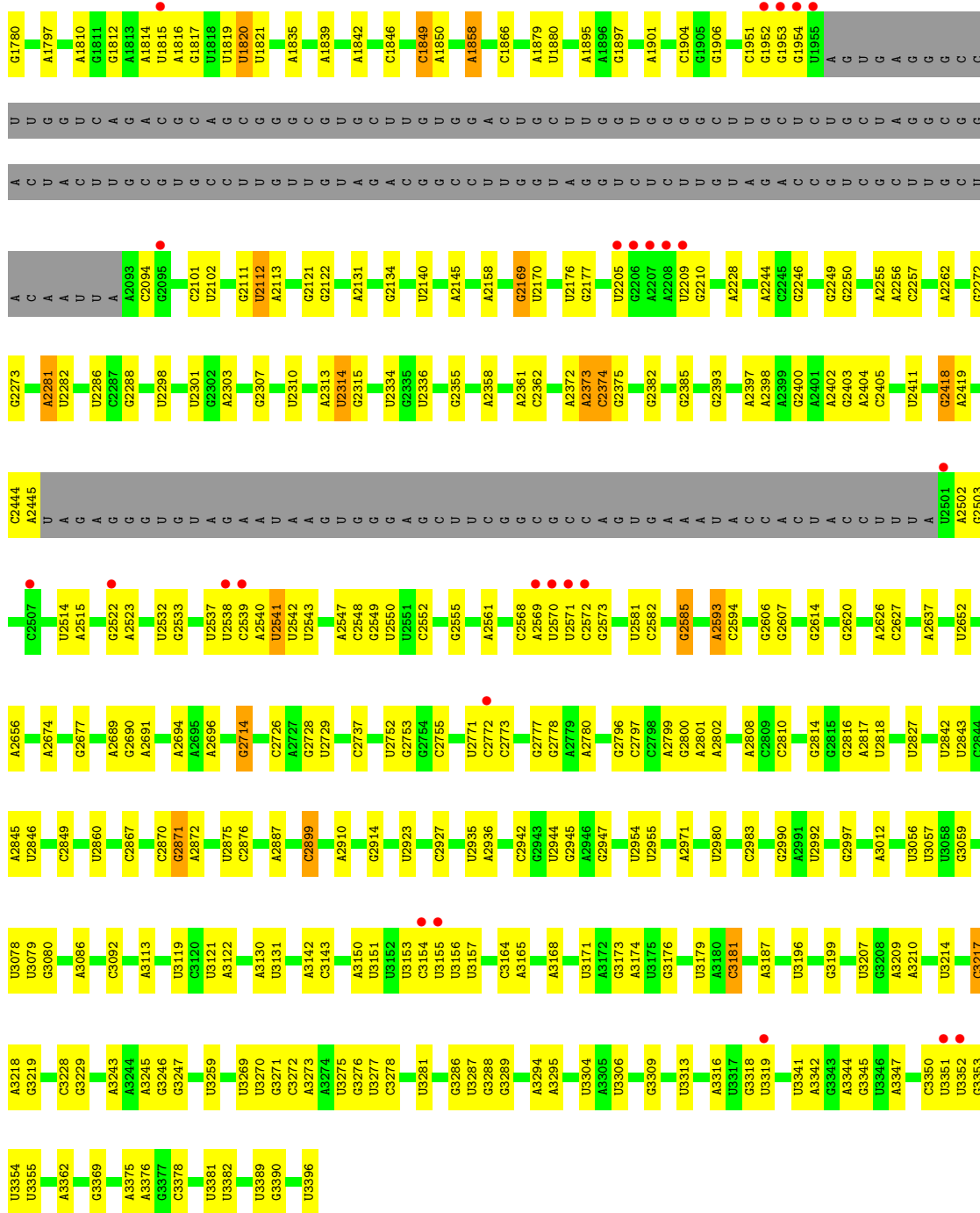
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|------------|--------------|-----------------|--------------|----|----------------|----------------|
| 88 | e1 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

3 Residue-property plots

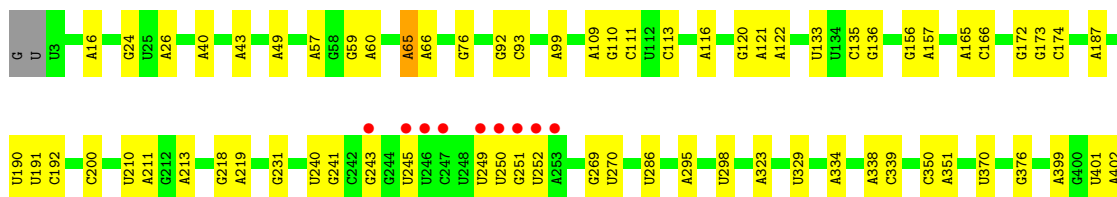
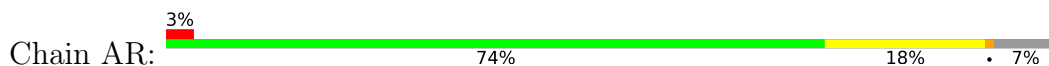
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

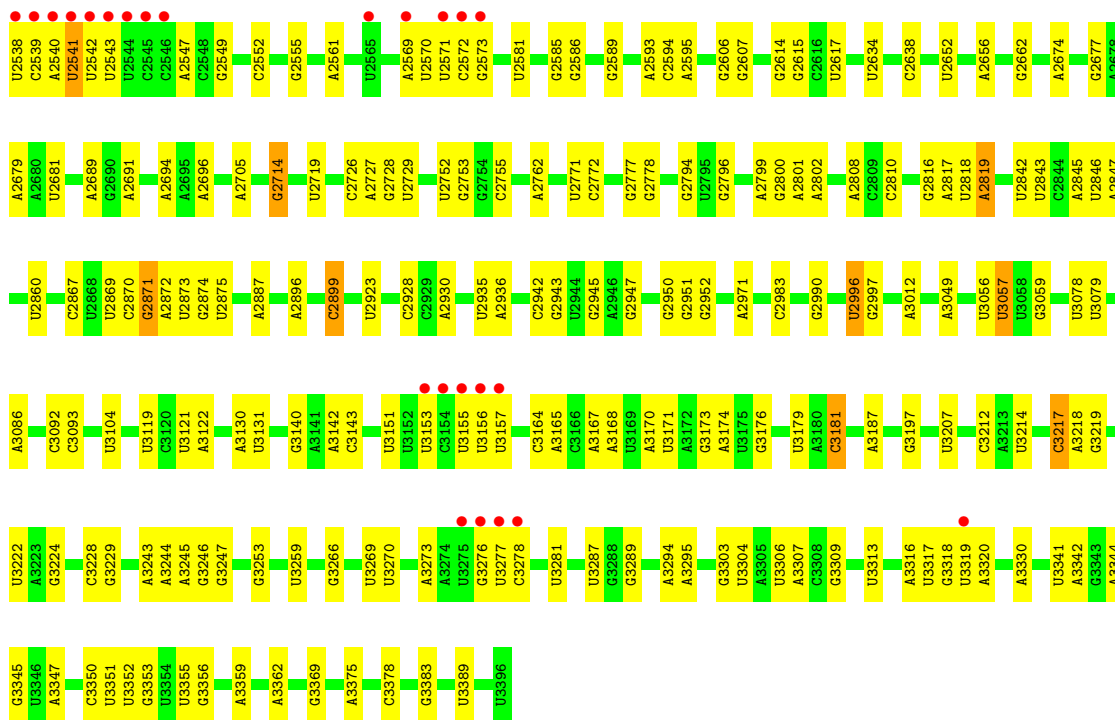
• Molecule 1: 25S ribosomal RNA



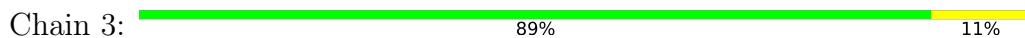


● Molecule 1: 25S ribosomal RNA

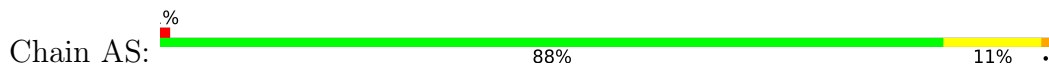




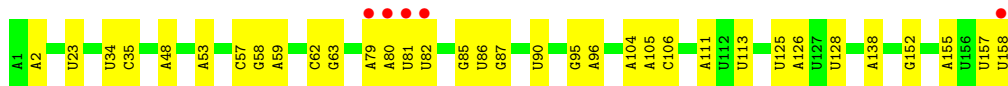
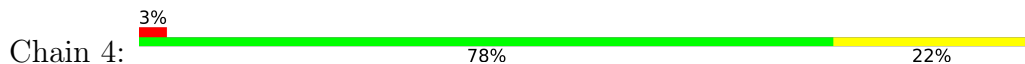
• Molecule 2: 5S ribosomal RNA



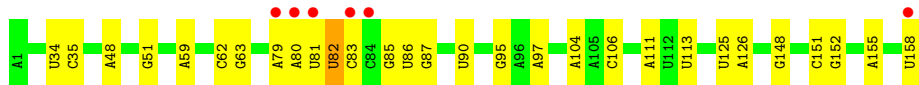
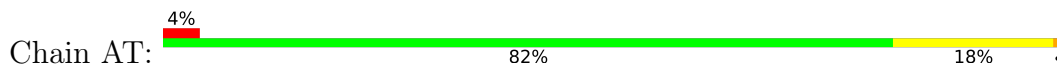
• Molecule 2: 5S ribosomal RNA



• Molecule 3: 5.8S ribosomal RNA



• Molecule 3: 5.8S ribosomal RNA



- Molecule 4: 60S ribosomal protein L2-A

Chain j: 89% 11%



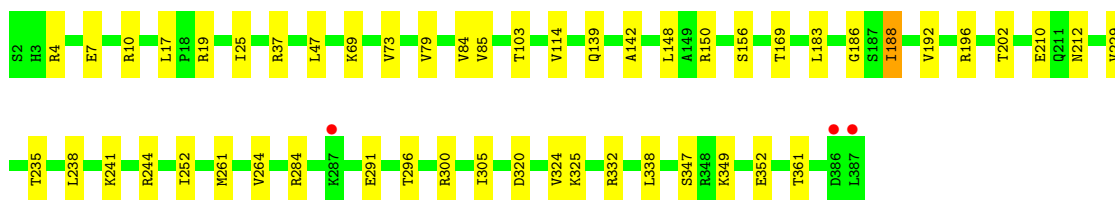
- Molecule 4: 60S ribosomal protein L2-A

Chain CD: 90% 10%



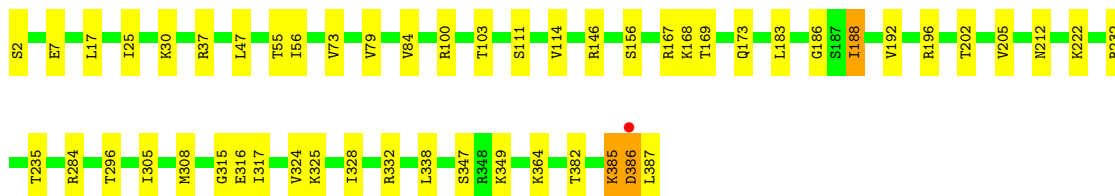
- Molecule 5: 60S ribosomal protein L3

Chain k: 87% 13%



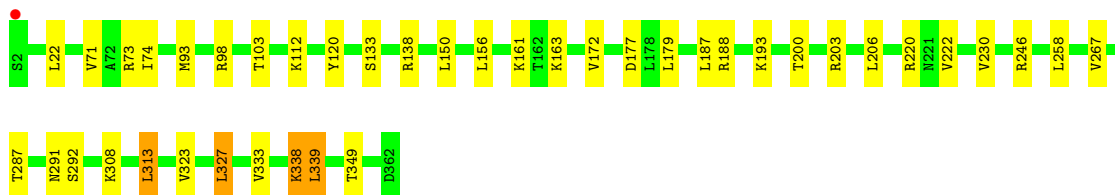
- Molecule 5: 60S ribosomal protein L3

Chain CE: 87% 13%



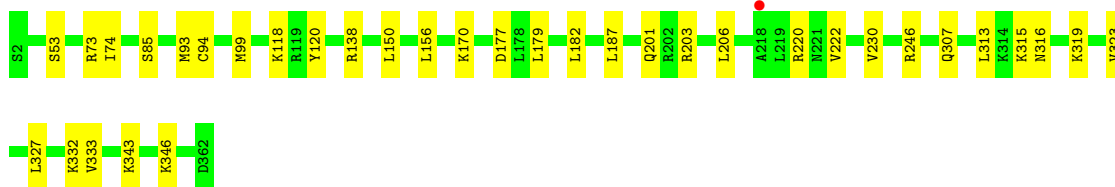
- Molecule 6: 60S ribosomal protein L4-A

Chain l: 89% 10%

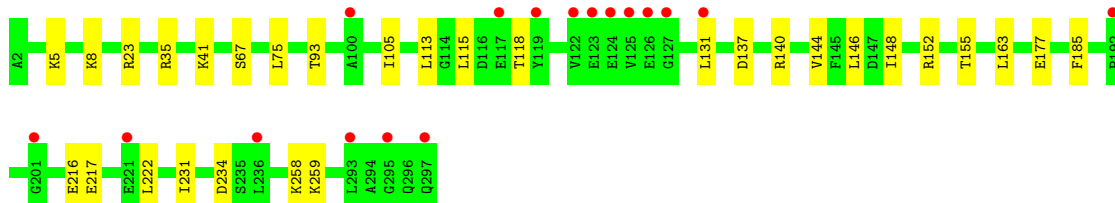
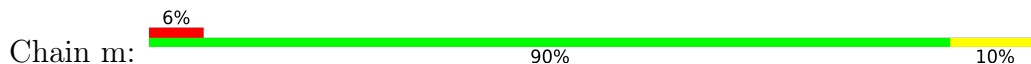


- Molecule 6: 60S ribosomal protein L4-A

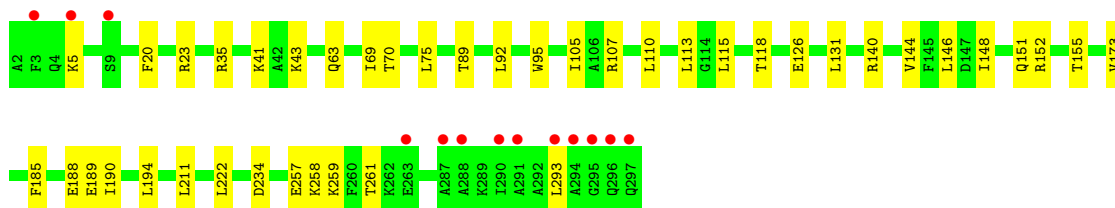
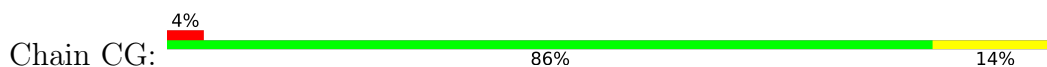
Chain CF: 90% 10%



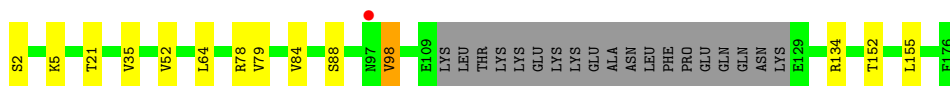
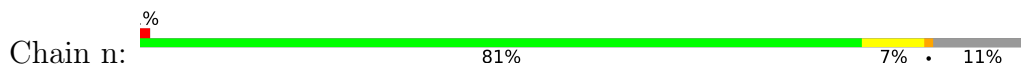
- Molecule 7: 60S ribosomal protein L5



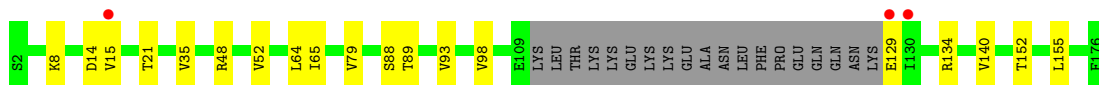
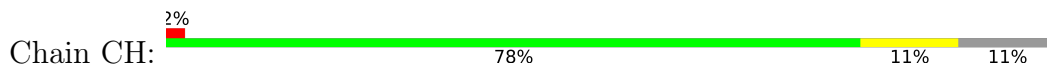
- Molecule 7: 60S ribosomal protein L5



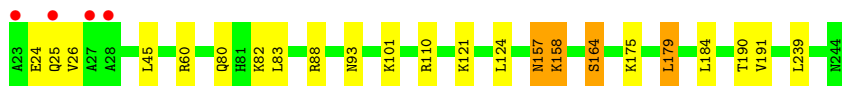
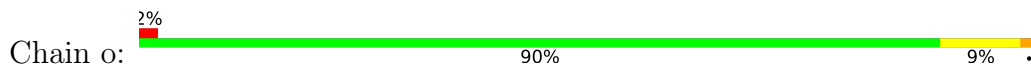
- Molecule 8: 60S ribosomal protein L6-A



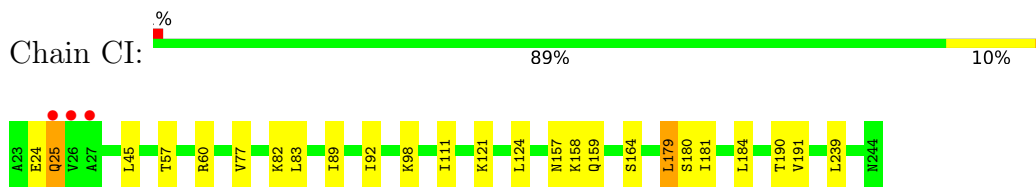
- Molecule 8: 60S ribosomal protein L6-A



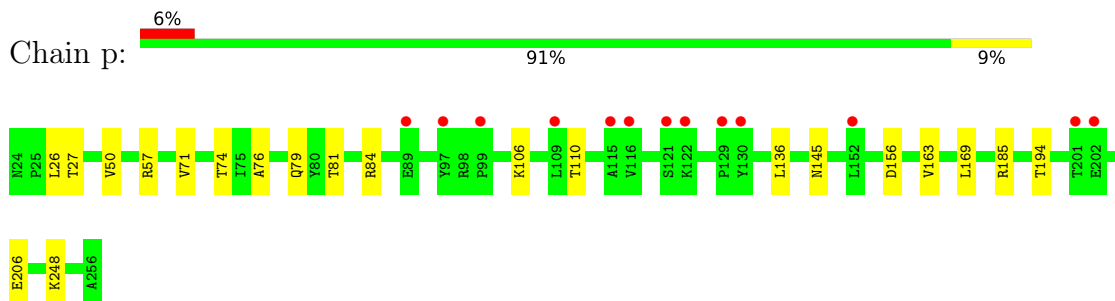
- Molecule 9: 60S ribosomal protein L7-A



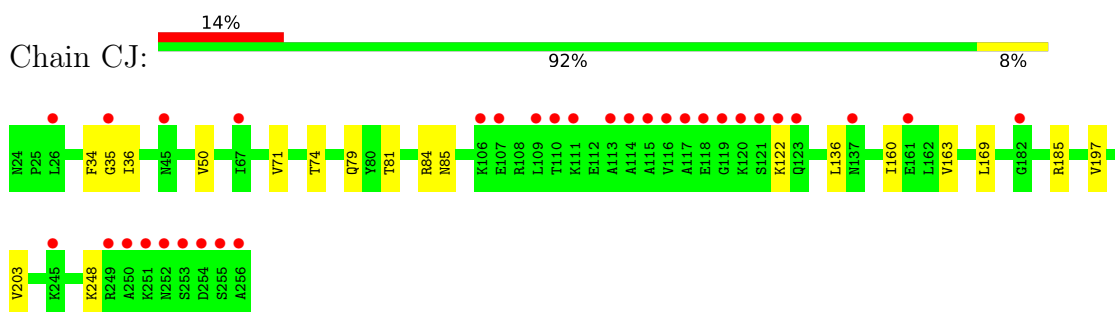
- Molecule 9: 60S ribosomal protein L7-A



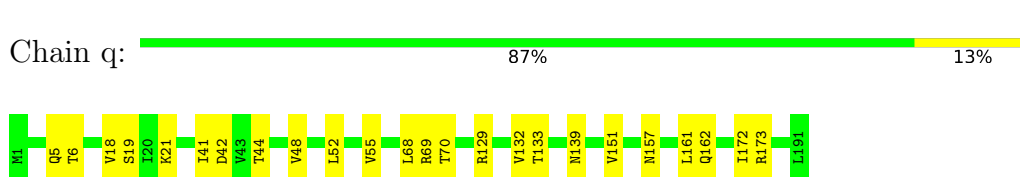
- Molecule 10: 60S ribosomal protein L8-A



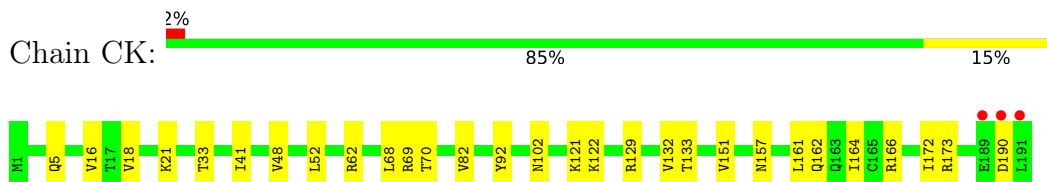
- Molecule 10: 60S ribosomal protein L8-A



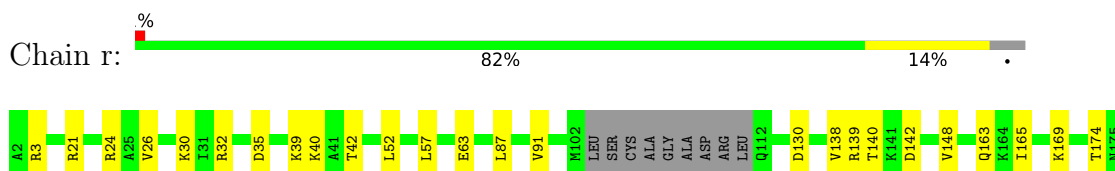
- Molecule 11: 60S ribosomal protein L9-A

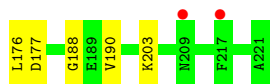


- Molecule 11: 60S ribosomal protein L9-A

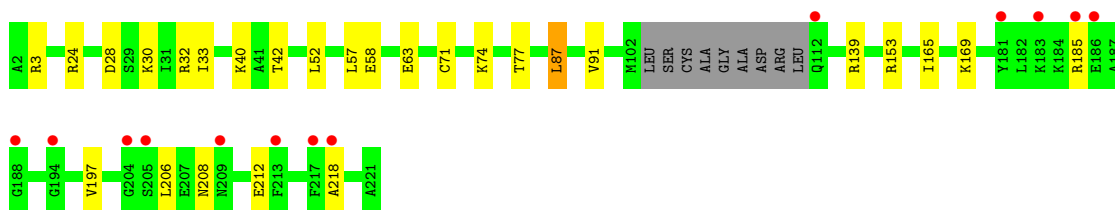
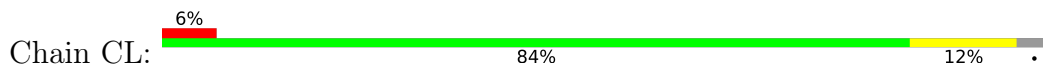


- Molecule 12: 60S ribosomal protein L10

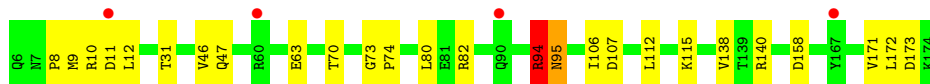
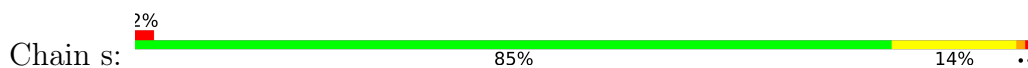




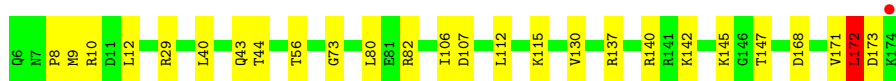
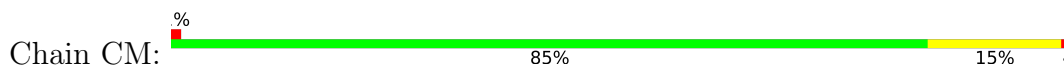
- Molecule 12: 60S ribosomal protein L10



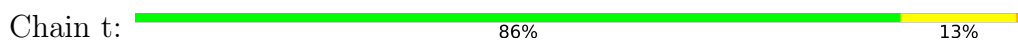
- Molecule 13: 60S ribosomal protein L11-B



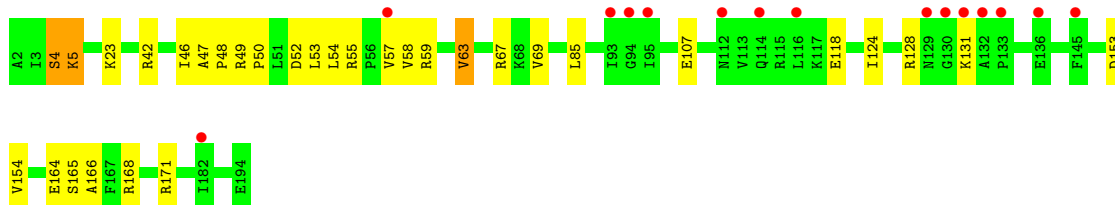
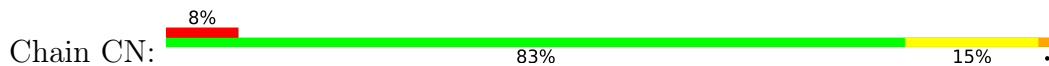
- Molecule 13: 60S ribosomal protein L11-B



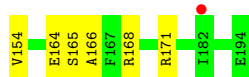
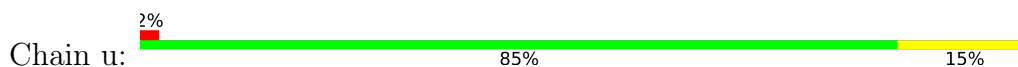
- Molecule 14: 60S ribosomal protein L13-A



- Molecule 14: 60S ribosomal protein L13-A

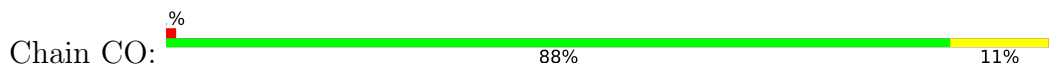


- Molecule 15: 60S ribosomal protein L14-A

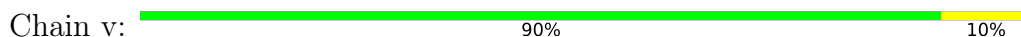




- Molecule 15: 60S ribosomal protein L14-A



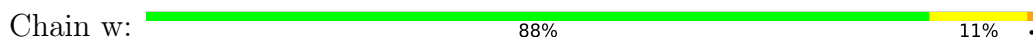
- Molecule 16: 60S ribosomal protein L15-A



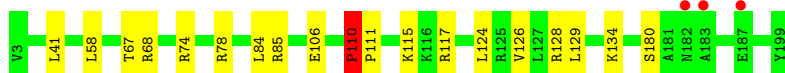
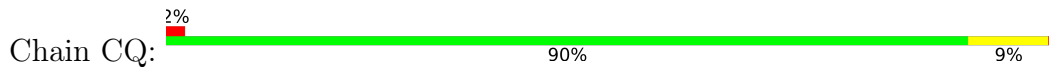
- Molecule 16: 60S ribosomal protein L15-A



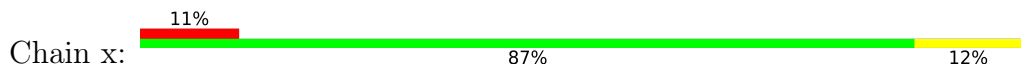
- Molecule 17: 60S ribosomal protein L16-A



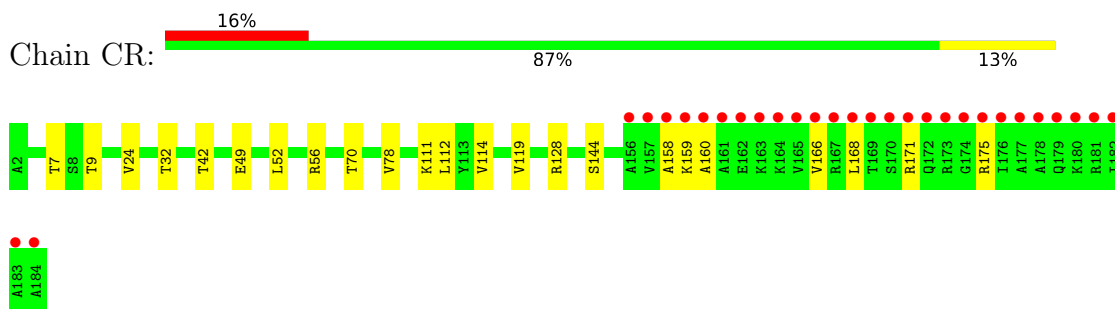
- Molecule 17: 60S ribosomal protein L16-A



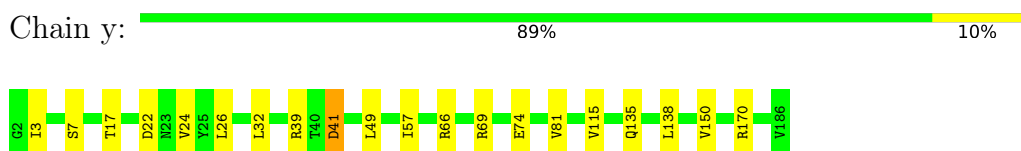
- Molecule 18: 60S ribosomal protein L17-A



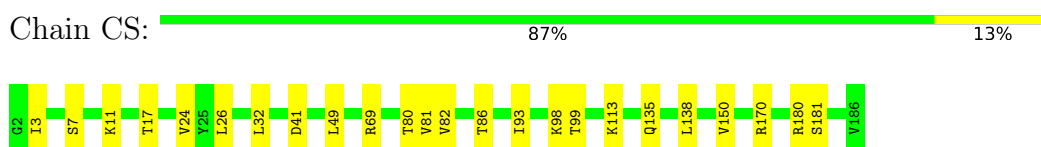
- Molecule 18: 60S ribosomal protein L17-A



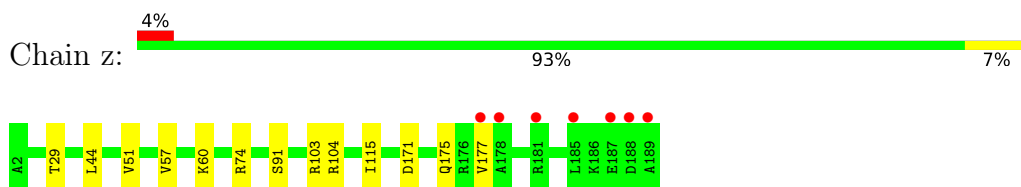
- Molecule 19: 60S ribosomal protein L18-A



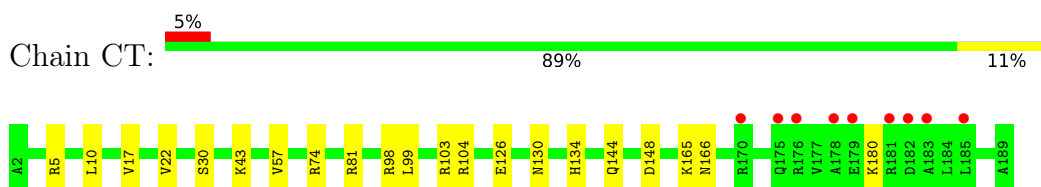
- Molecule 19: 60S ribosomal protein L18-A



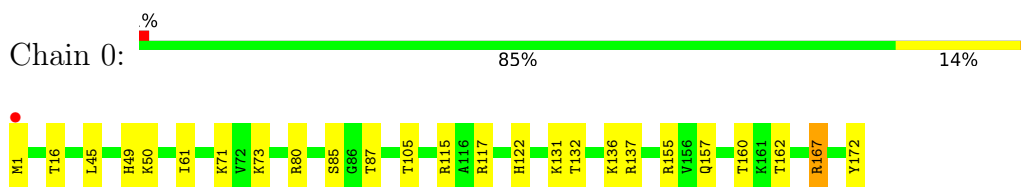
- Molecule 20: 60S ribosomal protein L19-A




- Molecule 20: 60S ribosomal protein L19-A



- Molecule 21: 60S ribosomal protein L20-A




- Molecule 21: 60S ribosomal protein L20-A

Chain CU:  85% 15%




- Molecule 22: 60S ribosomal protein L21-A

Chain 2:  86% 14%



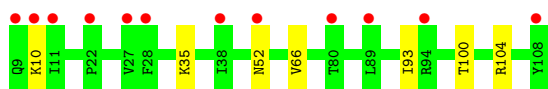
- Molecule 22: 60S ribosomal protein L21-A

Chain CV:  84% 16%

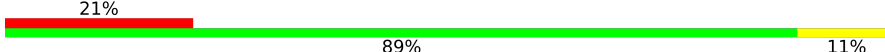


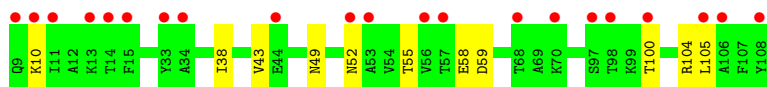
- Molecule 23: 60S ribosomal protein L22-A

Chain 5:  12% 93% 7%




- Molecule 23: 60S ribosomal protein L22-A

Chain CW:  21% 89% 11%



- Molecule 24: 60S ribosomal protein L23-A

Chain LR:  3% 89% 11%

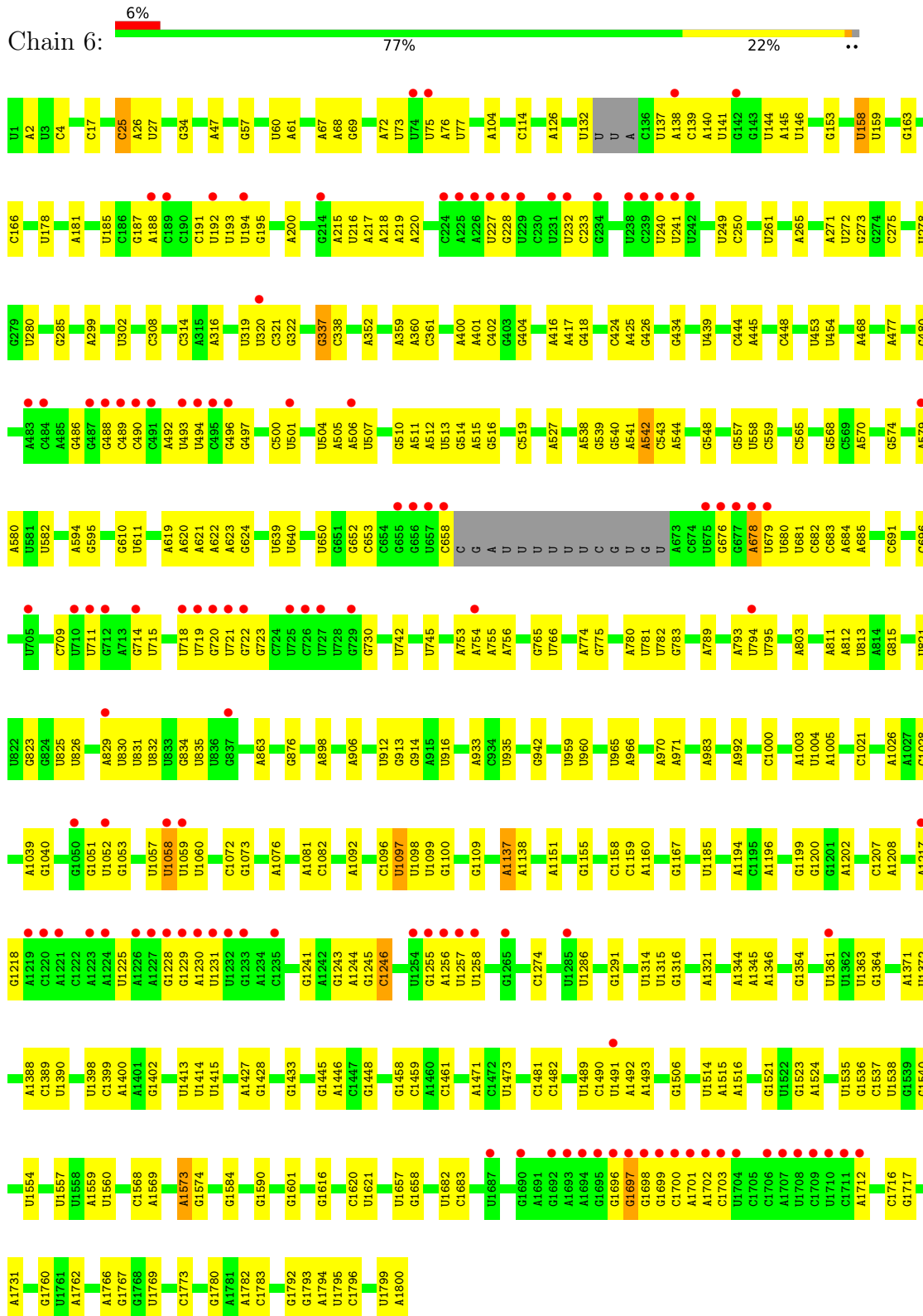


- Molecule 24: 60S ribosomal protein L23-A

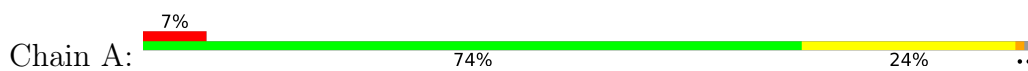
Chain CX:  92% 8%

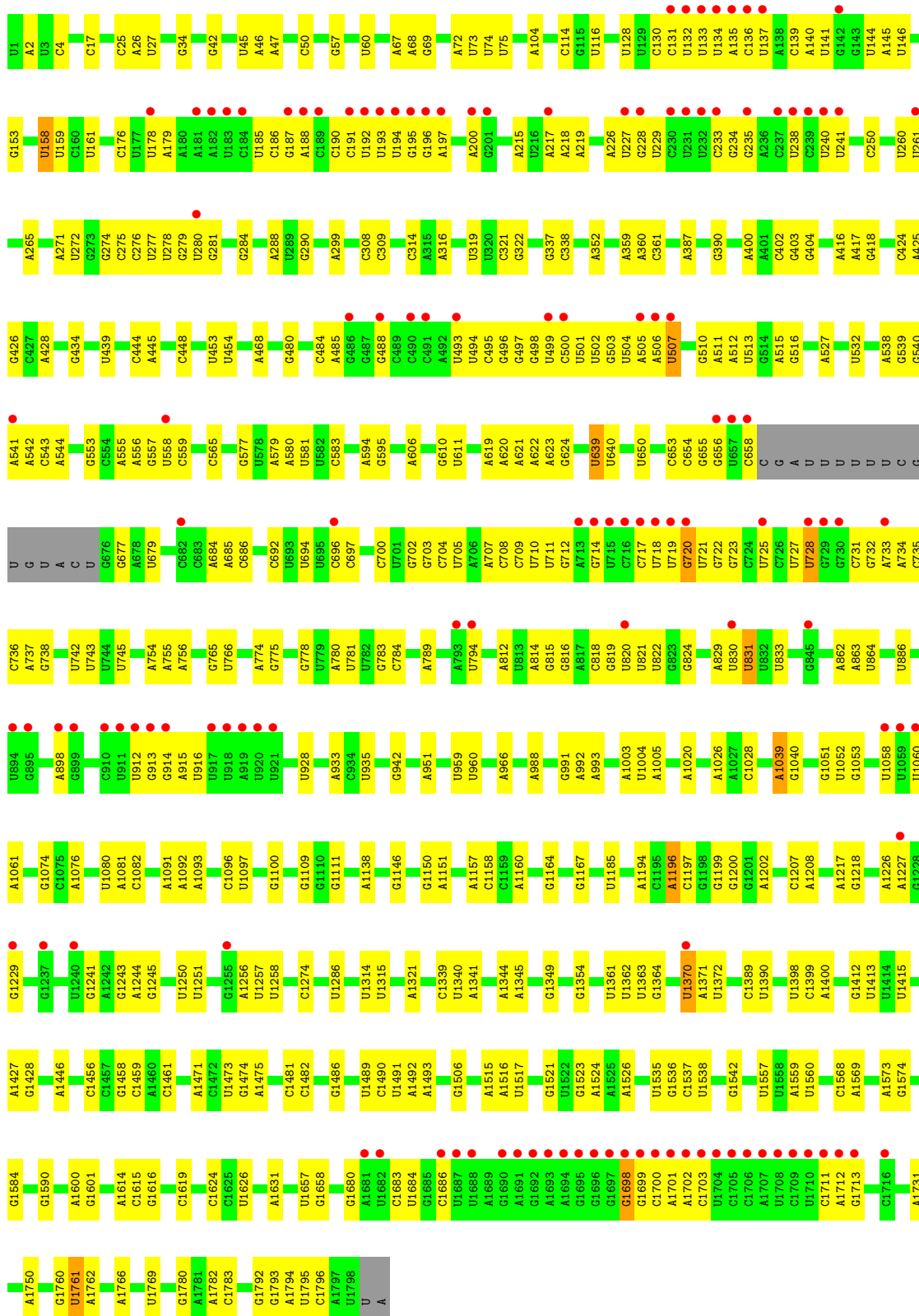


- Molecule 25: 18S ribosomal RNA

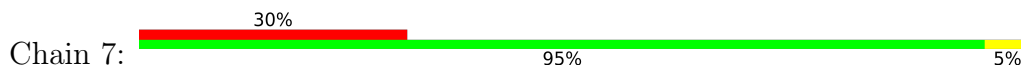


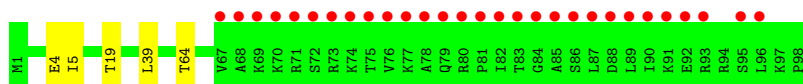
- Molecule 25: 18S ribosomal RNA



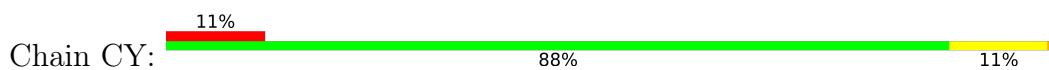


• Molecule 26: 60S ribosomal protein L24-A

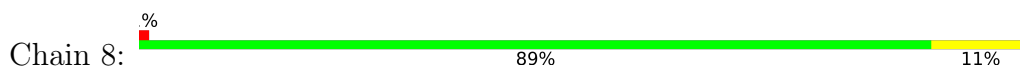




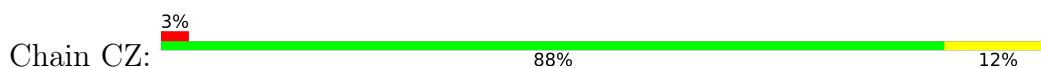
- Molecule 26: 60S ribosomal protein L24-A



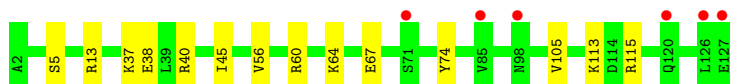
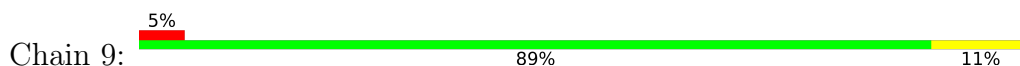
- Molecule 27: 60S ribosomal protein L25



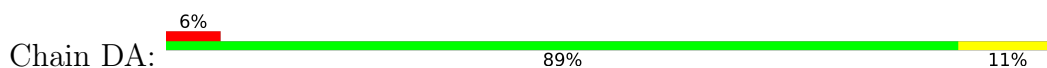
- Molecule 27: 60S ribosomal protein L25



- Molecule 28: 60S ribosomal protein L26-A

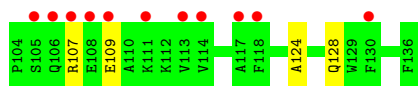


- Molecule 28: 60S ribosomal protein L26-A

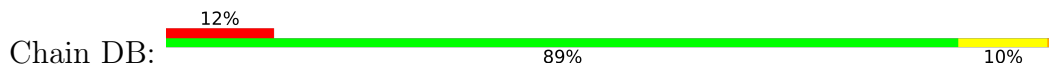


- Molecule 29: 60S ribosomal protein L27-A

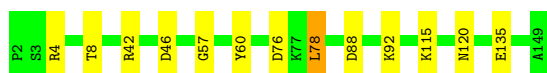




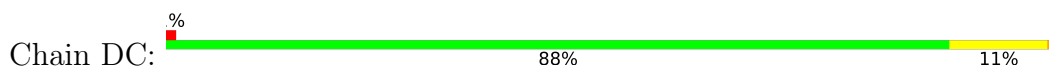
- Molecule 29: 60S ribosomal protein L27-A



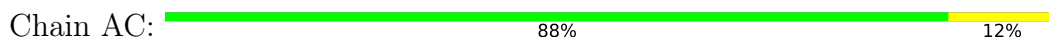
- Molecule 30: 60S ribosomal protein L28



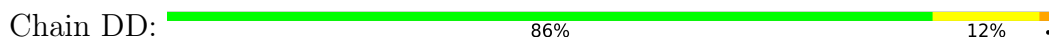
- Molecule 30: 60S ribosomal protein L28



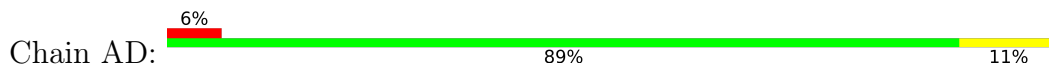
- Molecule 31: 60S ribosomal protein L29



- Molecule 31: 60S ribosomal protein L29

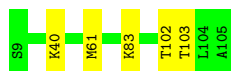


- Molecule 32: 60S ribosomal protein L30

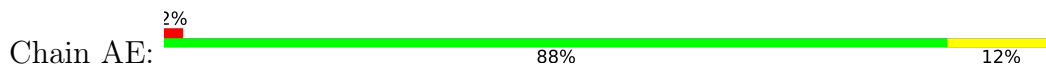


- Molecule 32: 60S ribosomal protein L30

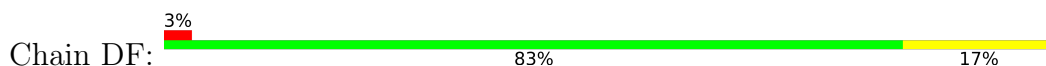




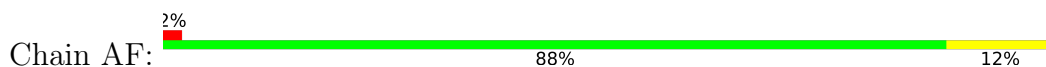
- Molecule 33: 60S ribosomal protein L31-A



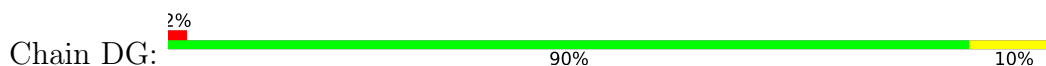
- Molecule 33: 60S ribosomal protein L31-A



- Molecule 34: 60S ribosomal protein L32



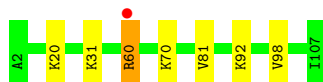
- Molecule 34: 60S ribosomal protein L32



- Molecule 35: 60S ribosomal protein L33-A



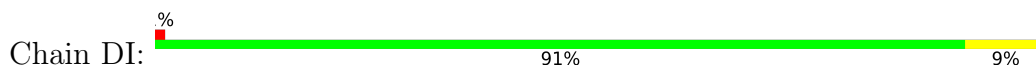
- Molecule 35: 60S ribosomal protein L33-A



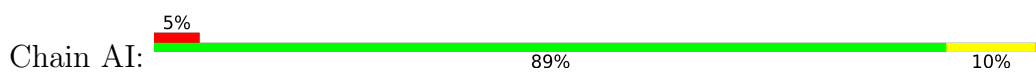
- Molecule 36: 60S ribosomal protein L34-A



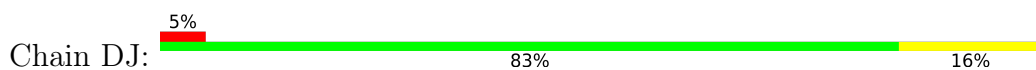
- Molecule 36: 60S ribosomal protein L34-A



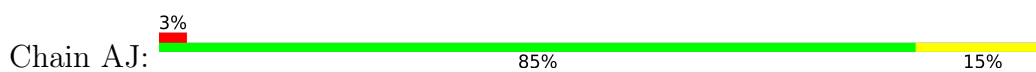
- Molecule 37: 60S ribosomal protein L35-A



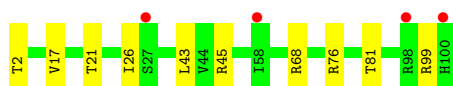
- Molecule 37: 60S ribosomal protein L35-A



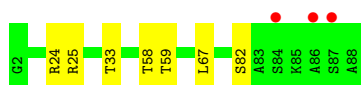
- Molecule 38: 60S ribosomal protein L36-A



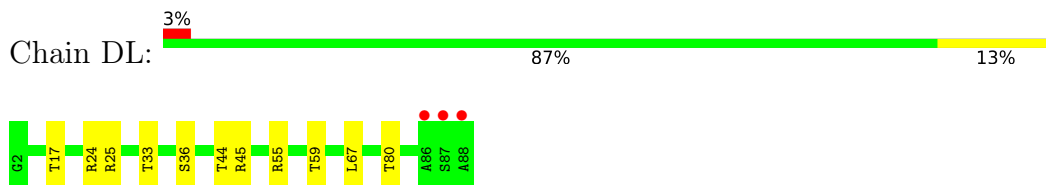
- Molecule 38: 60S ribosomal protein L36-A



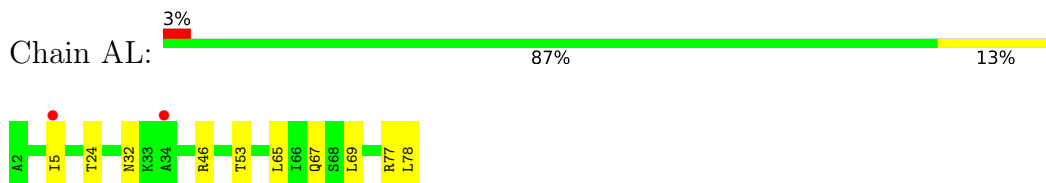
- Molecule 39: 60S ribosomal protein L37-A



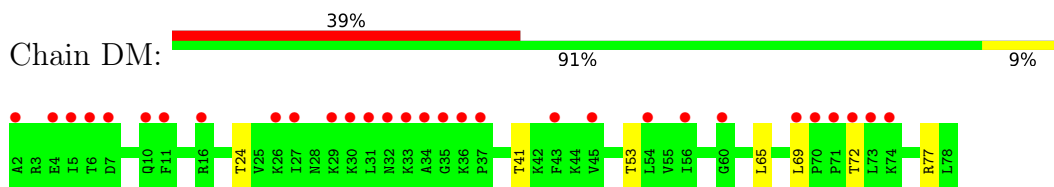
- Molecule 39: 60S ribosomal protein L37-A



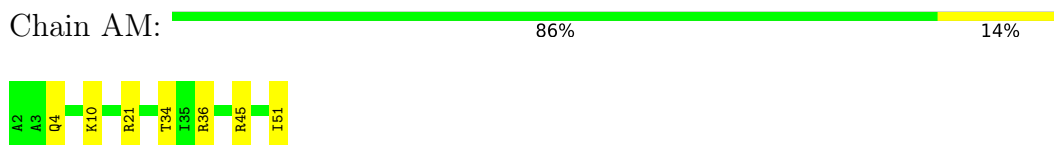
- Molecule 40: 60S ribosomal protein L38



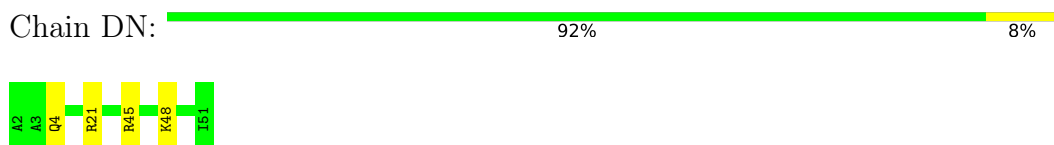
- Molecule 40: 60S ribosomal protein L38



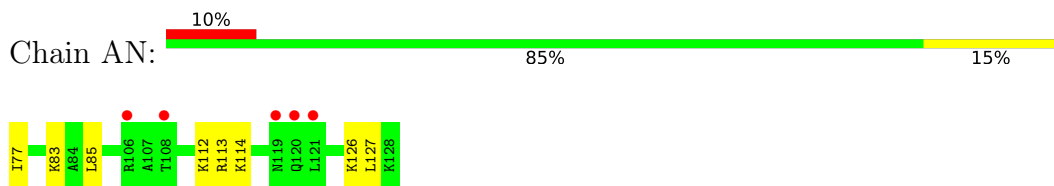
- Molecule 41: 60S ribosomal protein L39



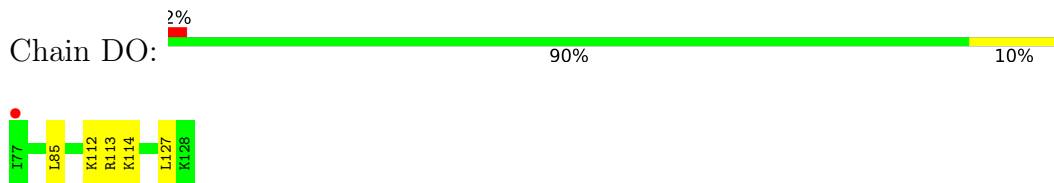
- Molecule 41: 60S ribosomal protein L39



- Molecule 42: Ubiquitin-60S ribosomal protein L40

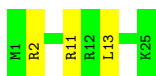


- Molecule 42: Ubiquitin-60S ribosomal protein L40




- Molecule 43: 60S ribosomal protein L41-B

Chain AO:  88% 12%

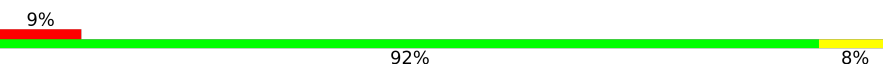


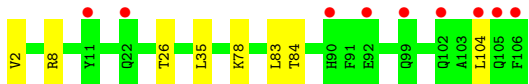
- Molecule 43: 60S ribosomal protein L41-B

Chain DP:  84% 16%



- Molecule 44: 60S ribosomal protein L42-A

Chain AP:  9% 92% 8%




- Molecule 44: 60S ribosomal protein L42-A

Chain DQ:  91% 9%



- Molecule 45: 60S ribosomal protein L43-A

Chain AQ:  87% 13%



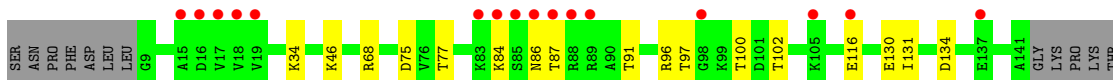
- Molecule 45: 60S ribosomal protein L43-A

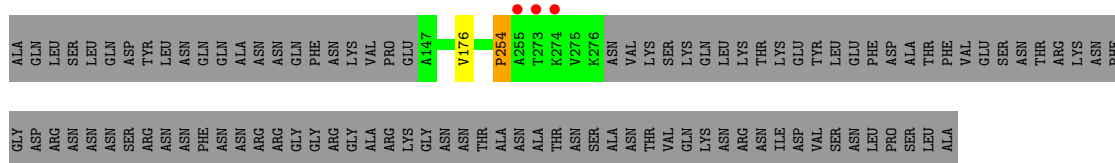
Chain DR:  91% 9%



- Molecule 46: Suppressor protein STM1

Chain i:  7% 51% 7% 42%



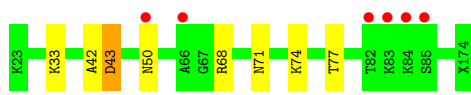


- Molecule 47: 60S ribosomal protein L12

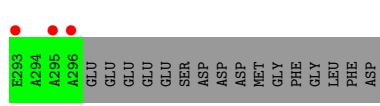
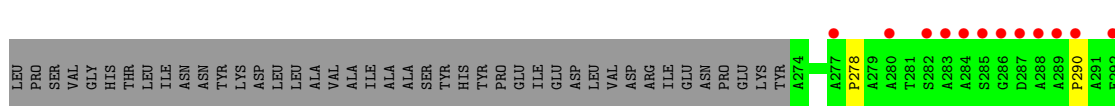
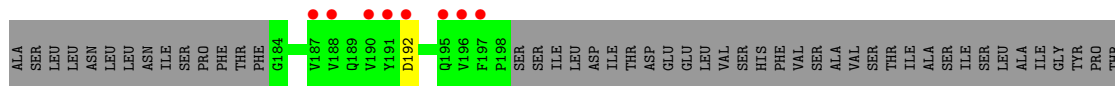
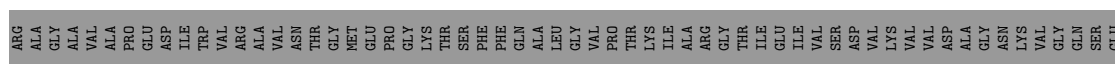
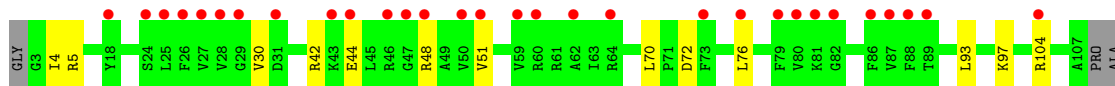
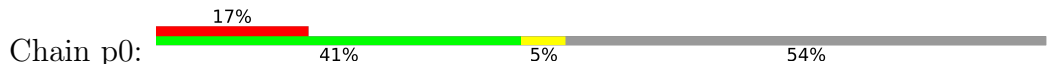


There are no outlier residues recorded for this chain.

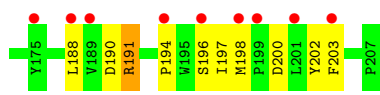
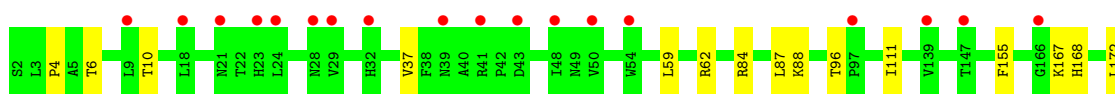
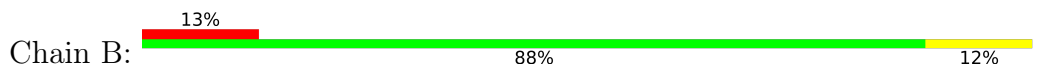
- Molecule 48: Suppressor protein STM1, Suppressor protein STM1



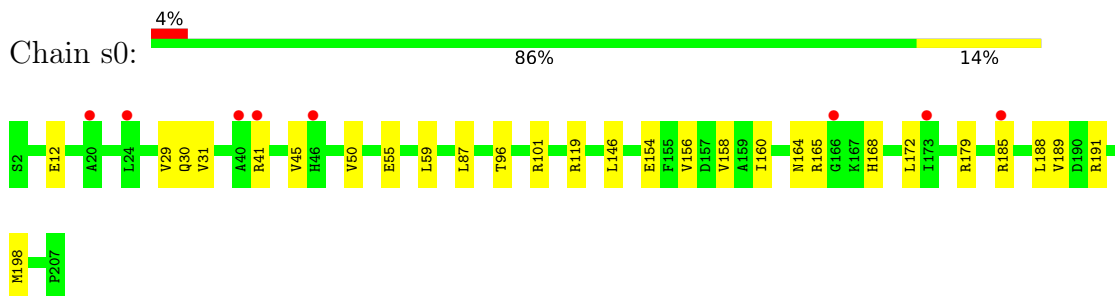
- Molecule 49: 60S acidic ribosomal protein P0



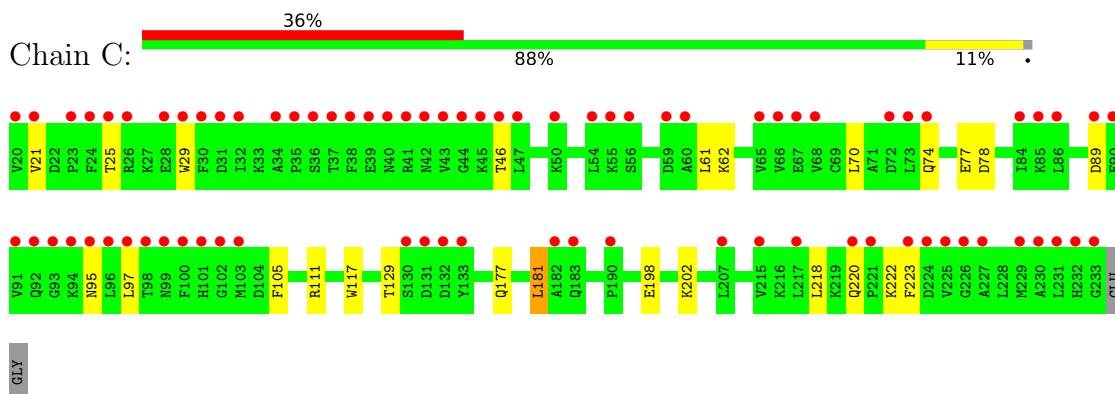
- Molecule 50: 40S ribosomal protein S0-A



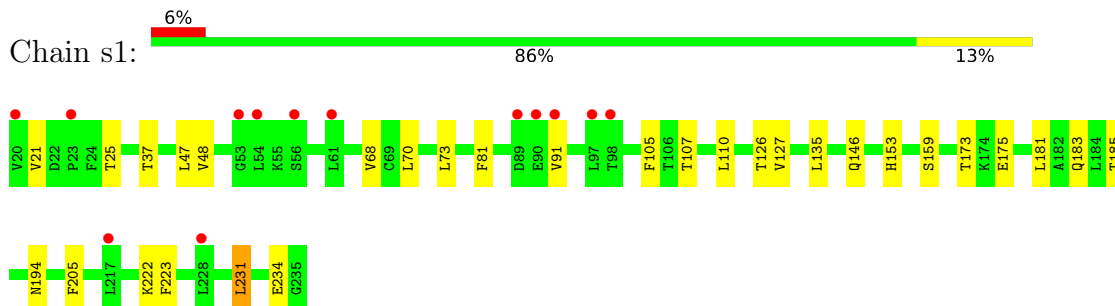
- Molecule 50: 40S ribosomal protein S0-A



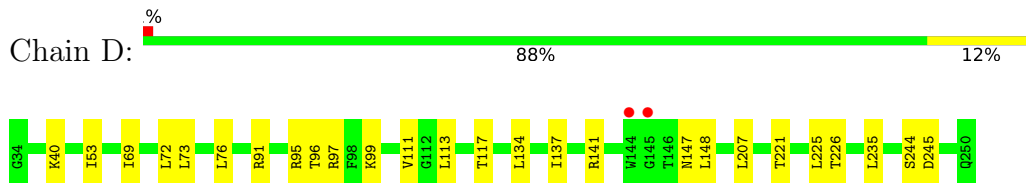
- Molecule 51: 40S ribosomal protein S1-A



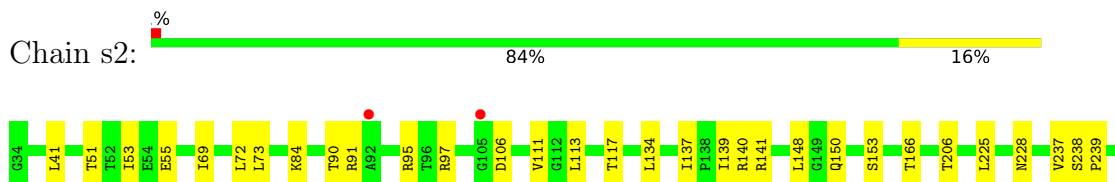
- Molecule 51: 40S ribosomal protein S1-A



- Molecule 52: 40S ribosomal protein S2

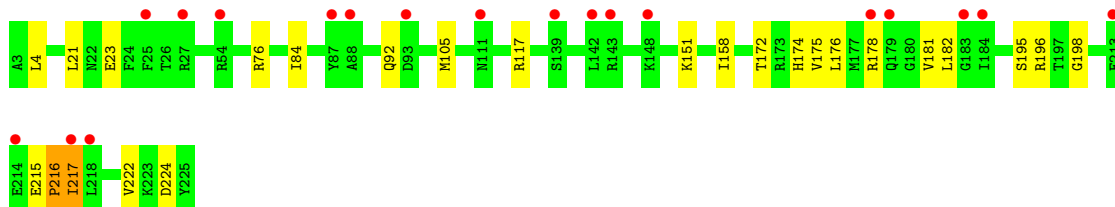
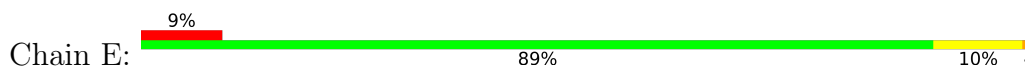


- Molecule 52: 40S ribosomal protein S2

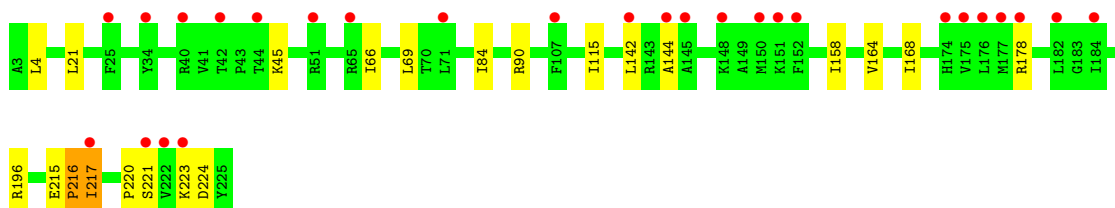
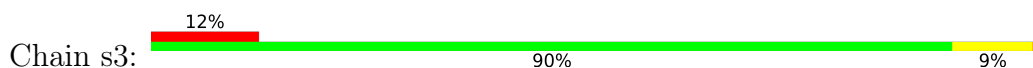




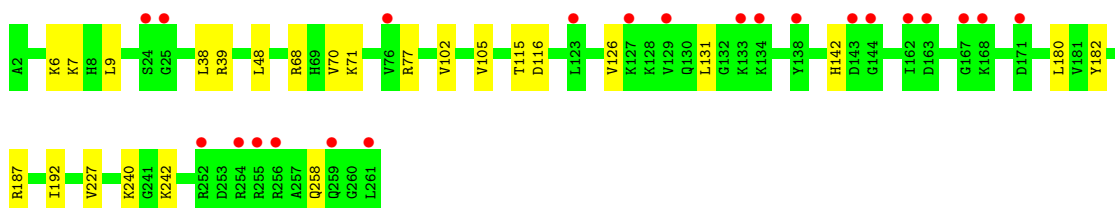
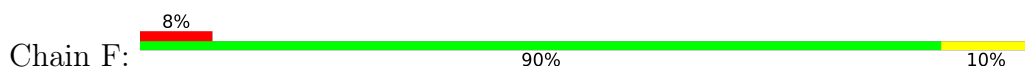
- Molecule 53: 40S ribosomal protein S3



- Molecule 53: 40S ribosomal protein S3



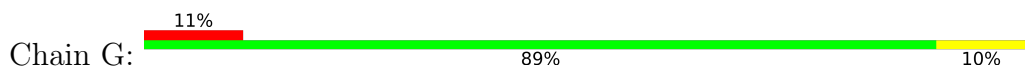
- Molecule 54: 40S ribosomal protein S4-A



- Molecule 54: 40S ribosomal protein S4-A

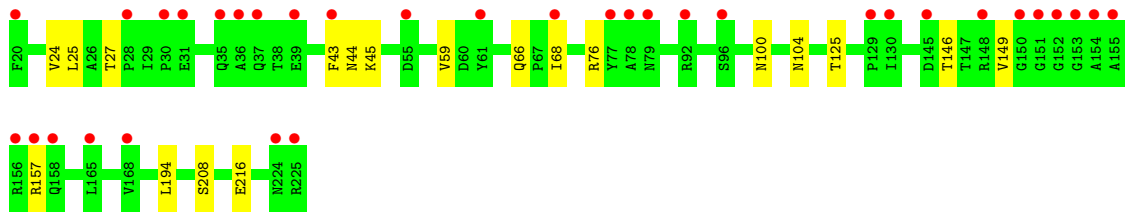
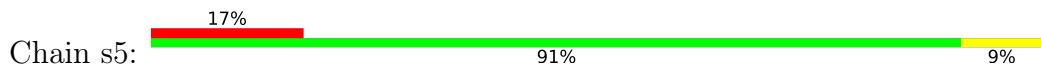


- Molecule 55: 40S ribosomal protein S5

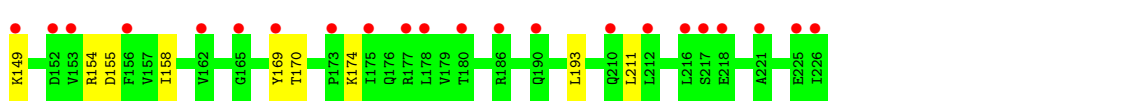
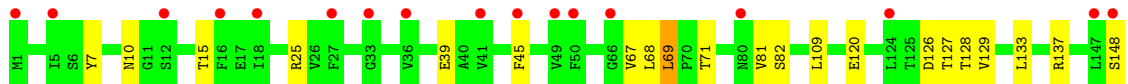
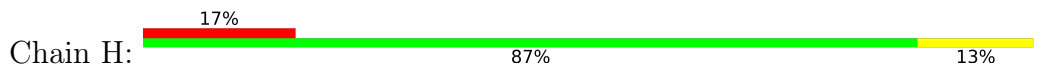




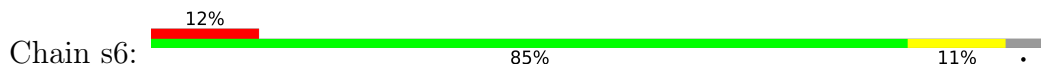
• Molecule 55: 40S ribosomal protein S5



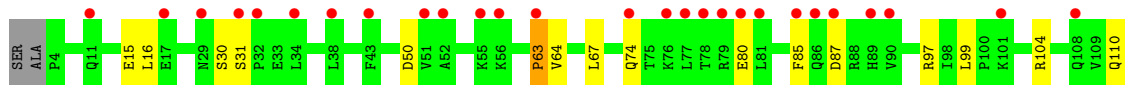
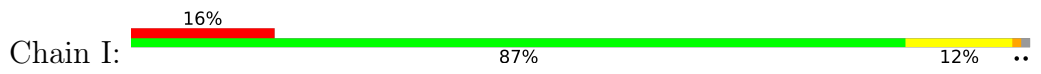
• Molecule 56: 40S ribosomal protein S6-A



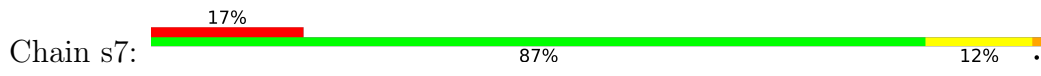
• Molecule 56: 40S ribosomal protein S6-A

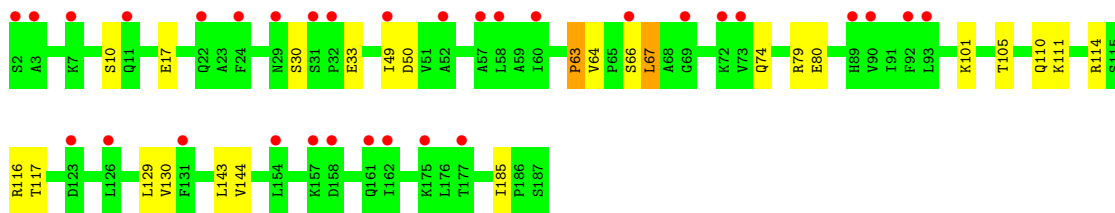


• Molecule 57: 40S ribosomal protein S7-A

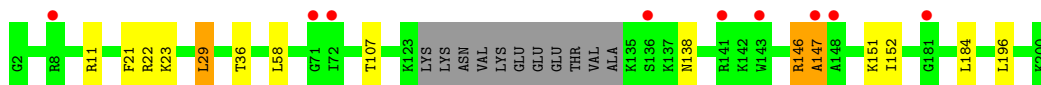
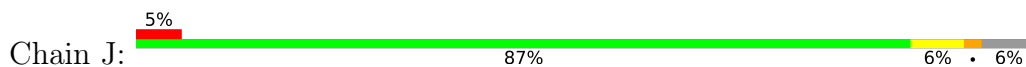


• Molecule 57: 40S ribosomal protein S7-A

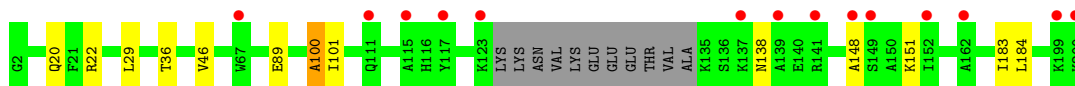
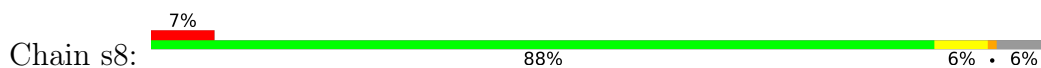




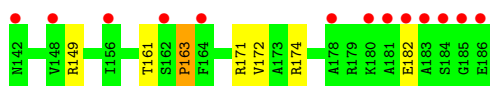
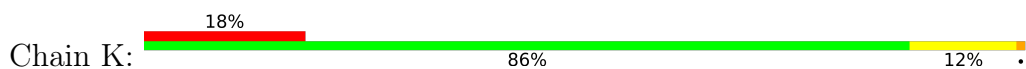
- Molecule 58: 40S ribosomal protein S8-A



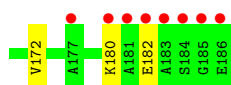
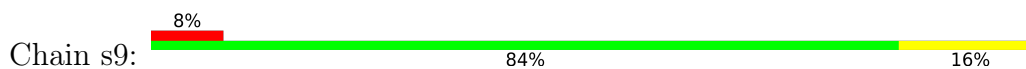
- Molecule 58: 40S ribosomal protein S8-A



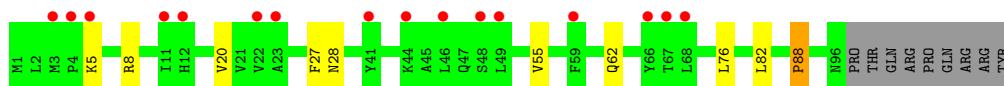
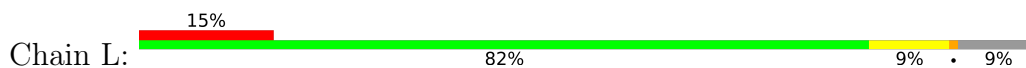
- Molecule 59: 40S ribosomal protein S9-A



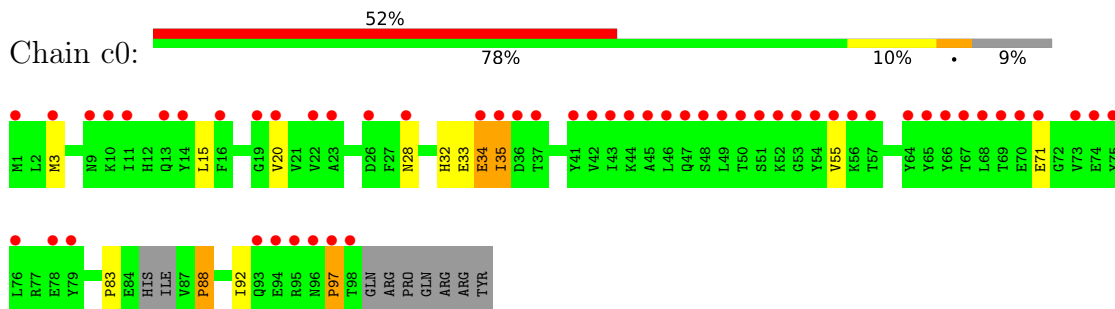
- Molecule 59: 40S ribosomal protein S9-A



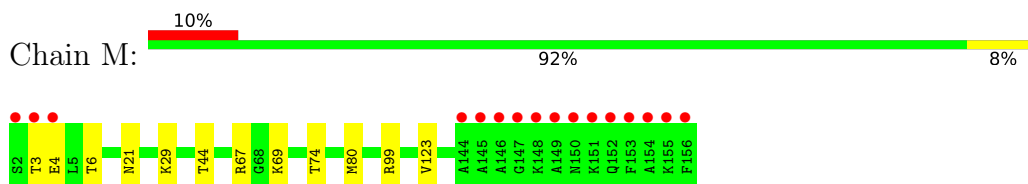
- Molecule 60: 40S ribosomal protein S10-A



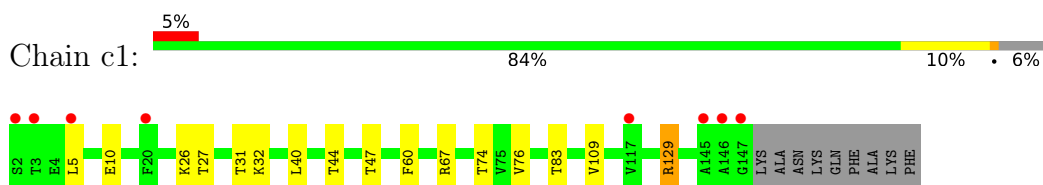
- Molecule 60: 40S ribosomal protein S10-A



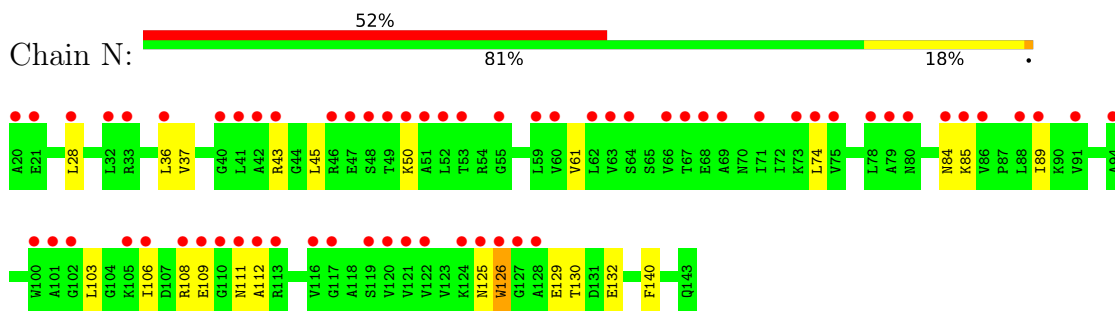
- Molecule 61: 40S ribosomal protein S11-A



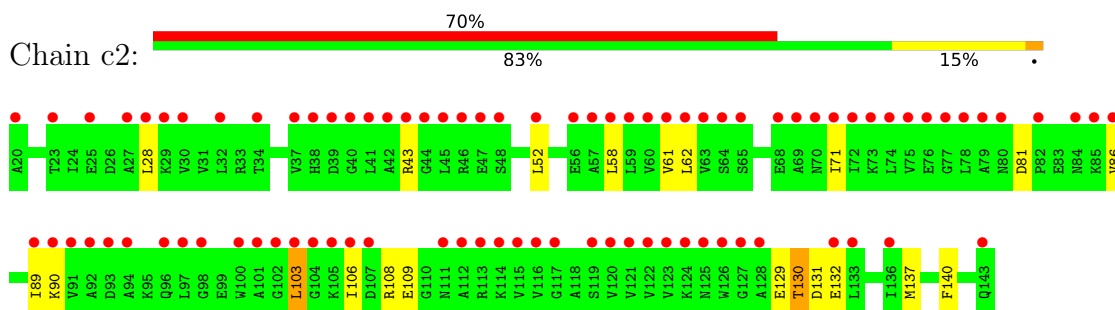
- Molecule 61: 40S ribosomal protein S11-A



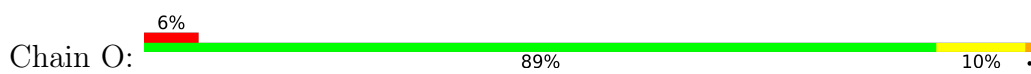
- Molecule 62: 40S ribosomal protein S12



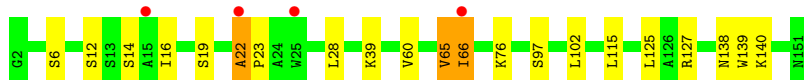
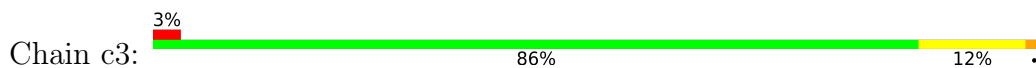
- Molecule 62: 40S ribosomal protein S12



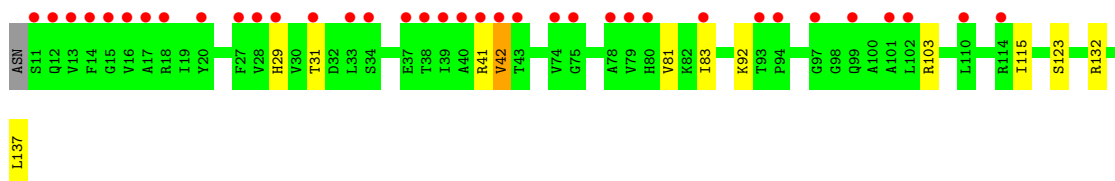
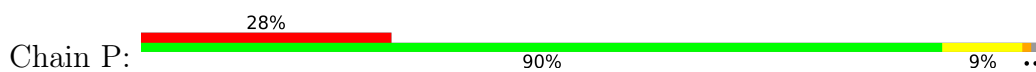
- Molecule 63: 40S ribosomal protein S13



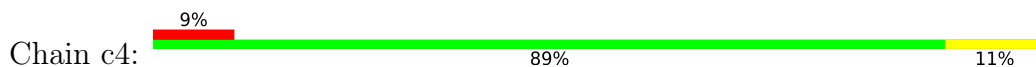
- Molecule 63: 40S ribosomal protein S13



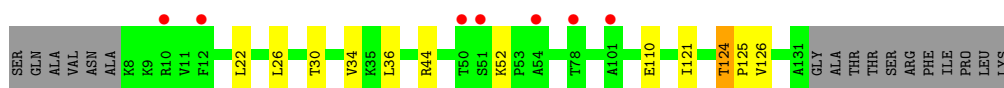
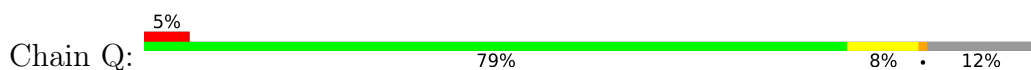
- Molecule 64: 40S ribosomal protein S14-B



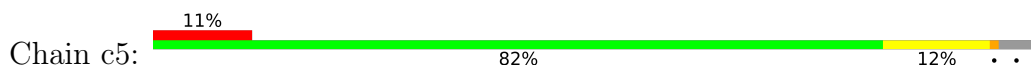
- Molecule 64: 40S ribosomal protein S14-B



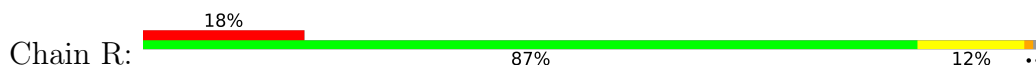
- Molecule 65: 40S ribosomal protein S15

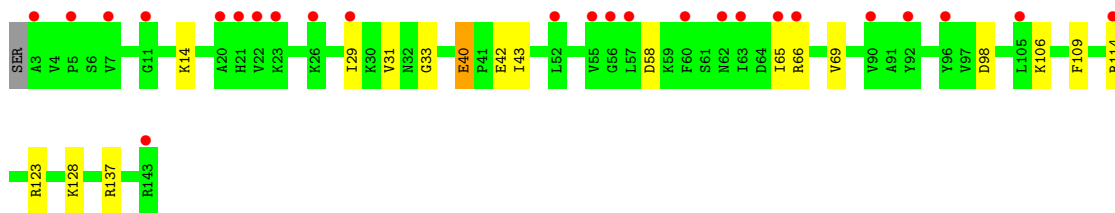


- Molecule 65: 40S ribosomal protein S15

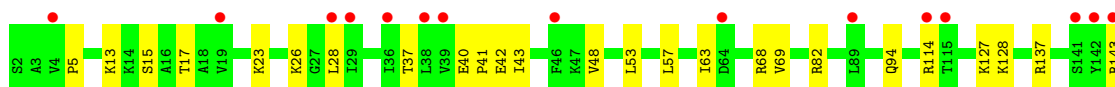
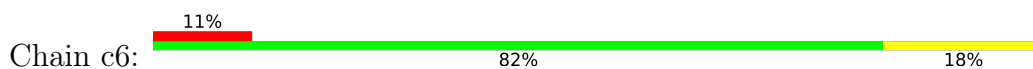


- Molecule 66: 40S ribosomal protein S16-A

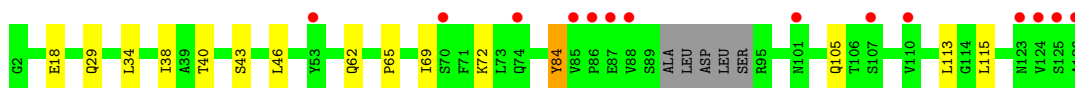
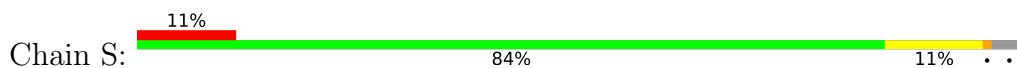




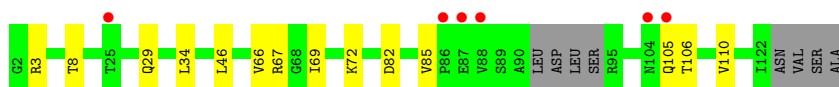
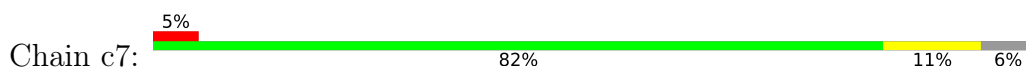
- Molecule 66: 40S ribosomal protein S16-A



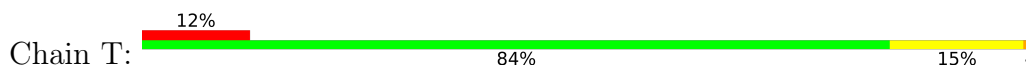
- Molecule 67: 40S ribosomal protein S17-A



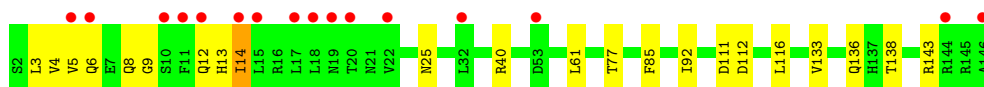
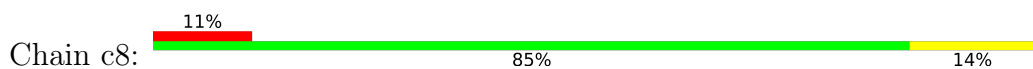
- Molecule 67: 40S ribosomal protein S17-A



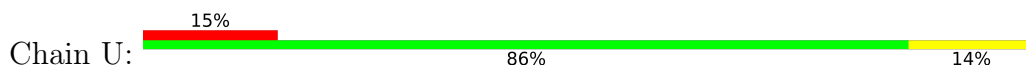
- Molecule 68: 40S ribosomal protein S18-A

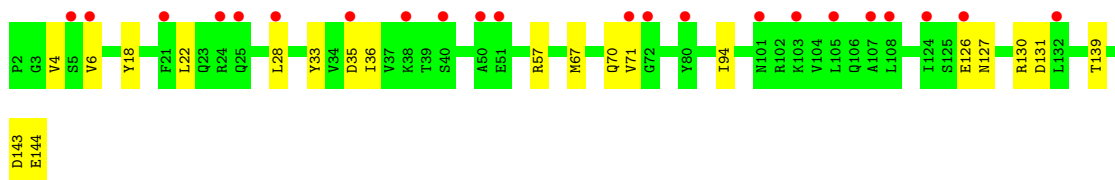


- Molecule 68: 40S ribosomal protein S18-A

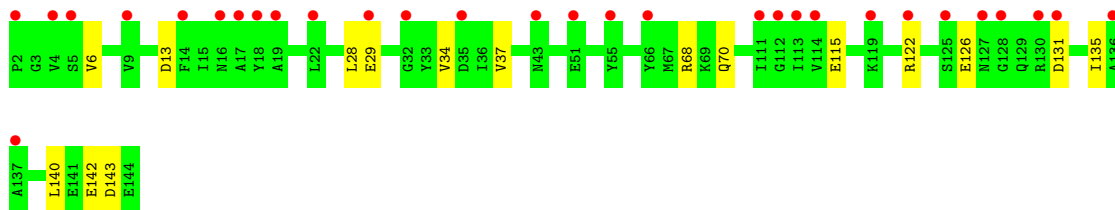
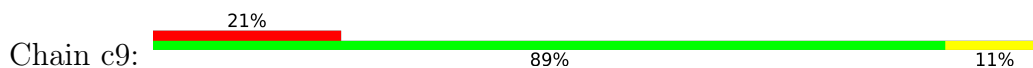


- Molecule 69: 40S ribosomal protein S19-A

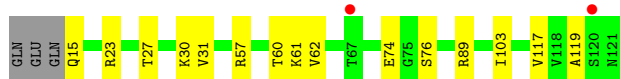
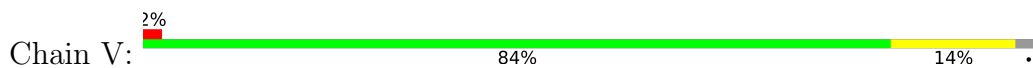




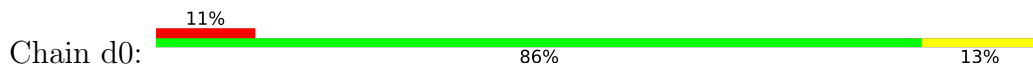
- Molecule 69: 40S ribosomal protein S19-A



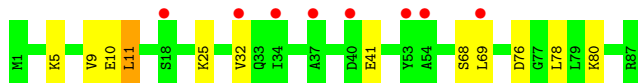
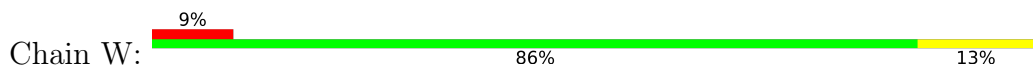
- Molecule 70: 40S ribosomal protein S20



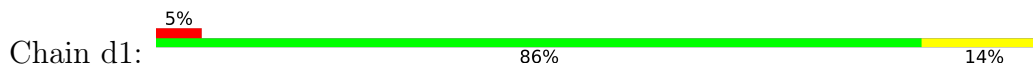
- Molecule 70: 40S ribosomal protein S20



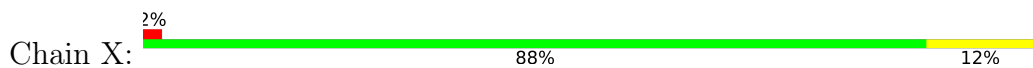
- Molecule 71: 40S ribosomal protein S21-A



- Molecule 71: 40S ribosomal protein S21-A

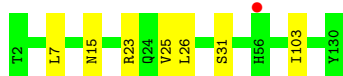


- Molecule 72: 40S ribosomal protein S22-A

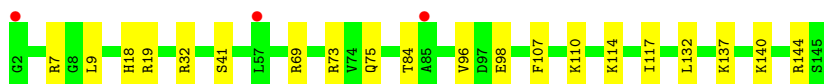
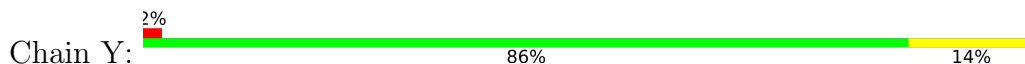




- Molecule 72: 40S ribosomal protein S22-A



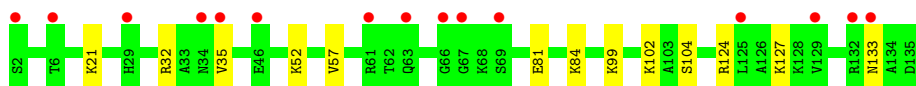
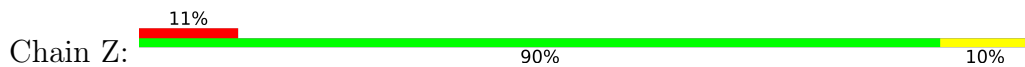
- Molecule 73: 40S ribosomal protein S23-A



- Molecule 73: 40S ribosomal protein S23-A



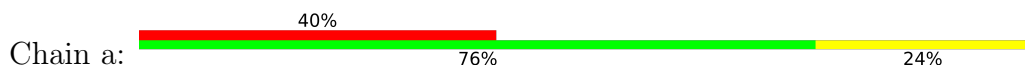
- Molecule 74: 40S ribosomal protein S24-A



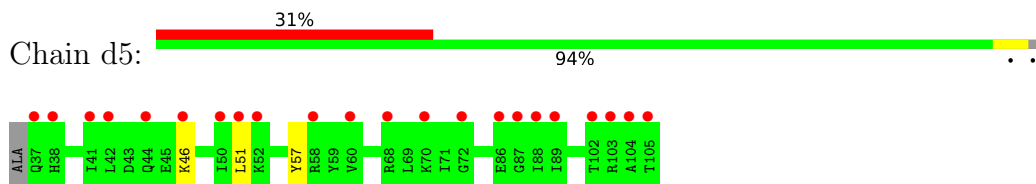
- Molecule 74: 40S ribosomal protein S24-A



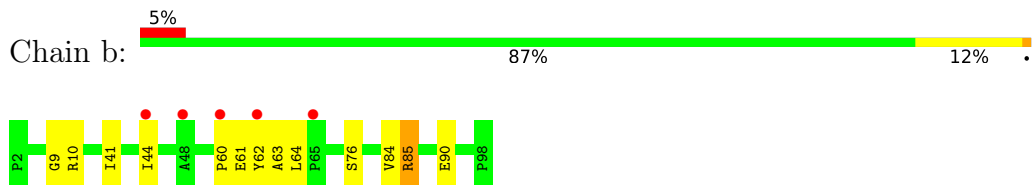
- Molecule 75: 40S ribosomal protein S25-A



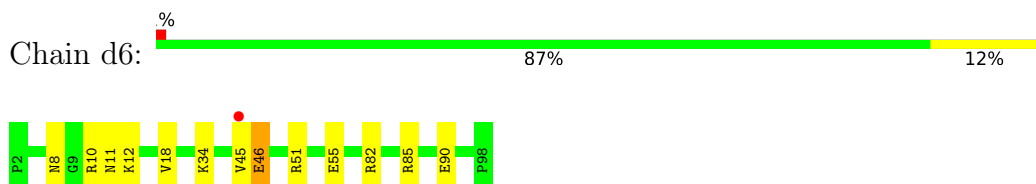
- Molecule 75: 40S ribosomal protein S25-A



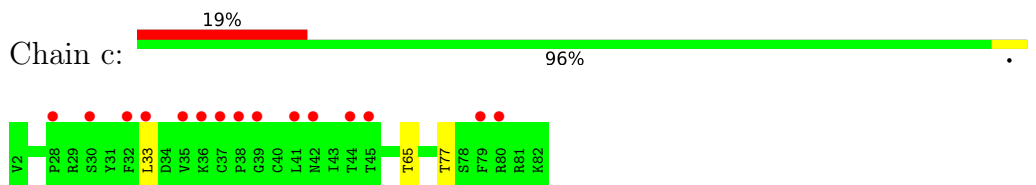
- Molecule 76: 40S ribosomal protein S26-B



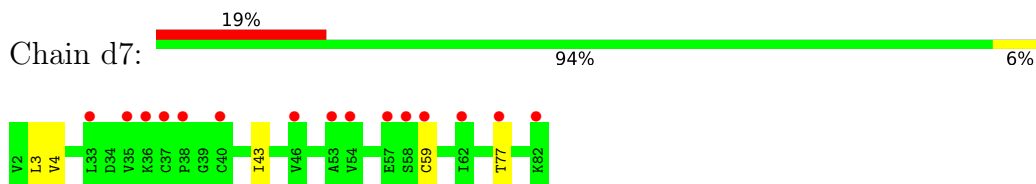
- Molecule 76: 40S ribosomal protein S26-B



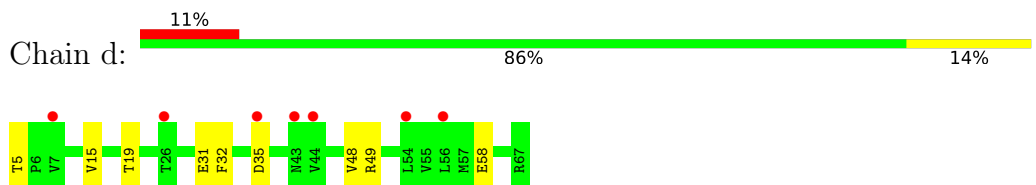
- Molecule 77: 40S ribosomal protein S27-A



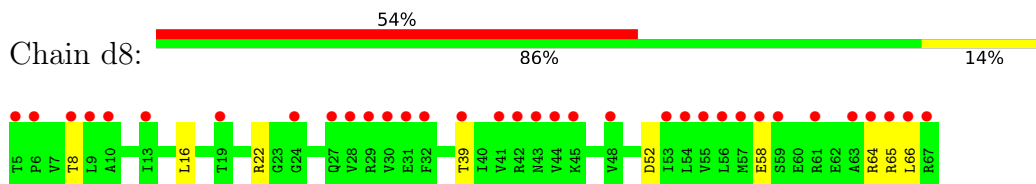
- Molecule 77: 40S ribosomal protein S27-A



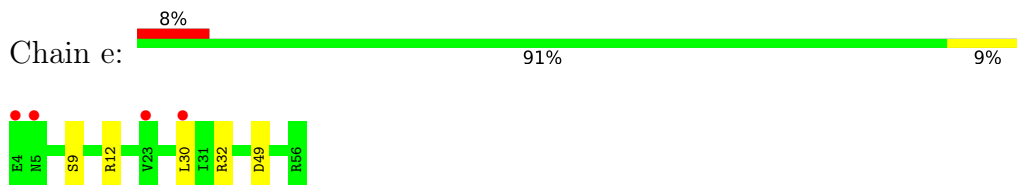
- Molecule 78: 40S ribosomal protein S28-A



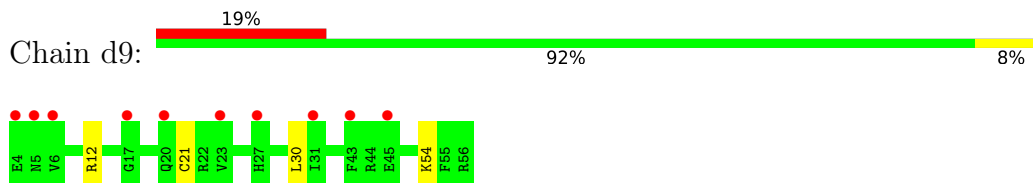
- Molecule 78: 40S ribosomal protein S28-A



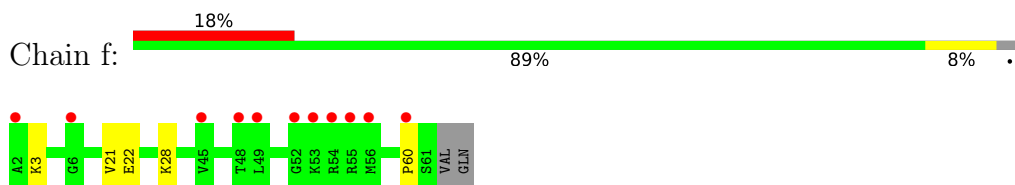
- Molecule 79: 40S ribosomal protein S29-A



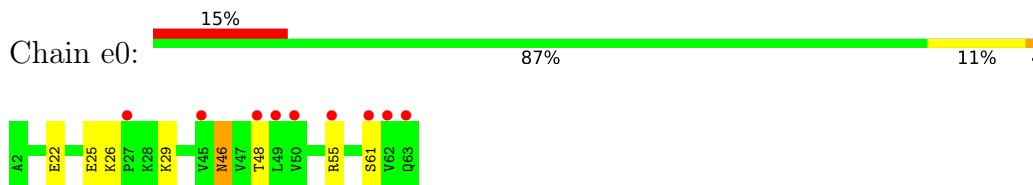
- Molecule 79: 40S ribosomal protein S29-A



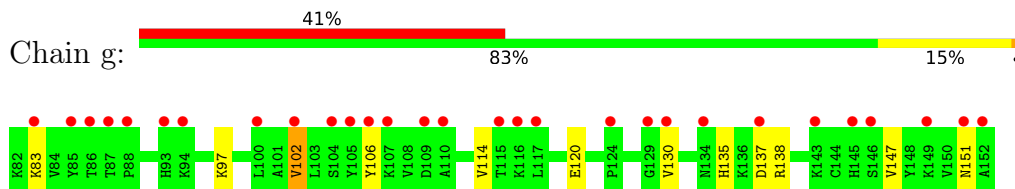
- Molecule 80: 40S ribosomal protein S30-A



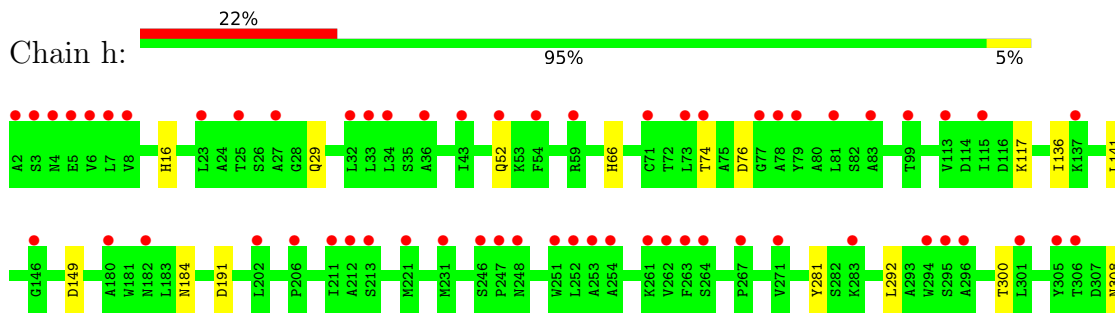
- Molecule 80: 40S ribosomal protein S30-A

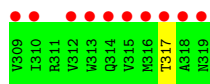


- Molecule 81: Ubiquitin-40S ribosomal protein S31

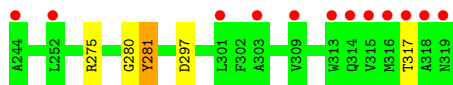


- Molecule 82: Guanine nucleotide-binding protein subunit beta-like protein

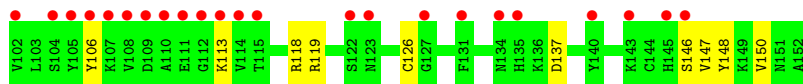
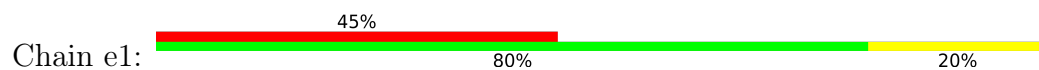




- Molecule 82: Guanine nucleotide-binding protein subunit beta-like protein



- Molecule 83: Ubiquitin-40S ribosomal protein S31



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 303.13Å 286.50Å 435.66Å 90.00° 98.87° 90.00° | Depositor |
| Resolution (Å) | 99.84 – 3.10 99.94 – 3.10 | Depositor EDS |
| % Data completeness (in resolution range) | 99.5 (99.84-3.10) 99.5 (99.94-3.10) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.64 (at 3.13Å) | Xtrriage |
| Refinement program | PHENIX dev_2450 | Depositor |
| R, R_{free} | 0.222 , 0.252 0.222 , 0.252 | Depositor DCC |
| R_{free} test set | 26196 reflections (1.99%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 67.3 | Xtrriage |
| Anisotropy | 0.134 | Xtrriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.29 , 69.9 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$ | Xtrriage |
| Estimated twinning fraction | No twinning to report. | Xtrriage |
| F_o, F_c correlation | 0.90 | EDS |
| Total number of atoms | 410383 | wwPDB-VP |
| Average B, all atoms (Å ²) | 72.0 | wwPDB-VP |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: HN8, OHX, MG, GOL, ZN

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | 1 | 0.60 | 1/75394 (0.0%) | 1.02 | 117/117545 (0.1%) |
| 1 | AR | 0.61 | 0/75394 | 1.03 | 127/117545 (0.1%) |
| 2 | 3 | 0.51 | 0/2883 | 0.88 | 0/4491 |
| 2 | AS | 0.57 | 0/2883 | 0.97 | 1/4491 (0.0%) |
| 3 | 4 | 0.57 | 0/3746 | 0.97 | 0/5832 |
| 3 | AT | 0.50 | 0/3746 | 0.90 | 2/5832 (0.0%) |
| 4 | CD | 0.36 | 0/1948 | 0.55 | 0/2617 |
| 4 | j | 0.39 | 0/1948 | 0.60 | 0/2617 |
| 5 | CE | 0.44 | 1/3146 (0.0%) | 0.61 | 0/4228 |
| 5 | k | 0.39 | 0/3146 | 0.58 | 0/4228 |
| 6 | CF | 0.40 | 1/2800 (0.0%) | 0.62 | 2/3790 (0.1%) |
| 6 | l | 0.41 | 0/2800 | 0.62 | 2/3790 (0.1%) |
| 7 | CG | 0.40 | 0/2425 | 0.55 | 0/3271 |
| 7 | m | 0.34 | 0/2425 | 0.53 | 0/3271 |
| 8 | CH | 0.41 | 0/1260 | 0.56 | 0/1694 |
| 8 | n | 0.39 | 0/1260 | 0.53 | 0/1694 |
| 9 | CI | 0.44 | 0/1821 | 0.61 | 1/2451 (0.0%) |
| 9 | o | 0.43 | 0/1821 | 0.60 | 1/2451 (0.0%) |
| 10 | CJ | 0.32 | 0/1836 | 0.48 | 0/2481 |
| 10 | p | 0.32 | 0/1836 | 0.49 | 0/2481 |
| 11 | CK | 0.40 | 0/1539 | 0.57 | 0/2073 |
| 11 | q | 0.39 | 0/1539 | 0.56 | 0/2073 |
| 12 | CL | 0.42 | 0/1741 | 0.57 | 1/2335 (0.0%) |
| 12 | r | 0.42 | 0/1741 | 0.57 | 1/2335 (0.0%) |
| 13 | CM | 0.41 | 1/1374 (0.1%) | 0.60 | 1/1842 (0.1%) |
| 13 | s | 0.33 | 0/1374 | 0.56 | 0/1842 |
| 14 | CN | 0.39 | 1/1568 (0.1%) | 0.58 | 1/2106 (0.0%) |
| 14 | t | 0.42 | 1/1568 (0.1%) | 0.57 | 0/2106 |
| 15 | CO | 0.40 | 0/1068 | 0.59 | 1/1438 (0.1%) |
| 15 | u | 0.40 | 0/1068 | 0.55 | 0/1438 |
| 16 | CP | 0.35 | 0/1757 | 0.53 | 0/2354 |
| 16 | v | 0.39 | 0/1757 | 0.58 | 0/2354 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | CQ | 0.51 | 0/1585 | 0.61 | 2/2128 (0.1%) |
| 17 | w | 0.46 | 0/1585 | 0.59 | 0/2128 |
| 18 | CR | 0.45 | 0/1443 | 0.61 | 0/1944 |
| 18 | x | 0.42 | 0/1443 | 0.61 | 1/1944 (0.1%) |
| 19 | CS | 0.41 | 0/1465 | 0.58 | 0/1965 |
| 19 | y | 0.40 | 0/1465 | 0.60 | 1/1965 (0.1%) |
| 20 | CT | 0.34 | 0/1538 | 0.49 | 0/2050 |
| 20 | z | 0.32 | 0/1538 | 0.47 | 0/2050 |
| 21 | 0 | 0.40 | 0/1481 | 0.58 | 0/1990 |
| 21 | CU | 0.44 | 0/1481 | 0.59 | 0/1990 |
| 22 | 2 | 0.40 | 0/1300 | 0.57 | 0/1743 |
| 22 | CV | 0.46 | 0/1300 | 0.58 | 0/1743 |
| 23 | 5 | 0.30 | 0/812 | 0.47 | 0/1099 |
| 23 | CW | 0.35 | 0/812 | 0.51 | 0/1099 |
| 24 | CX | 0.46 | 0/1018 | 0.59 | 0/1369 |
| 24 | IR | 0.41 | 0/1018 | 0.58 | 0/1369 |
| 25 | 6 | 0.43 | 0/42490 | 0.88 | 37/66207 (0.1%) |
| 25 | A | 0.39 | 0/42443 | 0.87 | 34/66134 (0.1%) |
| 26 | 7 | 0.35 | 0/712 | 0.50 | 0/958 |
| 26 | CY | 0.38 | 0/712 | 0.54 | 0/958 |
| 27 | 8 | 0.35 | 0/979 | 0.55 | 0/1321 |
| 27 | CZ | 0.35 | 0/979 | 0.52 | 0/1321 |
| 28 | 9 | 0.37 | 0/1004 | 0.58 | 0/1341 |
| 28 | DA | 0.38 | 0/1004 | 0.55 | 0/1341 |
| 29 | AA | 0.36 | 0/1118 | 0.50 | 0/1497 |
| 29 | DB | 0.47 | 1/1118 (0.1%) | 0.48 | 0/1497 |
| 30 | AB | 0.43 | 0/1204 | 0.64 | 0/1612 |
| 30 | DC | 0.39 | 0/1204 | 0.62 | 0/1612 |
| 31 | AC | 0.34 | 0/473 | 0.54 | 0/629 |
| 31 | DD | 0.39 | 0/473 | 0.57 | 0/629 |
| 32 | AD | 0.30 | 0/751 | 0.48 | 0/1008 |
| 32 | DE | 0.30 | 0/751 | 0.47 | 0/1008 |
| 33 | AE | 0.39 | 0/890 | 0.54 | 0/1196 |
| 33 | DF | 0.37 | 0/890 | 0.55 | 0/1196 |
| 34 | AF | 0.42 | 0/1041 | 0.59 | 0/1394 |
| 34 | DG | 0.42 | 0/1041 | 0.57 | 0/1394 |
| 35 | AG | 0.47 | 0/868 | 0.57 | 0/1168 |
| 35 | DH | 0.46 | 0/868 | 0.62 | 0/1168 |
| 36 | AH | 0.36 | 0/890 | 0.57 | 1/1189 (0.1%) |
| 36 | DI | 0.35 | 0/890 | 0.54 | 0/1189 |
| 37 | AI | 0.37 | 0/978 | 0.53 | 0/1301 |
| 37 | DJ | 0.35 | 0/978 | 0.52 | 1/1301 (0.1%) |
| 38 | AJ | 0.33 | 0/778 | 0.52 | 0/1034 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 38 | DK | 0.32 | 0/778 | 0.51 | 0/1034 |
| 39 | AK | 0.39 | 0/696 | 0.60 | 0/923 |
| 39 | DL | 0.39 | 0/696 | 0.58 | 0/923 |
| 40 | AL | 0.34 | 0/618 | 0.50 | 0/826 |
| 40 | DM | 0.32 | 0/618 | 0.49 | 0/826 |
| 41 | AM | 0.40 | 0/443 | 0.59 | 0/588 |
| 41 | DN | 0.36 | 0/443 | 0.59 | 0/588 |
| 42 | AN | 0.44 | 0/423 | 0.56 | 0/562 |
| 42 | DO | 0.43 | 0/423 | 0.60 | 0/562 |
| 43 | AO | 0.36 | 0/234 | 0.62 | 0/300 |
| 43 | DP | 0.39 | 0/234 | 0.51 | 0/300 |
| 44 | AP | 0.41 | 0/860 | 0.59 | 0/1136 |
| 44 | DQ | 0.41 | 0/860 | 0.59 | 0/1136 |
| 45 | AQ | 0.40 | 0/701 | 0.56 | 0/934 |
| 45 | DR | 0.39 | 0/701 | 0.58 | 0/934 |
| 46 | i | 0.31 | 0/1113 | 0.54 | 1/1502 (0.1%) |
| 48 | sM | 0.34 | 0/480 | 0.58 | 0/642 |
| 49 | p0 | 0.30 | 0/1091 | 0.53 | 2/1472 (0.1%) |
| 50 | B | 0.29 | 0/1617 | 0.51 | 0/2215 |
| 50 | s0 | 0.36 | 1/1623 (0.1%) | 0.49 | 0/2222 |
| 51 | C | 0.27 | 0/1735 | 0.54 | 0/2335 |
| 51 | s1 | 0.30 | 0/1748 | 0.55 | 1/2352 (0.0%) |
| 52 | D | 0.30 | 0/1665 | 0.50 | 0/2263 |
| 52 | s2 | 0.31 | 0/1665 | 0.52 | 0/2263 |
| 53 | E | 0.30 | 0/1759 | 0.51 | 0/2368 |
| 53 | s3 | 0.28 | 0/1759 | 0.50 | 0/2368 |
| 54 | F | 0.31 | 0/2109 | 0.53 | 0/2839 |
| 54 | s4 | 0.36 | 1/2109 (0.0%) | 0.52 | 0/2839 |
| 55 | G | 0.27 | 0/1629 | 0.50 | 0/2202 |
| 55 | s5 | 0.29 | 0/1629 | 0.47 | 0/2202 |
| 56 | H | 0.32 | 0/1823 | 0.51 | 1/2439 (0.0%) |
| 56 | s6 | 0.32 | 0/1779 | 0.53 | 0/2379 |
| 57 | I | 0.30 | 0/1506 | 0.52 | 0/2028 |
| 57 | s7 | 0.30 | 0/1516 | 0.51 | 0/2043 |
| 58 | J | 0.31 | 0/1514 | 0.57 | 1/2021 (0.0%) |
| 58 | s8 | 0.33 | 0/1514 | 0.53 | 0/2021 |
| 59 | K | 0.29 | 0/1519 | 0.49 | 0/2035 |
| 59 | s9 | 0.30 | 0/1519 | 0.49 | 0/2035 |
| 60 | L | 0.29 | 0/789 | 0.57 | 1/1067 (0.1%) |
| 60 | c0 | 0.27 | 0/775 | 0.62 | 3/1045 (0.3%) |
| 61 | M | 0.33 | 0/1239 | 0.52 | 0/1673 |
| 61 | c1 | 0.34 | 0/1194 | 0.52 | 0/1610 |
| 62 | N | 0.30 | 0/898 | 0.62 | 0/1220 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 62 | c2 | 0.35 | 1/898 (0.1%) | 0.62 | 1/1220 (0.1%) |
| 63 | O | 0.31 | 0/1215 | 0.49 | 0/1638 |
| 63 | c3 | 0.32 | 0/1215 | 0.53 | 0/1638 |
| 64 | P | 0.28 | 0/901 | 0.54 | 0/1217 |
| 64 | c4 | 0.32 | 0/960 | 0.55 | 0/1290 |
| 65 | Q | 0.31 | 0/998 | 0.49 | 0/1341 |
| 65 | c5 | 0.29 | 0/1060 | 0.60 | 0/1426 |
| 66 | R | 0.29 | 0/1125 | 0.55 | 0/1510 |
| 66 | c6 | 0.29 | 0/1131 | 0.54 | 0/1518 |
| 67 | S | 0.29 | 0/935 | 0.52 | 0/1254 |
| 67 | c7 | 0.28 | 0/914 | 0.48 | 0/1224 |
| 68 | T | 0.29 | 0/1211 | 0.50 | 0/1628 |
| 68 | c8 | 0.29 | 0/1211 | 0.50 | 0/1628 |
| 69 | U | 0.29 | 0/1130 | 0.46 | 0/1517 |
| 69 | c9 | 0.29 | 0/1130 | 0.46 | 0/1517 |
| 70 | V | 0.27 | 0/865 | 0.51 | 0/1169 |
| 70 | d0 | 0.29 | 0/892 | 0.52 | 0/1205 |
| 71 | W | 0.31 | 0/693 | 0.50 | 0/935 |
| 71 | d1 | 0.30 | 0/693 | 0.51 | 0/935 |
| 72 | X | 0.30 | 0/1038 | 0.55 | 0/1395 |
| 72 | d2 | 0.31 | 0/1038 | 0.52 | 0/1395 |
| 73 | Y | 0.33 | 0/1139 | 0.55 | 0/1518 |
| 73 | d3 | 0.35 | 0/1139 | 0.54 | 0/1518 |
| 74 | Z | 0.31 | 0/1087 | 0.49 | 0/1449 |
| 74 | d4 | 0.32 | 0/1087 | 0.54 | 0/1449 |
| 75 | a | 0.29 | 0/571 | 0.53 | 0/768 |
| 75 | d5 | 0.27 | 0/566 | 0.46 | 0/761 |
| 76 | b | 0.34 | 0/782 | 0.61 | 0/1047 |
| 76 | d6 | 0.33 | 0/782 | 0.60 | 0/1047 |
| 77 | c | 0.27 | 0/620 | 0.54 | 0/838 |
| 77 | d7 | 0.28 | 0/620 | 0.54 | 0/838 |
| 78 | d | 0.43 | 1/499 (0.2%) | 0.53 | 0/670 |
| 78 | d8 | 0.28 | 0/499 | 0.62 | 0/670 |
| 79 | d9 | 0.33 | 0/452 | 0.51 | 0/600 |
| 79 | e | 0.30 | 0/452 | 0.50 | 0/600 |
| 80 | e0 | 0.32 | 0/499 | 0.49 | 0/665 |
| 80 | f | 0.29 | 0/483 | 0.48 | 0/643 |
| 81 | g | 0.29 | 0/577 | 0.58 | 0/770 |
| 82 | h | 0.26 | 0/2494 | 0.49 | 0/3393 |
| 82 | sR | 0.27 | 0/2495 | 0.50 | 0/3395 |
| 83 | e1 | 0.27 | 0/404 | 0.56 | 0/542 |
| All | All | 0.47 | 11/429967 (0.0%) | 0.83 | 346/631328 (0.1%) |

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 |
|-----|-------|---------------------|---------------------|
| 5 | CE | 0 | 3 |
| 5 | k | 0 | 2 |
| 6 | l | 0 | 2 |
| 7 | CG | 0 | 3 |
| 7 | m | 0 | 1 |
| 9 | CI | 0 | 2 |
| 9 | o | 0 | 2 |
| 10 | CJ | 0 | 2 |
| 10 | p | 0 | 1 |
| 11 | CK | 0 | 1 |
| 11 | q | 0 | 1 |
| 12 | CL | 0 | 1 |
| 13 | CM | 0 | 2 |
| 13 | s | 0 | 2 |
| 14 | CN | 0 | 1 |
| 14 | t | 0 | 2 |
| 15 | CO | 0 | 1 |
| 15 | u | 0 | 1 |
| 16 | CP | 0 | 1 |
| 17 | CQ | 0 | 1 |
| 17 | w | 0 | 1 |
| 18 | x | 0 | 1 |
| 19 | CS | 0 | 1 |
| 21 | CU | 0 | 2 |
| 26 | CY | 0 | 1 |
| 29 | AA | 0 | 2 |
| 30 | DC | 0 | 2 |
| 31 | AC | 0 | 1 |
| 31 | DD | 0 | 1 |
| 37 | AI | 0 | 1 |
| 37 | DJ | 0 | 1 |
| 50 | B | 0 | 1 |
| 51 | s1 | 0 | 1 |
| 53 | E | 0 | 2 |
| 53 | s3 | 0 | 2 |
| 55 | G | 0 | 3 |
| 55 | s5 | 0 | 1 |
| 56 | H | 0 | 2 |
| 57 | I | 0 | 2 |

Continued on next page...

Continued from previous page...

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 57 | s7 | 0 | 2 |
| 58 | J | 0 | 2 |
| 58 | s8 | 0 | 2 |
| 59 | K | 0 | 1 |
| 60 | c0 | 0 | 1 |
| 61 | M | 0 | 1 |
| 62 | N | 0 | 1 |
| 62 | c2 | 0 | 2 |
| 63 | c3 | 0 | 2 |
| 64 | P | 0 | 1 |
| 64 | c4 | 0 | 2 |
| 65 | Q | 0 | 1 |
| 65 | c5 | 0 | 2 |
| 66 | R | 0 | 2 |
| 66 | c6 | 0 | 4 |
| 67 | S | 0 | 1 |
| 67 | c7 | 0 | 2 |
| 68 | T | 0 | 3 |
| 68 | c8 | 0 | 1 |
| 70 | d0 | 0 | 1 |
| 74 | d4 | 0 | 1 |
| 75 | a | 0 | 2 |
| 76 | b | 0 | 2 |
| 80 | e0 | 0 | 1 |
| 81 | g | 0 | 1 |
| 82 | sR | 0 | 1 |
| 83 | e1 | 0 | 1 |
| All | All | 0 | 103 |

All (11) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 29 | DB | 36 | HIS | C-N | 11.46 | 1.56 | 1.34 |
| 54 | s4 | 82 | TYR | C-N | -8.48 | 1.18 | 1.34 |
| 14 | t | 132 | ALA | C-N | 8.06 | 1.49 | 1.34 |
| 50 | s0 | 160 | ILE | C-N | -7.98 | 1.19 | 1.34 |
| 78 | d | 5 | THR | C-N | 7.62 | 1.48 | 1.34 |
| 62 | c2 | 81 | ASP | C-N | 6.82 | 1.47 | 1.34 |
| 5 | CE | 168 | LYS | C-N | -6.50 | 1.19 | 1.34 |
| 13 | CM | 43 | GLN | C-N | 6.35 | 1.48 | 1.34 |
| 6 | CF | 94 | CYS | CB-SG | -5.58 | 1.72 | 1.81 |
| 14 | CN | 49 | ARG | C-N | 5.20 | 1.44 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 1 | 1308 | A | N7-C5 | -5.02 | 1.36 | 1.39 |

All (346) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 1 | 3278 | C | N1-C2-O2 | 10.14 | 124.98 | 118.90 |
| 1 | 1 | 2373 | A | O5'-P-OP1 | -9.82 | 96.86 | 105.70 |
| 1 | 1 | 1308 | A | C8-N9-C4 | -8.98 | 102.21 | 105.80 |
| 1 | AR | 2846 | U | N3-C2-O2 | -8.79 | 116.05 | 122.20 |
| 1 | AR | 2714 | G | N3-C4-C5 | 8.71 | 132.95 | 128.60 |
| 1 | AR | 2870 | C | C2-N1-C1' | -8.67 | 109.26 | 118.80 |
| 1 | 1 | 3278 | C | N3-C2-O2 | -8.64 | 115.86 | 121.90 |
| 1 | 1 | 2870 | C | C2-N1-C1' | -8.61 | 109.33 | 118.80 |
| 1 | AR | 1307 | G | P-O3'-C3' | 8.57 | 129.98 | 119.70 |
| 1 | AR | 3217 | C | N1-C2-O2 | 8.51 | 124.01 | 118.90 |
| 1 | AR | 3344 | A | N7-C8-N9 | 8.48 | 118.04 | 113.80 |
| 1 | AR | 2726 | C | C6-N1-C2 | -8.34 | 116.96 | 120.30 |
| 1 | 1 | 3217 | C | C2-N1-C1' | 8.29 | 127.91 | 118.80 |
| 1 | 1 | 1308 | A | N7-C8-N9 | 8.01 | 117.81 | 113.80 |
| 1 | 1 | 1192 | C | N1-C2-O2 | 8.00 | 123.70 | 118.90 |
| 1 | 1 | 1495 | U | C5-C6-N1 | -7.96 | 118.72 | 122.70 |
| 25 | 6 | 453 | U | N1-C2-O2 | 7.92 | 128.34 | 122.80 |
| 1 | AR | 2714 | G | N3-C4-N9 | -7.89 | 121.27 | 126.00 |
| 1 | 1 | 406 | G | O4'-C1'-N9 | 7.88 | 114.51 | 108.20 |
| 1 | AR | 2846 | U | C5-C4-O4 | 7.85 | 130.61 | 125.90 |
| 1 | 1 | 3217 | C | N3-C2-O2 | -7.85 | 116.41 | 121.90 |
| 1 | 1 | 1495 | U | N1-C2-O2 | -7.85 | 117.31 | 122.80 |
| 1 | AR | 2404 | A | N1-C6-N6 | 7.82 | 123.29 | 118.60 |
| 1 | AR | 3344 | A | C8-N9-C4 | -7.77 | 102.69 | 105.80 |
| 1 | 1 | 2870 | C | C6-N1-C1' | 7.60 | 129.92 | 120.80 |
| 1 | 1 | 3217 | C | N1-C2-O2 | 7.53 | 123.42 | 118.90 |
| 1 | AR | 1149 | G | N1-C6-O6 | 7.53 | 124.42 | 119.90 |
| 1 | AR | 2871 | G | O5'-P-OP2 | -7.52 | 98.93 | 105.70 |
| 1 | 1 | 3278 | C | C2-N1-C1' | 7.51 | 127.06 | 118.80 |
| 1 | 1 | 3306 | U | C5-C4-O4 | 7.47 | 130.38 | 125.90 |
| 1 | AR | 2870 | C | C6-N1-C1' | 7.43 | 129.71 | 120.80 |
| 1 | AR | 1495 | U | C5-C6-N1 | -7.36 | 119.02 | 122.70 |
| 25 | 6 | 453 | U | C2-N1-C1' | 7.32 | 126.48 | 117.70 |
| 1 | AR | 3217 | C | C2-N1-C1' | 7.27 | 126.79 | 118.80 |
| 1 | AR | 3306 | U | N3-C2-O2 | -7.22 | 117.14 | 122.20 |
| 25 | 6 | 163 | G | N3-C4-N9 | -7.20 | 121.68 | 126.00 |
| 25 | 6 | 453 | U | N3-C2-O2 | -7.19 | 117.17 | 122.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 1 | 2846 | U | N3-C2-O2 | -7.18 | 117.17 | 122.20 |
| 1 | 1 | 1858 | A | C2-N3-C4 | 7.11 | 114.15 | 110.60 |
| 51 | s1 | 231 | LEU | CA-CB-CG | 6.98 | 131.35 | 115.30 |
| 60 | c0 | 97 | PRO | N-CA-CB | 6.97 | 111.67 | 103.30 |
| 1 | AR | 3057 | U | C5-C4-O4 | 6.95 | 130.07 | 125.90 |
| 25 | A | 553 | G | N1-C6-O6 | 6.95 | 124.07 | 119.90 |
| 25 | A | 507 | U | C2-N1-C1' | 6.91 | 125.99 | 117.70 |
| 1 | 1 | 3306 | U | N3-C2-O2 | -6.91 | 117.37 | 122.20 |
| 1 | AR | 3217 | C | N3-C2-O2 | -6.87 | 117.09 | 121.90 |
| 1 | 1 | 937 | G | C5-C6-O6 | -6.86 | 124.48 | 128.60 |
| 1 | 1 | 1269 | U | C2-N1-C1' | 6.84 | 125.91 | 117.70 |
| 25 | 6 | 1274 | C | N1-C2-O2 | 6.75 | 122.95 | 118.90 |
| 1 | AR | 2263 | C | C4-C5-C6 | -6.73 | 114.04 | 117.40 |
| 1 | AR | 3093 | C | N1-C2-O2 | -6.71 | 114.87 | 118.90 |
| 1 | 1 | 2726 | C | C6-N1-C2 | -6.69 | 117.62 | 120.30 |
| 1 | 1 | 1849 | C | O5'-P-OP1 | -6.68 | 99.69 | 105.70 |
| 60 | c0 | 88 | PRO | N-CA-CB | 6.67 | 111.30 | 103.30 |
| 1 | AR | 2726 | C | N3-C2-O2 | -6.65 | 117.24 | 121.90 |
| 25 | 6 | 1274 | C | C2-N1-C1' | 6.65 | 126.11 | 118.80 |
| 1 | AR | 2819 | A | O5'-P-OP2 | -6.64 | 99.72 | 105.70 |
| 25 | A | 577 | G | N1-C6-O6 | 6.62 | 123.87 | 119.90 |
| 1 | AR | 2808 | A | C8-N9-C4 | 6.59 | 108.44 | 105.80 |
| 1 | 1 | 3217 | C | C6-N1-C2 | -6.58 | 117.67 | 120.30 |
| 1 | 1 | 1307 | G | P-O3'-C3' | 6.57 | 127.58 | 119.70 |
| 1 | AR | 2617 | U | C4-C5-C6 | 6.57 | 123.64 | 119.70 |
| 1 | 1 | 407 | A | N1-C6-N6 | 6.56 | 122.54 | 118.60 |
| 1 | AR | 2257 | C | C2-N1-C1' | 6.55 | 126.00 | 118.80 |
| 1 | AR | 2404 | A | N7-C8-N9 | 6.55 | 117.07 | 113.80 |
| 6 | 1 | 327 | LEU | CA-CB-CG | 6.50 | 130.26 | 115.30 |
| 25 | A | 553 | G | C5-C6-O6 | -6.49 | 124.71 | 128.60 |
| 25 | A | 728 | U | C2-N1-C1' | 6.47 | 125.46 | 117.70 |
| 1 | 1 | 2726 | C | C5-C4-N4 | 6.45 | 124.72 | 120.20 |
| 25 | A | 577 | G | C5-C6-O6 | -6.45 | 124.73 | 128.60 |
| 1 | AR | 1495 | U | C5-C4-O4 | 6.43 | 129.76 | 125.90 |
| 1 | AR | 2272 | G | O4'-C1'-N9 | 6.43 | 113.35 | 108.20 |
| 1 | 1 | 2620 | G | N1-C6-O6 | 6.42 | 123.75 | 119.90 |
| 25 | A | 639 | U | N3-C2-O2 | -6.41 | 117.71 | 122.20 |
| 1 | 1 | 3306 | U | N3-C4-O4 | -6.40 | 114.92 | 119.40 |
| 25 | 6 | 813 | U | N1-C2-O2 | 6.40 | 127.28 | 122.80 |
| 1 | AR | 3344 | A | C5-N7-C8 | -6.38 | 100.71 | 103.90 |
| 1 | 1 | 1192 | C | C2-N1-C1' | 6.38 | 125.81 | 118.80 |
| 1 | AR | 2870 | C | N3-C4-C5 | 6.37 | 124.45 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 1 | 1160 | C | C6-N1-C2 | 6.37 | 122.85 | 120.30 |
| 1 | 1 | 2827 | U | C5-C6-N1 | -6.37 | 119.52 | 122.70 |
| 25 | A | 507 | U | N1-C2-O2 | 6.34 | 127.24 | 122.80 |
| 49 | p0 | 278 | PRO | N-CA-CB | 6.33 | 110.89 | 103.30 |
| 1 | 1 | 1556 | C | N1-C2-O2 | 6.32 | 122.69 | 118.90 |
| 25 | A | 507 | U | N3-C2-O2 | -6.31 | 117.78 | 122.20 |
| 1 | 1 | 2870 | C | N1-C2-O2 | -6.31 | 115.12 | 118.90 |
| 1 | 1 | 65 | A | P-O3'-C3' | 6.29 | 127.25 | 119.70 |
| 60 | L | 88 | PRO | N-CA-CB | 6.26 | 110.81 | 103.30 |
| 25 | 6 | 813 | U | C2-N1-C1' | 6.25 | 125.21 | 117.70 |
| 1 | 1 | 1495 | U | N1-C2-N3 | 6.25 | 118.65 | 114.90 |
| 1 | 1 | 3278 | C | C6-N1-C2 | -6.22 | 117.81 | 120.30 |
| 1 | AR | 1311 | G | O5'-P-OP2 | -6.21 | 100.11 | 105.70 |
| 56 | H | 69 | LEU | CA-CB-CG | 6.20 | 129.56 | 115.30 |
| 6 | CF | 182 | LEU | CA-CB-CG | 6.20 | 129.56 | 115.30 |
| 1 | 1 | 3181 | C | N3-C2-O2 | -6.17 | 117.58 | 121.90 |
| 1 | 1 | 1495 | U | C2-N1-C1' | -6.16 | 110.31 | 117.70 |
| 1 | 1 | 353 | G | C5-C6-O6 | -6.15 | 124.91 | 128.60 |
| 1 | AR | 2257 | C | C6-N1-C2 | -6.14 | 117.84 | 120.30 |
| 25 | A | 959 | U | C2-N1-C1' | 6.14 | 125.07 | 117.70 |
| 1 | AR | 3309 | G | N3-C4-N9 | 6.14 | 129.68 | 126.00 |
| 1 | AR | 3057 | U | N3-C2-O2 | -6.13 | 117.91 | 122.20 |
| 12 | r | 57 | LEU | CA-CB-CG | 6.12 | 129.37 | 115.30 |
| 1 | 1 | 2281 | A | O4'-C1'-N9 | 6.09 | 113.07 | 108.20 |
| 1 | AR | 3309 | G | C4-N9-C1' | 6.09 | 134.41 | 126.50 |
| 1 | AR | 2899 | C | C6-N1-C2 | -6.08 | 117.87 | 120.30 |
| 46 | i | 254 | PRO | N-CA-CB | 6.07 | 110.58 | 103.30 |
| 1 | AR | 637 | C | C6-N1-C2 | -6.06 | 117.88 | 120.30 |
| 25 | A | 1389 | C | C2-N1-C1' | 6.06 | 125.46 | 118.80 |
| 1 | AR | 1495 | U | C4-C5-C6 | 6.04 | 123.33 | 119.70 |
| 14 | CN | 46 | ILE | C-N-CA | 6.04 | 136.81 | 121.70 |
| 1 | AR | 3057 | U | N3-C4-O4 | -6.04 | 115.17 | 119.40 |
| 1 | 1 | 2257 | C | C2-N1-C1' | 6.03 | 125.43 | 118.80 |
| 1 | AR | 2950 | G | O4'-C1'-N9 | 6.03 | 113.02 | 108.20 |
| 25 | 6 | 1389 | C | C2-N1-C1' | 6.02 | 125.42 | 118.80 |
| 1 | AR | 637 | C | C2-N1-C1' | 6.02 | 125.42 | 118.80 |
| 1 | 1 | 1329 | U | C2-N1-C1' | 6.01 | 124.91 | 117.70 |
| 1 | 1 | 3344 | A | N7-C8-N9 | 5.99 | 116.79 | 113.80 |
| 1 | AR | 1103 | A | O4'-C1'-N9 | 5.98 | 112.98 | 108.20 |
| 1 | AR | 2726 | C | C5-C4-N4 | 5.96 | 124.37 | 120.20 |
| 1 | 1 | 2355 | G | N1-C6-O6 | 5.95 | 123.47 | 119.90 |
| 1 | 1 | 1820 | U | P-O3'-C3' | 5.95 | 126.84 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AR | 2343 | C | C6-N1-C2 | 5.94 | 122.68 | 120.30 |
| 1 | AR | 437 | G | N7-C8-N9 | 5.94 | 116.07 | 113.10 |
| 1 | AR | 2846 | U | N3-C4-O4 | -5.93 | 115.25 | 119.40 |
| 1 | AR | 2714 | G | C2-N3-C4 | -5.91 | 108.94 | 111.90 |
| 25 | A | 1274 | C | C6-N1-C2 | -5.91 | 117.94 | 120.30 |
| 1 | AR | 2404 | A | C5-N7-C8 | -5.90 | 100.95 | 103.90 |
| 1 | 1 | 1269 | U | N1-C2-O2 | 5.90 | 126.93 | 122.80 |
| 25 | A | 1560 | U | N3-C2-O2 | -5.90 | 118.07 | 122.20 |
| 25 | 6 | 163 | G | N3-C4-C5 | 5.89 | 131.54 | 128.60 |
| 1 | AR | 2996 | U | N1-C2-O2 | 5.88 | 126.92 | 122.80 |
| 1 | 1 | 1858 | A | C8-N9-C4 | -5.87 | 103.45 | 105.80 |
| 49 | p0 | 290 | PRO | N-CA-CB | 5.84 | 110.31 | 103.30 |
| 25 | A | 728 | U | N1-C2-O2 | 5.82 | 126.88 | 122.80 |
| 1 | 1 | 835 | G | O4'-C1'-N9 | 5.82 | 112.86 | 108.20 |
| 17 | CQ | 68 | ARG | NE-CZ-NH1 | -5.81 | 117.40 | 120.30 |
| 1 | AR | 3309 | G | C6-C5-N7 | -5.80 | 126.92 | 130.40 |
| 1 | AR | 637 | C | P-O3'-C3' | 5.79 | 126.65 | 119.70 |
| 1 | AR | 2899 | C | N3-C2-O2 | -5.79 | 117.85 | 121.90 |
| 1 | 1 | 3214 | U | N3-C2-O2 | -5.79 | 118.15 | 122.20 |
| 1 | AR | 2385 | G | N3-C4-C5 | 5.79 | 131.49 | 128.60 |
| 1 | 1 | 1858 | A | N3-C4-C5 | -5.78 | 122.76 | 126.80 |
| 1 | AR | 2404 | A | C6-C5-N7 | -5.77 | 128.26 | 132.30 |
| 25 | 6 | 795 | U | N3-C2-O2 | -5.76 | 118.17 | 122.20 |
| 25 | A | 720 | G | OP1-P-O3' | 5.76 | 117.86 | 105.20 |
| 1 | 1 | 895 | A | N1-C6-N6 | 5.75 | 122.05 | 118.60 |
| 1 | 1 | 2714 | G | N3-C4-C5 | 5.75 | 131.47 | 128.60 |
| 1 | AR | 637 | C | C5-C6-N1 | 5.74 | 123.87 | 121.00 |
| 25 | A | 959 | U | N3-C2-O2 | -5.72 | 118.19 | 122.20 |
| 1 | 1 | 1556 | C | N3-C2-O2 | -5.72 | 117.90 | 121.90 |
| 1 | AR | 407 | A | N1-C6-N6 | 5.71 | 122.03 | 118.60 |
| 25 | 6 | 965 | U | N1-C2-O2 | 5.70 | 126.79 | 122.80 |
| 1 | AR | 1556 | C | C2-N1-C1' | 5.70 | 125.07 | 118.80 |
| 1 | AR | 1149 | G | C5-C6-O6 | -5.70 | 125.18 | 128.60 |
| 1 | 1 | 1581 | C | N1-C2-O2 | 5.69 | 122.32 | 118.90 |
| 1 | AR | 2662 | G | N1-C6-O6 | -5.69 | 116.49 | 119.90 |
| 1 | 1 | 895 | A | C6-C5-N7 | -5.68 | 128.32 | 132.30 |
| 1 | 1 | 2871 | G | O5'-P-OP2 | -5.68 | 100.58 | 105.70 |
| 25 | A | 453 | U | C2-N1-C1' | 5.68 | 124.52 | 117.70 |
| 25 | A | 959 | U | N1-C2-O2 | 5.68 | 126.78 | 122.80 |
| 1 | 1 | 2169 | G | N1-C6-O6 | -5.67 | 116.50 | 119.90 |
| 1 | AR | 3344 | A | O4'-C1'-N9 | 5.67 | 112.73 | 108.20 |
| 1 | 1 | 2808 | A | N1-C6-N6 | 5.66 | 122.00 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 25 | A | 1456 | C | C2-N1-C1' | 5.66 | 125.03 | 118.80 |
| 1 | 1 | 3344 | A | O4'-C1'-N9 | 5.66 | 112.73 | 108.20 |
| 15 | CO | 72 | LEU | CA-CB-CG | 5.65 | 128.29 | 115.30 |
| 1 | 1 | 218 | G | O5'-P-OP2 | -5.64 | 100.62 | 105.70 |
| 25 | A | 639 | U | N1-C2-O2 | 5.64 | 126.75 | 122.80 |
| 25 | A | 1698 | G | P-O3'-C3' | 5.62 | 126.44 | 119.70 |
| 1 | AR | 1103 | A | P-O3'-C3' | 5.62 | 126.44 | 119.70 |
| 1 | AR | 2617 | U | C5-C6-N1 | -5.62 | 119.89 | 122.70 |
| 1 | 1 | 2314 | U | C5-C4-O4 | -5.59 | 122.55 | 125.90 |
| 1 | 1 | 1149 | G | N1-C6-O6 | 5.58 | 123.25 | 119.90 |
| 25 | A | 1039 | A | O4'-C1'-N9 | 5.57 | 112.66 | 108.20 |
| 1 | 1 | 2899 | C | C6-N1-C2 | -5.57 | 118.07 | 120.30 |
| 25 | A | 75 | U | N1-C2-O2 | 5.56 | 126.69 | 122.80 |
| 1 | 1 | 2726 | C | N3-C2-O2 | -5.55 | 118.01 | 121.90 |
| 1 | 1 | 770 | G | O4'-C1'-N9 | 5.55 | 112.64 | 108.20 |
| 1 | AR | 2808 | A | N9-C4-C5 | -5.54 | 103.58 | 105.80 |
| 1 | 1 | 1377 | G | C5-C6-O6 | -5.53 | 125.28 | 128.60 |
| 1 | AR | 2714 | G | C5-N7-C8 | -5.53 | 101.53 | 104.30 |
| 1 | AR | 2334 | U | N3-C2-O2 | -5.53 | 118.33 | 122.20 |
| 1 | AR | 3309 | G | C8-N9-C1' | -5.51 | 119.84 | 127.00 |
| 25 | 6 | 337 | G | C4-N9-C1' | 5.50 | 133.66 | 126.50 |
| 1 | AR | 2358 | A | C8-N9-C4 | 5.50 | 108.00 | 105.80 |
| 1 | 1 | 2627 | C | C6-N1-C2 | 5.49 | 122.50 | 120.30 |
| 1 | AR | 3212 | C | N1-C2-O2 | -5.49 | 115.61 | 118.90 |
| 1 | AR | 2870 | C | N1-C2-O2 | -5.48 | 115.61 | 118.90 |
| 1 | 1 | 979 | U | P-O3'-C3' | 5.48 | 126.27 | 119.70 |
| 25 | 6 | 1473 | U | C2-N1-C1' | 5.47 | 124.27 | 117.70 |
| 25 | 6 | 1473 | U | N1-C2-O2 | 5.47 | 126.63 | 122.80 |
| 1 | AR | 3217 | C | C6-N1-C1' | -5.46 | 114.24 | 120.80 |
| 1 | AR | 3181 | C | N3-C2-O2 | -5.46 | 118.08 | 121.90 |
| 1 | AR | 2281 | A | O4'-C1'-N9 | 5.46 | 112.56 | 108.20 |
| 1 | AR | 1588 | A | N1-C6-N6 | -5.45 | 115.33 | 118.60 |
| 25 | 6 | 1097 | U | P-O3'-C3' | 5.45 | 126.24 | 119.70 |
| 60 | c0 | 83 | PRO | N-CA-CB | 5.45 | 109.84 | 103.30 |
| 1 | 1 | 2550 | U | N1-C2-O2 | 5.45 | 126.61 | 122.80 |
| 1 | 1 | 2944 | U | C5-C4-O4 | -5.45 | 122.63 | 125.90 |
| 1 | AR | 979 | U | P-O3'-C3' | 5.45 | 126.23 | 119.70 |
| 25 | 6 | 1473 | U | N3-C2-O2 | -5.44 | 118.39 | 122.20 |
| 1 | AR | 1605 | A | O4'-C1'-N9 | 5.44 | 112.55 | 108.20 |
| 1 | 1 | 2286 | U | O5'-P-OP2 | -5.44 | 100.81 | 105.70 |
| 1 | AR | 2617 | U | N3-C2-O2 | -5.44 | 118.39 | 122.20 |
| 25 | A | 1761 | U | P-O3'-C3' | 5.44 | 126.22 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 1 | 3057 | U | N3-C2-O2 | -5.43 | 118.40 | 122.20 |
| 1 | AR | 2263 | C | N3-C4-C5 | 5.43 | 124.07 | 121.90 |
| 1 | 1 | 646 | A | O5'-P-OP2 | -5.43 | 100.82 | 105.70 |
| 25 | 6 | 610 | G | C4-N9-C1' | 5.42 | 133.55 | 126.50 |
| 25 | 6 | 1000 | C | C2-N1-C1' | 5.42 | 124.77 | 118.80 |
| 25 | 6 | 1389 | C | N1-C2-O2 | 5.42 | 122.16 | 118.90 |
| 1 | AR | 2816 | G | C8-N9-C4 | 5.42 | 108.57 | 106.40 |
| 17 | CQ | 84 | LEU | CB-CG-CD1 | -5.42 | 101.79 | 111.00 |
| 1 | AR | 881 | C | N1-C2-O2 | 5.42 | 122.15 | 118.90 |
| 1 | 1 | 2374 | C | N3-C2-O2 | -5.41 | 118.11 | 121.90 |
| 25 | A | 1241 | G | O4'-C1'-N9 | 5.41 | 112.53 | 108.20 |
| 25 | A | 1370 | U | P-O3'-C3' | 5.41 | 126.19 | 119.70 |
| 25 | 6 | 25 | C | P-O3'-C3' | 5.41 | 126.19 | 119.70 |
| 1 | 1 | 776 | U | C4-C5-C6 | 5.40 | 122.94 | 119.70 |
| 1 | 1 | 1556 | C | C2-N1-C1' | 5.40 | 124.74 | 118.80 |
| 1 | AR | 895 | A | C6-C5-N7 | -5.40 | 128.52 | 132.30 |
| 1 | 1 | 937 | G | N1-C6-O6 | 5.40 | 123.14 | 119.90 |
| 1 | 1 | 66 | A | O5'-P-OP1 | -5.39 | 100.85 | 105.70 |
| 1 | 1 | 1604 | G | C4-N9-C1' | 5.39 | 133.51 | 126.50 |
| 1 | AR | 65 | A | P-O3'-C3' | 5.39 | 126.17 | 119.70 |
| 1 | AR | 3057 | U | N1-C2-N3 | 5.39 | 118.14 | 114.90 |
| 25 | 6 | 1560 | U | C2-N1-C1' | 5.39 | 124.16 | 117.70 |
| 1 | AR | 2541 | U | P-O3'-C3' | 5.38 | 126.16 | 119.70 |
| 1 | AR | 406 | G | O4'-C1'-N9 | 5.38 | 112.50 | 108.20 |
| 1 | AR | 1097 | G | P-O3'-C3' | 5.38 | 126.16 | 119.70 |
| 25 | A | 610 | G | C4-N9-C1' | 5.38 | 133.49 | 126.50 |
| 1 | 1 | 3217 | C | C6-N1-C1' | -5.37 | 114.35 | 120.80 |
| 1 | AR | 3344 | A | C6-C5-N7 | -5.37 | 128.54 | 132.30 |
| 1 | 1 | 1367 | G | N1-C6-O6 | 5.36 | 123.12 | 119.90 |
| 9 | o | 179 | LEU | CA-CB-CG | 5.35 | 127.61 | 115.30 |
| 1 | AR | 1495 | U | N1-C2-N3 | 5.35 | 118.11 | 114.90 |
| 25 | A | 158 | U | P-O3'-C3' | 5.35 | 126.12 | 119.70 |
| 25 | 6 | 158 | U | P-O3'-C3' | 5.35 | 126.12 | 119.70 |
| 36 | AH | 51 | LEU | CA-CB-CG | 5.35 | 127.60 | 115.30 |
| 1 | AR | 1192 | C | N1-C2-O2 | 5.34 | 122.10 | 118.90 |
| 1 | AR | 1886 | A | O5'-P-OP2 | -5.34 | 100.89 | 105.70 |
| 1 | 1 | 1269 | U | N3-C2-O2 | -5.33 | 118.47 | 122.20 |
| 1 | AR | 2273 | G | C8-N9-C4 | 5.33 | 108.53 | 106.40 |
| 1 | 1 | 353 | G | N1-C6-O6 | 5.33 | 123.10 | 119.90 |
| 1 | AR | 437 | G | C8-N9-C4 | -5.33 | 104.27 | 106.40 |
| 1 | 1 | 1114 | U | N1-C2-O2 | 5.32 | 126.52 | 122.80 |
| 25 | 6 | 1773 | C | N3-C4-C5 | -5.31 | 119.78 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 1 | 422 | A | N1-C6-N6 | -5.31 | 115.41 | 118.60 |
| 1 | AR | 2257 | C | O4'-C1'-N1 | 5.30 | 112.44 | 108.20 |
| 1 | 1 | 1495 | U | C4-C5-C6 | 5.30 | 122.88 | 119.70 |
| 25 | A | 1196 | A | P-O3'-C3' | 5.30 | 126.06 | 119.70 |
| 25 | 6 | 542 | A | P-O3'-C3' | 5.30 | 126.06 | 119.70 |
| 1 | 1 | 1196 | C | C6-N1-C2 | 5.29 | 122.42 | 120.30 |
| 1 | AR | 1556 | C | N1-C2-O2 | 5.29 | 122.07 | 118.90 |
| 25 | 6 | 1137 | A | C8-N9-C4 | 5.27 | 107.91 | 105.80 |
| 1 | 1 | 497 | C | N1-C2-O2 | -5.27 | 115.74 | 118.90 |
| 1 | AR | 2679 | A | C2-N3-C4 | -5.27 | 107.97 | 110.60 |
| 1 | 1 | 3275 | U | OP1-P-O3' | 5.26 | 116.78 | 105.20 |
| 25 | 6 | 610 | G | C8-N9-C1' | -5.26 | 120.16 | 127.00 |
| 13 | CM | 172 | LEU | C-N-CA | 5.26 | 134.85 | 121.70 |
| 1 | AR | 3309 | G | N3-C4-C5 | -5.26 | 125.97 | 128.60 |
| 1 | 1 | 3362 | A | O4'-C1'-N9 | 5.25 | 112.40 | 108.20 |
| 1 | 1 | 651 | G | N3-C4-N9 | 5.25 | 129.15 | 126.00 |
| 19 | y | 41 | ASP | CB-CG-OD1 | 5.25 | 123.02 | 118.30 |
| 1 | 1 | 1897 | G | C5-C6-O6 | -5.25 | 125.45 | 128.60 |
| 1 | AR | 2899 | C | N3-C4-C5 | -5.24 | 119.80 | 121.90 |
| 1 | 1 | 922 | U | N1-C2-O2 | 5.23 | 126.46 | 122.80 |
| 25 | 6 | 1058 | U | OP1-P-O3' | 5.23 | 116.70 | 105.20 |
| 1 | AR | 1149 | G | C4-C5-C6 | 5.22 | 121.93 | 118.80 |
| 6 | 1 | 313 | LEU | CA-CB-CG | 5.22 | 127.31 | 115.30 |
| 1 | AR | 878 | G | C8-N9-C4 | -5.22 | 104.31 | 106.40 |
| 1 | 1 | 2550 | U | N3-C2-O2 | -5.22 | 118.55 | 122.20 |
| 1 | 1 | 936 | A | P-O3'-C3' | 5.22 | 125.96 | 119.70 |
| 1 | AR | 2943 | G | N1-C6-O6 | 5.21 | 123.03 | 119.90 |
| 37 | DJ | 28 | LEU | CA-CB-CG | 5.21 | 127.29 | 115.30 |
| 25 | 6 | 1573 | A | P-O3'-C3' | 5.21 | 125.95 | 119.70 |
| 25 | A | 581 | U | C2-N1-C1' | 5.21 | 123.95 | 117.70 |
| 25 | A | 720 | G | P-O3'-C3' | 5.21 | 125.95 | 119.70 |
| 1 | 1 | 2358 | A | N1-C6-N6 | 5.21 | 121.72 | 118.60 |
| 1 | AR | 1858 | A | C4-N9-C1' | 5.20 | 135.66 | 126.30 |
| 1 | AR | 3306 | U | N3-C4-O4 | -5.19 | 115.77 | 119.40 |
| 1 | 1 | 2827 | U | C2-N3-C4 | -5.18 | 123.89 | 127.00 |
| 1 | AR | 942 | U | N3-C4-O4 | 5.18 | 123.03 | 119.40 |
| 58 | J | 29 | LEU | CA-CB-CG | 5.18 | 127.21 | 115.30 |
| 3 | AT | 82 | U | C2-N1-C1' | 5.18 | 123.91 | 117.70 |
| 1 | 1 | 2585 | G | N3-C4-C5 | -5.18 | 126.01 | 128.60 |
| 1 | 1 | 3344 | A | C8-N9-C4 | -5.17 | 103.73 | 105.80 |
| 1 | AR | 1521 | G | N1-C6-O6 | -5.17 | 116.80 | 119.90 |
| 1 | 1 | 1904 | C | C6-N1-C2 | -5.16 | 118.23 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2 | AS | 101 | G | N1-C6-O6 | 5.16 | 122.99 | 119.90 |
| 1 | AR | 3214 | U | C2-N1-C1' | 5.16 | 123.89 | 117.70 |
| 62 | c2 | 103 | LEU | CA-CB-CG | 5.16 | 127.16 | 115.30 |
| 1 | AR | 1496 | C | C2-N1-C1' | 5.15 | 124.47 | 118.80 |
| 1 | AR | 800 | G | N3-C4-N9 | 5.15 | 129.09 | 126.00 |
| 1 | 1 | 2418 | G | OP1-P-O3' | 5.14 | 116.51 | 105.20 |
| 25 | A | 831 | U | C5-C6-N1 | 5.14 | 125.27 | 122.70 |
| 25 | 6 | 1000 | C | N3-C2-O2 | -5.14 | 118.30 | 121.90 |
| 25 | A | 1060 | U | N1-C2-O2 | 5.13 | 126.39 | 122.80 |
| 18 | x | 41 | LEU | CA-CB-CG | 5.13 | 127.10 | 115.30 |
| 1 | 1 | 1897 | G | C6-C5-N7 | -5.13 | 127.32 | 130.40 |
| 1 | 1 | 3277 | U | N3-C2-O2 | -5.13 | 118.61 | 122.20 |
| 1 | AR | 1151 | U | N3-C2-O2 | 5.13 | 125.79 | 122.20 |
| 1 | AR | 2615 | G | N9-C4-C5 | -5.13 | 103.35 | 105.40 |
| 1 | AR | 1887 | A | O5'-P-OP2 | -5.12 | 101.09 | 105.70 |
| 3 | AT | 82 | U | P-O3'-C3' | 5.12 | 125.85 | 119.70 |
| 1 | 1 | 1002 | A | N1-C6-N6 | 5.12 | 121.67 | 118.60 |
| 9 | CI | 179 | LEU | CA-CB-CG | 5.11 | 127.05 | 115.30 |
| 1 | AR | 2679 | A | N1-C6-N6 | 5.11 | 121.67 | 118.60 |
| 1 | 1 | 2593 | A | P-O3'-C3' | 5.11 | 125.83 | 119.70 |
| 25 | 6 | 453 | U | C6-N1-C1' | -5.11 | 114.05 | 121.20 |
| 25 | 6 | 1246 | C | C2-N1-C1' | 5.11 | 124.42 | 118.80 |
| 1 | AR | 1047 | A | N1-C6-N6 | 5.11 | 121.66 | 118.60 |
| 1 | 1 | 2112 | U | P-O3'-C3' | 5.10 | 125.82 | 119.70 |
| 1 | 1 | 2400 | G | N1-C6-O6 | 5.10 | 122.96 | 119.90 |
| 1 | AR | 895 | A | C5-N7-C8 | -5.10 | 101.35 | 103.90 |
| 1 | AR | 2869 | U | C5-C4-O4 | -5.09 | 122.84 | 125.90 |
| 25 | 6 | 795 | U | C2-N1-C1' | 5.08 | 123.80 | 117.70 |
| 1 | AR | 2679 | A | O4'-C1'-N9 | 5.08 | 112.27 | 108.20 |
| 1 | AR | 3362 | A | O4'-C1'-N9 | 5.08 | 112.26 | 108.20 |
| 1 | AR | 2808 | A | N1-C6-N6 | 5.07 | 121.64 | 118.60 |
| 25 | 6 | 1274 | C | N3-C2-O2 | -5.07 | 118.35 | 121.90 |
| 1 | 1 | 2176 | U | N3-C2-O2 | -5.07 | 118.65 | 122.20 |
| 1 | 1 | 922 | U | C2-N1-C1' | 5.06 | 123.77 | 117.70 |
| 1 | 1 | 3209 | A | N1-C6-N6 | 5.06 | 121.64 | 118.60 |
| 1 | 1 | 109 | A | OP1-P-O3' | 5.05 | 116.32 | 105.20 |
| 1 | AR | 2846 | U | C6-N1-C2 | -5.05 | 117.97 | 121.00 |
| 1 | AR | 3306 | U | C5-C4-O4 | 5.05 | 128.93 | 125.90 |
| 25 | A | 1060 | U | N3-C2-O2 | -5.05 | 118.66 | 122.20 |
| 1 | AR | 2930 | A | O4'-C1'-N9 | 5.05 | 112.24 | 108.20 |
| 25 | 6 | 1697 | G | C4-N9-C1' | 5.04 | 133.06 | 126.50 |
| 1 | AR | 1437 | C | C2-N1-C1' | 5.04 | 124.35 | 118.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AR | 1483 | G | O4'-C1'-N9 | 5.04 | 112.23 | 108.20 |
| 1 | 1 | 1495 | U | C2-N3-C4 | -5.04 | 123.98 | 127.00 |
| 6 | CF | 315 | LYS | C-N-CA | -5.04 | 109.10 | 121.70 |
| 1 | AR | 2794 | G | O4'-C1'-N9 | 5.04 | 112.23 | 108.20 |
| 1 | AR | 3278 | C | C2-N1-C1' | 5.04 | 124.34 | 118.80 |
| 12 | CL | 87 | LEU | CA-CB-CG | 5.04 | 126.88 | 115.30 |
| 1 | AR | 648 | C | O5'-P-OP1 | -5.03 | 101.17 | 105.70 |
| 1 | 1 | 2808 | A | N9-C4-C5 | -5.03 | 103.79 | 105.80 |
| 25 | 6 | 678 | A | P-O3'-C3' | 5.03 | 125.73 | 119.70 |
| 1 | 1 | 936 | A | O4'-C1'-N9 | 5.02 | 112.21 | 108.20 |
| 1 | 1 | 2802 | A | OP2-P-O3' | 5.01 | 116.23 | 105.20 |
| 25 | 6 | 813 | U | N3-C2-O2 | -5.01 | 118.70 | 122.20 |
| 1 | AR | 2874 | G | C5-C6-O6 | 5.00 | 131.60 | 128.60 |
| 1 | 1 | 2541 | U | P-O3'-C3' | 5.00 | 125.70 | 119.70 |
| 1 | AR | 3140 | G | N1-C6-O6 | 5.00 | 122.90 | 119.90 |

There are no chirality outliers.

All (103) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 29 | AA | 102 | GLU | Peptide |
| 29 | AA | 124 | ALA | Peptide |
| 31 | AC | 19 | ASN | Peptide |
| 37 | AI | 83 | LYS | Peptide |
| 50 | B | 191 | ARG | Peptide |
| 5 | CE | 186 | GLY | Peptide |
| 5 | CE | 315 | GLY | Peptide |
| 5 | CE | 385 | LYS | Peptide |
| 7 | CG | 257 | GLU | Peptide |
| 7 | CG | 258 | LYS | Peptide |
| 7 | CG | 43 | LYS | Peptide |
| 9 | CI | 157 | ASN | Peptide |
| 9 | CI | 190 | THR | Peptide |
| 10 | CJ | 34 | PHE | Peptide |
| 10 | CJ | 35 | GLY | Peptide |
| 11 | CK | 21 | LYS | Peptide |
| 12 | CL | 218 | ALA | Peptide |
| 13 | CM | 172 | LEU | Peptide |
| 13 | CM | 73 | GLY | Peptide |
| 14 | CN | 4 | SER | Peptide |
| 15 | CO | 7 | VAL | Peptide |
| 16 | CP | 92 | LEU | Peptide |

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| Mol | Chain | Res | Type | Group |
|------------|--------------|------------|-------------|--------------|
| 17 | CQ | 110 | PRO | Peptide |
| 19 | CS | 98 | LYS | Peptide |
| 21 | CU | 133 | ALA | Peptide |
| 21 | CU | 22 | PRO | Peptide |
| 26 | CY | 80 | ARG | Peptide |
| 30 | DC | 115 | LYS | Peptide |
| 30 | DC | 45 | MET | Peptide |
| 31 | DD | 19 | ASN | Peptide |
| 37 | DJ | 118 | ILE | Peptide |
| 53 | E | 198 | GLY | Peptide |
| 53 | E | 216 | PRO | Peptide |
| 55 | G | 56 | ALA | Peptide |
| 55 | G | 58 | LEU | Peptide |
| 55 | G | 65 | ARG | Peptide |
| 56 | H | 148 | SER | Peptide |
| 56 | H | 67 | VAL | Peptide |
| 57 | I | 30 | SER | Peptide |
| 57 | I | 63 | PRO | Peptide |
| 58 | J | 146 | ARG | Peptide |
| 58 | J | 147 | ALA | Peptide |
| 59 | K | 163 | PRO | Peptide |
| 61 | M | 3 | THR | Peptide |
| 62 | N | 111 | ASN | Peptide |
| 64 | P | 41 | ARG | Peptide |
| 65 | Q | 124 | THR | Peptide |
| 66 | R | 14 | LYS | Peptide |
| 66 | R | 40 | GLU | Peptide |
| 67 | S | 84 | TYR | Peptide |
| 68 | T | 13 | HIS | Peptide |
| 68 | T | 144 | ARG | Peptide |
| 68 | T | 81 | ILE | Peptide |
| 75 | a | 87 | GLY | Peptide |
| 75 | a | 94 | LYS | Peptide |
| 76 | b | 10 | ARG | Peptide |
| 76 | b | 84 | VAL | Peptide |
| 60 | c0 | 34 | GLU | Peptide |
| 62 | c2 | 108 | ARG | Peptide |
| 62 | c2 | 130 | THR | Peptide |
| 63 | c3 | 22 | ALA | Peptide |
| 63 | c3 | 65 | VAL | Peptide |
| 64 | c4 | 11 | SER | Peptide |
| 64 | c4 | 125 | SER | Peptide |

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| Mol | Chain | Res | Type | Group |
|------------|--------------|------------|-------------|--------------|
| 65 | c5 | 134 | THR | Peptide |
| 65 | c5 | 52 | LYS | Peptide |
| 66 | c6 | 114 | ARG | Peptide |
| 66 | c6 | 13 | LYS | Peptide |
| 66 | c6 | 40 | GLU | Peptide |
| 66 | c6 | 41 | PRO | Peptide |
| 67 | c7 | 105 | GLN | Peptide |
| 67 | c7 | 66 | VAL | Peptide |
| 68 | c8 | 13 | HIS | Peptide |
| 70 | d0 | 70 | THR | Peptide |
| 74 | d4 | 29 | HIS | Peptide |
| 80 | e0 | 46 | ASN | Peptide |
| 83 | e1 | 146 | SER | Peptide |
| 81 | g | 102 | VAL | Peptide |
| 5 | k | 186 | GLY | Peptide |
| 5 | k | 349 | LYS | Peptide |
| 6 | l | 291 | ASN | Peptide |
| 6 | l | 338 | LYS | Peptide |
| 7 | m | 258 | LYS | Peptide |
| 9 | o | 157 | ASN | Peptide |
| 9 | o | 190 | THR | Peptide |
| 10 | p | 76 | ALA | Peptide |
| 11 | q | 21 | LYS | Peptide |
| 13 | s | 171 | VAL | Peptide |
| 13 | s | 94 | ARG | Peptide |
| 51 | s1 | 146 | GLN | Peptide |
| 53 | s3 | 144 | ALA | Peptide |
| 53 | s3 | 216 | PRO | Peptide |
| 55 | s5 | 44 | ASN | Peptide |
| 57 | s7 | 130 | VAL | Peptide |
| 57 | s7 | 63 | PRO | Peptide |
| 58 | s8 | 100 | ALA | Peptide |
| 58 | s8 | 148 | ALA | Peptide |
| 82 | sR | 280 | GLY | Peptide |
| 14 | t | 46 | ILE | Peptide |
| 14 | t | 47 | ALA | Peptide |
| 15 | u | 7 | VAL | Peptide |
| 17 | w | 110 | PRO | Peptide |
| 18 | x | 157 | VAL | Peptide |

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 4 | CD | 250/252 (99%) | 226 (90%) | 23 (9%) | 1 (0%) | 34 | 69 |
| 4 | j | 250/252 (99%) | 230 (92%) | 19 (8%) | 1 (0%) | 34 | 69 |
| 5 | CE | 384/386 (100%) | 349 (91%) | 31 (8%) | 4 (1%) | 15 | 49 |
| 5 | k | 384/386 (100%) | 348 (91%) | 33 (9%) | 3 (1%) | 19 | 54 |
| 6 | CF | 359/361 (99%) | 326 (91%) | 33 (9%) | 0 | 100 | 100 |
| 6 | l | 359/361 (99%) | 320 (89%) | 37 (10%) | 2 (1%) | 25 | 59 |
| 7 | CG | 294/296 (99%) | 254 (86%) | 38 (13%) | 2 (1%) | 22 | 57 |
| 7 | m | 294/296 (99%) | 263 (90%) | 30 (10%) | 1 (0%) | 41 | 73 |
| 8 | CH | 152/175 (87%) | 139 (91%) | 12 (8%) | 1 (1%) | 22 | 57 |
| 8 | n | 152/175 (87%) | 145 (95%) | 6 (4%) | 1 (1%) | 22 | 57 |
| 9 | CI | 220/222 (99%) | 199 (90%) | 16 (7%) | 5 (2%) | 6 | 28 |
| 9 | o | 220/222 (99%) | 204 (93%) | 13 (6%) | 3 (1%) | 11 | 40 |
| 10 | CJ | 231/233 (99%) | 201 (87%) | 28 (12%) | 2 (1%) | 17 | 52 |
| 10 | p | 231/233 (99%) | 207 (90%) | 24 (10%) | 0 | 100 | 100 |
| 11 | CK | 189/191 (99%) | 176 (93%) | 13 (7%) | 0 | 100 | 100 |
| 11 | q | 189/191 (99%) | 168 (89%) | 21 (11%) | 0 | 100 | 100 |
| 12 | CL | 207/220 (94%) | 188 (91%) | 19 (9%) | 0 | 100 | 100 |
| 12 | r | 207/220 (94%) | 189 (91%) | 17 (8%) | 1 (0%) | 29 | 64 |
| 13 | CM | 167/169 (99%) | 145 (87%) | 19 (11%) | 3 (2%) | 8 | 34 |
| 13 | s | 167/169 (99%) | 137 (82%) | 23 (14%) | 7 (4%) | 3 | 16 |
| 14 | CN | 191/193 (99%) | 168 (88%) | 17 (9%) | 6 (3%) | 4 | 23 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 14 | t | 191/193 (99%) | 171 (90%) | 13 (7%) | 7 (4%) | 3 | 19 |
| 15 | CO | 134/136 (98%) | 122 (91%) | 11 (8%) | 1 (1%) | 22 | 57 |
| 15 | u | 134/136 (98%) | 120 (90%) | 13 (10%) | 1 (1%) | 22 | 57 |
| 16 | CP | 201/203 (99%) | 188 (94%) | 13 (6%) | 0 | 100 | 100 |
| 16 | v | 201/203 (99%) | 177 (88%) | 23 (11%) | 1 (0%) | 29 | 64 |
| 17 | CQ | 195/197 (99%) | 185 (95%) | 8 (4%) | 2 (1%) | 15 | 49 |
| 17 | w | 195/197 (99%) | 187 (96%) | 6 (3%) | 2 (1%) | 15 | 49 |
| 18 | CR | 181/183 (99%) | 161 (89%) | 17 (9%) | 3 (2%) | 9 | 36 |
| 18 | x | 181/183 (99%) | 164 (91%) | 17 (9%) | 0 | 100 | 100 |
| 19 | CS | 183/185 (99%) | 166 (91%) | 16 (9%) | 1 (0%) | 29 | 64 |
| 19 | y | 183/185 (99%) | 167 (91%) | 16 (9%) | 0 | 100 | 100 |
| 20 | CT | 186/188 (99%) | 171 (92%) | 15 (8%) | 0 | 100 | 100 |
| 20 | z | 186/188 (99%) | 175 (94%) | 11 (6%) | 0 | 100 | 100 |
| 21 | 0 | 170/172 (99%) | 158 (93%) | 11 (6%) | 1 (1%) | 25 | 59 |
| 21 | CU | 170/172 (99%) | 160 (94%) | 10 (6%) | 0 | 100 | 100 |
| 22 | 2 | 157/159 (99%) | 142 (90%) | 13 (8%) | 2 (1%) | 12 | 42 |
| 22 | CV | 157/159 (99%) | 146 (93%) | 10 (6%) | 1 (1%) | 25 | 59 |
| 23 | 5 | 98/100 (98%) | 89 (91%) | 9 (9%) | 0 | 100 | 100 |
| 23 | CW | 98/100 (98%) | 81 (83%) | 16 (16%) | 1 (1%) | 15 | 49 |
| 24 | CX | 134/136 (98%) | 128 (96%) | 6 (4%) | 0 | 100 | 100 |
| 24 | IR | 134/136 (98%) | 129 (96%) | 5 (4%) | 0 | 100 | 100 |
| 26 | 7 | 96/98 (98%) | 83 (86%) | 13 (14%) | 0 | 100 | 100 |
| 26 | CY | 96/98 (98%) | 79 (82%) | 15 (16%) | 2 (2%) | 7 | 30 |
| 27 | 8 | 119/121 (98%) | 108 (91%) | 11 (9%) | 0 | 100 | 100 |
| 27 | CZ | 119/121 (98%) | 111 (93%) | 8 (7%) | 0 | 100 | 100 |
| 28 | 9 | 124/126 (98%) | 113 (91%) | 11 (9%) | 0 | 100 | 100 |
| 28 | DA | 124/126 (98%) | 119 (96%) | 5 (4%) | 0 | 100 | 100 |
| 29 | AA | 133/135 (98%) | 115 (86%) | 15 (11%) | 3 (2%) | 6 | 28 |
| 29 | DB | 133/135 (98%) | 119 (90%) | 10 (8%) | 4 (3%) | 4 | 23 |
| 30 | AB | 146/148 (99%) | 125 (86%) | 19 (13%) | 2 (1%) | 11 | 40 |
| 30 | DC | 146/148 (99%) | 123 (84%) | 21 (14%) | 2 (1%) | 11 | 40 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 31 | AC | 56/58 (97%) | 48 (86%) | 8 (14%) | 0 | 100 | 100 |
| 31 | DD | 56/58 (97%) | 50 (89%) | 5 (9%) | 1 (2%) | 8 | 34 |
| 32 | AD | 95/97 (98%) | 90 (95%) | 5 (5%) | 0 | 100 | 100 |
| 32 | DE | 95/97 (98%) | 90 (95%) | 5 (5%) | 0 | 100 | 100 |
| 33 | AE | 107/109 (98%) | 98 (92%) | 8 (8%) | 1 (1%) | 17 | 52 |
| 33 | DF | 107/109 (98%) | 99 (92%) | 7 (6%) | 1 (1%) | 17 | 52 |
| 34 | AF | 125/127 (98%) | 116 (93%) | 9 (7%) | 0 | 100 | 100 |
| 34 | DG | 125/127 (98%) | 119 (95%) | 6 (5%) | 0 | 100 | 100 |
| 35 | AG | 104/106 (98%) | 99 (95%) | 5 (5%) | 0 | 100 | 100 |
| 35 | DH | 104/106 (98%) | 99 (95%) | 4 (4%) | 1 (1%) | 15 | 49 |
| 36 | AH | 110/112 (98%) | 105 (96%) | 5 (4%) | 0 | 100 | 100 |
| 36 | DI | 110/112 (98%) | 105 (96%) | 5 (4%) | 0 | 100 | 100 |
| 37 | AI | 117/119 (98%) | 104 (89%) | 12 (10%) | 1 (1%) | 17 | 52 |
| 37 | DJ | 117/119 (98%) | 109 (93%) | 7 (6%) | 1 (1%) | 17 | 52 |
| 38 | AJ | 97/99 (98%) | 83 (86%) | 11 (11%) | 3 (3%) | 4 | 23 |
| 38 | DK | 97/99 (98%) | 84 (87%) | 13 (13%) | 0 | 100 | 100 |
| 39 | AK | 85/87 (98%) | 77 (91%) | 8 (9%) | 0 | 100 | 100 |
| 39 | DL | 85/87 (98%) | 79 (93%) | 6 (7%) | 0 | 100 | 100 |
| 40 | AL | 75/77 (97%) | 69 (92%) | 6 (8%) | 0 | 100 | 100 |
| 40 | DM | 75/77 (97%) | 67 (89%) | 8 (11%) | 0 | 100 | 100 |
| 41 | AM | 48/50 (96%) | 45 (94%) | 3 (6%) | 0 | 100 | 100 |
| 41 | DN | 48/50 (96%) | 46 (96%) | 2 (4%) | 0 | 100 | 100 |
| 42 | AN | 50/52 (96%) | 47 (94%) | 3 (6%) | 0 | 100 | 100 |
| 42 | DO | 50/52 (96%) | 47 (94%) | 3 (6%) | 0 | 100 | 100 |
| 43 | AO | 23/25 (92%) | 21 (91%) | 2 (9%) | 0 | 100 | 100 |
| 43 | DP | 23/25 (92%) | 23 (100%) | 0 | 0 | 100 | 100 |
| 44 | AP | 103/105 (98%) | 84 (82%) | 19 (18%) | 0 | 100 | 100 |
| 44 | DQ | 103/105 (98%) | 88 (85%) | 15 (15%) | 0 | 100 | 100 |
| 45 | AQ | 89/91 (98%) | 79 (89%) | 10 (11%) | 0 | 100 | 100 |
| 45 | DR | 89/91 (98%) | 82 (92%) | 7 (8%) | 0 | 100 | 100 |
| 46 | i | 155/272 (57%) | 121 (78%) | 30 (19%) | 4 (3%) | 5 | 26 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 48 | sM | 61/104 (59%) | 45 (74%) | 14 (23%) | 2 (3%) | 4 | 21 |
| 49 | p0 | 139/311 (45%) | 131 (94%) | 8 (6%) | 0 | 100 | 100 |
| 50 | B | 204/206 (99%) | 157 (77%) | 40 (20%) | 7 (3%) | 3 | 21 |
| 50 | s0 | 204/206 (99%) | 172 (84%) | 30 (15%) | 2 (1%) | 15 | 49 |
| 51 | C | 212/216 (98%) | 167 (79%) | 43 (20%) | 2 (1%) | 17 | 52 |
| 51 | s1 | 214/216 (99%) | 190 (89%) | 23 (11%) | 1 (0%) | 29 | 64 |
| 52 | D | 215/217 (99%) | 189 (88%) | 25 (12%) | 1 (0%) | 29 | 64 |
| 52 | s2 | 215/217 (99%) | 190 (88%) | 23 (11%) | 2 (1%) | 17 | 52 |
| 53 | E | 221/223 (99%) | 200 (90%) | 19 (9%) | 2 (1%) | 17 | 52 |
| 53 | s3 | 221/223 (99%) | 195 (88%) | 22 (10%) | 4 (2%) | 8 | 34 |
| 54 | F | 258/260 (99%) | 233 (90%) | 25 (10%) | 0 | 100 | 100 |
| 54 | s4 | 258/260 (99%) | 229 (89%) | 28 (11%) | 1 (0%) | 34 | 69 |
| 55 | G | 204/206 (99%) | 166 (81%) | 36 (18%) | 2 (1%) | 15 | 49 |
| 55 | s5 | 204/206 (99%) | 168 (82%) | 36 (18%) | 0 | 100 | 100 |
| 56 | H | 224/226 (99%) | 202 (90%) | 19 (8%) | 3 (1%) | 12 | 42 |
| 56 | s6 | 216/226 (96%) | 199 (92%) | 15 (7%) | 2 (1%) | 17 | 52 |
| 57 | I | 182/186 (98%) | 154 (85%) | 25 (14%) | 3 (2%) | 9 | 37 |
| 57 | s7 | 184/186 (99%) | 158 (86%) | 21 (11%) | 5 (3%) | 5 | 25 |
| 58 | J | 184/199 (92%) | 159 (86%) | 21 (11%) | 4 (2%) | 6 | 29 |
| 58 | s8 | 184/199 (92%) | 159 (86%) | 23 (12%) | 2 (1%) | 14 | 46 |
| 59 | K | 183/185 (99%) | 160 (87%) | 21 (12%) | 2 (1%) | 14 | 46 |
| 59 | s9 | 183/185 (99%) | 161 (88%) | 22 (12%) | 0 | 100 | 100 |
| 60 | L | 94/105 (90%) | 70 (74%) | 23 (24%) | 1 (1%) | 14 | 46 |
| 60 | c0 | 92/105 (88%) | 61 (66%) | 25 (27%) | 6 (6%) | 1 | 8 |
| 61 | M | 153/155 (99%) | 137 (90%) | 14 (9%) | 2 (1%) | 12 | 42 |
| 61 | c1 | 144/155 (93%) | 128 (89%) | 15 (10%) | 1 (1%) | 22 | 57 |
| 62 | N | 122/124 (98%) | 81 (66%) | 33 (27%) | 8 (7%) | 1 | 7 |
| 62 | c2 | 122/124 (98%) | 81 (66%) | 37 (30%) | 4 (3%) | 4 | 21 |
| 63 | O | 148/150 (99%) | 137 (93%) | 9 (6%) | 2 (1%) | 11 | 40 |
| 63 | c3 | 148/150 (99%) | 128 (86%) | 14 (10%) | 6 (4%) | 3 | 16 |
| 64 | P | 125/128 (98%) | 103 (82%) | 21 (17%) | 1 (1%) | 19 | 54 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 64 | c4 | 126/128 (98%) | 110 (87%) | 16 (13%) | 0 | 100 | 100 |
| 65 | Q | 122/141 (86%) | 100 (82%) | 19 (16%) | 3 (2%) | 5 | 27 |
| 65 | c5 | 133/141 (94%) | 99 (74%) | 27 (20%) | 7 (5%) | 2 | 12 |
| 66 | R | 139/142 (98%) | 122 (88%) | 16 (12%) | 1 (1%) | 22 | 57 |
| 66 | c6 | 140/142 (99%) | 124 (89%) | 15 (11%) | 1 (1%) | 22 | 57 |
| 67 | S | 116/125 (93%) | 93 (80%) | 22 (19%) | 1 (1%) | 17 | 52 |
| 67 | c7 | 113/125 (90%) | 91 (80%) | 21 (19%) | 1 (1%) | 17 | 52 |
| 68 | T | 143/145 (99%) | 126 (88%) | 16 (11%) | 1 (1%) | 22 | 57 |
| 68 | c8 | 143/145 (99%) | 121 (85%) | 19 (13%) | 3 (2%) | 7 | 30 |
| 69 | U | 141/143 (99%) | 127 (90%) | 14 (10%) | 0 | 100 | 100 |
| 69 | c9 | 141/143 (99%) | 130 (92%) | 11 (8%) | 0 | 100 | 100 |
| 70 | V | 105/110 (96%) | 89 (85%) | 15 (14%) | 1 (1%) | 15 | 49 |
| 70 | d0 | 108/110 (98%) | 92 (85%) | 14 (13%) | 2 (2%) | 8 | 33 |
| 71 | W | 85/87 (98%) | 62 (73%) | 22 (26%) | 1 (1%) | 13 | 44 |
| 71 | d1 | 85/87 (98%) | 77 (91%) | 7 (8%) | 1 (1%) | 13 | 44 |
| 72 | X | 127/129 (98%) | 118 (93%) | 8 (6%) | 1 (1%) | 19 | 54 |
| 72 | d2 | 127/129 (98%) | 121 (95%) | 6 (5%) | 0 | 100 | 100 |
| 73 | Y | 142/144 (99%) | 115 (81%) | 24 (17%) | 3 (2%) | 7 | 30 |
| 73 | d3 | 142/144 (99%) | 130 (92%) | 12 (8%) | 0 | 100 | 100 |
| 74 | Z | 132/134 (98%) | 120 (91%) | 10 (8%) | 2 (2%) | 10 | 39 |
| 74 | d4 | 132/134 (98%) | 114 (86%) | 16 (12%) | 2 (2%) | 10 | 39 |
| 75 | a | 68/70 (97%) | 51 (75%) | 14 (21%) | 3 (4%) | 2 | 15 |
| 75 | d5 | 67/70 (96%) | 56 (84%) | 11 (16%) | 0 | 100 | 100 |
| 76 | b | 95/97 (98%) | 66 (70%) | 24 (25%) | 5 (5%) | 2 | 12 |
| 76 | d6 | 95/97 (98%) | 73 (77%) | 20 (21%) | 2 (2%) | 7 | 30 |
| 77 | c | 79/81 (98%) | 65 (82%) | 14 (18%) | 0 | 100 | 100 |
| 77 | d7 | 79/81 (98%) | 70 (89%) | 9 (11%) | 0 | 100 | 100 |
| 78 | d | 61/63 (97%) | 51 (84%) | 10 (16%) | 0 | 100 | 100 |
| 78 | d8 | 61/63 (97%) | 47 (77%) | 14 (23%) | 0 | 100 | 100 |
| 79 | d9 | 51/53 (96%) | 47 (92%) | 4 (8%) | 0 | 100 | 100 |
| 79 | e | 51/53 (96%) | 46 (90%) | 5 (10%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|------------|----------|-------------|-----|
| 80 | e0 | 60/62 (97%) | 52 (87%) | 8 (13%) | 0 | 100 | 100 |
| 80 | f | 58/62 (94%) | 47 (81%) | 10 (17%) | 1 (2%) | 9 | 36 |
| 81 | g | 69/71 (97%) | 38 (55%) | 31 (45%) | 0 | 100 | 100 |
| 82 | h | 316/318 (99%) | 277 (88%) | 39 (12%) | 0 | 100 | 100 |
| 82 | sR | 316/318 (99%) | 285 (90%) | 30 (10%) | 1 (0%) | 41 | 73 |
| 83 | e1 | 49/51 (96%) | 30 (61%) | 18 (37%) | 1 (2%) | 7 | 31 |
| All | All | 22260/23067 (96%) | 19629 (88%) | 2417 (11%) | 214 (1%) | 15 | 49 |

All (214) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | l | 339 | LEU |
| 13 | s | 74 | PRO |
| 13 | s | 95 | ASN |
| 13 | s | 172 | LEU |
| 14 | t | 47 | ALA |
| 14 | t | 63 | VAL |
| 15 | u | 8 | LYS |
| 29 | AA | 128 | GLN |
| 46 | i | 176 | VAL |
| 46 | i | 254 | PRO |
| 13 | CM | 173 | ASP |
| 14 | CN | 5 | LYS |
| 14 | CN | 47 | ALA |
| 14 | CN | 48 | PRO |
| 14 | CN | 63 | VAL |
| 51 | C | 62 | LYS |
| 51 | C | 181 | LEU |
| 55 | G | 57 | SER |
| 55 | G | 126 | ASP |
| 56 | H | 68 | LEU |
| 56 | H | 149 | LYS |
| 57 | I | 63 | PRO |
| 57 | I | 74 | GLN |
| 58 | J | 147 | ALA |
| 60 | L | 88 | PRO |
| 62 | N | 106 | ILE |
| 63 | O | 28 | LEU |
| 74 | Z | 52 | LYS |
| 53 | s3 | 220 | PRO |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 56 | s6 | 68 | LEU |
| 57 | s7 | 63 | PRO |
| 57 | s7 | 67 | LEU |
| 60 | c0 | 88 | PRO |
| 60 | c0 | 97 | PRO |
| 62 | c2 | 130 | THR |
| 63 | c3 | 66 | ILE |
| 65 | c5 | 51 | SER |
| 65 | c5 | 128 | HIS |
| 74 | d4 | 52 | LYS |
| 5 | k | 347 | SER |
| 6 | l | 292 | SER |
| 9 | o | 158 | LYS |
| 14 | t | 77 | LEU |
| 17 | w | 111 | PRO |
| 30 | AB | 57 | GLY |
| 30 | AB | 78 | LEU |
| 37 | AI | 92 | LEU |
| 38 | AJ | 35 | ASN |
| 4 | CD | 144 | ASN |
| 5 | CE | 386 | ASP |
| 7 | CG | 20 | PHE |
| 9 | CI | 158 | LYS |
| 10 | CJ | 36 | ILE |
| 15 | CO | 8 | LYS |
| 19 | CS | 99 | THR |
| 29 | DB | 60 | LYS |
| 30 | DC | 78 | LEU |
| 35 | DH | 60 | ARG |
| 50 | B | 4 | PRO |
| 50 | B | 191 | ARG |
| 50 | B | 196 | SER |
| 61 | M | 4 | GLU |
| 62 | N | 109 | GLU |
| 62 | N | 112 | ALA |
| 63 | O | 27 | LYS |
| 64 | P | 42 | VAL |
| 65 | Q | 30 | THR |
| 73 | Y | 137 | LYS |
| 75 | a | 39 | ALA |
| 51 | s1 | 107 | THR |
| 52 | s2 | 106 | ASP |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 53 | s3 | 216 | PRO |
| 53 | s3 | 217 | ILE |
| 57 | s7 | 74 | GLN |
| 58 | s8 | 100 | ALA |
| 58 | s8 | 101 | ILE |
| 60 | c0 | 32 | HIS |
| 60 | c0 | 35 | ILE |
| 62 | c2 | 106 | ILE |
| 62 | c2 | 131 | ASP |
| 76 | d6 | 46 | GLU |
| 82 | sR | 281 | TYR |
| 7 | m | 259 | LYS |
| 9 | o | 191 | VAL |
| 13 | s | 94 | ARG |
| 14 | t | 48 | PRO |
| 14 | t | 166 | ALA |
| 38 | AJ | 77 | LEU |
| 46 | i | 86 | ASN |
| 7 | CG | 259 | LYS |
| 8 | CH | 98 | VAL |
| 9 | CI | 164 | SER |
| 9 | CI | 191 | VAL |
| 17 | CQ | 110 | PRO |
| 17 | CQ | 111 | PRO |
| 18 | CR | 159 | LYS |
| 30 | DC | 57 | GLY |
| 37 | DJ | 85 | THR |
| 48 | sM | 42 | ALA |
| 50 | B | 190 | ASP |
| 52 | D | 40 | LYS |
| 53 | E | 216 | PRO |
| 58 | J | 11 | ARG |
| 58 | J | 146 | ARG |
| 61 | M | 6 | THR |
| 62 | N | 85 | LYS |
| 62 | N | 108 | ARG |
| 62 | N | 126 | TRP |
| 62 | N | 130 | THR |
| 65 | Q | 125 | PRO |
| 71 | W | 11 | LEU |
| 76 | b | 63 | ALA |
| 60 | c0 | 34 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 63 | c3 | 23 | PRO |
| 63 | c3 | 65 | VAL |
| 65 | c5 | 68 | PRO |
| 67 | c7 | 67 | ARG |
| 68 | c8 | 9 | GLY |
| 71 | d1 | 11 | LEU |
| 4 | j | 250 | GLN |
| 9 | o | 164 | SER |
| 13 | s | 8 | PRO |
| 13 | s | 73 | GLY |
| 14 | t | 76 | THR |
| 17 | w | 110 | PRO |
| 5 | CE | 385 | LYS |
| 13 | CM | 172 | LEU |
| 18 | CR | 158 | ALA |
| 50 | B | 167 | LYS |
| 50 | B | 202 | TYR |
| 57 | I | 64 | VAL |
| 58 | J | 23 | LYS |
| 70 | V | 119 | ALA |
| 73 | Y | 98 | GLU |
| 75 | a | 38 | HIS |
| 76 | b | 61 | GLU |
| 76 | b | 85 | ARG |
| 57 | s7 | 64 | VAL |
| 57 | s7 | 66 | SER |
| 62 | c2 | 109 | GLU |
| 63 | c3 | 22 | ALA |
| 63 | c3 | 140 | LYS |
| 65 | c5 | 125 | PRO |
| 70 | d0 | 73 | GLY |
| 76 | d6 | 34 | LYS |
| 5 | k | 142 | ALA |
| 13 | s | 173 | ASP |
| 14 | t | 6 | ASN |
| 21 | 0 | 167 | ARG |
| 22 | 2 | 125 | ALA |
| 29 | AA | 102 | GLU |
| 29 | AA | 103 | GLN |
| 38 | AJ | 78 | GLY |
| 9 | CI | 25 | GLN |
| 9 | CI | 159 | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 14 | CN | 166 | ALA |
| 18 | CR | 160 | ALA |
| 26 | CY | 25 | ASP |
| 29 | DB | 59 | ALA |
| 29 | DB | 102 | GLU |
| 29 | DB | 103 | GLN |
| 48 | sM | 43 | ASP |
| 53 | E | 217 | ILE |
| 68 | T | 60 | GLU |
| 50 | s0 | 31 | VAL |
| 50 | s0 | 168 | HIS |
| 65 | c5 | 135 | THR |
| 68 | c8 | 8 | GLN |
| 33 | AE | 7 | VAL |
| 46 | i | 87 | THR |
| 10 | CJ | 122 | LYS |
| 13 | CM | 8 | PRO |
| 23 | CW | 52 | ASN |
| 26 | CY | 81 | PRO |
| 62 | N | 84 | ASN |
| 66 | R | 33 | GLY |
| 75 | a | 44 | GLN |
| 53 | s3 | 221 | SER |
| 63 | c3 | 139 | TRP |
| 65 | c5 | 52 | LYS |
| 70 | d0 | 52 | LYS |
| 83 | e1 | 118 | ARG |
| 5 | k | 188 | ILE |
| 8 | n | 98 | VAL |
| 31 | DD | 21 | ILE |
| 33 | DF | 7 | VAL |
| 50 | B | 194 | PRO |
| 56 | H | 69 | LEU |
| 59 | K | 134 | ILE |
| 59 | K | 163 | PRO |
| 65 | Q | 126 | VAL |
| 76 | b | 9 | GLY |
| 52 | s2 | 239 | PRO |
| 22 | 2 | 124 | VAL |
| 5 | CE | 188 | ILE |
| 14 | CN | 50 | PRO |
| 67 | S | 65 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 72 | X | 67 | GLY |
| 76 | b | 60 | PRO |
| 80 | f | 60 | PRO |
| 61 | c1 | 129 | ARG |
| 16 | v | 75 | VAL |
| 22 | CV | 124 | VAL |
| 73 | Y | 41 | SER |
| 74 | Z | 35 | VAL |
| 68 | c8 | 14 | ILE |
| 74 | d4 | 30 | PRO |
| 12 | r | 188 | GLY |
| 5 | CE | 317 | ILE |
| 54 | s4 | 90 | ILE |
| 56 | s6 | 70 | PRO |
| 66 | c6 | 5 | PRO |
| 60 | c0 | 92 | ILE |
| 65 | c5 | 126 | VAL |

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 4 | CD | 193/194 (100%) | 169 (88%) | 24 (12%) | 4 | 19 |
| 4 | j | 193/194 (100%) | 166 (86%) | 27 (14%) | 3 | 15 |
| 5 | CE | 319/322 (99%) | 272 (85%) | 47 (15%) | 3 | 13 |
| 5 | k | 321/322 (100%) | 274 (85%) | 47 (15%) | 3 | 13 |
| 6 | CF | 288/288 (100%) | 256 (89%) | 32 (11%) | 6 | 24 |
| 6 | l | 288/288 (100%) | 249 (86%) | 39 (14%) | 4 | 16 |
| 7 | CG | 244/244 (100%) | 207 (85%) | 37 (15%) | 3 | 12 |
| 7 | m | 244/244 (100%) | 216 (88%) | 28 (12%) | 5 | 22 |
| 8 | CH | 134/152 (88%) | 116 (87%) | 18 (13%) | 4 | 16 |
| 8 | n | 134/152 (88%) | 120 (90%) | 14 (10%) | 7 | 27 |
| 9 | CI | 186/186 (100%) | 167 (90%) | 19 (10%) | 7 | 27 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 9 | o | 186/186 (100%) | 165 (89%) | 21 (11%) | 6 | 23 |
| 10 | CJ | 187/191 (98%) | 172 (92%) | 15 (8%) | 12 | 40 |
| 10 | p | 187/191 (98%) | 167 (89%) | 20 (11%) | 6 | 26 |
| 11 | CK | 171/171 (100%) | 143 (84%) | 28 (16%) | 2 | 10 |
| 11 | q | 171/171 (100%) | 148 (86%) | 23 (14%) | 4 | 16 |
| 12 | CL | 177/186 (95%) | 151 (85%) | 26 (15%) | 3 | 13 |
| 12 | r | 177/186 (95%) | 149 (84%) | 28 (16%) | 2 | 11 |
| 13 | CM | 147/147 (100%) | 125 (85%) | 22 (15%) | 3 | 12 |
| 13 | s | 147/147 (100%) | 127 (86%) | 20 (14%) | 3 | 16 |
| 14 | CN | 154/154 (100%) | 128 (83%) | 26 (17%) | 2 | 9 |
| 14 | t | 154/154 (100%) | 136 (88%) | 18 (12%) | 5 | 22 |
| 15 | CO | 107/107 (100%) | 93 (87%) | 14 (13%) | 4 | 17 |
| 15 | u | 107/107 (100%) | 89 (83%) | 18 (17%) | 2 | 9 |
| 16 | CP | 175/175 (100%) | 160 (91%) | 15 (9%) | 10 | 37 |
| 16 | v | 175/175 (100%) | 155 (89%) | 20 (11%) | 5 | 23 |
| 17 | CQ | 160/160 (100%) | 144 (90%) | 16 (10%) | 7 | 28 |
| 17 | w | 160/160 (100%) | 139 (87%) | 21 (13%) | 4 | 17 |
| 18 | CR | 140/145 (97%) | 120 (86%) | 20 (14%) | 3 | 14 |
| 18 | x | 140/145 (97%) | 118 (84%) | 22 (16%) | 2 | 11 |
| 19 | CS | 150/150 (100%) | 128 (85%) | 22 (15%) | 3 | 13 |
| 19 | y | 150/150 (100%) | 130 (87%) | 20 (13%) | 4 | 16 |
| 20 | CT | 153/153 (100%) | 132 (86%) | 21 (14%) | 3 | 16 |
| 20 | z | 153/153 (100%) | 140 (92%) | 13 (8%) | 10 | 37 |
| 21 | 0 | 156/156 (100%) | 131 (84%) | 25 (16%) | 2 | 11 |
| 21 | CU | 156/156 (100%) | 133 (85%) | 23 (15%) | 3 | 13 |
| 22 | 2 | 136/136 (100%) | 116 (85%) | 20 (15%) | 3 | 13 |
| 22 | CV | 136/136 (100%) | 112 (82%) | 24 (18%) | 2 | 8 |
| 23 | 5 | 87/87 (100%) | 80 (92%) | 7 (8%) | 12 | 40 |
| 23 | CW | 87/87 (100%) | 77 (88%) | 10 (12%) | 5 | 22 |
| 24 | CX | 104/104 (100%) | 93 (89%) | 11 (11%) | 6 | 26 |
| 24 | IR | 104/104 (100%) | 89 (86%) | 15 (14%) | 3 | 14 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 26 | 7 | 57/86 (66%) | 52 (91%) | 5 (9%) | 10 | 36 |
| 26 | CY | 57/86 (66%) | 47 (82%) | 10 (18%) | 2 | 8 |
| 27 | 8 | 104/105 (99%) | 91 (88%) | 13 (12%) | 4 | 18 |
| 27 | CZ | 104/105 (99%) | 90 (86%) | 14 (14%) | 4 | 16 |
| 28 | 9 | 109/109 (100%) | 95 (87%) | 14 (13%) | 4 | 18 |
| 28 | DA | 109/109 (100%) | 95 (87%) | 14 (13%) | 4 | 18 |
| 29 | AA | 115/115 (100%) | 104 (90%) | 11 (10%) | 8 | 31 |
| 29 | DB | 115/115 (100%) | 104 (90%) | 11 (10%) | 8 | 31 |
| 30 | AB | 118/118 (100%) | 106 (90%) | 12 (10%) | 7 | 27 |
| 30 | DC | 118/118 (100%) | 103 (87%) | 15 (13%) | 4 | 18 |
| 31 | AC | 46/46 (100%) | 40 (87%) | 6 (13%) | 4 | 18 |
| 31 | DD | 46/46 (100%) | 39 (85%) | 7 (15%) | 3 | 12 |
| 32 | AD | 81/81 (100%) | 70 (86%) | 11 (14%) | 3 | 16 |
| 32 | DE | 81/81 (100%) | 76 (94%) | 5 (6%) | 18 | 49 |
| 33 | AE | 92/96 (96%) | 80 (87%) | 12 (13%) | 4 | 18 |
| 33 | DF | 92/96 (96%) | 75 (82%) | 17 (18%) | 1 | 7 |
| 34 | AF | 109/109 (100%) | 94 (86%) | 15 (14%) | 3 | 16 |
| 34 | DG | 109/109 (100%) | 96 (88%) | 13 (12%) | 5 | 20 |
| 35 | AG | 90/90 (100%) | 81 (90%) | 9 (10%) | 7 | 28 |
| 35 | DH | 90/90 (100%) | 83 (92%) | 7 (8%) | 12 | 40 |
| 36 | AH | 95/95 (100%) | 84 (88%) | 11 (12%) | 5 | 22 |
| 36 | DI | 95/95 (100%) | 85 (90%) | 10 (10%) | 7 | 26 |
| 37 | AI | 104/104 (100%) | 92 (88%) | 12 (12%) | 5 | 22 |
| 37 | DJ | 104/104 (100%) | 86 (83%) | 18 (17%) | 2 | 9 |
| 38 | AJ | 81/81 (100%) | 69 (85%) | 12 (15%) | 3 | 13 |
| 38 | DK | 81/81 (100%) | 71 (88%) | 10 (12%) | 4 | 19 |
| 39 | AK | 70/70 (100%) | 63 (90%) | 7 (10%) | 7 | 28 |
| 39 | DL | 70/70 (100%) | 59 (84%) | 11 (16%) | 2 | 11 |
| 40 | AL | 68/68 (100%) | 58 (85%) | 10 (15%) | 3 | 13 |
| 40 | DM | 68/68 (100%) | 61 (90%) | 7 (10%) | 7 | 27 |
| 41 | AM | 45/45 (100%) | 38 (84%) | 7 (16%) | 2 | 11 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 41 | DN | 45/45 (100%) | 41 (91%) | 4 (9%) | 9 | 34 |
| 42 | AN | 47/47 (100%) | 39 (83%) | 8 (17%) | 2 | 9 |
| 42 | DO | 47/47 (100%) | 42 (89%) | 5 (11%) | 6 | 26 |
| 43 | AO | 23/23 (100%) | 20 (87%) | 3 (13%) | 4 | 18 |
| 43 | DP | 23/23 (100%) | 19 (83%) | 4 (17%) | 2 | 9 |
| 44 | AP | 90/90 (100%) | 82 (91%) | 8 (9%) | 9 | 34 |
| 44 | DQ | 90/90 (100%) | 81 (90%) | 9 (10%) | 7 | 28 |
| 45 | AQ | 71/71 (100%) | 59 (83%) | 12 (17%) | 2 | 9 |
| 45 | DR | 71/71 (100%) | 63 (89%) | 8 (11%) | 6 | 23 |
| 46 | i | 97/227 (43%) | 82 (84%) | 15 (16%) | 2 | 11 |
| 48 | sM | 54/54 (100%) | 47 (87%) | 7 (13%) | 4 | 18 |
| 49 | p0 | 105/253 (42%) | 91 (87%) | 14 (13%) | 4 | 16 |
| 50 | B | 164/173 (95%) | 146 (89%) | 18 (11%) | 6 | 25 |
| 50 | s0 | 165/173 (95%) | 140 (85%) | 25 (15%) | 3 | 12 |
| 51 | C | 191/192 (100%) | 167 (87%) | 24 (13%) | 4 | 18 |
| 51 | s1 | 192/192 (100%) | 164 (85%) | 28 (15%) | 3 | 13 |
| 52 | D | 176/176 (100%) | 151 (86%) | 25 (14%) | 3 | 14 |
| 52 | s2 | 176/176 (100%) | 144 (82%) | 32 (18%) | 1 | 7 |
| 53 | E | 182/182 (100%) | 159 (87%) | 23 (13%) | 4 | 18 |
| 53 | s3 | 182/182 (100%) | 164 (90%) | 18 (10%) | 8 | 29 |
| 54 | F | 221/221 (100%) | 196 (89%) | 25 (11%) | 6 | 23 |
| 54 | s4 | 221/221 (100%) | 200 (90%) | 21 (10%) | 8 | 31 |
| 55 | G | 173/173 (100%) | 153 (88%) | 20 (12%) | 5 | 22 |
| 55 | s5 | 173/173 (100%) | 155 (90%) | 18 (10%) | 7 | 27 |
| 56 | H | 188/193 (97%) | 163 (87%) | 25 (13%) | 4 | 16 |
| 56 | s6 | 187/193 (97%) | 163 (87%) | 24 (13%) | 4 | 18 |
| 57 | I | 165/166 (99%) | 146 (88%) | 19 (12%) | 5 | 22 |
| 57 | s7 | 165/166 (99%) | 145 (88%) | 20 (12%) | 5 | 20 |
| 58 | J | 150/160 (94%) | 139 (93%) | 11 (7%) | 14 | 43 |
| 58 | s8 | 150/160 (94%) | 140 (93%) | 10 (7%) | 16 | 46 |
| 59 | K | 158/158 (100%) | 134 (85%) | 24 (15%) | 3 | 12 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 59 | s9 | 158/158 (100%) | 129 (82%) | 29 (18%) | 1 | 7 |
| 60 | L | 77/98 (79%) | 68 (88%) | 9 (12%) | 5 | 22 |
| 60 | c0 | 73/98 (74%) | 65 (89%) | 8 (11%) | 6 | 25 |
| 61 | M | 129/136 (95%) | 120 (93%) | 9 (7%) | 15 | 45 |
| 61 | c1 | 129/136 (95%) | 113 (88%) | 16 (12%) | 4 | 19 |
| 62 | N | 88/100 (88%) | 73 (83%) | 15 (17%) | 2 | 9 |
| 62 | c2 | 88/100 (88%) | 73 (83%) | 15 (17%) | 2 | 9 |
| 63 | O | 127/127 (100%) | 110 (87%) | 17 (13%) | 4 | 16 |
| 63 | c3 | 127/127 (100%) | 111 (87%) | 16 (13%) | 4 | 18 |
| 64 | P | 81/97 (84%) | 70 (86%) | 11 (14%) | 3 | 16 |
| 64 | c4 | 97/97 (100%) | 85 (88%) | 12 (12%) | 4 | 19 |
| 65 | Q | 101/117 (86%) | 92 (91%) | 9 (9%) | 9 | 34 |
| 65 | c5 | 103/117 (88%) | 91 (88%) | 12 (12%) | 5 | 22 |
| 66 | R | 117/118 (99%) | 101 (86%) | 16 (14%) | 3 | 16 |
| 66 | c6 | 118/118 (100%) | 98 (83%) | 20 (17%) | 2 | 9 |
| 67 | S | 94/113 (83%) | 80 (85%) | 14 (15%) | 3 | 13 |
| 67 | c7 | 92/113 (81%) | 81 (88%) | 11 (12%) | 5 | 20 |
| 68 | T | 128/128 (100%) | 108 (84%) | 20 (16%) | 2 | 11 |
| 68 | c8 | 128/128 (100%) | 109 (85%) | 19 (15%) | 3 | 13 |
| 69 | U | 115/115 (100%) | 95 (83%) | 20 (17%) | 2 | 9 |
| 69 | c9 | 115/115 (100%) | 99 (86%) | 16 (14%) | 3 | 15 |
| 70 | V | 100/103 (97%) | 86 (86%) | 14 (14%) | 3 | 15 |
| 70 | d0 | 103/103 (100%) | 90 (87%) | 13 (13%) | 4 | 18 |
| 71 | W | 74/74 (100%) | 62 (84%) | 12 (16%) | 2 | 10 |
| 71 | d1 | 74/74 (100%) | 63 (85%) | 11 (15%) | 3 | 13 |
| 72 | X | 110/110 (100%) | 95 (86%) | 15 (14%) | 3 | 16 |
| 72 | d2 | 110/110 (100%) | 103 (94%) | 7 (6%) | 17 | 48 |
| 73 | Y | 119/119 (100%) | 102 (86%) | 17 (14%) | 3 | 14 |
| 73 | d3 | 119/119 (100%) | 104 (87%) | 15 (13%) | 4 | 18 |
| 74 | Z | 112/112 (100%) | 101 (90%) | 11 (10%) | 8 | 29 |
| 74 | d4 | 112/112 (100%) | 105 (94%) | 7 (6%) | 18 | 48 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|------------|-------------|----|
| 75 | a | 61/61 (100%) | 49 (80%) | 12 (20%) | 1 | 6 |
| 75 | d5 | 61/61 (100%) | 58 (95%) | 3 (5%) | 25 | 57 |
| 76 | b | 83/83 (100%) | 76 (92%) | 7 (8%) | 11 | 38 |
| 76 | d6 | 83/83 (100%) | 71 (86%) | 12 (14%) | 3 | 13 |
| 77 | c | 70/70 (100%) | 67 (96%) | 3 (4%) | 29 | 62 |
| 77 | d7 | 70/70 (100%) | 65 (93%) | 5 (7%) | 14 | 44 |
| 78 | d | 56/56 (100%) | 48 (86%) | 8 (14%) | 3 | 14 |
| 78 | d8 | 56/56 (100%) | 47 (84%) | 9 (16%) | 2 | 10 |
| 79 | d9 | 47/47 (100%) | 43 (92%) | 4 (8%) | 10 | 37 |
| 79 | e | 47/47 (100%) | 42 (89%) | 5 (11%) | 6 | 26 |
| 80 | e0 | 53/53 (100%) | 45 (85%) | 8 (15%) | 3 | 12 |
| 80 | f | 51/53 (96%) | 47 (92%) | 4 (8%) | 12 | 40 |
| 81 | g | 62/62 (100%) | 50 (81%) | 12 (19%) | 1 | 6 |
| 82 | h | 260/261 (100%) | 243 (94%) | 17 (6%) | 17 | 47 |
| 82 | sR | 260/261 (100%) | 242 (93%) | 18 (7%) | 15 | 45 |
| 83 | e1 | 43/43 (100%) | 35 (81%) | 8 (19%) | 1 | 7 |
| All | All | 18684/19337 (97%) | 16334 (87%) | 2350 (13%) | 4 | 18 |

All (2350) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | j | 20 | THR |
| 4 | j | 23 | ARG |
| 4 | j | 32 | LEU |
| 4 | j | 44 | ILE |
| 4 | j | 45 | VAL |
| 4 | j | 48 | ILE |
| 4 | j | 49 | VAL |
| 4 | j | 62 | VAL |
| 4 | j | 72 | ARG |
| 4 | j | 74 | GLU |
| 4 | j | 84 | THR |
| 4 | j | 96 | LEU |
| 4 | j | 101 | VAL |
| 4 | j | 104 | LEU |
| 4 | j | 119 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 4 | j | 157 | VAL |
| 4 | j | 165 | VAL |
| 4 | j | 179 | LEU |
| 4 | j | 180 | LEU |
| 4 | j | 202 | VAL |
| 4 | j | 204 | MET |
| 4 | j | 207 | VAL |
| 4 | j | 226 | SER |
| 4 | j | 227 | ARG |
| 4 | j | 230 | VAL |
| 4 | j | 231 | SER |
| 4 | j | 247 | ARG |
| 5 | k | 4 | ARG |
| 5 | k | 7 | GLU |
| 5 | k | 10 | ARG |
| 5 | k | 17 | LEU |
| 5 | k | 19 | ARG |
| 5 | k | 25 | ILE |
| 5 | k | 37 | ARG |
| 5 | k | 47 | LEU |
| 5 | k | 69 | LYS |
| 5 | k | 73 | VAL |
| 5 | k | 79 | VAL |
| 5 | k | 84 | VAL |
| 5 | k | 85 | VAL |
| 5 | k | 103 | THR |
| 5 | k | 114 | VAL |
| 5 | k | 139 | GLN |
| 5 | k | 148 | LEU |
| 5 | k | 150 | ARG |
| 5 | k | 156 | SER |
| 5 | k | 169 | THR |
| 5 | k | 183 | LEU |
| 5 | k | 188 | ILE |
| 5 | k | 192 | VAL |
| 5 | k | 196 | ARG |
| 5 | k | 202 | THR |
| 5 | k | 210 | GLU |
| 5 | k | 212 | ASN |
| 5 | k | 229 | VAL |
| 5 | k | 235 | THR |
| 5 | k | 238 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 5 | k | 241 | LYS |
| 5 | k | 244 | ARG |
| 5 | k | 252 | ILE |
| 5 | k | 261 | MET |
| 5 | k | 264 | VAL |
| 5 | k | 284 | ARG |
| 5 | k | 291 | GLU |
| 5 | k | 296 | THR |
| 5 | k | 300 | ARG |
| 5 | k | 305 | ILE |
| 5 | k | 320 | ASP |
| 5 | k | 324 | VAL |
| 5 | k | 325 | LYS |
| 5 | k | 332 | ARG |
| 5 | k | 338 | LEU |
| 5 | k | 352 | GLU |
| 5 | k | 361 | THR |
| 6 | l | 22 | LEU |
| 6 | l | 71 | VAL |
| 6 | l | 73 | ARG |
| 6 | l | 74 | ILE |
| 6 | l | 93 | MET |
| 6 | l | 98 | ARG |
| 6 | l | 103 | THR |
| 6 | l | 112 | LYS |
| 6 | l | 120 | TYR |
| 6 | l | 133 | SER |
| 6 | l | 138 | ARG |
| 6 | l | 150 | LEU |
| 6 | l | 156 | LEU |
| 6 | l | 161 | LYS |
| 6 | l | 163 | LYS |
| 6 | l | 172 | VAL |
| 6 | l | 177 | ASP |
| 6 | l | 179 | LEU |
| 6 | l | 187 | LEU |
| 6 | l | 188 | ARG |
| 6 | l | 193 | LYS |
| 6 | l | 200 | THR |
| 6 | l | 203 | ARG |
| 6 | l | 206 | LEU |
| 6 | l | 220 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 6 | l | 222 | VAL |
| 6 | l | 230 | VAL |
| 6 | l | 246 | ARG |
| 6 | l | 258 | LEU |
| 6 | l | 267 | VAL |
| 6 | l | 287 | THR |
| 6 | l | 308 | LYS |
| 6 | l | 313 | LEU |
| 6 | l | 323 | VAL |
| 6 | l | 327 | LEU |
| 6 | l | 333 | VAL |
| 6 | l | 338 | LYS |
| 6 | l | 339 | LEU |
| 6 | l | 349 | THR |
| 7 | m | 5 | LYS |
| 7 | m | 8 | LYS |
| 7 | m | 23 | ARG |
| 7 | m | 35 | ARG |
| 7 | m | 41 | LYS |
| 7 | m | 67 | SER |
| 7 | m | 75 | LEU |
| 7 | m | 93 | THR |
| 7 | m | 105 | ILE |
| 7 | m | 113 | LEU |
| 7 | m | 115 | LEU |
| 7 | m | 118 | THR |
| 7 | m | 131 | LEU |
| 7 | m | 137 | ASP |
| 7 | m | 140 | ARG |
| 7 | m | 144 | VAL |
| 7 | m | 146 | LEU |
| 7 | m | 148 | ILE |
| 7 | m | 152 | ARG |
| 7 | m | 155 | THR |
| 7 | m | 163 | LEU |
| 7 | m | 177 | GLU |
| 7 | m | 185 | PHE |
| 7 | m | 216 | GLU |
| 7 | m | 217 | GLU |
| 7 | m | 222 | LEU |
| 7 | m | 231 | ILE |
| 7 | m | 234 | ASP |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 8 | n | 2 | SER |
| 8 | n | 5 | LYS |
| 8 | n | 21 | THR |
| 8 | n | 35 | VAL |
| 8 | n | 52 | VAL |
| 8 | n | 64 | LEU |
| 8 | n | 78 | ARG |
| 8 | n | 79 | VAL |
| 8 | n | 84 | VAL |
| 8 | n | 88 | SER |
| 8 | n | 98 | VAL |
| 8 | n | 134 | ARG |
| 8 | n | 152 | THR |
| 8 | n | 155 | LEU |
| 9 | o | 24 | GLU |
| 9 | o | 25 | GLN |
| 9 | o | 26 | VAL |
| 9 | o | 45 | LEU |
| 9 | o | 60 | ARG |
| 9 | o | 80 | GLN |
| 9 | o | 82 | LYS |
| 9 | o | 83 | LEU |
| 9 | o | 88 | ARG |
| 9 | o | 93 | ASN |
| 9 | o | 101 | LYS |
| 9 | o | 110 | ARG |
| 9 | o | 121 | LYS |
| 9 | o | 124 | LEU |
| 9 | o | 157 | ASN |
| 9 | o | 158 | LYS |
| 9 | o | 164 | SER |
| 9 | o | 175 | LYS |
| 9 | o | 179 | LEU |
| 9 | o | 184 | LEU |
| 9 | o | 239 | LEU |
| 10 | p | 26 | LEU |
| 10 | p | 27 | THR |
| 10 | p | 50 | VAL |
| 10 | p | 57 | ARG |
| 10 | p | 71 | VAL |
| 10 | p | 74 | THR |
| 10 | p | 79 | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 10 | p | 81 | THR |
| 10 | p | 84 | ARG |
| 10 | p | 106 | LYS |
| 10 | p | 110 | THR |
| 10 | p | 136 | LEU |
| 10 | p | 145 | ASN |
| 10 | p | 156 | ASP |
| 10 | p | 163 | VAL |
| 10 | p | 169 | LEU |
| 10 | p | 185 | ARG |
| 10 | p | 194 | THR |
| 10 | p | 206 | GLU |
| 10 | p | 248 | LYS |
| 11 | q | 5 | GLN |
| 11 | q | 6 | THR |
| 11 | q | 18 | VAL |
| 11 | q | 19 | SER |
| 11 | q | 41 | ILE |
| 11 | q | 42 | ASP |
| 11 | q | 44 | THR |
| 11 | q | 48 | VAL |
| 11 | q | 52 | LEU |
| 11 | q | 55 | VAL |
| 11 | q | 68 | LEU |
| 11 | q | 69 | ARG |
| 11 | q | 70 | THR |
| 11 | q | 129 | ARG |
| 11 | q | 132 | VAL |
| 11 | q | 133 | THR |
| 11 | q | 139 | ASN |
| 11 | q | 151 | VAL |
| 11 | q | 157 | ASN |
| 11 | q | 161 | LEU |
| 11 | q | 162 | GLN |
| 11 | q | 172 | ILE |
| 11 | q | 173 | ARG |
| 12 | r | 3 | ARG |
| 12 | r | 21 | ARG |
| 12 | r | 24 | ARG |
| 12 | r | 26 | VAL |
| 12 | r | 30 | LYS |
| 12 | r | 32 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 12 | r | 35 | ASP |
| 12 | r | 39 | LYS |
| 12 | r | 40 | LYS |
| 12 | r | 42 | THR |
| 12 | r | 52 | LEU |
| 12 | r | 63 | GLU |
| 12 | r | 87 | LEU |
| 12 | r | 91 | VAL |
| 12 | r | 130 | ASP |
| 12 | r | 138 | VAL |
| 12 | r | 139 | ARG |
| 12 | r | 140 | THR |
| 12 | r | 142 | ASP |
| 12 | r | 148 | VAL |
| 12 | r | 163 | GLN |
| 12 | r | 165 | ILE |
| 12 | r | 169 | LYS |
| 12 | r | 174 | THR |
| 12 | r | 176 | LEU |
| 12 | r | 177 | ASP |
| 12 | r | 190 | VAL |
| 12 | r | 203 | LYS |
| 13 | s | 9 | MET |
| 13 | s | 10 | ARG |
| 13 | s | 11 | ASP |
| 13 | s | 12 | LEU |
| 13 | s | 31 | THR |
| 13 | s | 46 | VAL |
| 13 | s | 47 | GLN |
| 13 | s | 63 | GLU |
| 13 | s | 70 | THR |
| 13 | s | 80 | LEU |
| 13 | s | 82 | ARG |
| 13 | s | 94 | ARG |
| 13 | s | 95 | ASN |
| 13 | s | 106 | ILE |
| 13 | s | 107 | ASP |
| 13 | s | 112 | LEU |
| 13 | s | 115 | LYS |
| 13 | s | 138 | VAL |
| 13 | s | 140 | ARG |
| 13 | s | 158 | ASP |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 14 | t | 13 | HIS |
| 14 | t | 23 | LYS |
| 14 | t | 24 | VAL |
| 14 | t | 34 | SER |
| 14 | t | 54 | LEU |
| 14 | t | 55 | ARG |
| 14 | t | 59 | ARG |
| 14 | t | 64 | LYS |
| 14 | t | 67 | ARG |
| 14 | t | 69 | VAL |
| 14 | t | 85 | LEU |
| 14 | t | 104 | ARG |
| 14 | t | 114 | GLN |
| 14 | t | 122 | LYS |
| 14 | t | 131 | LYS |
| 14 | t | 164 | GLU |
| 14 | t | 168 | ARG |
| 14 | t | 171 | ARG |
| 15 | u | 3 | THR |
| 15 | u | 5 | SER |
| 15 | u | 10 | SER |
| 15 | u | 15 | VAL |
| 15 | u | 27 | GLN |
| 15 | u | 38 | ILE |
| 15 | u | 50 | LYS |
| 15 | u | 53 | VAL |
| 15 | u | 58 | ILE |
| 15 | u | 63 | VAL |
| 15 | u | 66 | THR |
| 15 | u | 69 | THR |
| 15 | u | 90 | VAL |
| 15 | u | 91 | CYS |
| 15 | u | 102 | LYS |
| 15 | u | 107 | GLU |
| 15 | u | 135 | LEU |
| 15 | u | 137 | LYS |
| 16 | v | 10 | LEU |
| 16 | v | 15 | GLN |
| 16 | v | 19 | LEU |
| 16 | v | 22 | LEU |
| 16 | v | 38 | ARG |
| 16 | v | 49 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 16 | v | 50 | ARG |
| 16 | v | 80 | THR |
| 16 | v | 85 | THR |
| 16 | v | 96 | ARG |
| 16 | v | 106 | VAL |
| 16 | v | 109 | ARG |
| 16 | v | 117 | ASN |
| 16 | v | 132 | VAL |
| 16 | v | 133 | ILE |
| 16 | v | 151 | ILE |
| 16 | v | 182 | ASN |
| 16 | v | 183 | THR |
| 16 | v | 187 | ARG |
| 16 | v | 201 | ARG |
| 17 | w | 22 | VAL |
| 17 | w | 34 | VAL |
| 17 | w | 68 | ARG |
| 17 | w | 78 | ARG |
| 17 | w | 84 | LEU |
| 17 | w | 85 | ARG |
| 17 | w | 106 | GLU |
| 17 | w | 116 | LYS |
| 17 | w | 117 | ARG |
| 17 | w | 122 | GLN |
| 17 | w | 124 | LEU |
| 17 | w | 126 | VAL |
| 17 | w | 128 | ARG |
| 17 | w | 129 | LEU |
| 17 | w | 143 | THR |
| 17 | w | 160 | ARG |
| 17 | w | 161 | LYS |
| 17 | w | 180 | SER |
| 17 | w | 184 | THR |
| 17 | w | 188 | SER |
| 17 | w | 190 | VAL |
| 18 | x | 13 | LYS |
| 18 | x | 16 | SER |
| 18 | x | 20 | SER |
| 18 | x | 23 | ARG |
| 18 | x | 24 | VAL |
| 18 | x | 29 | THR |
| 18 | x | 32 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 18 | x | 36 | ILE |
| 18 | x | 41 | LEU |
| 18 | x | 49 | GLU |
| 18 | x | 52 | LEU |
| 18 | x | 53 | ASP |
| 18 | x | 69 | ARG |
| 18 | x | 94 | LEU |
| 18 | x | 103 | GLU |
| 18 | x | 112 | LEU |
| 18 | x | 119 | VAL |
| 18 | x | 127 | ARG |
| 18 | x | 142 | SER |
| 18 | x | 168 | LEU |
| 18 | x | 180 | LYS |
| 18 | x | 181 | ARG |
| 19 | y | 3 | ILE |
| 19 | y | 7 | SER |
| 19 | y | 17 | THR |
| 19 | y | 22 | ASP |
| 19 | y | 24 | VAL |
| 19 | y | 26 | LEU |
| 19 | y | 32 | LEU |
| 19 | y | 39 | ARG |
| 19 | y | 41 | ASP |
| 19 | y | 49 | LEU |
| 19 | y | 57 | ILE |
| 19 | y | 66 | ARG |
| 19 | y | 69 | ARG |
| 19 | y | 74 | GLU |
| 19 | y | 81 | VAL |
| 19 | y | 115 | VAL |
| 19 | y | 135 | GLN |
| 19 | y | 138 | LEU |
| 19 | y | 150 | VAL |
| 19 | y | 170 | ARG |
| 20 | z | 29 | THR |
| 20 | z | 44 | LEU |
| 20 | z | 51 | VAL |
| 20 | z | 57 | VAL |
| 20 | z | 60 | LYS |
| 20 | z | 74 | ARG |
| 20 | z | 91 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 20 | z | 103 | ARG |
| 20 | z | 104 | ARG |
| 20 | z | 115 | ILE |
| 20 | z | 171 | ASP |
| 20 | z | 175 | GLN |
| 20 | z | 177 | VAL |
| 21 | 0 | 1 | MET |
| 21 | 0 | 16 | THR |
| 21 | 0 | 45 | LEU |
| 21 | 0 | 49 | HIS |
| 21 | 0 | 50 | LYS |
| 21 | 0 | 61 | ILE |
| 21 | 0 | 71 | LYS |
| 21 | 0 | 73 | LYS |
| 21 | 0 | 80 | ARG |
| 21 | 0 | 85 | SER |
| 21 | 0 | 87 | THR |
| 21 | 0 | 105 | THR |
| 21 | 0 | 115 | ARG |
| 21 | 0 | 117 | ARG |
| 21 | 0 | 122 | HIS |
| 21 | 0 | 131 | LYS |
| 21 | 0 | 132 | THR |
| 21 | 0 | 136 | LYS |
| 21 | 0 | 137 | ARG |
| 21 | 0 | 155 | ARG |
| 21 | 0 | 157 | GLN |
| 21 | 0 | 160 | THR |
| 21 | 0 | 162 | THR |
| 21 | 0 | 167 | ARG |
| 21 | 0 | 172 | TYR |
| 22 | 2 | 12 | ARG |
| 22 | 2 | 18 | ASP |
| 22 | 2 | 25 | VAL |
| 22 | 2 | 27 | LEU |
| 22 | 2 | 32 | LYS |
| 22 | 2 | 52 | MET |
| 22 | 2 | 75 | ILE |
| 22 | 2 | 78 | LYS |
| 22 | 2 | 79 | MET |
| 22 | 2 | 80 | VAL |
| 22 | 2 | 83 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 22 | 2 | 88 | ARG |
| 22 | 2 | 96 | ILE |
| 22 | 2 | 103 | GLN |
| 22 | 2 | 122 | GLN |
| 22 | 2 | 126 | VAL |
| 22 | 2 | 128 | LEU |
| 22 | 2 | 139 | ARG |
| 22 | 2 | 143 | THR |
| 22 | 2 | 160 | ILE |
| 23 | 5 | 10 | LYS |
| 23 | 5 | 35 | LYS |
| 23 | 5 | 52 | ASN |
| 23 | 5 | 66 | VAL |
| 23 | 5 | 93 | ILE |
| 23 | 5 | 100 | THR |
| 23 | 5 | 104 | ARG |
| 24 | 1R | 12 | ARG |
| 24 | 1R | 13 | ILE |
| 24 | 1R | 14 | SER |
| 24 | 1R | 32 | ARG |
| 24 | 1R | 45 | ARG |
| 24 | 1R | 48 | ARG |
| 24 | 1R | 63 | LYS |
| 24 | 1R | 64 | LYS |
| 24 | 1R | 69 | LEU |
| 24 | 1R | 72 | LYS |
| 24 | 1R | 83 | LYS |
| 24 | 1R | 102 | ILE |
| 24 | 1R | 106 | LYS |
| 24 | 1R | 115 | THR |
| 24 | 1R | 120 | LYS |
| 26 | 7 | 4 | GLU |
| 26 | 7 | 5 | ILE |
| 26 | 7 | 19 | THR |
| 26 | 7 | 39 | LEU |
| 26 | 7 | 64 | THR |
| 27 | 8 | 27 | ARG |
| 27 | 8 | 28 | THR |
| 27 | 8 | 36 | LYS |
| 27 | 8 | 63 | ILE |
| 27 | 8 | 92 | LYS |
| 27 | 8 | 104 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 27 | 8 | 108 | LEU |
| 27 | 8 | 115 | ARG |
| 27 | 8 | 125 | ARG |
| 27 | 8 | 129 | ASP |
| 27 | 8 | 135 | ILE |
| 27 | 8 | 139 | ILE |
| 27 | 8 | 142 | ILE |
| 28 | 9 | 5 | SER |
| 28 | 9 | 13 | ARG |
| 28 | 9 | 37 | LYS |
| 28 | 9 | 38 | GLU |
| 28 | 9 | 40 | ARG |
| 28 | 9 | 45 | ILE |
| 28 | 9 | 56 | VAL |
| 28 | 9 | 60 | ARG |
| 28 | 9 | 64 | LYS |
| 28 | 9 | 67 | GLU |
| 28 | 9 | 74 | TYR |
| 28 | 9 | 105 | VAL |
| 28 | 9 | 113 | LYS |
| 28 | 9 | 115 | ARG |
| 29 | AA | 14 | VAL |
| 29 | AA | 24 | VAL |
| 29 | AA | 46 | ILE |
| 29 | AA | 52 | LYS |
| 29 | AA | 81 | LEU |
| 29 | AA | 83 | THR |
| 29 | AA | 90 | GLU |
| 29 | AA | 102 | GLU |
| 29 | AA | 103 | GLN |
| 29 | AA | 107 | ARG |
| 29 | AA | 109 | GLU |
| 30 | AB | 4 | ARG |
| 30 | AB | 8 | THR |
| 30 | AB | 42 | ARG |
| 30 | AB | 46 | ASP |
| 30 | AB | 60 | TYR |
| 30 | AB | 76 | ASP |
| 30 | AB | 78 | LEU |
| 30 | AB | 88 | ASP |
| 30 | AB | 92 | LYS |
| 30 | AB | 115 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 30 | AB | 120 | ASN |
| 30 | AB | 135 | GLU |
| 31 | AC | 13 | THR |
| 31 | AC | 14 | ARG |
| 31 | AC | 25 | LYS |
| 31 | AC | 31 | SER |
| 31 | AC | 50 | THR |
| 31 | AC | 59 | LYS |
| 32 | AD | 14 | LEU |
| 32 | AD | 16 | LEU |
| 32 | AD | 18 | ILE |
| 32 | AD | 34 | LEU |
| 32 | AD | 54 | SER |
| 32 | AD | 61 | MET |
| 32 | AD | 76 | GLU |
| 32 | AD | 99 | ASP |
| 32 | AD | 101 | LEU |
| 32 | AD | 103 | THR |
| 32 | AD | 104 | LEU |
| 33 | AE | 8 | VAL |
| 33 | AE | 16 | LEU |
| 33 | AE | 26 | LYS |
| 33 | AE | 31 | ARG |
| 33 | AE | 55 | LEU |
| 33 | AE | 79 | ARG |
| 33 | AE | 86 | LYS |
| 33 | AE | 96 | VAL |
| 33 | AE | 100 | SER |
| 33 | AE | 106 | THR |
| 33 | AE | 107 | VAL |
| 33 | AE | 110 | GLU |
| 34 | AF | 14 | THR |
| 34 | AF | 16 | LYS |
| 34 | AF | 19 | ARG |
| 34 | AF | 27 | ARG |
| 34 | AF | 33 | ARG |
| 34 | AF | 44 | ARG |
| 34 | AF | 51 | SER |
| 34 | AF | 61 | LYS |
| 34 | AF | 62 | LYS |
| 34 | AF | 73 | THR |
| 34 | AF | 89 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 34 | AF | 106 | VAL |
| 34 | AF | 109 | LEU |
| 34 | AF | 111 | ARG |
| 34 | AF | 128 | LEU |
| 35 | AG | 15 | SER |
| 35 | AG | 20 | LYS |
| 35 | AG | 22 | VAL |
| 35 | AG | 49 | ILE |
| 35 | AG | 59 | VAL |
| 35 | AG | 70 | LYS |
| 35 | AG | 81 | VAL |
| 35 | AG | 98 | VAL |
| 35 | AG | 105 | SER |
| 36 | AH | 8 | ARG |
| 36 | AH | 20 | ILE |
| 36 | AH | 24 | LYS |
| 36 | AH | 29 | ILE |
| 36 | AH | 31 | ARG |
| 36 | AH | 51 | LEU |
| 36 | AH | 58 | ARG |
| 36 | AH | 65 | VAL |
| 36 | AH | 71 | THR |
| 36 | AH | 102 | LYS |
| 36 | AH | 104 | VAL |
| 37 | AI | 15 | GLU |
| 37 | AI | 20 | GLN |
| 37 | AI | 21 | LEU |
| 37 | AI | 30 | GLU |
| 37 | AI | 31 | LEU |
| 37 | AI | 46 | THR |
| 37 | AI | 84 | LYS |
| 37 | AI | 89 | ARG |
| 37 | AI | 90 | ARG |
| 37 | AI | 92 | LEU |
| 37 | AI | 96 | GLU |
| 37 | AI | 101 | THR |
| 38 | AJ | 11 | LEU |
| 38 | AJ | 18 | THR |
| 38 | AJ | 25 | LYS |
| 38 | AJ | 26 | ILE |
| 38 | AJ | 34 | SER |
| 38 | AJ | 45 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 38 | AJ | 57 | LEU |
| 38 | AJ | 60 | LEU |
| 38 | AJ | 62 | ARG |
| 38 | AJ | 68 | ARG |
| 38 | AJ | 88 | GLU |
| 38 | AJ | 90 | MET |
| 39 | AK | 24 | ARG |
| 39 | AK | 25 | ARG |
| 39 | AK | 33 | THR |
| 39 | AK | 58 | THR |
| 39 | AK | 59 | THR |
| 39 | AK | 67 | LEU |
| 39 | AK | 82 | SER |
| 40 | AL | 5 | ILE |
| 40 | AL | 24 | THR |
| 40 | AL | 32 | ASN |
| 40 | AL | 46 | ARG |
| 40 | AL | 53 | THR |
| 40 | AL | 65 | LEU |
| 40 | AL | 67 | GLN |
| 40 | AL | 69 | LEU |
| 40 | AL | 77 | ARG |
| 40 | AL | 78 | LEU |
| 41 | AM | 4 | GLN |
| 41 | AM | 10 | LYS |
| 41 | AM | 21 | ARG |
| 41 | AM | 34 | THR |
| 41 | AM | 36 | ARG |
| 41 | AM | 45 | ARG |
| 41 | AM | 51 | ILE |
| 42 | AN | 77 | ILE |
| 42 | AN | 83 | LYS |
| 42 | AN | 85 | LEU |
| 42 | AN | 112 | LYS |
| 42 | AN | 113 | ARG |
| 42 | AN | 114 | LYS |
| 42 | AN | 126 | LYS |
| 42 | AN | 127 | LEU |
| 43 | AO | 2 | ARG |
| 43 | AO | 11 | ARG |
| 43 | AO | 13 | LEU |
| 44 | AP | 2 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 44 | AP | 8 | ARG |
| 44 | AP | 26 | THR |
| 44 | AP | 35 | LEU |
| 44 | AP | 78 | LYS |
| 44 | AP | 83 | LEU |
| 44 | AP | 84 | THR |
| 44 | AP | 104 | LEU |
| 45 | AQ | 11 | THR |
| 45 | AQ | 16 | VAL |
| 45 | AQ | 25 | GLN |
| 45 | AQ | 45 | LYS |
| 45 | AQ | 46 | THR |
| 45 | AQ | 49 | ARG |
| 45 | AQ | 56 | THR |
| 45 | AQ | 59 | CYS |
| 45 | AQ | 60 | CYS |
| 45 | AQ | 84 | ARG |
| 45 | AQ | 90 | VAL |
| 45 | AQ | 91 | GLU |
| 46 | i | 34 | LYS |
| 46 | i | 46 | LYS |
| 46 | i | 68 | ARG |
| 46 | i | 75 | ASP |
| 46 | i | 77 | THR |
| 46 | i | 84 | LYS |
| 46 | i | 91 | THR |
| 46 | i | 96 | ARG |
| 46 | i | 97 | THR |
| 46 | i | 100 | THR |
| 46 | i | 102 | THR |
| 46 | i | 116 | GLU |
| 46 | i | 130 | GLU |
| 46 | i | 131 | ILE |
| 46 | i | 134 | ASP |
| 4 | CD | 10 | LYS |
| 4 | CD | 19 | HIS |
| 4 | CD | 20 | THR |
| 4 | CD | 32 | LEU |
| 4 | CD | 44 | ILE |
| 4 | CD | 45 | VAL |
| 4 | CD | 48 | ILE |
| 4 | CD | 62 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 4 | CD | 64 | ARG |
| 4 | CD | 70 | ARG |
| 4 | CD | 82 | VAL |
| 4 | CD | 96 | LEU |
| 4 | CD | 101 | VAL |
| 4 | CD | 137 | ILE |
| 4 | CD | 142 | ASP |
| 4 | CD | 149 | ARG |
| 4 | CD | 179 | LEU |
| 4 | CD | 180 | LEU |
| 4 | CD | 204 | MET |
| 4 | CD | 207 | VAL |
| 4 | CD | 227 | ARG |
| 4 | CD | 230 | VAL |
| 4 | CD | 250 | GLN |
| 4 | CD | 252 | THR |
| 5 | CE | 2 | SER |
| 5 | CE | 7 | GLU |
| 5 | CE | 17 | LEU |
| 5 | CE | 25 | ILE |
| 5 | CE | 30 | LYS |
| 5 | CE | 37 | ARG |
| 5 | CE | 47 | LEU |
| 5 | CE | 55 | THR |
| 5 | CE | 56 | ILE |
| 5 | CE | 73 | VAL |
| 5 | CE | 79 | VAL |
| 5 | CE | 84 | VAL |
| 5 | CE | 100 | ARG |
| 5 | CE | 103 | THR |
| 5 | CE | 111 | SER |
| 5 | CE | 114 | VAL |
| 5 | CE | 146 | ARG |
| 5 | CE | 156 | SER |
| 5 | CE | 167 | ARG |
| 5 | CE | 169 | THR |
| 5 | CE | 173 | GLN |
| 5 | CE | 183 | LEU |
| 5 | CE | 188 | ILE |
| 5 | CE | 192 | VAL |
| 5 | CE | 196 | ARG |
| 5 | CE | 202 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 5 | CE | 205 | VAL |
| 5 | CE | 212 | ASN |
| 5 | CE | 222 | LYS |
| 5 | CE | 232 | ARG |
| 5 | CE | 235 | THR |
| 5 | CE | 284 | ARG |
| 5 | CE | 296 | THR |
| 5 | CE | 305 | ILE |
| 5 | CE | 308 | MET |
| 5 | CE | 316 | GLU |
| 5 | CE | 324 | VAL |
| 5 | CE | 325 | LYS |
| 5 | CE | 328 | ILE |
| 5 | CE | 332 | ARG |
| 5 | CE | 338 | LEU |
| 5 | CE | 347 | SER |
| 5 | CE | 349 | LYS |
| 5 | CE | 364 | LYS |
| 5 | CE | 382 | THR |
| 5 | CE | 386 | ASP |
| 5 | CE | 387 | LEU |
| 6 | CF | 53 | SER |
| 6 | CF | 73 | ARG |
| 6 | CF | 74 | ILE |
| 6 | CF | 85 | SER |
| 6 | CF | 93 | MET |
| 6 | CF | 99 | MET |
| 6 | CF | 118 | LYS |
| 6 | CF | 120 | TYR |
| 6 | CF | 138 | ARG |
| 6 | CF | 150 | LEU |
| 6 | CF | 156 | LEU |
| 6 | CF | 170 | LYS |
| 6 | CF | 177 | ASP |
| 6 | CF | 179 | LEU |
| 6 | CF | 187 | LEU |
| 6 | CF | 201 | GLN |
| 6 | CF | 203 | ARG |
| 6 | CF | 206 | LEU |
| 6 | CF | 220 | ARG |
| 6 | CF | 222 | VAL |
| 6 | CF | 230 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 6 | CF | 246 | ARG |
| 6 | CF | 307 | GLN |
| 6 | CF | 313 | LEU |
| 6 | CF | 316 | ASN |
| 6 | CF | 319 | LYS |
| 6 | CF | 323 | VAL |
| 6 | CF | 327 | LEU |
| 6 | CF | 332 | LYS |
| 6 | CF | 333 | VAL |
| 6 | CF | 343 | LYS |
| 6 | CF | 346 | LYS |
| 7 | CG | 5 | LYS |
| 7 | CG | 23 | ARG |
| 7 | CG | 35 | ARG |
| 7 | CG | 41 | LYS |
| 7 | CG | 63 | GLN |
| 7 | CG | 69 | ILE |
| 7 | CG | 70 | THR |
| 7 | CG | 75 | LEU |
| 7 | CG | 89 | THR |
| 7 | CG | 92 | LEU |
| 7 | CG | 95 | TRP |
| 7 | CG | 105 | ILE |
| 7 | CG | 107 | ARG |
| 7 | CG | 110 | LEU |
| 7 | CG | 113 | LEU |
| 7 | CG | 115 | LEU |
| 7 | CG | 118 | THR |
| 7 | CG | 126 | GLU |
| 7 | CG | 131 | LEU |
| 7 | CG | 140 | ARG |
| 7 | CG | 144 | VAL |
| 7 | CG | 146 | LEU |
| 7 | CG | 148 | ILE |
| 7 | CG | 151 | GLN |
| 7 | CG | 152 | ARG |
| 7 | CG | 155 | THR |
| 7 | CG | 173 | VAL |
| 7 | CG | 185 | PHE |
| 7 | CG | 188 | GLU |
| 7 | CG | 189 | GLU |
| 7 | CG | 190 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 7 | CG | 194 | LEU |
| 7 | CG | 211 | LEU |
| 7 | CG | 222 | LEU |
| 7 | CG | 234 | ASP |
| 7 | CG | 261 | THR |
| 7 | CG | 293 | LEU |
| 8 | CH | 8 | LYS |
| 8 | CH | 14 | ASP |
| 8 | CH | 15 | VAL |
| 8 | CH | 21 | THR |
| 8 | CH | 35 | VAL |
| 8 | CH | 48 | ARG |
| 8 | CH | 52 | VAL |
| 8 | CH | 64 | LEU |
| 8 | CH | 65 | ILE |
| 8 | CH | 79 | VAL |
| 8 | CH | 88 | SER |
| 8 | CH | 89 | THR |
| 8 | CH | 93 | VAL |
| 8 | CH | 129 | GLU |
| 8 | CH | 134 | ARG |
| 8 | CH | 140 | VAL |
| 8 | CH | 152 | THR |
| 8 | CH | 155 | LEU |
| 9 | CI | 24 | GLU |
| 9 | CI | 25 | GLN |
| 9 | CI | 45 | LEU |
| 9 | CI | 57 | THR |
| 9 | CI | 60 | ARG |
| 9 | CI | 77 | VAL |
| 9 | CI | 82 | LYS |
| 9 | CI | 83 | LEU |
| 9 | CI | 89 | ILE |
| 9 | CI | 92 | ILE |
| 9 | CI | 98 | LYS |
| 9 | CI | 111 | ILE |
| 9 | CI | 121 | LYS |
| 9 | CI | 124 | LEU |
| 9 | CI | 179 | LEU |
| 9 | CI | 180 | SER |
| 9 | CI | 181 | ILE |
| 9 | CI | 184 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 9 | CI | 239 | LEU |
| 10 | CJ | 50 | VAL |
| 10 | CJ | 71 | VAL |
| 10 | CJ | 74 | THR |
| 10 | CJ | 79 | GLN |
| 10 | CJ | 81 | THR |
| 10 | CJ | 84 | ARG |
| 10 | CJ | 85 | ASN |
| 10 | CJ | 136 | LEU |
| 10 | CJ | 160 | ILE |
| 10 | CJ | 163 | VAL |
| 10 | CJ | 169 | LEU |
| 10 | CJ | 185 | ARG |
| 10 | CJ | 197 | VAL |
| 10 | CJ | 203 | VAL |
| 10 | CJ | 248 | LYS |
| 11 | CK | 5 | GLN |
| 11 | CK | 16 | VAL |
| 11 | CK | 18 | VAL |
| 11 | CK | 33 | THR |
| 11 | CK | 41 | ILE |
| 11 | CK | 48 | VAL |
| 11 | CK | 52 | LEU |
| 11 | CK | 62 | ARG |
| 11 | CK | 68 | LEU |
| 11 | CK | 69 | ARG |
| 11 | CK | 70 | THR |
| 11 | CK | 82 | VAL |
| 11 | CK | 92 | TYR |
| 11 | CK | 102 | ASN |
| 11 | CK | 121 | LYS |
| 11 | CK | 122 | LYS |
| 11 | CK | 129 | ARG |
| 11 | CK | 132 | VAL |
| 11 | CK | 133 | THR |
| 11 | CK | 151 | VAL |
| 11 | CK | 157 | ASN |
| 11 | CK | 161 | LEU |
| 11 | CK | 162 | GLN |
| 11 | CK | 164 | ILE |
| 11 | CK | 166 | ARG |
| 11 | CK | 172 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 11 | CK | 173 | ARG |
| 11 | CK | 190 | ASP |
| 12 | CL | 3 | ARG |
| 12 | CL | 24 | ARG |
| 12 | CL | 28 | ASP |
| 12 | CL | 30 | LYS |
| 12 | CL | 32 | ARG |
| 12 | CL | 33 | ILE |
| 12 | CL | 40 | LYS |
| 12 | CL | 42 | THR |
| 12 | CL | 52 | LEU |
| 12 | CL | 57 | LEU |
| 12 | CL | 58 | GLU |
| 12 | CL | 63 | GLU |
| 12 | CL | 71 | CYS |
| 12 | CL | 74 | LYS |
| 12 | CL | 77 | THR |
| 12 | CL | 87 | LEU |
| 12 | CL | 91 | VAL |
| 12 | CL | 139 | ARG |
| 12 | CL | 153 | ARG |
| 12 | CL | 165 | ILE |
| 12 | CL | 169 | LYS |
| 12 | CL | 185 | ARG |
| 12 | CL | 197 | VAL |
| 12 | CL | 206 | LEU |
| 12 | CL | 208 | ASN |
| 12 | CL | 212 | GLU |
| 13 | CM | 9 | MET |
| 13 | CM | 10 | ARG |
| 13 | CM | 12 | LEU |
| 13 | CM | 29 | ARG |
| 13 | CM | 40 | LEU |
| 13 | CM | 44 | THR |
| 13 | CM | 56 | THR |
| 13 | CM | 80 | LEU |
| 13 | CM | 82 | ARG |
| 13 | CM | 106 | ILE |
| 13 | CM | 107 | ASP |
| 13 | CM | 112 | LEU |
| 13 | CM | 115 | LYS |
| 13 | CM | 130 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 13 | CM | 137 | ARG |
| 13 | CM | 140 | ARG |
| 13 | CM | 142 | LYS |
| 13 | CM | 145 | LYS |
| 13 | CM | 147 | THR |
| 13 | CM | 168 | ASP |
| 13 | CM | 171 | VAL |
| 13 | CM | 172 | LEU |
| 14 | CN | 4 | SER |
| 14 | CN | 5 | LYS |
| 14 | CN | 23 | LYS |
| 14 | CN | 42 | ARG |
| 14 | CN | 52 | ASP |
| 14 | CN | 53 | LEU |
| 14 | CN | 54 | LEU |
| 14 | CN | 55 | ARG |
| 14 | CN | 57 | VAL |
| 14 | CN | 58 | VAL |
| 14 | CN | 59 | ARG |
| 14 | CN | 63 | VAL |
| 14 | CN | 67 | ARG |
| 14 | CN | 69 | VAL |
| 14 | CN | 85 | LEU |
| 14 | CN | 107 | GLU |
| 14 | CN | 118 | GLU |
| 14 | CN | 124 | ILE |
| 14 | CN | 128 | ARG |
| 14 | CN | 131 | LYS |
| 14 | CN | 153 | ASP |
| 14 | CN | 154 | VAL |
| 14 | CN | 164 | GLU |
| 14 | CN | 165 | SER |
| 14 | CN | 168 | ARG |
| 14 | CN | 171 | ARG |
| 15 | CO | 4 | ASP |
| 15 | CO | 5 | SER |
| 15 | CO | 8 | LYS |
| 15 | CO | 15 | VAL |
| 15 | CO | 38 | ILE |
| 15 | CO | 45 | LEU |
| 15 | CO | 53 | VAL |
| 15 | CO | 63 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 15 | CO | 66 | THR |
| 15 | CO | 90 | VAL |
| 15 | CO | 121 | MET |
| 15 | CO | 123 | LEU |
| 15 | CO | 124 | ARG |
| 15 | CO | 130 | THR |
| 16 | CP | 10 | LEU |
| 16 | CP | 17 | ASP |
| 16 | CP | 20 | ARG |
| 16 | CP | 22 | LEU |
| 16 | CP | 68 | ARG |
| 16 | CP | 80 | THR |
| 16 | CP | 85 | THR |
| 16 | CP | 133 | ILE |
| 16 | CP | 138 | GLN |
| 16 | CP | 151 | ILE |
| 16 | CP | 153 | ASP |
| 16 | CP | 182 | ASN |
| 16 | CP | 183 | THR |
| 16 | CP | 190 | THR |
| 16 | CP | 198 | SER |
| 17 | CQ | 41 | LEU |
| 17 | CQ | 58 | LEU |
| 17 | CQ | 67 | THR |
| 17 | CQ | 74 | ARG |
| 17 | CQ | 78 | ARG |
| 17 | CQ | 85 | ARG |
| 17 | CQ | 106 | GLU |
| 17 | CQ | 110 | PRO |
| 17 | CQ | 115 | LYS |
| 17 | CQ | 117 | ARG |
| 17 | CQ | 124 | LEU |
| 17 | CQ | 126 | VAL |
| 17 | CQ | 128 | ARG |
| 17 | CQ | 129 | LEU |
| 17 | CQ | 134 | LYS |
| 17 | CQ | 180 | SER |
| 18 | CR | 7 | THR |
| 18 | CR | 9 | THR |
| 18 | CR | 24 | VAL |
| 18 | CR | 32 | THR |
| 18 | CR | 42 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 18 | CR | 49 | GLU |
| 18 | CR | 52 | LEU |
| 18 | CR | 56 | ARG |
| 18 | CR | 70 | THR |
| 18 | CR | 78 | VAL |
| 18 | CR | 111 | LYS |
| 18 | CR | 112 | LEU |
| 18 | CR | 114 | VAL |
| 18 | CR | 119 | VAL |
| 18 | CR | 128 | ARG |
| 18 | CR | 144 | SER |
| 18 | CR | 166 | VAL |
| 18 | CR | 168 | LEU |
| 18 | CR | 171 | ARG |
| 18 | CR | 175 | ARG |
| 19 | CS | 3 | ILE |
| 19 | CS | 7 | SER |
| 19 | CS | 11 | LYS |
| 19 | CS | 17 | THR |
| 19 | CS | 24 | VAL |
| 19 | CS | 26 | LEU |
| 19 | CS | 32 | LEU |
| 19 | CS | 41 | ASP |
| 19 | CS | 49 | LEU |
| 19 | CS | 69 | ARG |
| 19 | CS | 80 | THR |
| 19 | CS | 81 | VAL |
| 19 | CS | 82 | VAL |
| 19 | CS | 86 | THR |
| 19 | CS | 93 | ILE |
| 19 | CS | 113 | LYS |
| 19 | CS | 135 | GLN |
| 19 | CS | 138 | LEU |
| 19 | CS | 150 | VAL |
| 19 | CS | 170 | ARG |
| 19 | CS | 180 | ARG |
| 19 | CS | 181 | SER |
| 20 | CT | 5 | ARG |
| 20 | CT | 10 | LEU |
| 20 | CT | 17 | VAL |
| 20 | CT | 22 | VAL |
| 20 | CT | 30 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 20 | CT | 43 | LYS |
| 20 | CT | 57 | VAL |
| 20 | CT | 74 | ARG |
| 20 | CT | 81 | ARG |
| 20 | CT | 98 | ARG |
| 20 | CT | 99 | LEU |
| 20 | CT | 103 | ARG |
| 20 | CT | 104 | ARG |
| 20 | CT | 126 | GLU |
| 20 | CT | 130 | ASN |
| 20 | CT | 134 | HIS |
| 20 | CT | 144 | GLN |
| 20 | CT | 148 | ASP |
| 20 | CT | 165 | LYS |
| 20 | CT | 166 | ASN |
| 20 | CT | 180 | LYS |
| 21 | CU | 1 | MET |
| 21 | CU | 24 | LEU |
| 21 | CU | 45 | LEU |
| 21 | CU | 58 | ILE |
| 21 | CU | 61 | ILE |
| 21 | CU | 71 | LYS |
| 21 | CU | 80 | ARG |
| 21 | CU | 81 | TYR |
| 21 | CU | 82 | ASP |
| 21 | CU | 97 | VAL |
| 21 | CU | 100 | VAL |
| 21 | CU | 104 | GLU |
| 21 | CU | 117 | ARG |
| 21 | CU | 132 | THR |
| 21 | CU | 137 | ARG |
| 21 | CU | 145 | THR |
| 21 | CU | 149 | LYS |
| 21 | CU | 155 | ARG |
| 21 | CU | 156 | VAL |
| 21 | CU | 160 | THR |
| 21 | CU | 162 | THR |
| 21 | CU | 167 | ARG |
| 21 | CU | 172 | TYR |
| 22 | CV | 9 | SER |
| 22 | CV | 16 | GLN |
| 22 | CV | 25 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 22 | CV | 26 | HIS |
| 22 | CV | 27 | LEU |
| 22 | CV | 32 | LYS |
| 22 | CV | 75 | ILE |
| 22 | CV | 78 | LYS |
| 22 | CV | 79 | MET |
| 22 | CV | 80 | VAL |
| 22 | CV | 88 | ARG |
| 22 | CV | 92 | ARG |
| 22 | CV | 96 | ILE |
| 22 | CV | 97 | LYS |
| 22 | CV | 100 | LYS |
| 22 | CV | 101 | CYS |
| 22 | CV | 102 | ARG |
| 22 | CV | 103 | GLN |
| 22 | CV | 106 | LEU |
| 22 | CV | 126 | VAL |
| 22 | CV | 127 | GLN |
| 22 | CV | 128 | LEU |
| 22 | CV | 139 | ARG |
| 22 | CV | 143 | THR |
| 23 | CW | 10 | LYS |
| 23 | CW | 38 | ILE |
| 23 | CW | 43 | VAL |
| 23 | CW | 49 | ASN |
| 23 | CW | 55 | THR |
| 23 | CW | 58 | GLU |
| 23 | CW | 59 | ASP |
| 23 | CW | 100 | THR |
| 23 | CW | 104 | ARG |
| 23 | CW | 105 | LEU |
| 24 | CX | 13 | ILE |
| 24 | CX | 32 | ARG |
| 24 | CX | 45 | ARG |
| 24 | CX | 69 | LEU |
| 24 | CX | 73 | VAL |
| 24 | CX | 83 | LYS |
| 24 | CX | 88 | ARG |
| 24 | CX | 93 | LEU |
| 24 | CX | 102 | ILE |
| 24 | CX | 120 | LYS |
| 24 | CX | 128 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 26 | CY | 1 | MET |
| 26 | CY | 4 | GLU |
| 26 | CY | 5 | ILE |
| 26 | CY | 19 | THR |
| 26 | CY | 25 | ASP |
| 26 | CY | 34 | SER |
| 26 | CY | 39 | LEU |
| 26 | CY | 43 | ARG |
| 26 | CY | 54 | LEU |
| 26 | CY | 63 | ILE |
| 27 | CZ | 26 | VAL |
| 27 | CZ | 27 | ARG |
| 27 | CZ | 37 | THR |
| 27 | CZ | 38 | LEU |
| 27 | CZ | 39 | LYS |
| 27 | CZ | 63 | ILE |
| 27 | CZ | 71 | THR |
| 27 | CZ | 92 | LYS |
| 27 | CZ | 108 | LEU |
| 27 | CZ | 115 | ARG |
| 27 | CZ | 117 | ASN |
| 27 | CZ | 125 | ARG |
| 27 | CZ | 133 | LEU |
| 27 | CZ | 135 | ILE |
| 28 | DA | 8 | VAL |
| 28 | DA | 9 | SER |
| 28 | DA | 13 | ARG |
| 28 | DA | 17 | LYS |
| 28 | DA | 37 | LYS |
| 28 | DA | 45 | ILE |
| 28 | DA | 50 | ILE |
| 28 | DA | 56 | VAL |
| 28 | DA | 57 | LEU |
| 28 | DA | 59 | VAL |
| 28 | DA | 67 | GLU |
| 28 | DA | 74 | TYR |
| 28 | DA | 76 | LEU |
| 28 | DA | 105 | VAL |
| 29 | DB | 14 | VAL |
| 29 | DB | 17 | ARG |
| 29 | DB | 24 | VAL |
| 29 | DB | 26 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 29 | DB | 30 | ASP |
| 29 | DB | 46 | ILE |
| 29 | DB | 66 | THR |
| 29 | DB | 81 | LEU |
| 29 | DB | 86 | THR |
| 29 | DB | 92 | PHE |
| 29 | DB | 103 | GLN |
| 30 | DC | 4 | ARG |
| 30 | DC | 8 | THR |
| 30 | DC | 10 | LYS |
| 30 | DC | 14 | HIS |
| 30 | DC | 42 | ARG |
| 30 | DC | 46 | ASP |
| 30 | DC | 56 | VAL |
| 30 | DC | 60 | TYR |
| 30 | DC | 76 | ASP |
| 30 | DC | 77 | LYS |
| 30 | DC | 85 | ASP |
| 30 | DC | 88 | ASP |
| 30 | DC | 91 | LEU |
| 30 | DC | 115 | LYS |
| 30 | DC | 139 | ARG |
| 31 | DD | 13 | THR |
| 31 | DD | 14 | ARG |
| 31 | DD | 21 | ILE |
| 31 | DD | 22 | LYS |
| 31 | DD | 23 | LYS |
| 31 | DD | 26 | THR |
| 31 | DD | 59 | LYS |
| 32 | DE | 40 | LYS |
| 32 | DE | 61 | MET |
| 32 | DE | 83 | LYS |
| 32 | DE | 102 | THR |
| 32 | DE | 103 | THR |
| 33 | DF | 8 | VAL |
| 33 | DF | 13 | THR |
| 33 | DF | 16 | LEU |
| 33 | DF | 26 | LYS |
| 33 | DF | 31 | ARG |
| 33 | DF | 46 | THR |
| 33 | DF | 64 | VAL |
| 33 | DF | 68 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 33 | DF | 76 | SER |
| 33 | DF | 79 | ARG |
| 33 | DF | 86 | LYS |
| 33 | DF | 93 | VAL |
| 33 | DF | 96 | VAL |
| 33 | DF | 100 | SER |
| 33 | DF | 104 | LEU |
| 33 | DF | 106 | THR |
| 33 | DF | 110 | GLU |
| 34 | DG | 4 | LEU |
| 34 | DG | 19 | ARG |
| 34 | DG | 31 | ASN |
| 34 | DG | 33 | ARG |
| 34 | DG | 34 | LYS |
| 34 | DG | 40 | SER |
| 34 | DG | 73 | THR |
| 34 | DG | 75 | LEU |
| 34 | DG | 82 | LEU |
| 34 | DG | 91 | THR |
| 34 | DG | 109 | LEU |
| 34 | DG | 125 | ARG |
| 34 | DG | 128 | LEU |
| 35 | DH | 20 | LYS |
| 35 | DH | 31 | LYS |
| 35 | DH | 60 | ARG |
| 35 | DH | 70 | LYS |
| 35 | DH | 81 | VAL |
| 35 | DH | 92 | LYS |
| 35 | DH | 98 | VAL |
| 36 | DI | 5 | VAL |
| 36 | DI | 20 | ILE |
| 36 | DI | 23 | VAL |
| 36 | DI | 29 | ILE |
| 36 | DI | 31 | ARG |
| 36 | DI | 36 | LYS |
| 36 | DI | 58 | ARG |
| 36 | DI | 64 | THR |
| 36 | DI | 65 | VAL |
| 36 | DI | 71 | THR |
| 37 | DJ | 11 | THR |
| 37 | DJ | 20 | GLN |
| 37 | DJ | 21 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 37 | DJ | 27 | GLU |
| 37 | DJ | 28 | LEU |
| 37 | DJ | 36 | LEU |
| 37 | DJ | 46 | THR |
| 37 | DJ | 48 | ARG |
| 37 | DJ | 49 | LYS |
| 37 | DJ | 59 | ASN |
| 37 | DJ | 64 | GLU |
| 37 | DJ | 68 | GLN |
| 37 | DJ | 69 | LEU |
| 37 | DJ | 71 | LYS |
| 37 | DJ | 89 | ARG |
| 37 | DJ | 101 | THR |
| 37 | DJ | 107 | LYS |
| 37 | DJ | 119 | LYS |
| 38 | DK | 2 | THR |
| 38 | DK | 17 | VAL |
| 38 | DK | 21 | THR |
| 38 | DK | 26 | ILE |
| 38 | DK | 43 | LEU |
| 38 | DK | 45 | ARG |
| 38 | DK | 68 | ARG |
| 38 | DK | 76 | ARG |
| 38 | DK | 81 | THR |
| 38 | DK | 99 | ARG |
| 39 | DL | 17 | THR |
| 39 | DL | 24 | ARG |
| 39 | DL | 25 | ARG |
| 39 | DL | 33 | THR |
| 39 | DL | 36 | SER |
| 39 | DL | 44 | THR |
| 39 | DL | 45 | ARG |
| 39 | DL | 55 | ARG |
| 39 | DL | 59 | THR |
| 39 | DL | 67 | LEU |
| 39 | DL | 80 | THR |
| 40 | DM | 24 | THR |
| 40 | DM | 41 | THR |
| 40 | DM | 53 | THR |
| 40 | DM | 65 | LEU |
| 40 | DM | 69 | LEU |
| 40 | DM | 72 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 40 | DM | 77 | ARG |
| 41 | DN | 4 | GLN |
| 41 | DN | 21 | ARG |
| 41 | DN | 45 | ARG |
| 41 | DN | 48 | LYS |
| 42 | DO | 85 | LEU |
| 42 | DO | 112 | LYS |
| 42 | DO | 113 | ARG |
| 42 | DO | 114 | LYS |
| 42 | DO | 127 | LEU |
| 43 | DP | 6 | ARG |
| 43 | DP | 9 | ARG |
| 43 | DP | 11 | ARG |
| 43 | DP | 13 | LEU |
| 44 | DQ | 7 | THR |
| 44 | DQ | 35 | LEU |
| 44 | DQ | 78 | LYS |
| 44 | DQ | 79 | THR |
| 44 | DQ | 83 | LEU |
| 44 | DQ | 84 | THR |
| 44 | DQ | 85 | LEU |
| 44 | DQ | 100 | LYS |
| 44 | DQ | 105 | GLN |
| 45 | DR | 7 | LYS |
| 45 | DR | 10 | ILE |
| 45 | DR | 11 | THR |
| 45 | DR | 25 | GLN |
| 45 | DR | 49 | ARG |
| 45 | DR | 56 | THR |
| 45 | DR | 60 | CYS |
| 45 | DR | 70 | THR |
| 48 | sM | 33 | LYS |
| 48 | sM | 43 | ASP |
| 48 | sM | 50 | ASN |
| 48 | sM | 68 | ARG |
| 48 | sM | 71 | ASN |
| 48 | sM | 74 | LYS |
| 48 | sM | 77 | THR |
| 49 | p0 | 4 | ILE |
| 49 | p0 | 5 | ARG |
| 49 | p0 | 30 | VAL |
| 49 | p0 | 42 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 49 | p0 | 44 | GLU |
| 49 | p0 | 48 | ARG |
| 49 | p0 | 51 | VAL |
| 49 | p0 | 70 | LEU |
| 49 | p0 | 72 | ASP |
| 49 | p0 | 76 | LEU |
| 49 | p0 | 93 | LEU |
| 49 | p0 | 97 | LYS |
| 49 | p0 | 104 | ARG |
| 49 | p0 | 192 | ASP |
| 50 | B | 6 | THR |
| 50 | B | 10 | THR |
| 50 | B | 37 | VAL |
| 50 | B | 59 | LEU |
| 50 | B | 62 | ARG |
| 50 | B | 84 | ARG |
| 50 | B | 87 | LEU |
| 50 | B | 88 | LYS |
| 50 | B | 96 | THR |
| 50 | B | 111 | ILE |
| 50 | B | 155 | PHE |
| 50 | B | 168 | HIS |
| 50 | B | 172 | LEU |
| 50 | B | 188 | LEU |
| 50 | B | 197 | ILE |
| 50 | B | 198 | MET |
| 50 | B | 200 | ASP |
| 50 | B | 203 | PHE |
| 51 | C | 21 | VAL |
| 51 | C | 25 | THR |
| 51 | C | 29 | TRP |
| 51 | C | 46 | THR |
| 51 | C | 61 | LEU |
| 51 | C | 70 | LEU |
| 51 | C | 74 | GLN |
| 51 | C | 77 | GLU |
| 51 | C | 78 | ASP |
| 51 | C | 89 | ASP |
| 51 | C | 95 | ASN |
| 51 | C | 97 | LEU |
| 51 | C | 105 | PHE |
| 51 | C | 111 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 51 | C | 117 | TRP |
| 51 | C | 129 | THR |
| 51 | C | 177 | GLN |
| 51 | C | 181 | LEU |
| 51 | C | 198 | GLU |
| 51 | C | 202 | LYS |
| 51 | C | 218 | LEU |
| 51 | C | 220 | GLN |
| 51 | C | 222 | LYS |
| 51 | C | 223 | PHE |
| 52 | D | 53 | ILE |
| 52 | D | 69 | ILE |
| 52 | D | 72 | LEU |
| 52 | D | 73 | LEU |
| 52 | D | 76 | LEU |
| 52 | D | 91 | ARG |
| 52 | D | 95 | ARG |
| 52 | D | 96 | THR |
| 52 | D | 97 | ARG |
| 52 | D | 99 | LYS |
| 52 | D | 111 | VAL |
| 52 | D | 113 | LEU |
| 52 | D | 117 | THR |
| 52 | D | 134 | LEU |
| 52 | D | 137 | ILE |
| 52 | D | 141 | ARG |
| 52 | D | 147 | ASN |
| 52 | D | 148 | LEU |
| 52 | D | 207 | LEU |
| 52 | D | 221 | THR |
| 52 | D | 225 | LEU |
| 52 | D | 226 | THR |
| 52 | D | 235 | LEU |
| 52 | D | 244 | SER |
| 52 | D | 245 | ASP |
| 53 | E | 4 | LEU |
| 53 | E | 21 | LEU |
| 53 | E | 23 | GLU |
| 53 | E | 76 | ARG |
| 53 | E | 84 | ILE |
| 53 | E | 92 | GLN |
| 53 | E | 105 | MET |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 53 | E | 117 | ARG |
| 53 | E | 151 | LYS |
| 53 | E | 158 | ILE |
| 53 | E | 172 | THR |
| 53 | E | 174 | HIS |
| 53 | E | 175 | VAL |
| 53 | E | 176 | LEU |
| 53 | E | 178 | ARG |
| 53 | E | 181 | VAL |
| 53 | E | 182 | LEU |
| 53 | E | 195 | SER |
| 53 | E | 196 | ARG |
| 53 | E | 215 | GLU |
| 53 | E | 217 | ILE |
| 53 | E | 222 | VAL |
| 53 | E | 224 | ASP |
| 54 | F | 6 | LYS |
| 54 | F | 7 | LYS |
| 54 | F | 9 | LEU |
| 54 | F | 38 | LEU |
| 54 | F | 39 | ARG |
| 54 | F | 48 | LEU |
| 54 | F | 68 | ARG |
| 54 | F | 70 | VAL |
| 54 | F | 71 | LYS |
| 54 | F | 77 | ARG |
| 54 | F | 102 | VAL |
| 54 | F | 105 | VAL |
| 54 | F | 115 | THR |
| 54 | F | 116 | ASP |
| 54 | F | 126 | VAL |
| 54 | F | 131 | LEU |
| 54 | F | 142 | HIS |
| 54 | F | 180 | LEU |
| 54 | F | 182 | TYR |
| 54 | F | 187 | ARG |
| 54 | F | 192 | ILE |
| 54 | F | 227 | VAL |
| 54 | F | 240 | LYS |
| 54 | F | 242 | LYS |
| 54 | F | 258 | GLN |
| 55 | G | 25 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 55 | G | 32 | GLU |
| 55 | G | 38 | THR |
| 55 | G | 40 | ILE |
| 55 | G | 41 | LYS |
| 55 | G | 43 | PHE |
| 55 | G | 45 | LYS |
| 55 | G | 48 | PHE |
| 55 | G | 58 | LEU |
| 55 | G | 65 | ARG |
| 55 | G | 76 | ARG |
| 55 | G | 79 | ASN |
| 55 | G | 93 | LEU |
| 55 | G | 146 | THR |
| 55 | G | 149 | VAL |
| 55 | G | 156 | ARG |
| 55 | G | 162 | VAL |
| 55 | G | 186 | ASN |
| 55 | G | 194 | LEU |
| 55 | G | 216 | GLU |
| 56 | H | 7 | TYR |
| 56 | H | 10 | ASN |
| 56 | H | 15 | THR |
| 56 | H | 25 | ARG |
| 56 | H | 39 | GLU |
| 56 | H | 45 | PHE |
| 56 | H | 71 | THR |
| 56 | H | 81 | VAL |
| 56 | H | 82 | SER |
| 56 | H | 109 | LEU |
| 56 | H | 120 | GLU |
| 56 | H | 126 | ASP |
| 56 | H | 127 | THR |
| 56 | H | 128 | THR |
| 56 | H | 129 | VAL |
| 56 | H | 133 | LEU |
| 56 | H | 137 | ARG |
| 56 | H | 154 | ARG |
| 56 | H | 155 | ASP |
| 56 | H | 158 | ILE |
| 56 | H | 169 | TYR |
| 56 | H | 170 | THR |
| 56 | H | 174 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 56 | H | 193 | LEU |
| 56 | H | 211 | LEU |
| 57 | I | 15 | GLU |
| 57 | I | 16 | LEU |
| 57 | I | 31 | SER |
| 57 | I | 50 | ASP |
| 57 | I | 67 | LEU |
| 57 | I | 80 | GLU |
| 57 | I | 85 | PHE |
| 57 | I | 87 | ASP |
| 57 | I | 97 | ARG |
| 57 | I | 99 | LEU |
| 57 | I | 104 | ARG |
| 57 | I | 110 | GLN |
| 57 | I | 114 | ARG |
| 57 | I | 116 | ARG |
| 57 | I | 126 | LEU |
| 57 | I | 133 | THR |
| 57 | I | 147 | ASN |
| 57 | I | 166 | LEU |
| 57 | I | 185 | ILE |
| 58 | J | 21 | PHE |
| 58 | J | 22 | ARG |
| 58 | J | 29 | LEU |
| 58 | J | 36 | THR |
| 58 | J | 58 | LEU |
| 58 | J | 107 | THR |
| 58 | J | 138 | ASN |
| 58 | J | 151 | LYS |
| 58 | J | 152 | ILE |
| 58 | J | 184 | LEU |
| 58 | J | 196 | LEU |
| 59 | K | 3 | ARG |
| 59 | K | 6 | ARG |
| 59 | K | 7 | THR |
| 59 | K | 14 | THR |
| 59 | K | 28 | LEU |
| 59 | K | 39 | LYS |
| 59 | K | 40 | LYS |
| 59 | K | 78 | ARG |
| 59 | K | 89 | ASP |
| 59 | K | 92 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 59 | K | 93 | LEU |
| 59 | K | 97 | LEU |
| 59 | K | 99 | LEU |
| 59 | K | 101 | VAL |
| 59 | K | 109 | LEU |
| 59 | K | 110 | GLN |
| 59 | K | 134 | ILE |
| 59 | K | 138 | LYS |
| 59 | K | 149 | ARG |
| 59 | K | 161 | THR |
| 59 | K | 171 | ARG |
| 59 | K | 172 | VAL |
| 59 | K | 174 | ARG |
| 59 | K | 182 | GLU |
| 60 | L | 5 | LYS |
| 60 | L | 8 | ARG |
| 60 | L | 20 | VAL |
| 60 | L | 27 | PHE |
| 60 | L | 28 | ASN |
| 60 | L | 55 | VAL |
| 60 | L | 62 | GLN |
| 60 | L | 76 | LEU |
| 60 | L | 82 | LEU |
| 61 | M | 21 | ASN |
| 61 | M | 29 | LYS |
| 61 | M | 44 | THR |
| 61 | M | 67 | ARG |
| 61 | M | 69 | LYS |
| 61 | M | 74 | THR |
| 61 | M | 80 | MET |
| 61 | M | 99 | ARG |
| 61 | M | 123 | VAL |
| 62 | N | 28 | LEU |
| 62 | N | 36 | LEU |
| 62 | N | 37 | VAL |
| 62 | N | 43 | ARG |
| 62 | N | 45 | LEU |
| 62 | N | 50 | LYS |
| 62 | N | 61 | VAL |
| 62 | N | 74 | LEU |
| 62 | N | 89 | ILE |
| 62 | N | 103 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 62 | N | 125 | ASN |
| 62 | N | 126 | TRP |
| 62 | N | 129 | GLU |
| 62 | N | 132 | GLU |
| 62 | N | 140 | PHE |
| 63 | O | 3 | ARG |
| 63 | O | 6 | SER |
| 63 | O | 9 | LYS |
| 63 | O | 27 | LYS |
| 63 | O | 28 | LEU |
| 63 | O | 32 | SER |
| 63 | O | 39 | LYS |
| 63 | O | 64 | ARG |
| 63 | O | 66 | ILE |
| 63 | O | 76 | LYS |
| 63 | O | 83 | GLU |
| 63 | O | 88 | LEU |
| 63 | O | 102 | LEU |
| 63 | O | 115 | LEU |
| 63 | O | 125 | LEU |
| 63 | O | 134 | VAL |
| 63 | O | 149 | LEU |
| 64 | P | 29 | HIS |
| 64 | P | 31 | THR |
| 64 | P | 42 | VAL |
| 64 | P | 81 | VAL |
| 64 | P | 83 | ILE |
| 64 | P | 92 | LYS |
| 64 | P | 103 | ARG |
| 64 | P | 115 | ILE |
| 64 | P | 123 | SER |
| 64 | P | 132 | ARG |
| 64 | P | 137 | LEU |
| 65 | Q | 22 | LEU |
| 65 | Q | 26 | LEU |
| 65 | Q | 34 | VAL |
| 65 | Q | 36 | LEU |
| 65 | Q | 44 | ARG |
| 65 | Q | 52 | LYS |
| 65 | Q | 110 | GLU |
| 65 | Q | 121 | ILE |
| 65 | Q | 124 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 66 | R | 29 | ILE |
| 66 | R | 31 | VAL |
| 66 | R | 40 | GLU |
| 66 | R | 42 | GLU |
| 66 | R | 43 | ILE |
| 66 | R | 58 | ASP |
| 66 | R | 65 | ILE |
| 66 | R | 66 | ARG |
| 66 | R | 69 | VAL |
| 66 | R | 98 | ASP |
| 66 | R | 106 | LYS |
| 66 | R | 109 | PHE |
| 66 | R | 114 | ARG |
| 66 | R | 123 | ARG |
| 66 | R | 128 | LYS |
| 66 | R | 137 | ARG |
| 67 | S | 18 | GLU |
| 67 | S | 29 | GLN |
| 67 | S | 34 | LEU |
| 67 | S | 38 | ILE |
| 67 | S | 40 | THR |
| 67 | S | 43 | SER |
| 67 | S | 46 | LEU |
| 67 | S | 62 | GLN |
| 67 | S | 69 | ILE |
| 67 | S | 72 | LYS |
| 67 | S | 84 | TYR |
| 67 | S | 105 | GLN |
| 67 | S | 113 | LEU |
| 67 | S | 115 | LEU |
| 68 | T | 3 | LEU |
| 68 | T | 5 | VAL |
| 68 | T | 6 | GLN |
| 68 | T | 7 | GLU |
| 68 | T | 8 | GLN |
| 68 | T | 11 | PHE |
| 68 | T | 12 | GLN |
| 68 | T | 13 | HIS |
| 68 | T | 15 | LEU |
| 68 | T | 26 | ILE |
| 68 | T | 28 | ILE |
| 68 | T | 40 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 68 | T | 71 | GLN |
| 68 | T | 77 | THR |
| 68 | T | 80 | LYS |
| 68 | T | 136 | GLN |
| 68 | T | 138 | THR |
| 68 | T | 140 | THR |
| 68 | T | 143 | ARG |
| 68 | T | 145 | ARG |
| 69 | U | 4 | VAL |
| 69 | U | 6 | VAL |
| 69 | U | 18 | TYR |
| 69 | U | 22 | LEU |
| 69 | U | 28 | LEU |
| 69 | U | 33 | TYR |
| 69 | U | 35 | ASP |
| 69 | U | 36 | ILE |
| 69 | U | 57 | ARG |
| 69 | U | 67 | MET |
| 69 | U | 70 | GLN |
| 69 | U | 71 | VAL |
| 69 | U | 94 | ILE |
| 69 | U | 126 | GLU |
| 69 | U | 127 | ASN |
| 69 | U | 130 | ARG |
| 69 | U | 131 | ASP |
| 69 | U | 139 | THR |
| 69 | U | 143 | ASP |
| 69 | U | 144 | GLU |
| 70 | V | 15 | GLN |
| 70 | V | 23 | ARG |
| 70 | V | 27 | THR |
| 70 | V | 30 | LYS |
| 70 | V | 31 | VAL |
| 70 | V | 57 | ARG |
| 70 | V | 60 | THR |
| 70 | V | 61 | LYS |
| 70 | V | 62 | VAL |
| 70 | V | 74 | GLU |
| 70 | V | 76 | SER |
| 70 | V | 89 | ARG |
| 70 | V | 103 | ILE |
| 70 | V | 117 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 71 | W | 5 | LYS |
| 71 | W | 9 | VAL |
| 71 | W | 10 | GLU |
| 71 | W | 11 | LEU |
| 71 | W | 25 | LYS |
| 71 | W | 32 | VAL |
| 71 | W | 41 | GLU |
| 71 | W | 68 | SER |
| 71 | W | 69 | LEU |
| 71 | W | 76 | ASP |
| 71 | W | 78 | LEU |
| 71 | W | 80 | LYS |
| 72 | X | 4 | SER |
| 72 | X | 7 | LEU |
| 72 | X | 24 | GLN |
| 72 | X | 25 | VAL |
| 72 | X | 26 | LEU |
| 72 | X | 53 | ILE |
| 72 | X | 65 | LEU |
| 72 | X | 76 | SER |
| 72 | X | 81 | VAL |
| 72 | X | 87 | GLU |
| 72 | X | 98 | GLN |
| 72 | X | 103 | ILE |
| 72 | X | 119 | LYS |
| 72 | X | 121 | VAL |
| 72 | X | 126 | LEU |
| 73 | Y | 7 | ARG |
| 73 | Y | 9 | LEU |
| 73 | Y | 18 | HIS |
| 73 | Y | 19 | ARG |
| 73 | Y | 32 | ARG |
| 73 | Y | 69 | ARG |
| 73 | Y | 73 | ARG |
| 73 | Y | 75 | GLN |
| 73 | Y | 84 | THR |
| 73 | Y | 96 | VAL |
| 73 | Y | 107 | PHE |
| 73 | Y | 110 | LYS |
| 73 | Y | 114 | LYS |
| 73 | Y | 117 | ILE |
| 73 | Y | 132 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 73 | Y | 140 | LYS |
| 73 | Y | 144 | ARG |
| 74 | Z | 21 | LYS |
| 74 | Z | 32 | ARG |
| 74 | Z | 57 | VAL |
| 74 | Z | 81 | GLU |
| 74 | Z | 84 | LYS |
| 74 | Z | 99 | LYS |
| 74 | Z | 102 | LYS |
| 74 | Z | 104 | SER |
| 74 | Z | 124 | ARG |
| 74 | Z | 127 | LYS |
| 74 | Z | 133 | ASN |
| 75 | a | 40 | VAL |
| 75 | a | 42 | LEU |
| 75 | a | 43 | ASP |
| 75 | a | 58 | ARG |
| 75 | a | 60 | VAL |
| 75 | a | 69 | LEU |
| 75 | a | 71 | ILE |
| 75 | a | 75 | LEU |
| 75 | a | 78 | ILE |
| 75 | a | 85 | LYS |
| 75 | a | 92 | ILE |
| 75 | a | 96 | SER |
| 76 | b | 41 | ILE |
| 76 | b | 44 | ILE |
| 76 | b | 62 | TYR |
| 76 | b | 64 | LEU |
| 76 | b | 76 | SER |
| 76 | b | 85 | ARG |
| 76 | b | 90 | GLU |
| 77 | c | 33 | LEU |
| 77 | c | 65 | THR |
| 77 | c | 77 | THR |
| 78 | d | 15 | VAL |
| 78 | d | 19 | THR |
| 78 | d | 31 | GLU |
| 78 | d | 32 | PHE |
| 78 | d | 35 | ASP |
| 78 | d | 48 | VAL |
| 78 | d | 49 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 78 | d | 58 | GLU |
| 79 | e | 9 | SER |
| 79 | e | 12 | ARG |
| 79 | e | 30 | LEU |
| 79 | e | 32 | ARG |
| 79 | e | 49 | ASP |
| 80 | f | 3 | LYS |
| 80 | f | 21 | VAL |
| 80 | f | 22 | GLU |
| 80 | f | 28 | LYS |
| 81 | g | 83 | LYS |
| 81 | g | 97 | LYS |
| 81 | g | 102 | VAL |
| 81 | g | 106 | TYR |
| 81 | g | 114 | VAL |
| 81 | g | 120 | GLU |
| 81 | g | 130 | VAL |
| 81 | g | 135 | HIS |
| 81 | g | 137 | ASP |
| 81 | g | 138 | ARG |
| 81 | g | 147 | VAL |
| 81 | g | 151 | ASN |
| 82 | h | 16 | HIS |
| 82 | h | 29 | GLN |
| 82 | h | 52 | GLN |
| 82 | h | 66 | HIS |
| 82 | h | 74 | THR |
| 82 | h | 76 | ASP |
| 82 | h | 117 | LYS |
| 82 | h | 136 | ILE |
| 82 | h | 141 | LEU |
| 82 | h | 149 | ASP |
| 82 | h | 184 | ASN |
| 82 | h | 191 | ASP |
| 82 | h | 281 | TYR |
| 82 | h | 292 | LEU |
| 82 | h | 300 | THR |
| 82 | h | 308 | ASN |
| 82 | h | 317 | THR |
| 50 | s0 | 12 | GLU |
| 50 | s0 | 29 | VAL |
| 50 | s0 | 30 | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 50 | s0 | 41 | ARG |
| 50 | s0 | 45 | VAL |
| 50 | s0 | 50 | VAL |
| 50 | s0 | 55 | GLU |
| 50 | s0 | 59 | LEU |
| 50 | s0 | 87 | LEU |
| 50 | s0 | 96 | THR |
| 50 | s0 | 101 | ARG |
| 50 | s0 | 119 | ARG |
| 50 | s0 | 146 | LEU |
| 50 | s0 | 154 | GLU |
| 50 | s0 | 156 | VAL |
| 50 | s0 | 158 | VAL |
| 50 | s0 | 164 | ASN |
| 50 | s0 | 165 | ARG |
| 50 | s0 | 172 | LEU |
| 50 | s0 | 179 | ARG |
| 50 | s0 | 185 | ARG |
| 50 | s0 | 188 | LEU |
| 50 | s0 | 189 | VAL |
| 50 | s0 | 191 | ARG |
| 50 | s0 | 198 | MET |
| 51 | s1 | 21 | VAL |
| 51 | s1 | 25 | THR |
| 51 | s1 | 37 | THR |
| 51 | s1 | 47 | LEU |
| 51 | s1 | 48 | VAL |
| 51 | s1 | 68 | VAL |
| 51 | s1 | 70 | LEU |
| 51 | s1 | 73 | LEU |
| 51 | s1 | 81 | PHE |
| 51 | s1 | 91 | VAL |
| 51 | s1 | 105 | PHE |
| 51 | s1 | 110 | LEU |
| 51 | s1 | 126 | THR |
| 51 | s1 | 127 | VAL |
| 51 | s1 | 135 | LEU |
| 51 | s1 | 153 | HIS |
| 51 | s1 | 159 | SER |
| 51 | s1 | 173 | THR |
| 51 | s1 | 175 | GLU |
| 51 | s1 | 181 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 51 | s1 | 183 | GLN |
| 51 | s1 | 185 | THR |
| 51 | s1 | 194 | ASN |
| 51 | s1 | 205 | PHE |
| 51 | s1 | 222 | LYS |
| 51 | s1 | 223 | PHE |
| 51 | s1 | 231 | LEU |
| 51 | s1 | 234 | GLU |
| 52 | s2 | 41 | LEU |
| 52 | s2 | 51 | THR |
| 52 | s2 | 53 | ILE |
| 52 | s2 | 55 | GLU |
| 52 | s2 | 69 | ILE |
| 52 | s2 | 72 | LEU |
| 52 | s2 | 73 | LEU |
| 52 | s2 | 84 | LYS |
| 52 | s2 | 90 | THR |
| 52 | s2 | 91 | ARG |
| 52 | s2 | 95 | ARG |
| 52 | s2 | 97 | ARG |
| 52 | s2 | 111 | VAL |
| 52 | s2 | 113 | LEU |
| 52 | s2 | 117 | THR |
| 52 | s2 | 134 | LEU |
| 52 | s2 | 137 | ILE |
| 52 | s2 | 139 | ILE |
| 52 | s2 | 140 | ARG |
| 52 | s2 | 141 | ARG |
| 52 | s2 | 148 | LEU |
| 52 | s2 | 150 | GLN |
| 52 | s2 | 153 | SER |
| 52 | s2 | 166 | THR |
| 52 | s2 | 206 | THR |
| 52 | s2 | 225 | LEU |
| 52 | s2 | 228 | ASN |
| 52 | s2 | 237 | VAL |
| 52 | s2 | 238 | SER |
| 52 | s2 | 245 | ASP |
| 52 | s2 | 246 | GLU |
| 52 | s2 | 250 | GLN |
| 53 | s3 | 4 | LEU |
| 53 | s3 | 21 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 53 | s3 | 45 | LYS |
| 53 | s3 | 66 | ILE |
| 53 | s3 | 69 | LEU |
| 53 | s3 | 84 | ILE |
| 53 | s3 | 90 | ARG |
| 53 | s3 | 115 | ILE |
| 53 | s3 | 142 | LEU |
| 53 | s3 | 158 | ILE |
| 53 | s3 | 164 | VAL |
| 53 | s3 | 168 | ILE |
| 53 | s3 | 178 | ARG |
| 53 | s3 | 196 | ARG |
| 53 | s3 | 215 | GLU |
| 53 | s3 | 217 | ILE |
| 53 | s3 | 223 | LYS |
| 53 | s3 | 224 | ASP |
| 54 | s4 | 9 | LEU |
| 54 | s4 | 38 | LEU |
| 54 | s4 | 42 | LEU |
| 54 | s4 | 49 | ARG |
| 54 | s4 | 51 | ARG |
| 54 | s4 | 67 | GLN |
| 54 | s4 | 70 | VAL |
| 54 | s4 | 78 | THR |
| 54 | s4 | 89 | VAL |
| 54 | s4 | 95 | THR |
| 54 | s4 | 104 | ASP |
| 54 | s4 | 131 | LEU |
| 54 | s4 | 156 | VAL |
| 54 | s4 | 176 | ASP |
| 54 | s4 | 180 | LEU |
| 54 | s4 | 181 | VAL |
| 54 | s4 | 182 | TYR |
| 54 | s4 | 221 | ARG |
| 54 | s4 | 222 | LEU |
| 54 | s4 | 227 | VAL |
| 54 | s4 | 245 | LYS |
| 55 | s5 | 24 | VAL |
| 55 | s5 | 25 | LEU |
| 55 | s5 | 27 | THR |
| 55 | s5 | 43 | PHE |
| 55 | s5 | 45 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 55 | s5 | 59 | VAL |
| 55 | s5 | 66 | GLN |
| 55 | s5 | 68 | ILE |
| 55 | s5 | 76 | ARG |
| 55 | s5 | 100 | ASN |
| 55 | s5 | 104 | ASN |
| 55 | s5 | 125 | THR |
| 55 | s5 | 146 | THR |
| 55 | s5 | 149 | VAL |
| 55 | s5 | 157 | ARG |
| 55 | s5 | 194 | LEU |
| 55 | s5 | 208 | SER |
| 55 | s5 | 216 | GLU |
| 56 | s6 | 9 | VAL |
| 56 | s6 | 65 | GLN |
| 56 | s6 | 67 | VAL |
| 56 | s6 | 68 | LEU |
| 56 | s6 | 71 | THR |
| 56 | s6 | 76 | LEU |
| 56 | s6 | 78 | THR |
| 56 | s6 | 97 | VAL |
| 56 | s6 | 98 | ARG |
| 56 | s6 | 108 | VAL |
| 56 | s6 | 120 | GLU |
| 56 | s6 | 121 | LEU |
| 56 | s6 | 126 | ASP |
| 56 | s6 | 128 | THR |
| 56 | s6 | 129 | VAL |
| 56 | s6 | 133 | LEU |
| 56 | s6 | 143 | LYS |
| 56 | s6 | 151 | ASP |
| 56 | s6 | 177 | ARG |
| 56 | s6 | 179 | VAL |
| 56 | s6 | 182 | GLN |
| 56 | s6 | 193 | LEU |
| 56 | s6 | 215 | ARG |
| 56 | s6 | 216 | LEU |
| 57 | s7 | 10 | SER |
| 57 | s7 | 17 | GLU |
| 57 | s7 | 30 | SER |
| 57 | s7 | 33 | GLU |
| 57 | s7 | 49 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 57 | s7 | 50 | ASP |
| 57 | s7 | 67 | LEU |
| 57 | s7 | 79 | ARG |
| 57 | s7 | 80 | GLU |
| 57 | s7 | 101 | LYS |
| 57 | s7 | 105 | THR |
| 57 | s7 | 110 | GLN |
| 57 | s7 | 111 | LYS |
| 57 | s7 | 114 | ARG |
| 57 | s7 | 116 | ARG |
| 57 | s7 | 117 | THR |
| 57 | s7 | 129 | LEU |
| 57 | s7 | 143 | LEU |
| 57 | s7 | 144 | VAL |
| 57 | s7 | 185 | ILE |
| 58 | s8 | 20 | GLN |
| 58 | s8 | 22 | ARG |
| 58 | s8 | 29 | LEU |
| 58 | s8 | 36 | THR |
| 58 | s8 | 46 | VAL |
| 58 | s8 | 89 | GLU |
| 58 | s8 | 138 | ASN |
| 58 | s8 | 151 | LYS |
| 58 | s8 | 183 | ILE |
| 58 | s8 | 184 | LEU |
| 59 | s9 | 3 | ARG |
| 59 | s9 | 6 | ARG |
| 59 | s9 | 7 | THR |
| 59 | s9 | 16 | LYS |
| 59 | s9 | 20 | GLU |
| 59 | s9 | 21 | SER |
| 59 | s9 | 28 | LEU |
| 59 | s9 | 37 | LYS |
| 59 | s9 | 39 | LYS |
| 59 | s9 | 49 | LEU |
| 59 | s9 | 54 | ARG |
| 59 | s9 | 78 | ARG |
| 59 | s9 | 89 | ASP |
| 59 | s9 | 93 | LEU |
| 59 | s9 | 96 | VAL |
| 59 | s9 | 99 | LEU |
| 59 | s9 | 103 | ASP |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 59 | s9 | 109 | LEU |
| 59 | s9 | 111 | THR |
| 59 | s9 | 116 | LEU |
| 59 | s9 | 118 | LEU |
| 59 | s9 | 130 | THR |
| 59 | s9 | 132 | ARG |
| 59 | s9 | 134 | ILE |
| 59 | s9 | 145 | SER |
| 59 | s9 | 151 | ASP |
| 59 | s9 | 172 | VAL |
| 59 | s9 | 180 | LYS |
| 59 | s9 | 182 | GLU |
| 60 | c0 | 3 | MET |
| 60 | c0 | 15 | LEU |
| 60 | c0 | 20 | VAL |
| 60 | c0 | 28 | ASN |
| 60 | c0 | 33 | GLU |
| 60 | c0 | 35 | ILE |
| 60 | c0 | 55 | VAL |
| 60 | c0 | 71 | GLU |
| 61 | c1 | 5 | LEU |
| 61 | c1 | 10 | GLU |
| 61 | c1 | 26 | LYS |
| 61 | c1 | 27 | THR |
| 61 | c1 | 31 | THR |
| 61 | c1 | 32 | LYS |
| 61 | c1 | 40 | LEU |
| 61 | c1 | 44 | THR |
| 61 | c1 | 47 | THR |
| 61 | c1 | 60 | PHE |
| 61 | c1 | 67 | ARG |
| 61 | c1 | 74 | THR |
| 61 | c1 | 76 | VAL |
| 61 | c1 | 83 | THR |
| 61 | c1 | 109 | VAL |
| 61 | c1 | 129 | ARG |
| 62 | c2 | 28 | LEU |
| 62 | c2 | 43 | ARG |
| 62 | c2 | 52 | LEU |
| 62 | c2 | 58 | LEU |
| 62 | c2 | 61 | VAL |
| 62 | c2 | 62 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 62 | c2 | 71 | ILE |
| 62 | c2 | 86 | VAL |
| 62 | c2 | 89 | ILE |
| 62 | c2 | 90 | LYS |
| 62 | c2 | 103 | LEU |
| 62 | c2 | 129 | GLU |
| 62 | c2 | 132 | GLU |
| 62 | c2 | 137 | MET |
| 62 | c2 | 140 | PHE |
| 63 | c3 | 6 | SER |
| 63 | c3 | 12 | SER |
| 63 | c3 | 14 | SER |
| 63 | c3 | 16 | ILE |
| 63 | c3 | 19 | SER |
| 63 | c3 | 28 | LEU |
| 63 | c3 | 39 | LYS |
| 63 | c3 | 60 | VAL |
| 63 | c3 | 66 | ILE |
| 63 | c3 | 76 | LYS |
| 63 | c3 | 97 | SER |
| 63 | c3 | 102 | LEU |
| 63 | c3 | 115 | LEU |
| 63 | c3 | 125 | LEU |
| 63 | c3 | 127 | ARG |
| 63 | c3 | 138 | ASN |
| 64 | c4 | 18 | ARG |
| 64 | c4 | 49 | LYS |
| 64 | c4 | 51 | ASP |
| 64 | c4 | 52 | ARG |
| 64 | c4 | 81 | VAL |
| 64 | c4 | 91 | THR |
| 64 | c4 | 107 | ARG |
| 64 | c4 | 114 | ARG |
| 64 | c4 | 119 | THR |
| 64 | c4 | 124 | ASP |
| 64 | c4 | 133 | ARG |
| 64 | c4 | 136 | ARG |
| 65 | c5 | 12 | PHE |
| 65 | c5 | 28 | MET |
| 65 | c5 | 36 | LEU |
| 65 | c5 | 60 | LEU |
| 65 | c5 | 65 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 65 | c5 | 69 | GLU |
| 65 | c5 | 72 | LYS |
| 65 | c5 | 84 | ILE |
| 65 | c5 | 110 | GLU |
| 65 | c5 | 122 | THR |
| 65 | c5 | 127 | ARG |
| 65 | c5 | 128 | HIS |
| 66 | c6 | 15 | SER |
| 66 | c6 | 17 | THR |
| 66 | c6 | 23 | LYS |
| 66 | c6 | 26 | LYS |
| 66 | c6 | 28 | LEU |
| 66 | c6 | 37 | THR |
| 66 | c6 | 42 | GLU |
| 66 | c6 | 43 | ILE |
| 66 | c6 | 48 | VAL |
| 66 | c6 | 53 | LEU |
| 66 | c6 | 57 | LEU |
| 66 | c6 | 63 | ILE |
| 66 | c6 | 68 | ARG |
| 66 | c6 | 69 | VAL |
| 66 | c6 | 82 | ARG |
| 66 | c6 | 94 | GLN |
| 66 | c6 | 127 | LYS |
| 66 | c6 | 128 | LYS |
| 66 | c6 | 137 | ARG |
| 66 | c6 | 143 | ARG |
| 67 | c7 | 3 | ARG |
| 67 | c7 | 8 | THR |
| 67 | c7 | 29 | GLN |
| 67 | c7 | 34 | LEU |
| 67 | c7 | 46 | LEU |
| 67 | c7 | 69 | ILE |
| 67 | c7 | 72 | LYS |
| 67 | c7 | 82 | ASP |
| 67 | c7 | 85 | VAL |
| 67 | c7 | 106 | THR |
| 67 | c7 | 110 | VAL |
| 68 | c8 | 3 | LEU |
| 68 | c8 | 4 | VAL |
| 68 | c8 | 5 | VAL |
| 68 | c8 | 6 | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 68 | c8 | 12 | GLN |
| 68 | c8 | 14 | ILE |
| 68 | c8 | 25 | ASN |
| 68 | c8 | 40 | ARG |
| 68 | c8 | 61 | LEU |
| 68 | c8 | 77 | THR |
| 68 | c8 | 85 | PHE |
| 68 | c8 | 92 | ILE |
| 68 | c8 | 111 | ASP |
| 68 | c8 | 112 | ASP |
| 68 | c8 | 116 | LEU |
| 68 | c8 | 133 | VAL |
| 68 | c8 | 136 | GLN |
| 68 | c8 | 138 | THR |
| 68 | c8 | 143 | ARG |
| 69 | c9 | 6 | VAL |
| 69 | c9 | 13 | ASP |
| 69 | c9 | 28 | LEU |
| 69 | c9 | 29 | GLU |
| 69 | c9 | 34 | VAL |
| 69 | c9 | 37 | VAL |
| 69 | c9 | 68 | ARG |
| 69 | c9 | 70 | GLN |
| 69 | c9 | 115 | GLU |
| 69 | c9 | 122 | ARG |
| 69 | c9 | 126 | GLU |
| 69 | c9 | 131 | ASP |
| 69 | c9 | 135 | ILE |
| 69 | c9 | 140 | LEU |
| 69 | c9 | 142 | GLU |
| 69 | c9 | 143 | ASP |
| 70 | d0 | 21 | LYS |
| 70 | d0 | 23 | ARG |
| 70 | d0 | 27 | THR |
| 70 | d0 | 30 | LYS |
| 70 | d0 | 51 | VAL |
| 70 | d0 | 57 | ARG |
| 70 | d0 | 60 | THR |
| 70 | d0 | 70 | THR |
| 70 | d0 | 72 | ASN |
| 70 | d0 | 74 | GLU |
| 70 | d0 | 103 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 70 | d0 | 107 | THR |
| 70 | d0 | 108 | ILE |
| 71 | d1 | 2 | GLU |
| 71 | d1 | 4 | ASP |
| 71 | d1 | 5 | LYS |
| 71 | d1 | 12 | TYR |
| 71 | d1 | 17 | CYS |
| 71 | d1 | 32 | VAL |
| 71 | d1 | 44 | ARG |
| 71 | d1 | 50 | TYR |
| 71 | d1 | 52 | THR |
| 71 | d1 | 78 | LEU |
| 71 | d1 | 80 | LYS |
| 72 | d2 | 7 | LEU |
| 72 | d2 | 15 | ASN |
| 72 | d2 | 23 | ARG |
| 72 | d2 | 25 | VAL |
| 72 | d2 | 26 | LEU |
| 72 | d2 | 31 | SER |
| 72 | d2 | 103 | ILE |
| 73 | d3 | 9 | LEU |
| 73 | d3 | 16 | ARG |
| 73 | d3 | 19 | ARG |
| 73 | d3 | 27 | ASN |
| 73 | d3 | 28 | ASN |
| 73 | d3 | 33 | LEU |
| 73 | d3 | 52 | ILE |
| 73 | d3 | 55 | GLU |
| 73 | d3 | 73 | ARG |
| 73 | d3 | 84 | THR |
| 73 | d3 | 96 | VAL |
| 73 | d3 | 100 | ASP |
| 73 | d3 | 103 | LEU |
| 73 | d3 | 107 | PHE |
| 73 | d3 | 132 | LEU |
| 74 | d4 | 5 | VAL |
| 74 | d4 | 34 | ASN |
| 74 | d4 | 43 | LYS |
| 74 | d4 | 47 | VAL |
| 74 | d4 | 49 | LYS |
| 74 | d4 | 62 | THR |
| 74 | d4 | 105 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 75 | d5 | 46 | LYS |
| 75 | d5 | 51 | LEU |
| 75 | d5 | 57 | TYR |
| 76 | d6 | 8 | ASN |
| 76 | d6 | 10 | ARG |
| 76 | d6 | 11 | ASN |
| 76 | d6 | 12 | LYS |
| 76 | d6 | 18 | VAL |
| 76 | d6 | 45 | VAL |
| 76 | d6 | 46 | GLU |
| 76 | d6 | 51 | ARG |
| 76 | d6 | 55 | GLU |
| 76 | d6 | 82 | ARG |
| 76 | d6 | 85 | ARG |
| 76 | d6 | 90 | GLU |
| 77 | d7 | 3 | LEU |
| 77 | d7 | 4 | VAL |
| 77 | d7 | 43 | ILE |
| 77 | d7 | 59 | CYS |
| 77 | d7 | 77 | THR |
| 78 | d8 | 8 | THR |
| 78 | d8 | 16 | LEU |
| 78 | d8 | 22 | ARG |
| 78 | d8 | 39 | THR |
| 78 | d8 | 52 | ASP |
| 78 | d8 | 58 | GLU |
| 78 | d8 | 64 | ARG |
| 78 | d8 | 65 | ARG |
| 78 | d8 | 66 | LEU |
| 79 | d9 | 12 | ARG |
| 79 | d9 | 21 | CYS |
| 79 | d9 | 30 | LEU |
| 79 | d9 | 54 | LYS |
| 80 | e0 | 22 | GLU |
| 80 | e0 | 25 | GLU |
| 80 | e0 | 26 | LYS |
| 80 | e0 | 29 | LYS |
| 80 | e0 | 46 | ASN |
| 80 | e0 | 48 | THR |
| 80 | e0 | 55 | ARG |
| 80 | e0 | 61 | SER |
| 83 | e1 | 106 | TYR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 83 | e1 | 113 | LYS |
| 83 | e1 | 119 | ARG |
| 83 | e1 | 126 | CYS |
| 83 | e1 | 137 | ASP |
| 83 | e1 | 147 | VAL |
| 83 | e1 | 148 | TYR |
| 83 | e1 | 150 | VAL |
| 82 | sR | 16 | HIS |
| 82 | sR | 48 | THR |
| 82 | sR | 52 | GLN |
| 82 | sR | 66 | HIS |
| 82 | sR | 70 | ASP |
| 82 | sR | 76 | ASP |
| 82 | sR | 96 | THR |
| 82 | sR | 145 | LEU |
| 82 | sR | 149 | ASP |
| 82 | sR | 159 | ASN |
| 82 | sR | 166 | SER |
| 82 | sR | 167 | VAL |
| 82 | sR | 201 | THR |
| 82 | sR | 232 | TYR |
| 82 | sR | 275 | ARG |
| 82 | sR | 281 | TYR |
| 82 | sR | 297 | ASP |
| 82 | sR | 317 | THR |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 4 | j | 132 | ASN |
| 6 | l | 307 | GLN |
| 7 | m | 40 | HIS |
| 12 | r | 144 | ASN |
| 12 | r | 163 | GLN |
| 29 | AA | 29 | HIS |
| 29 | AA | 57 | HIS |
| 6 | CF | 110 | ASN |
| 7 | CG | 40 | HIS |
| 11 | CK | 49 | ASN |
| 11 | CK | 51 | GLN |
| 18 | CR | 137 | ASN |
| 40 | DM | 32 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51 | C | 177 | GLN |
| 55 | G | 103 | ASN |
| 57 | I | 74 | GLN |
| 59 | K | 110 | GLN |
| 62 | N | 125 | ASN |
| 67 | S | 105 | GLN |
| 68 | T | 136 | GLN |
| 69 | U | 16 | ASN |
| 74 | Z | 107 | GLN |
| 82 | h | 159 | ASN |
| 56 | s6 | 34 | GLN |
| 57 | s7 | 71 | HIS |
| 64 | c4 | 10 | ASN |
| 65 | c5 | 103 | ASN |

5.3.3 RNA [i](#)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------------|-------------------|-----------------|
| 1 | 1 | 3145/3396 (92%) | 559 (17%) | 46 (1%) |
| 1 | AR | 3145/3396 (92%) | 562 (17%) | 58 (1%) |
| 2 | 3 | 120/121 (99%) | 13 (10%) | 0 |
| 2 | AS | 120/121 (99%) | 14 (11%) | 1 (0%) |
| 25 | 6 | 1780/1800 (98%) | 376 (21%) | 32 (1%) |
| 25 | A | 1778/1800 (98%) | 419 (23%) | 45 (2%) |
| 3 | 4 | 157/158 (99%) | 34 (21%) | 2 (1%) |
| 3 | AT | 157/158 (99%) | 29 (18%) | 2 (1%) |
| All | All | 10402/10950 (94%) | 2006 (19%) | 186 (1%) |

All (2006) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1 | 26 | A |
| 1 | 1 | 40 | A |
| 1 | 1 | 43 | A |
| 1 | 1 | 45 | A |
| 1 | 1 | 49 | A |
| 1 | 1 | 57 | A |
| 1 | 1 | 59 | G |
| 1 | 1 | 60 | A |
| 1 | 1 | 65 | A |
| 1 | 1 | 66 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 72 | C |
| 1 | 1 | 73 | C |
| 1 | 1 | 76 | G |
| 1 | 1 | 83 | U |
| 1 | 1 | 92 | G |
| 1 | 1 | 93 | C |
| 1 | 1 | 99 | A |
| 1 | 1 | 109 | A |
| 1 | 1 | 110 | G |
| 1 | 1 | 113 | C |
| 1 | 1 | 117 | U |
| 1 | 1 | 121 | A |
| 1 | 1 | 122 | A |
| 1 | 1 | 133 | U |
| 1 | 1 | 135 | C |
| 1 | 1 | 136 | G |
| 1 | 1 | 156 | G |
| 1 | 1 | 157 | A |
| 1 | 1 | 166 | C |
| 1 | 1 | 170 | G |
| 1 | 1 | 187 | A |
| 1 | 1 | 190 | U |
| 1 | 1 | 191 | U |
| 1 | 1 | 192 | C |
| 1 | 1 | 210 | U |
| 1 | 1 | 213 | A |
| 1 | 1 | 218 | G |
| 1 | 1 | 219 | A |
| 1 | 1 | 240 | U |
| 1 | 1 | 243 | G |
| 1 | 1 | 247 | C |
| 1 | 1 | 249 | U |
| 1 | 1 | 250 | U |
| 1 | 1 | 251 | G |
| 1 | 1 | 252 | U |
| 1 | 1 | 269 | G |
| 1 | 1 | 282 | G |
| 1 | 1 | 283 | G |
| 1 | 1 | 284 | A |
| 1 | 1 | 286 | U |
| 1 | 1 | 295 | A |
| 1 | 1 | 298 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 315 | C |
| 1 | 1 | 323 | A |
| 1 | 1 | 329 | U |
| 1 | 1 | 337 | G |
| 1 | 1 | 338 | A |
| 1 | 1 | 339 | C |
| 1 | 1 | 349 | A |
| 1 | 1 | 350 | C |
| 1 | 1 | 351 | A |
| 1 | 1 | 352 | A |
| 1 | 1 | 376 | G |
| 1 | 1 | 398 | A |
| 1 | 1 | 401 | U |
| 1 | 1 | 402 | A |
| 1 | 1 | 403 | C |
| 1 | 1 | 414 | U |
| 1 | 1 | 421 | G |
| 1 | 1 | 422 | A |
| 1 | 1 | 438 | A |
| 1 | 1 | 439 | C |
| 1 | 1 | 440 | A |
| 1 | 1 | 495 | G |
| 1 | 1 | 498 | A |
| 1 | 1 | 507 | U |
| 1 | 1 | 520 | U |
| 1 | 1 | 521 | A |
| 1 | 1 | 535 | G |
| 1 | 1 | 544 | C |
| 1 | 1 | 546 | C |
| 1 | 1 | 547 | G |
| 1 | 1 | 548 | G |
| 1 | 1 | 552 | G |
| 1 | 1 | 555 | U |
| 1 | 1 | 557 | A |
| 1 | 1 | 559 | A |
| 1 | 1 | 578 | A |
| 1 | 1 | 579 | G |
| 1 | 1 | 592 | A |
| 1 | 1 | 604 | G |
| 1 | 1 | 609 | G |
| 1 | 1 | 611 | A |
| 1 | 1 | 619 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 620 | U |
| 1 | 1 | 621 | A |
| 1 | 1 | 636 | C |
| 1 | 1 | 649 | A |
| 1 | 1 | 651 | G |
| 1 | 1 | 658 | G |
| 1 | 1 | 660 | A |
| 1 | 1 | 677 | A |
| 1 | 1 | 681 | U |
| 1 | 1 | 691 | A |
| 1 | 1 | 705 | A |
| 1 | 1 | 712 | G |
| 1 | 1 | 715 | A |
| 1 | 1 | 716 | A |
| 1 | 1 | 727 | G |
| 1 | 1 | 764 | U |
| 1 | 1 | 766 | U |
| 1 | 1 | 767 | U |
| 1 | 1 | 776 | U |
| 1 | 1 | 777 | U |
| 1 | 1 | 780 | A |
| 1 | 1 | 781 | G |
| 1 | 1 | 785 | G |
| 1 | 1 | 806 | A |
| 1 | 1 | 817 | A |
| 1 | 1 | 830 | A |
| 1 | 1 | 849 | C |
| 1 | 1 | 861 | C |
| 1 | 1 | 869 | G |
| 1 | 1 | 874 | U |
| 1 | 1 | 879 | U |
| 1 | 1 | 890 | C |
| 1 | 1 | 896 | A |
| 1 | 1 | 907 | G |
| 1 | 1 | 908 | G |
| 1 | 1 | 914 | A |
| 1 | 1 | 916 | G |
| 1 | 1 | 917 | A |
| 1 | 1 | 921 | A |
| 1 | 1 | 923 | C |
| 1 | 1 | 924 | G |
| 1 | 1 | 925 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 937 | G |
| 1 | 1 | 938 | C |
| 1 | 1 | 943 | U |
| 1 | 1 | 944 | C |
| 1 | 1 | 959 | C |
| 1 | 1 | 960 | U |
| 1 | 1 | 979 | U |
| 1 | 1 | 980 | A |
| 1 | 1 | 981 | U |
| 1 | 1 | 982 | C |
| 1 | 1 | 994 | G |
| 1 | 1 | 1001 | G |
| 1 | 1 | 1002 | A |
| 1 | 1 | 1010 | G |
| 1 | 1 | 1017 | C |
| 1 | 1 | 1018 | G |
| 1 | 1 | 1020 | G |
| 1 | 1 | 1024 | G |
| 1 | 1 | 1025 | A |
| 1 | 1 | 1029 | G |
| 1 | 1 | 1036 | A |
| 1 | 1 | 1037 | C |
| 1 | 1 | 1047 | A |
| 1 | 1 | 1049 | C |
| 1 | 1 | 1052 | U |
| 1 | 1 | 1064 | A |
| 1 | 1 | 1065 | A |
| 1 | 1 | 1072 | G |
| 1 | 1 | 1081 | U |
| 1 | 1 | 1082 | U |
| 1 | 1 | 1083 | G |
| 1 | 1 | 1087 | G |
| 1 | 1 | 1093 | A |
| 1 | 1 | 1094 | U |
| 1 | 1 | 1095 | U |
| 1 | 1 | 1097 | G |
| 1 | 1 | 1098 | A |
| 1 | 1 | 1102 | A |
| 1 | 1 | 1103 | A |
| 1 | 1 | 1104 | G |
| 1 | 1 | 1116 | G |
| 1 | 1 | 1117 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 1131 | G |
| 1 | 1 | 1153 | A |
| 1 | 1 | 1159 | A |
| 1 | 1 | 1160 | C |
| 1 | 1 | 1168 | U |
| 1 | 1 | 1180 | A |
| 1 | 1 | 1181 | U |
| 1 | 1 | 1185 | C |
| 1 | 1 | 1190 | A |
| 1 | 1 | 1191 | U |
| 1 | 1 | 1192 | C |
| 1 | 1 | 1201 | C |
| 1 | 1 | 1209 | G |
| 1 | 1 | 1217 | A |
| 1 | 1 | 1222 | G |
| 1 | 1 | 1227 | C |
| 1 | 1 | 1232 | C |
| 1 | 1 | 1235 | U |
| 1 | 1 | 1236 | G |
| 1 | 1 | 1237 | G |
| 1 | 1 | 1243 | G |
| 1 | 1 | 1245 | A |
| 1 | 1 | 1246 | G |
| 1 | 1 | 1248 | C |
| 1 | 1 | 1249 | G |
| 1 | 1 | 1258 | U |
| 1 | 1 | 1262 | G |
| 1 | 1 | 1263 | A |
| 1 | 1 | 1264 | G |
| 1 | 1 | 1265 | U |
| 1 | 1 | 1267 | U |
| 1 | 1 | 1269 | U |
| 1 | 1 | 1270 | A |
| 1 | 1 | 1271 | A |
| 1 | 1 | 1274 | A |
| 1 | 1 | 1278 | A |
| 1 | 1 | 1279 | C |
| 1 | 1 | 1285 | G |
| 1 | 1 | 1286 | A |
| 1 | 1 | 1287 | A |
| 1 | 1 | 1292 | C |
| 1 | 1 | 1308 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 1309 | U |
| 1 | 1 | 1313 | G |
| 1 | 1 | 1330 | A |
| 1 | 1 | 1348 | U |
| 1 | 1 | 1349 | G |
| 1 | 1 | 1351 | U |
| 1 | 1 | 1352 | A |
| 1 | 1 | 1353 | U |
| 1 | 1 | 1355 | A |
| 1 | 1 | 1356 | U |
| 1 | 1 | 1357 | G |
| 1 | 1 | 1386 | A |
| 1 | 1 | 1399 | A |
| 1 | 1 | 1400 | G |
| 1 | 1 | 1418 | A |
| 1 | 1 | 1419 | A |
| 1 | 1 | 1421 | G |
| 1 | 1 | 1429 | G |
| 1 | 1 | 1433 | A |
| 1 | 1 | 1434 | G |
| 1 | 1 | 1437 | C |
| 1 | 1 | 1443 | G |
| 1 | 1 | 1446 | A |
| 1 | 1 | 1450 | G |
| 1 | 1 | 1481 | A |
| 1 | 1 | 1482 | A |
| 1 | 1 | 1485 | G |
| 1 | 1 | 1491 | A |
| 1 | 1 | 1508 | C |
| 1 | 1 | 1527 | C |
| 1 | 1 | 1533 | U |
| 1 | 1 | 1536 | G |
| 1 | 1 | 1556 | C |
| 1 | 1 | 1560 | G |
| 1 | 1 | 1561 | G |
| 1 | 1 | 1562 | C |
| 1 | 1 | 1563 | C |
| 1 | 1 | 1564 | U |
| 1 | 1 | 1567 | U |
| 1 | 1 | 1568 | U |
| 1 | 1 | 1569 | U |
| 1 | 1 | 1570 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 1576 | G |
| 1 | 1 | 1580 | A |
| 1 | 1 | 1582 | C |
| 1 | 1 | 1583 | A |
| 1 | 1 | 1587 | A |
| 1 | 1 | 1589 | A |
| 1 | 1 | 1605 | A |
| 1 | 1 | 1620 | U |
| 1 | 1 | 1629 | U |
| 1 | 1 | 1639 | C |
| 1 | 1 | 1643 | A |
| 1 | 1 | 1655 | G |
| 1 | 1 | 1656 | A |
| 1 | 1 | 1657 | C |
| 1 | 1 | 1658 | G |
| 1 | 1 | 1683 | A |
| 1 | 1 | 1716 | U |
| 1 | 1 | 1717 | U |
| 1 | 1 | 1724 | U |
| 1 | 1 | 1729 | A |
| 1 | 1 | 1736 | G |
| 1 | 1 | 1741 | A |
| 1 | 1 | 1750 | A |
| 1 | 1 | 1751 | G |
| 1 | 1 | 1765 | U |
| 1 | 1 | 1766 | G |
| 1 | 1 | 1769 | G |
| 1 | 1 | 1770 | G |
| 1 | 1 | 1780 | G |
| 1 | 1 | 1797 | A |
| 1 | 1 | 1810 | A |
| 1 | 1 | 1812 | G |
| 1 | 1 | 1814 | A |
| 1 | 1 | 1815 | U |
| 1 | 1 | 1816 | A |
| 1 | 1 | 1817 | G |
| 1 | 1 | 1819 | U |
| 1 | 1 | 1820 | U |
| 1 | 1 | 1821 | U |
| 1 | 1 | 1835 | A |
| 1 | 1 | 1839 | A |
| 1 | 1 | 1842 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 1846 | C |
| 1 | 1 | 1849 | C |
| 1 | 1 | 1850 | A |
| 1 | 1 | 1858 | A |
| 1 | 1 | 1866 | C |
| 1 | 1 | 1879 | A |
| 1 | 1 | 1880 | U |
| 1 | 1 | 1895 | A |
| 1 | 1 | 1901 | A |
| 1 | 1 | 1906 | G |
| 1 | 1 | 1951 | C |
| 1 | 1 | 1952 | G |
| 1 | 1 | 1953 | G |
| 1 | 1 | 1954 | G |
| 1 | 1 | 2094 | C |
| 1 | 1 | 2101 | C |
| 1 | 1 | 2102 | U |
| 1 | 1 | 2111 | G |
| 1 | 1 | 2112 | U |
| 1 | 1 | 2113 | A |
| 1 | 1 | 2121 | G |
| 1 | 1 | 2122 | G |
| 1 | 1 | 2131 | A |
| 1 | 1 | 2134 | G |
| 1 | 1 | 2140 | U |
| 1 | 1 | 2145 | A |
| 1 | 1 | 2158 | A |
| 1 | 1 | 2169 | G |
| 1 | 1 | 2170 | U |
| 1 | 1 | 2177 | G |
| 1 | 1 | 2205 | U |
| 1 | 1 | 2210 | G |
| 1 | 1 | 2228 | A |
| 1 | 1 | 2244 | A |
| 1 | 1 | 2246 | G |
| 1 | 1 | 2249 | G |
| 1 | 1 | 2250 | G |
| 1 | 1 | 2255 | A |
| 1 | 1 | 2256 | A |
| 1 | 1 | 2262 | A |
| 1 | 1 | 2272 | G |
| 1 | 1 | 2273 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 2281 | A |
| 1 | 1 | 2282 | U |
| 1 | 1 | 2288 | G |
| 1 | 1 | 2298 | U |
| 1 | 1 | 2301 | U |
| 1 | 1 | 2303 | A |
| 1 | 1 | 2307 | G |
| 1 | 1 | 2310 | U |
| 1 | 1 | 2313 | A |
| 1 | 1 | 2314 | U |
| 1 | 1 | 2315 | G |
| 1 | 1 | 2334 | U |
| 1 | 1 | 2336 | U |
| 1 | 1 | 2361 | A |
| 1 | 1 | 2362 | C |
| 1 | 1 | 2372 | A |
| 1 | 1 | 2373 | A |
| 1 | 1 | 2374 | C |
| 1 | 1 | 2375 | G |
| 1 | 1 | 2382 | G |
| 1 | 1 | 2385 | G |
| 1 | 1 | 2393 | G |
| 1 | 1 | 2397 | A |
| 1 | 1 | 2398 | A |
| 1 | 1 | 2402 | A |
| 1 | 1 | 2403 | G |
| 1 | 1 | 2404 | A |
| 1 | 1 | 2405 | C |
| 1 | 1 | 2411 | U |
| 1 | 1 | 2418 | G |
| 1 | 1 | 2419 | A |
| 1 | 1 | 2444 | C |
| 1 | 1 | 2445 | A |
| 1 | 1 | 2502 | A |
| 1 | 1 | 2503 | G |
| 1 | 1 | 2514 | U |
| 1 | 1 | 2515 | A |
| 1 | 1 | 2522 | G |
| 1 | 1 | 2523 | A |
| 1 | 1 | 2532 | U |
| 1 | 1 | 2533 | G |
| 1 | 1 | 2537 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 2538 | U |
| 1 | 1 | 2539 | C |
| 1 | 1 | 2540 | A |
| 1 | 1 | 2541 | U |
| 1 | 1 | 2542 | U |
| 1 | 1 | 2543 | U |
| 1 | 1 | 2547 | A |
| 1 | 1 | 2548 | C |
| 1 | 1 | 2549 | G |
| 1 | 1 | 2552 | C |
| 1 | 1 | 2555 | G |
| 1 | 1 | 2561 | A |
| 1 | 1 | 2568 | C |
| 1 | 1 | 2569 | A |
| 1 | 1 | 2570 | U |
| 1 | 1 | 2571 | U |
| 1 | 1 | 2572 | C |
| 1 | 1 | 2573 | G |
| 1 | 1 | 2581 | U |
| 1 | 1 | 2582 | C |
| 1 | 1 | 2585 | G |
| 1 | 1 | 2593 | A |
| 1 | 1 | 2594 | C |
| 1 | 1 | 2606 | G |
| 1 | 1 | 2607 | G |
| 1 | 1 | 2614 | G |
| 1 | 1 | 2626 | A |
| 1 | 1 | 2637 | A |
| 1 | 1 | 2652 | U |
| 1 | 1 | 2656 | A |
| 1 | 1 | 2674 | A |
| 1 | 1 | 2677 | G |
| 1 | 1 | 2689 | A |
| 1 | 1 | 2690 | G |
| 1 | 1 | 2691 | A |
| 1 | 1 | 2694 | A |
| 1 | 1 | 2696 | A |
| 1 | 1 | 2714 | G |
| 1 | 1 | 2728 | G |
| 1 | 1 | 2729 | U |
| 1 | 1 | 2737 | C |
| 1 | 1 | 2752 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 2753 | G |
| 1 | 1 | 2755 | C |
| 1 | 1 | 2771 | U |
| 1 | 1 | 2772 | C |
| 1 | 1 | 2773 | C |
| 1 | 1 | 2777 | G |
| 1 | 1 | 2778 | G |
| 1 | 1 | 2780 | A |
| 1 | 1 | 2796 | G |
| 1 | 1 | 2797 | C |
| 1 | 1 | 2799 | A |
| 1 | 1 | 2800 | G |
| 1 | 1 | 2801 | A |
| 1 | 1 | 2810 | C |
| 1 | 1 | 2814 | G |
| 1 | 1 | 2816 | G |
| 1 | 1 | 2817 | A |
| 1 | 1 | 2818 | U |
| 1 | 1 | 2842 | U |
| 1 | 1 | 2843 | U |
| 1 | 1 | 2845 | A |
| 1 | 1 | 2849 | C |
| 1 | 1 | 2860 | U |
| 1 | 1 | 2867 | C |
| 1 | 1 | 2871 | G |
| 1 | 1 | 2872 | A |
| 1 | 1 | 2875 | U |
| 1 | 1 | 2876 | C |
| 1 | 1 | 2887 | A |
| 1 | 1 | 2899 | C |
| 1 | 1 | 2910 | A |
| 1 | 1 | 2914 | G |
| 1 | 1 | 2923 | U |
| 1 | 1 | 2927 | C |
| 1 | 1 | 2935 | U |
| 1 | 1 | 2936 | A |
| 1 | 1 | 2942 | C |
| 1 | 1 | 2945 | G |
| 1 | 1 | 2947 | G |
| 1 | 1 | 2954 | U |
| 1 | 1 | 2955 | U |
| 1 | 1 | 2971 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 2980 | U |
| 1 | 1 | 2983 | C |
| 1 | 1 | 2990 | G |
| 1 | 1 | 2992 | U |
| 1 | 1 | 2997 | G |
| 1 | 1 | 3012 | A |
| 1 | 1 | 3056 | U |
| 1 | 1 | 3059 | G |
| 1 | 1 | 3078 | U |
| 1 | 1 | 3079 | U |
| 1 | 1 | 3080 | G |
| 1 | 1 | 3086 | A |
| 1 | 1 | 3092 | C |
| 1 | 1 | 3113 | A |
| 1 | 1 | 3119 | U |
| 1 | 1 | 3122 | A |
| 1 | 1 | 3130 | A |
| 1 | 1 | 3131 | U |
| 1 | 1 | 3142 | A |
| 1 | 1 | 3143 | C |
| 1 | 1 | 3150 | A |
| 1 | 1 | 3151 | U |
| 1 | 1 | 3153 | U |
| 1 | 1 | 3154 | C |
| 1 | 1 | 3155 | U |
| 1 | 1 | 3156 | U |
| 1 | 1 | 3157 | U |
| 1 | 1 | 3164 | C |
| 1 | 1 | 3165 | A |
| 1 | 1 | 3168 | A |
| 1 | 1 | 3171 | U |
| 1 | 1 | 3173 | G |
| 1 | 1 | 3174 | A |
| 1 | 1 | 3176 | G |
| 1 | 1 | 3179 | U |
| 1 | 1 | 3181 | C |
| 1 | 1 | 3187 | A |
| 1 | 1 | 3196 | U |
| 1 | 1 | 3199 | G |
| 1 | 1 | 3207 | U |
| 1 | 1 | 3210 | A |
| 1 | 1 | 3217 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 3218 | A |
| 1 | 1 | 3219 | G |
| 1 | 1 | 3228 | C |
| 1 | 1 | 3229 | G |
| 1 | 1 | 3243 | A |
| 1 | 1 | 3245 | A |
| 1 | 1 | 3246 | G |
| 1 | 1 | 3247 | G |
| 1 | 1 | 3259 | U |
| 1 | 1 | 3270 | U |
| 1 | 1 | 3271 | G |
| 1 | 1 | 3272 | C |
| 1 | 1 | 3273 | A |
| 1 | 1 | 3276 | G |
| 1 | 1 | 3281 | U |
| 1 | 1 | 3286 | G |
| 1 | 1 | 3287 | U |
| 1 | 1 | 3288 | G |
| 1 | 1 | 3289 | G |
| 1 | 1 | 3294 | A |
| 1 | 1 | 3295 | A |
| 1 | 1 | 3304 | U |
| 1 | 1 | 3309 | G |
| 1 | 1 | 3313 | U |
| 1 | 1 | 3316 | A |
| 1 | 1 | 3318 | G |
| 1 | 1 | 3319 | U |
| 1 | 1 | 3341 | U |
| 1 | 1 | 3342 | A |
| 1 | 1 | 3345 | G |
| 1 | 1 | 3347 | A |
| 1 | 1 | 3351 | U |
| 1 | 1 | 3352 | U |
| 1 | 1 | 3353 | G |
| 1 | 1 | 3354 | U |
| 1 | 1 | 3355 | U |
| 1 | 1 | 3369 | G |
| 1 | 1 | 3375 | A |
| 1 | 1 | 3376 | A |
| 1 | 1 | 3378 | C |
| 1 | 1 | 3381 | U |
| 1 | 1 | 3382 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 3389 | U |
| 1 | 1 | 3390 | G |
| 1 | 1 | 3396 | U |
| 2 | 3 | 7 | G |
| 2 | 3 | 11 | A |
| 2 | 3 | 13 | A |
| 2 | 3 | 22 | A |
| 2 | 3 | 54 | U |
| 2 | 3 | 65 | G |
| 2 | 3 | 73 | C |
| 2 | 3 | 74 | C |
| 2 | 3 | 76 | A |
| 2 | 3 | 95 | A |
| 2 | 3 | 102 | A |
| 2 | 3 | 112 | G |
| 2 | 3 | 121 | U |
| 3 | 4 | 2 | A |
| 3 | 4 | 23 | U |
| 3 | 4 | 34 | U |
| 3 | 4 | 35 | C |
| 3 | 4 | 48 | A |
| 3 | 4 | 53 | A |
| 3 | 4 | 57 | C |
| 3 | 4 | 58 | G |
| 3 | 4 | 59 | A |
| 3 | 4 | 62 | C |
| 3 | 4 | 63 | G |
| 3 | 4 | 79 | A |
| 3 | 4 | 80 | A |
| 3 | 4 | 81 | U |
| 3 | 4 | 82 | U |
| 3 | 4 | 85 | G |
| 3 | 4 | 86 | U |
| 3 | 4 | 87 | G |
| 3 | 4 | 90 | U |
| 3 | 4 | 95 | G |
| 3 | 4 | 96 | A |
| 3 | 4 | 104 | A |
| 3 | 4 | 105 | A |
| 3 | 4 | 106 | C |
| 3 | 4 | 111 | A |
| 3 | 4 | 113 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 3 | 4 | 125 | U |
| 3 | 4 | 126 | A |
| 3 | 4 | 128 | U |
| 3 | 4 | 138 | A |
| 3 | 4 | 152 | G |
| 3 | 4 | 155 | A |
| 3 | 4 | 157 | U |
| 3 | 4 | 158 | U |
| 25 | 6 | 2 | A |
| 25 | 6 | 4 | C |
| 25 | 6 | 17 | C |
| 25 | 6 | 25 | C |
| 25 | 6 | 26 | A |
| 25 | 6 | 27 | U |
| 25 | 6 | 34 | G |
| 25 | 6 | 47 | A |
| 25 | 6 | 57 | G |
| 25 | 6 | 60 | U |
| 25 | 6 | 61 | A |
| 25 | 6 | 67 | A |
| 25 | 6 | 68 | A |
| 25 | 6 | 69 | G |
| 25 | 6 | 72 | A |
| 25 | 6 | 73 | U |
| 25 | 6 | 75 | U |
| 25 | 6 | 76 | A |
| 25 | 6 | 77 | U |
| 25 | 6 | 104 | A |
| 25 | 6 | 114 | C |
| 25 | 6 | 126 | A |
| 25 | 6 | 132 | U |
| 25 | 6 | 137 | U |
| 25 | 6 | 138 | A |
| 25 | 6 | 140 | A |
| 25 | 6 | 141 | U |
| 25 | 6 | 144 | U |
| 25 | 6 | 145 | A |
| 25 | 6 | 146 | U |
| 25 | 6 | 153 | G |
| 25 | 6 | 159 | U |
| 25 | 6 | 166 | C |
| 25 | 6 | 178 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | 6 | 181 | A |
| 25 | 6 | 185 | U |
| 25 | 6 | 188 | A |
| 25 | 6 | 191 | C |
| 25 | 6 | 192 | U |
| 25 | 6 | 193 | U |
| 25 | 6 | 194 | U |
| 25 | 6 | 195 | G |
| 25 | 6 | 200 | A |
| 25 | 6 | 215 | A |
| 25 | 6 | 216 | U |
| 25 | 6 | 217 | A |
| 25 | 6 | 218 | A |
| 25 | 6 | 219 | A |
| 25 | 6 | 220 | A |
| 25 | 6 | 227 | U |
| 25 | 6 | 228 | G |
| 25 | 6 | 232 | U |
| 25 | 6 | 233 | C |
| 25 | 6 | 240 | U |
| 25 | 6 | 241 | U |
| 25 | 6 | 249 | U |
| 25 | 6 | 250 | C |
| 25 | 6 | 261 | U |
| 25 | 6 | 265 | A |
| 25 | 6 | 271 | A |
| 25 | 6 | 272 | U |
| 25 | 6 | 273 | G |
| 25 | 6 | 275 | C |
| 25 | 6 | 278 | U |
| 25 | 6 | 280 | U |
| 25 | 6 | 285 | G |
| 25 | 6 | 299 | A |
| 25 | 6 | 302 | U |
| 25 | 6 | 308 | C |
| 25 | 6 | 314 | C |
| 25 | 6 | 316 | A |
| 25 | 6 | 319 | U |
| 25 | 6 | 320 | U |
| 25 | 6 | 321 | C |
| 25 | 6 | 322 | G |
| 25 | 6 | 337 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | 6 | 338 | C |
| 25 | 6 | 352 | A |
| 25 | 6 | 359 | A |
| 25 | 6 | 360 | A |
| 25 | 6 | 361 | C |
| 25 | 6 | 400 | A |
| 25 | 6 | 401 | A |
| 25 | 6 | 402 | C |
| 25 | 6 | 404 | G |
| 25 | 6 | 416 | A |
| 25 | 6 | 418 | G |
| 25 | 6 | 424 | C |
| 25 | 6 | 425 | A |
| 25 | 6 | 426 | G |
| 25 | 6 | 434 | G |
| 25 | 6 | 439 | U |
| 25 | 6 | 444 | C |
| 25 | 6 | 445 | A |
| 25 | 6 | 448 | C |
| 25 | 6 | 454 | U |
| 25 | 6 | 468 | A |
| 25 | 6 | 477 | A |
| 25 | 6 | 480 | G |
| 25 | 6 | 486 | G |
| 25 | 6 | 488 | G |
| 25 | 6 | 489 | C |
| 25 | 6 | 490 | C |
| 25 | 6 | 492 | A |
| 25 | 6 | 493 | U |
| 25 | 6 | 494 | U |
| 25 | 6 | 496 | G |
| 25 | 6 | 497 | G |
| 25 | 6 | 500 | C |
| 25 | 6 | 501 | U |
| 25 | 6 | 504 | U |
| 25 | 6 | 505 | A |
| 25 | 6 | 506 | A |
| 25 | 6 | 507 | U |
| 25 | 6 | 510 | G |
| 25 | 6 | 511 | A |
| 25 | 6 | 512 | A |
| 25 | 6 | 513 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | 6 | 514 | G |
| 25 | 6 | 515 | A |
| 25 | 6 | 516 | G |
| 25 | 6 | 519 | C |
| 25 | 6 | 527 | A |
| 25 | 6 | 538 | A |
| 25 | 6 | 539 | G |
| 25 | 6 | 540 | G |
| 25 | 6 | 541 | A |
| 25 | 6 | 542 | A |
| 25 | 6 | 543 | C |
| 25 | 6 | 544 | A |
| 25 | 6 | 548 | G |
| 25 | 6 | 557 | G |
| 25 | 6 | 558 | U |
| 25 | 6 | 559 | C |
| 25 | 6 | 565 | C |
| 25 | 6 | 568 | G |
| 25 | 6 | 570 | A |
| 25 | 6 | 574 | G |
| 25 | 6 | 579 | A |
| 25 | 6 | 580 | A |
| 25 | 6 | 582 | U |
| 25 | 6 | 594 | A |
| 25 | 6 | 595 | G |
| 25 | 6 | 611 | U |
| 25 | 6 | 619 | A |
| 25 | 6 | 620 | A |
| 25 | 6 | 621 | A |
| 25 | 6 | 622 | A |
| 25 | 6 | 623 | A |
| 25 | 6 | 624 | G |
| 25 | 6 | 639 | U |
| 25 | 6 | 640 | U |
| 25 | 6 | 650 | U |
| 25 | 6 | 652 | G |
| 25 | 6 | 653 | C |
| 25 | 6 | 658 | C |
| 25 | 6 | 676 | G |
| 25 | 6 | 679 | U |
| 25 | 6 | 680 | U |
| 25 | 6 | 681 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | 6 | 682 | C |
| 25 | 6 | 683 | C |
| 25 | 6 | 684 | A |
| 25 | 6 | 685 | A |
| 25 | 6 | 691 | C |
| 25 | 6 | 696 | C |
| 25 | 6 | 709 | C |
| 25 | 6 | 711 | U |
| 25 | 6 | 714 | G |
| 25 | 6 | 715 | U |
| 25 | 6 | 718 | U |
| 25 | 6 | 719 | U |
| 25 | 6 | 720 | G |
| 25 | 6 | 721 | U |
| 25 | 6 | 722 | G |
| 25 | 6 | 723 | G |
| 25 | 6 | 730 | G |
| 25 | 6 | 742 | U |
| 25 | 6 | 745 | U |
| 25 | 6 | 753 | A |
| 25 | 6 | 754 | A |
| 25 | 6 | 755 | A |
| 25 | 6 | 756 | A |
| 25 | 6 | 765 | G |
| 25 | 6 | 766 | U |
| 25 | 6 | 774 | A |
| 25 | 6 | 775 | G |
| 25 | 6 | 780 | A |
| 25 | 6 | 781 | U |
| 25 | 6 | 782 | U |
| 25 | 6 | 783 | G |
| 25 | 6 | 789 | A |
| 25 | 6 | 793 | A |
| 25 | 6 | 794 | U |
| 25 | 6 | 803 | A |
| 25 | 6 | 811 | A |
| 25 | 6 | 812 | A |
| 25 | 6 | 815 | G |
| 25 | 6 | 821 | U |
| 25 | 6 | 823 | G |
| 25 | 6 | 825 | U |
| 25 | 6 | 826 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | 6 | 829 | A |
| 25 | 6 | 830 | U |
| 25 | 6 | 831 | U |
| 25 | 6 | 832 | U |
| 25 | 6 | 834 | G |
| 25 | 6 | 835 | U |
| 25 | 6 | 863 | A |
| 25 | 6 | 876 | G |
| 25 | 6 | 898 | A |
| 25 | 6 | 906 | A |
| 25 | 6 | 912 | U |
| 25 | 6 | 913 | G |
| 25 | 6 | 914 | G |
| 25 | 6 | 916 | U |
| 25 | 6 | 933 | A |
| 25 | 6 | 935 | U |
| 25 | 6 | 942 | G |
| 25 | 6 | 959 | U |
| 25 | 6 | 960 | U |
| 25 | 6 | 966 | A |
| 25 | 6 | 970 | A |
| 25 | 6 | 971 | A |
| 25 | 6 | 983 | A |
| 25 | 6 | 992 | A |
| 25 | 6 | 1003 | A |
| 25 | 6 | 1004 | U |
| 25 | 6 | 1005 | A |
| 25 | 6 | 1021 | C |
| 25 | 6 | 1026 | A |
| 25 | 6 | 1028 | C |
| 25 | 6 | 1039 | A |
| 25 | 6 | 1040 | G |
| 25 | 6 | 1052 | U |
| 25 | 6 | 1053 | G |
| 25 | 6 | 1057 | U |
| 25 | 6 | 1058 | U |
| 25 | 6 | 1059 | U |
| 25 | 6 | 1060 | U |
| 25 | 6 | 1072 | C |
| 25 | 6 | 1073 | G |
| 25 | 6 | 1076 | A |
| 25 | 6 | 1082 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | 6 | 1092 | A |
| 25 | 6 | 1096 | C |
| 25 | 6 | 1097 | U |
| 25 | 6 | 1098 | U |
| 25 | 6 | 1099 | U |
| 25 | 6 | 1100 | G |
| 25 | 6 | 1109 | G |
| 25 | 6 | 1137 | A |
| 25 | 6 | 1138 | A |
| 25 | 6 | 1151 | A |
| 25 | 6 | 1155 | G |
| 25 | 6 | 1158 | C |
| 25 | 6 | 1159 | C |
| 25 | 6 | 1160 | A |
| 25 | 6 | 1167 | G |
| 25 | 6 | 1185 | U |
| 25 | 6 | 1194 | A |
| 25 | 6 | 1196 | A |
| 25 | 6 | 1199 | G |
| 25 | 6 | 1200 | G |
| 25 | 6 | 1202 | A |
| 25 | 6 | 1208 | A |
| 25 | 6 | 1217 | A |
| 25 | 6 | 1218 | G |
| 25 | 6 | 1225 | U |
| 25 | 6 | 1228 | G |
| 25 | 6 | 1229 | G |
| 25 | 6 | 1230 | A |
| 25 | 6 | 1231 | U |
| 25 | 6 | 1241 | G |
| 25 | 6 | 1243 | G |
| 25 | 6 | 1244 | A |
| 25 | 6 | 1245 | G |
| 25 | 6 | 1246 | C |
| 25 | 6 | 1255 | G |
| 25 | 6 | 1256 | A |
| 25 | 6 | 1257 | U |
| 25 | 6 | 1258 | U |
| 25 | 6 | 1286 | U |
| 25 | 6 | 1291 | G |
| 25 | 6 | 1314 | U |
| 25 | 6 | 1315 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | 6 | 1316 | G |
| 25 | 6 | 1321 | A |
| 25 | 6 | 1344 | A |
| 25 | 6 | 1345 | A |
| 25 | 6 | 1346 | A |
| 25 | 6 | 1354 | G |
| 25 | 6 | 1361 | U |
| 25 | 6 | 1363 | U |
| 25 | 6 | 1364 | G |
| 25 | 6 | 1371 | A |
| 25 | 6 | 1372 | U |
| 25 | 6 | 1388 | A |
| 25 | 6 | 1390 | U |
| 25 | 6 | 1398 | U |
| 25 | 6 | 1399 | C |
| 25 | 6 | 1400 | A |
| 25 | 6 | 1402 | G |
| 25 | 6 | 1413 | U |
| 25 | 6 | 1414 | U |
| 25 | 6 | 1415 | U |
| 25 | 6 | 1427 | A |
| 25 | 6 | 1428 | G |
| 25 | 6 | 1433 | G |
| 25 | 6 | 1445 | G |
| 25 | 6 | 1446 | A |
| 25 | 6 | 1448 | G |
| 25 | 6 | 1458 | G |
| 25 | 6 | 1459 | C |
| 25 | 6 | 1461 | C |
| 25 | 6 | 1471 | A |
| 25 | 6 | 1481 | C |
| 25 | 6 | 1482 | C |
| 25 | 6 | 1490 | C |
| 25 | 6 | 1491 | U |
| 25 | 6 | 1492 | A |
| 25 | 6 | 1493 | A |
| 25 | 6 | 1506 | G |
| 25 | 6 | 1514 | U |
| 25 | 6 | 1515 | A |
| 25 | 6 | 1516 | A |
| 25 | 6 | 1521 | G |
| 25 | 6 | 1523 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | 6 | 1524 | A |
| 25 | 6 | 1535 | U |
| 25 | 6 | 1536 | G |
| 25 | 6 | 1537 | C |
| 25 | 6 | 1538 | U |
| 25 | 6 | 1540 | G |
| 25 | 6 | 1554 | U |
| 25 | 6 | 1557 | U |
| 25 | 6 | 1559 | A |
| 25 | 6 | 1569 | A |
| 25 | 6 | 1573 | A |
| 25 | 6 | 1574 | G |
| 25 | 6 | 1584 | G |
| 25 | 6 | 1590 | G |
| 25 | 6 | 1601 | G |
| 25 | 6 | 1616 | G |
| 25 | 6 | 1621 | U |
| 25 | 6 | 1657 | U |
| 25 | 6 | 1658 | G |
| 25 | 6 | 1682 | U |
| 25 | 6 | 1683 | C |
| 25 | 6 | 1696 | G |
| 25 | 6 | 1697 | G |
| 25 | 6 | 1698 | G |
| 25 | 6 | 1699 | G |
| 25 | 6 | 1700 | C |
| 25 | 6 | 1701 | A |
| 25 | 6 | 1702 | A |
| 25 | 6 | 1703 | C |
| 25 | 6 | 1712 | A |
| 25 | 6 | 1716 | C |
| 25 | 6 | 1717 | G |
| 25 | 6 | 1731 | A |
| 25 | 6 | 1760 | G |
| 25 | 6 | 1762 | A |
| 25 | 6 | 1766 | A |
| 25 | 6 | 1767 | G |
| 25 | 6 | 1769 | U |
| 25 | 6 | 1780 | G |
| 25 | 6 | 1782 | A |
| 25 | 6 | 1783 | C |
| 25 | 6 | 1792 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | 6 | 1793 | G |
| 25 | 6 | 1794 | A |
| 25 | 6 | 1795 | U |
| 25 | 6 | 1796 | C |
| 25 | 6 | 1799 | U |
| 25 | 6 | 1800 | A |
| 1 | AR | 16 | A |
| 1 | AR | 24 | G |
| 1 | AR | 26 | A |
| 1 | AR | 40 | A |
| 1 | AR | 43 | A |
| 1 | AR | 49 | A |
| 1 | AR | 57 | A |
| 1 | AR | 59 | G |
| 1 | AR | 60 | A |
| 1 | AR | 65 | A |
| 1 | AR | 66 | A |
| 1 | AR | 76 | G |
| 1 | AR | 92 | G |
| 1 | AR | 93 | C |
| 1 | AR | 99 | A |
| 1 | AR | 109 | A |
| 1 | AR | 110 | G |
| 1 | AR | 111 | C |
| 1 | AR | 113 | C |
| 1 | AR | 116 | A |
| 1 | AR | 120 | G |
| 1 | AR | 121 | A |
| 1 | AR | 122 | A |
| 1 | AR | 133 | U |
| 1 | AR | 135 | C |
| 1 | AR | 136 | G |
| 1 | AR | 156 | G |
| 1 | AR | 157 | A |
| 1 | AR | 165 | A |
| 1 | AR | 166 | C |
| 1 | AR | 172 | G |
| 1 | AR | 173 | G |
| 1 | AR | 174 | C |
| 1 | AR | 187 | A |
| 1 | AR | 190 | U |
| 1 | AR | 191 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | AR | 192 | C |
| 1 | AR | 200 | C |
| 1 | AR | 210 | U |
| 1 | AR | 211 | A |
| 1 | AR | 213 | A |
| 1 | AR | 218 | G |
| 1 | AR | 219 | A |
| 1 | AR | 231 | G |
| 1 | AR | 240 | U |
| 1 | AR | 241 | G |
| 1 | AR | 243 | G |
| 1 | AR | 245 | U |
| 1 | AR | 249 | U |
| 1 | AR | 250 | U |
| 1 | AR | 251 | G |
| 1 | AR | 252 | U |
| 1 | AR | 269 | G |
| 1 | AR | 270 | U |
| 1 | AR | 286 | U |
| 1 | AR | 295 | A |
| 1 | AR | 298 | U |
| 1 | AR | 323 | A |
| 1 | AR | 329 | U |
| 1 | AR | 334 | A |
| 1 | AR | 338 | A |
| 1 | AR | 339 | C |
| 1 | AR | 350 | C |
| 1 | AR | 351 | A |
| 1 | AR | 370 | U |
| 1 | AR | 376 | G |
| 1 | AR | 399 | A |
| 1 | AR | 401 | U |
| 1 | AR | 402 | A |
| 1 | AR | 403 | C |
| 1 | AR | 404 | G |
| 1 | AR | 409 | A |
| 1 | AR | 421 | G |
| 1 | AR | 422 | A |
| 1 | AR | 439 | C |
| 1 | AR | 440 | A |
| 1 | AR | 495 | G |
| 1 | AR | 516 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | AR | 521 | A |
| 1 | AR | 535 | G |
| 1 | AR | 544 | C |
| 1 | AR | 546 | C |
| 1 | AR | 548 | G |
| 1 | AR | 551 | A |
| 1 | AR | 552 | G |
| 1 | AR | 555 | U |
| 1 | AR | 557 | A |
| 1 | AR | 558 | U |
| 1 | AR | 559 | A |
| 1 | AR | 578 | A |
| 1 | AR | 579 | G |
| 1 | AR | 592 | A |
| 1 | AR | 600 | G |
| 1 | AR | 604 | G |
| 1 | AR | 607 | A |
| 1 | AR | 609 | G |
| 1 | AR | 611 | A |
| 1 | AR | 621 | A |
| 1 | AR | 622 | A |
| 1 | AR | 636 | C |
| 1 | AR | 638 | C |
| 1 | AR | 649 | A |
| 1 | AR | 651 | G |
| 1 | AR | 660 | A |
| 1 | AR | 677 | A |
| 1 | AR | 681 | U |
| 1 | AR | 691 | A |
| 1 | AR | 705 | A |
| 1 | AR | 712 | G |
| 1 | AR | 715 | A |
| 1 | AR | 716 | A |
| 1 | AR | 726 | G |
| 1 | AR | 727 | G |
| 1 | AR | 758 | C |
| 1 | AR | 764 | U |
| 1 | AR | 765 | C |
| 1 | AR | 766 | U |
| 1 | AR | 767 | U |
| 1 | AR | 776 | U |
| 1 | AR | 777 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | AR | 780 | A |
| 1 | AR | 781 | G |
| 1 | AR | 785 | G |
| 1 | AR | 806 | A |
| 1 | AR | 817 | A |
| 1 | AR | 830 | A |
| 1 | AR | 849 | C |
| 1 | AR | 861 | C |
| 1 | AR | 874 | U |
| 1 | AR | 879 | U |
| 1 | AR | 896 | A |
| 1 | AR | 907 | G |
| 1 | AR | 908 | G |
| 1 | AR | 914 | A |
| 1 | AR | 916 | G |
| 1 | AR | 917 | A |
| 1 | AR | 921 | A |
| 1 | AR | 923 | C |
| 1 | AR | 924 | G |
| 1 | AR | 937 | G |
| 1 | AR | 944 | C |
| 1 | AR | 959 | C |
| 1 | AR | 960 | U |
| 1 | AR | 964 | G |
| 1 | AR | 979 | U |
| 1 | AR | 980 | A |
| 1 | AR | 981 | U |
| 1 | AR | 982 | C |
| 1 | AR | 984 | G |
| 1 | AR | 994 | G |
| 1 | AR | 1001 | G |
| 1 | AR | 1002 | A |
| 1 | AR | 1006 | A |
| 1 | AR | 1010 | G |
| 1 | AR | 1015 | U |
| 1 | AR | 1016 | C |
| 1 | AR | 1017 | C |
| 1 | AR | 1018 | G |
| 1 | AR | 1020 | G |
| 1 | AR | 1021 | G |
| 1 | AR | 1024 | G |
| 1 | AR | 1029 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | AR | 1036 | A |
| 1 | AR | 1037 | C |
| 1 | AR | 1047 | A |
| 1 | AR | 1049 | C |
| 1 | AR | 1064 | A |
| 1 | AR | 1065 | A |
| 1 | AR | 1072 | G |
| 1 | AR | 1081 | U |
| 1 | AR | 1082 | U |
| 1 | AR | 1093 | A |
| 1 | AR | 1094 | U |
| 1 | AR | 1095 | U |
| 1 | AR | 1096 | U |
| 1 | AR | 1097 | G |
| 1 | AR | 1098 | A |
| 1 | AR | 1103 | A |
| 1 | AR | 1104 | G |
| 1 | AR | 1117 | G |
| 1 | AR | 1131 | G |
| 1 | AR | 1143 | A |
| 1 | AR | 1153 | A |
| 1 | AR | 1159 | A |
| 1 | AR | 1180 | A |
| 1 | AR | 1181 | U |
| 1 | AR | 1190 | A |
| 1 | AR | 1192 | C |
| 1 | AR | 1196 | C |
| 1 | AR | 1201 | C |
| 1 | AR | 1202 | A |
| 1 | AR | 1209 | G |
| 1 | AR | 1214 | U |
| 1 | AR | 1216 | C |
| 1 | AR | 1217 | A |
| 1 | AR | 1222 | G |
| 1 | AR | 1235 | U |
| 1 | AR | 1236 | G |
| 1 | AR | 1237 | G |
| 1 | AR | 1239 | C |
| 1 | AR | 1241 | U |
| 1 | AR | 1242 | G |
| 1 | AR | 1244 | A |
| 1 | AR | 1245 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | AR | 1246 | G |
| 1 | AR | 1252 | A |
| 1 | AR | 1258 | U |
| 1 | AR | 1262 | G |
| 1 | AR | 1263 | A |
| 1 | AR | 1285 | G |
| 1 | AR | 1292 | C |
| 1 | AR | 1295 | G |
| 1 | AR | 1307 | G |
| 1 | AR | 1308 | A |
| 1 | AR | 1309 | U |
| 1 | AR | 1313 | G |
| 1 | AR | 1330 | A |
| 1 | AR | 1348 | U |
| 1 | AR | 1349 | G |
| 1 | AR | 1351 | U |
| 1 | AR | 1352 | A |
| 1 | AR | 1353 | U |
| 1 | AR | 1355 | A |
| 1 | AR | 1356 | U |
| 1 | AR | 1357 | G |
| 1 | AR | 1385 | C |
| 1 | AR | 1386 | A |
| 1 | AR | 1399 | A |
| 1 | AR | 1400 | G |
| 1 | AR | 1418 | A |
| 1 | AR | 1419 | A |
| 1 | AR | 1421 | G |
| 1 | AR | 1431 | G |
| 1 | AR | 1434 | G |
| 1 | AR | 1437 | C |
| 1 | AR | 1446 | A |
| 1 | AR | 1450 | G |
| 1 | AR | 1453 | A |
| 1 | AR | 1481 | A |
| 1 | AR | 1482 | A |
| 1 | AR | 1488 | G |
| 1 | AR | 1508 | C |
| 1 | AR | 1536 | G |
| 1 | AR | 1555 | U |
| 1 | AR | 1556 | C |
| 1 | AR | 1560 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | AR | 1562 | C |
| 1 | AR | 1563 | C |
| 1 | AR | 1566 | A |
| 1 | AR | 1567 | U |
| 1 | AR | 1568 | U |
| 1 | AR | 1569 | U |
| 1 | AR | 1570 | U |
| 1 | AR | 1572 | U |
| 1 | AR | 1576 | G |
| 1 | AR | 1578 | C |
| 1 | AR | 1579 | C |
| 1 | AR | 1580 | A |
| 1 | AR | 1581 | C |
| 1 | AR | 1582 | C |
| 1 | AR | 1583 | A |
| 1 | AR | 1589 | A |
| 1 | AR | 1593 | A |
| 1 | AR | 1605 | A |
| 1 | AR | 1607 | U |
| 1 | AR | 1620 | U |
| 1 | AR | 1629 | U |
| 1 | AR | 1639 | C |
| 1 | AR | 1643 | A |
| 1 | AR | 1645 | U |
| 1 | AR | 1657 | C |
| 1 | AR | 1658 | G |
| 1 | AR | 1683 | A |
| 1 | AR | 1716 | U |
| 1 | AR | 1717 | U |
| 1 | AR | 1724 | U |
| 1 | AR | 1725 | C |
| 1 | AR | 1736 | G |
| 1 | AR | 1741 | A |
| 1 | AR | 1742 | U |
| 1 | AR | 1750 | A |
| 1 | AR | 1751 | G |
| 1 | AR | 1762 | C |
| 1 | AR | 1765 | U |
| 1 | AR | 1766 | G |
| 1 | AR | 1769 | G |
| 1 | AR | 1770 | G |
| 1 | AR | 1780 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | AR | 1797 | A |
| 1 | AR | 1809 | A |
| 1 | AR | 1810 | A |
| 1 | AR | 1814 | A |
| 1 | AR | 1815 | U |
| 1 | AR | 1816 | A |
| 1 | AR | 1817 | G |
| 1 | AR | 1820 | U |
| 1 | AR | 1821 | U |
| 1 | AR | 1835 | A |
| 1 | AR | 1839 | A |
| 1 | AR | 1841 | A |
| 1 | AR | 1842 | A |
| 1 | AR | 1846 | C |
| 1 | AR | 1849 | C |
| 1 | AR | 1878 | G |
| 1 | AR | 1879 | A |
| 1 | AR | 1893 | A |
| 1 | AR | 1906 | G |
| 1 | AR | 1952 | G |
| 1 | AR | 1953 | G |
| 1 | AR | 1954 | G |
| 1 | AR | 2094 | C |
| 1 | AR | 2101 | C |
| 1 | AR | 2102 | U |
| 1 | AR | 2111 | G |
| 1 | AR | 2112 | U |
| 1 | AR | 2113 | A |
| 1 | AR | 2114 | C |
| 1 | AR | 2121 | G |
| 1 | AR | 2122 | G |
| 1 | AR | 2131 | A |
| 1 | AR | 2134 | G |
| 1 | AR | 2140 | U |
| 1 | AR | 2144 | A |
| 1 | AR | 2158 | A |
| 1 | AR | 2169 | G |
| 1 | AR | 2187 | G |
| 1 | AR | 2198 | A |
| 1 | AR | 2201 | G |
| 1 | AR | 2205 | U |
| 1 | AR | 2209 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | AR | 2210 | G |
| 1 | AR | 2223 | A |
| 1 | AR | 2225 | U |
| 1 | AR | 2228 | A |
| 1 | AR | 2244 | A |
| 1 | AR | 2252 | A |
| 1 | AR | 2253 | G |
| 1 | AR | 2254 | U |
| 1 | AR | 2255 | A |
| 1 | AR | 2256 | A |
| 1 | AR | 2261 | G |
| 1 | AR | 2264 | U |
| 1 | AR | 2269 | U |
| 1 | AR | 2270 | A |
| 1 | AR | 2271 | A |
| 1 | AR | 2272 | G |
| 1 | AR | 2273 | G |
| 1 | AR | 2279 | A |
| 1 | AR | 2280 | A |
| 1 | AR | 2281 | A |
| 1 | AR | 2282 | U |
| 1 | AR | 2288 | G |
| 1 | AR | 2307 | G |
| 1 | AR | 2310 | U |
| 1 | AR | 2313 | A |
| 1 | AR | 2314 | U |
| 1 | AR | 2315 | G |
| 1 | AR | 2334 | U |
| 1 | AR | 2336 | U |
| 1 | AR | 2372 | A |
| 1 | AR | 2373 | A |
| 1 | AR | 2374 | C |
| 1 | AR | 2375 | G |
| 1 | AR | 2385 | G |
| 1 | AR | 2393 | G |
| 1 | AR | 2397 | A |
| 1 | AR | 2401 | A |
| 1 | AR | 2402 | A |
| 1 | AR | 2403 | G |
| 1 | AR | 2404 | A |
| 1 | AR | 2411 | U |
| 1 | AR | 2418 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | AR | 2419 | A |
| 1 | AR | 2435 | G |
| 1 | AR | 2443 | A |
| 1 | AR | 2444 | C |
| 1 | AR | 2445 | A |
| 1 | AR | 2502 | A |
| 1 | AR | 2503 | G |
| 1 | AR | 2504 | U |
| 1 | AR | 2507 | C |
| 1 | AR | 2508 | U |
| 1 | AR | 2514 | U |
| 1 | AR | 2515 | A |
| 1 | AR | 2522 | G |
| 1 | AR | 2523 | A |
| 1 | AR | 2524 | A |
| 1 | AR | 2530 | G |
| 1 | AR | 2533 | G |
| 1 | AR | 2536 | A |
| 1 | AR | 2538 | U |
| 1 | AR | 2539 | C |
| 1 | AR | 2540 | A |
| 1 | AR | 2541 | U |
| 1 | AR | 2542 | U |
| 1 | AR | 2543 | U |
| 1 | AR | 2547 | A |
| 1 | AR | 2549 | G |
| 1 | AR | 2552 | C |
| 1 | AR | 2555 | G |
| 1 | AR | 2561 | A |
| 1 | AR | 2569 | A |
| 1 | AR | 2570 | U |
| 1 | AR | 2571 | U |
| 1 | AR | 2572 | C |
| 1 | AR | 2573 | G |
| 1 | AR | 2581 | U |
| 1 | AR | 2585 | G |
| 1 | AR | 2586 | G |
| 1 | AR | 2589 | G |
| 1 | AR | 2593 | A |
| 1 | AR | 2594 | C |
| 1 | AR | 2595 | A |
| 1 | AR | 2606 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | AR | 2607 | G |
| 1 | AR | 2614 | G |
| 1 | AR | 2634 | U |
| 1 | AR | 2638 | C |
| 1 | AR | 2652 | U |
| 1 | AR | 2656 | A |
| 1 | AR | 2674 | A |
| 1 | AR | 2677 | G |
| 1 | AR | 2681 | U |
| 1 | AR | 2689 | A |
| 1 | AR | 2691 | A |
| 1 | AR | 2694 | A |
| 1 | AR | 2696 | A |
| 1 | AR | 2705 | A |
| 1 | AR | 2714 | G |
| 1 | AR | 2719 | U |
| 1 | AR | 2727 | A |
| 1 | AR | 2728 | G |
| 1 | AR | 2729 | U |
| 1 | AR | 2752 | U |
| 1 | AR | 2753 | G |
| 1 | AR | 2755 | C |
| 1 | AR | 2762 | A |
| 1 | AR | 2771 | U |
| 1 | AR | 2772 | C |
| 1 | AR | 2777 | G |
| 1 | AR | 2778 | G |
| 1 | AR | 2796 | G |
| 1 | AR | 2799 | A |
| 1 | AR | 2800 | G |
| 1 | AR | 2801 | A |
| 1 | AR | 2802 | A |
| 1 | AR | 2810 | C |
| 1 | AR | 2817 | A |
| 1 | AR | 2818 | U |
| 1 | AR | 2819 | A |
| 1 | AR | 2842 | U |
| 1 | AR | 2843 | U |
| 1 | AR | 2845 | A |
| 1 | AR | 2847 | A |
| 1 | AR | 2860 | U |
| 1 | AR | 2867 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | AR | 2871 | G |
| 1 | AR | 2872 | A |
| 1 | AR | 2873 | U |
| 1 | AR | 2875 | U |
| 1 | AR | 2887 | A |
| 1 | AR | 2896 | A |
| 1 | AR | 2899 | C |
| 1 | AR | 2923 | U |
| 1 | AR | 2928 | C |
| 1 | AR | 2935 | U |
| 1 | AR | 2936 | A |
| 1 | AR | 2942 | C |
| 1 | AR | 2945 | G |
| 1 | AR | 2947 | G |
| 1 | AR | 2951 | G |
| 1 | AR | 2952 | G |
| 1 | AR | 2971 | A |
| 1 | AR | 2983 | C |
| 1 | AR | 2990 | G |
| 1 | AR | 2996 | U |
| 1 | AR | 2997 | G |
| 1 | AR | 3012 | A |
| 1 | AR | 3049 | A |
| 1 | AR | 3056 | U |
| 1 | AR | 3057 | U |
| 1 | AR | 3059 | G |
| 1 | AR | 3078 | U |
| 1 | AR | 3079 | U |
| 1 | AR | 3086 | A |
| 1 | AR | 3092 | C |
| 1 | AR | 3104 | U |
| 1 | AR | 3119 | U |
| 1 | AR | 3122 | A |
| 1 | AR | 3130 | A |
| 1 | AR | 3131 | U |
| 1 | AR | 3142 | A |
| 1 | AR | 3143 | C |
| 1 | AR | 3151 | U |
| 1 | AR | 3153 | U |
| 1 | AR | 3155 | U |
| 1 | AR | 3156 | U |
| 1 | AR | 3157 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | AR | 3164 | C |
| 1 | AR | 3165 | A |
| 1 | AR | 3167 | A |
| 1 | AR | 3168 | A |
| 1 | AR | 3170 | A |
| 1 | AR | 3171 | U |
| 1 | AR | 3173 | G |
| 1 | AR | 3174 | A |
| 1 | AR | 3176 | G |
| 1 | AR | 3179 | U |
| 1 | AR | 3181 | C |
| 1 | AR | 3187 | A |
| 1 | AR | 3197 | G |
| 1 | AR | 3207 | U |
| 1 | AR | 3217 | C |
| 1 | AR | 3218 | A |
| 1 | AR | 3219 | G |
| 1 | AR | 3222 | U |
| 1 | AR | 3224 | G |
| 1 | AR | 3229 | G |
| 1 | AR | 3243 | A |
| 1 | AR | 3244 | A |
| 1 | AR | 3245 | A |
| 1 | AR | 3246 | G |
| 1 | AR | 3247 | G |
| 1 | AR | 3253 | G |
| 1 | AR | 3259 | U |
| 1 | AR | 3266 | G |
| 1 | AR | 3269 | U |
| 1 | AR | 3270 | U |
| 1 | AR | 3273 | A |
| 1 | AR | 3276 | G |
| 1 | AR | 3277 | U |
| 1 | AR | 3281 | U |
| 1 | AR | 3287 | U |
| 1 | AR | 3289 | G |
| 1 | AR | 3294 | A |
| 1 | AR | 3295 | A |
| 1 | AR | 3303 | G |
| 1 | AR | 3304 | U |
| 1 | AR | 3307 | A |
| 1 | AR | 3313 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | AR | 3316 | A |
| 1 | AR | 3317 | U |
| 1 | AR | 3318 | G |
| 1 | AR | 3319 | U |
| 1 | AR | 3320 | A |
| 1 | AR | 3330 | A |
| 1 | AR | 3341 | U |
| 1 | AR | 3342 | A |
| 1 | AR | 3345 | G |
| 1 | AR | 3347 | A |
| 1 | AR | 3350 | C |
| 1 | AR | 3351 | U |
| 1 | AR | 3352 | U |
| 1 | AR | 3353 | G |
| 1 | AR | 3355 | U |
| 1 | AR | 3356 | G |
| 1 | AR | 3359 | A |
| 1 | AR | 3369 | G |
| 1 | AR | 3375 | A |
| 1 | AR | 3378 | C |
| 1 | AR | 3383 | G |
| 1 | AR | 3389 | U |
| 2 | AS | 7 | G |
| 2 | AS | 22 | A |
| 2 | AS | 52 | G |
| 2 | AS | 53 | U |
| 2 | AS | 54 | U |
| 2 | AS | 60 | G |
| 2 | AS | 65 | G |
| 2 | AS | 73 | C |
| 2 | AS | 74 | C |
| 2 | AS | 99 | G |
| 2 | AS | 101 | G |
| 2 | AS | 102 | A |
| 2 | AS | 112 | G |
| 2 | AS | 121 | U |
| 3 | AT | 34 | U |
| 3 | AT | 35 | C |
| 3 | AT | 48 | A |
| 3 | AT | 51 | G |
| 3 | AT | 59 | A |
| 3 | AT | 62 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 3 | AT | 63 | G |
| 3 | AT | 79 | A |
| 3 | AT | 80 | A |
| 3 | AT | 81 | U |
| 3 | AT | 82 | U |
| 3 | AT | 83 | C |
| 3 | AT | 85 | G |
| 3 | AT | 86 | U |
| 3 | AT | 87 | G |
| 3 | AT | 90 | U |
| 3 | AT | 95 | G |
| 3 | AT | 97 | A |
| 3 | AT | 104 | A |
| 3 | AT | 106 | C |
| 3 | AT | 111 | A |
| 3 | AT | 113 | U |
| 3 | AT | 125 | U |
| 3 | AT | 126 | A |
| 3 | AT | 148 | G |
| 3 | AT | 151 | C |
| 3 | AT | 152 | G |
| 3 | AT | 155 | A |
| 3 | AT | 158 | U |
| 25 | A | 2 | A |
| 25 | A | 4 | C |
| 25 | A | 17 | C |
| 25 | A | 25 | C |
| 25 | A | 26 | A |
| 25 | A | 27 | U |
| 25 | A | 34 | G |
| 25 | A | 42 | G |
| 25 | A | 45 | U |
| 25 | A | 46 | A |
| 25 | A | 47 | A |
| 25 | A | 50 | C |
| 25 | A | 57 | G |
| 25 | A | 60 | U |
| 25 | A | 67 | A |
| 25 | A | 68 | A |
| 25 | A | 69 | G |
| 25 | A | 72 | A |
| 25 | A | 73 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | A | 74 | U |
| 25 | A | 104 | A |
| 25 | A | 114 | C |
| 25 | A | 116 | U |
| 25 | A | 128 | U |
| 25 | A | 130 | C |
| 25 | A | 131 | C |
| 25 | A | 132 | U |
| 25 | A | 133 | U |
| 25 | A | 134 | U |
| 25 | A | 135 | A |
| 25 | A | 136 | C |
| 25 | A | 137 | U |
| 25 | A | 140 | A |
| 25 | A | 141 | U |
| 25 | A | 144 | U |
| 25 | A | 145 | A |
| 25 | A | 146 | U |
| 25 | A | 153 | G |
| 25 | A | 158 | U |
| 25 | A | 159 | U |
| 25 | A | 161 | U |
| 25 | A | 176 | C |
| 25 | A | 178 | U |
| 25 | A | 179 | A |
| 25 | A | 185 | U |
| 25 | A | 186 | C |
| 25 | A | 187 | G |
| 25 | A | 188 | A |
| 25 | A | 190 | C |
| 25 | A | 191 | C |
| 25 | A | 192 | U |
| 25 | A | 193 | U |
| 25 | A | 194 | U |
| 25 | A | 195 | G |
| 25 | A | 196 | G |
| 25 | A | 197 | A |
| 25 | A | 200 | A |
| 25 | A | 215 | A |
| 25 | A | 217 | A |
| 25 | A | 218 | A |
| 25 | A | 219 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | A | 226 | A |
| 25 | A | 227 | U |
| 25 | A | 228 | G |
| 25 | A | 229 | U |
| 25 | A | 233 | C |
| 25 | A | 234 | G |
| 25 | A | 235 | G |
| 25 | A | 238 | U |
| 25 | A | 240 | U |
| 25 | A | 241 | U |
| 25 | A | 250 | C |
| 25 | A | 260 | U |
| 25 | A | 261 | U |
| 25 | A | 265 | A |
| 25 | A | 271 | A |
| 25 | A | 272 | U |
| 25 | A | 274 | G |
| 25 | A | 275 | C |
| 25 | A | 276 | C |
| 25 | A | 277 | U |
| 25 | A | 278 | U |
| 25 | A | 279 | G |
| 25 | A | 280 | U |
| 25 | A | 281 | G |
| 25 | A | 284 | G |
| 25 | A | 288 | A |
| 25 | A | 290 | G |
| 25 | A | 299 | A |
| 25 | A | 308 | C |
| 25 | A | 309 | C |
| 25 | A | 314 | C |
| 25 | A | 316 | A |
| 25 | A | 319 | U |
| 25 | A | 321 | C |
| 25 | A | 322 | G |
| 25 | A | 337 | G |
| 25 | A | 338 | C |
| 25 | A | 352 | A |
| 25 | A | 359 | A |
| 25 | A | 360 | A |
| 25 | A | 361 | C |
| 25 | A | 387 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | A | 390 | G |
| 25 | A | 400 | A |
| 25 | A | 402 | C |
| 25 | A | 403 | G |
| 25 | A | 404 | G |
| 25 | A | 416 | A |
| 25 | A | 418 | G |
| 25 | A | 424 | C |
| 25 | A | 425 | A |
| 25 | A | 426 | G |
| 25 | A | 428 | A |
| 25 | A | 434 | G |
| 25 | A | 439 | U |
| 25 | A | 444 | C |
| 25 | A | 445 | A |
| 25 | A | 448 | C |
| 25 | A | 454 | U |
| 25 | A | 468 | A |
| 25 | A | 480 | G |
| 25 | A | 484 | C |
| 25 | A | 485 | A |
| 25 | A | 488 | G |
| 25 | A | 493 | U |
| 25 | A | 494 | U |
| 25 | A | 495 | C |
| 25 | A | 496 | G |
| 25 | A | 497 | G |
| 25 | A | 498 | G |
| 25 | A | 499 | U |
| 25 | A | 500 | C |
| 25 | A | 502 | U |
| 25 | A | 503 | G |
| 25 | A | 504 | U |
| 25 | A | 505 | A |
| 25 | A | 506 | A |
| 25 | A | 507 | U |
| 25 | A | 510 | G |
| 25 | A | 511 | A |
| 25 | A | 512 | A |
| 25 | A | 513 | U |
| 25 | A | 515 | A |
| 25 | A | 516 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | A | 527 | A |
| 25 | A | 532 | U |
| 25 | A | 538 | A |
| 25 | A | 539 | G |
| 25 | A | 540 | G |
| 25 | A | 541 | A |
| 25 | A | 542 | A |
| 25 | A | 543 | C |
| 25 | A | 544 | A |
| 25 | A | 555 | A |
| 25 | A | 556 | A |
| 25 | A | 557 | G |
| 25 | A | 558 | U |
| 25 | A | 559 | C |
| 25 | A | 565 | C |
| 25 | A | 579 | A |
| 25 | A | 580 | A |
| 25 | A | 583 | C |
| 25 | A | 594 | A |
| 25 | A | 595 | G |
| 25 | A | 606 | A |
| 25 | A | 611 | U |
| 25 | A | 619 | A |
| 25 | A | 620 | A |
| 25 | A | 621 | A |
| 25 | A | 622 | A |
| 25 | A | 623 | A |
| 25 | A | 624 | G |
| 25 | A | 639 | U |
| 25 | A | 640 | U |
| 25 | A | 650 | U |
| 25 | A | 653 | C |
| 25 | A | 654 | C |
| 25 | A | 655 | G |
| 25 | A | 656 | G |
| 25 | A | 658 | C |
| 25 | A | 677 | G |
| 25 | A | 679 | U |
| 25 | A | 684 | A |
| 25 | A | 685 | A |
| 25 | A | 686 | C |
| 25 | A | 692 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | A | 694 | U |
| 25 | A | 696 | C |
| 25 | A | 697 | C |
| 25 | A | 700 | C |
| 25 | A | 702 | G |
| 25 | A | 703 | G |
| 25 | A | 704 | C |
| 25 | A | 705 | U |
| 25 | A | 707 | A |
| 25 | A | 708 | C |
| 25 | A | 709 | C |
| 25 | A | 710 | U |
| 25 | A | 711 | U |
| 25 | A | 712 | G |
| 25 | A | 714 | G |
| 25 | A | 717 | C |
| 25 | A | 718 | U |
| 25 | A | 719 | U |
| 25 | A | 721 | U |
| 25 | A | 722 | G |
| 25 | A | 723 | G |
| 25 | A | 725 | U |
| 25 | A | 727 | U |
| 25 | A | 728 | U |
| 25 | A | 731 | C |
| 25 | A | 732 | G |
| 25 | A | 733 | A |
| 25 | A | 734 | A |
| 25 | A | 735 | C |
| 25 | A | 736 | C |
| 25 | A | 737 | A |
| 25 | A | 738 | G |
| 25 | A | 742 | U |
| 25 | A | 743 | U |
| 25 | A | 745 | U |
| 25 | A | 754 | A |
| 25 | A | 755 | A |
| 25 | A | 756 | A |
| 25 | A | 765 | G |
| 25 | A | 766 | U |
| 25 | A | 774 | A |
| 25 | A | 775 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | A | 778 | G |
| 25 | A | 780 | A |
| 25 | A | 781 | U |
| 25 | A | 783 | G |
| 25 | A | 784 | C |
| 25 | A | 789 | A |
| 25 | A | 794 | U |
| 25 | A | 812 | A |
| 25 | A | 814 | A |
| 25 | A | 815 | G |
| 25 | A | 816 | G |
| 25 | A | 818 | C |
| 25 | A | 819 | G |
| 25 | A | 820 | U |
| 25 | A | 821 | U |
| 25 | A | 822 | U |
| 25 | A | 824 | G |
| 25 | A | 830 | U |
| 25 | A | 831 | U |
| 25 | A | 833 | U |
| 25 | A | 862 | A |
| 25 | A | 863 | A |
| 25 | A | 864 | U |
| 25 | A | 886 | U |
| 25 | A | 898 | A |
| 25 | A | 912 | U |
| 25 | A | 913 | G |
| 25 | A | 914 | G |
| 25 | A | 915 | A |
| 25 | A | 916 | U |
| 25 | A | 928 | U |
| 25 | A | 933 | A |
| 25 | A | 935 | U |
| 25 | A | 942 | G |
| 25 | A | 951 | A |
| 25 | A | 960 | U |
| 25 | A | 966 | A |
| 25 | A | 988 | A |
| 25 | A | 991 | G |
| 25 | A | 992 | A |
| 25 | A | 993 | A |
| 25 | A | 1003 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | A | 1004 | U |
| 25 | A | 1005 | A |
| 25 | A | 1020 | A |
| 25 | A | 1026 | A |
| 25 | A | 1028 | C |
| 25 | A | 1039 | A |
| 25 | A | 1040 | G |
| 25 | A | 1052 | U |
| 25 | A | 1053 | G |
| 25 | A | 1058 | U |
| 25 | A | 1061 | A |
| 25 | A | 1074 | G |
| 25 | A | 1076 | A |
| 25 | A | 1080 | U |
| 25 | A | 1082 | C |
| 25 | A | 1091 | A |
| 25 | A | 1092 | A |
| 25 | A | 1093 | A |
| 25 | A | 1096 | C |
| 25 | A | 1097 | U |
| 25 | A | 1100 | G |
| 25 | A | 1109 | G |
| 25 | A | 1111 | G |
| 25 | A | 1138 | A |
| 25 | A | 1146 | G |
| 25 | A | 1150 | G |
| 25 | A | 1151 | A |
| 25 | A | 1157 | A |
| 25 | A | 1158 | C |
| 25 | A | 1160 | A |
| 25 | A | 1164 | G |
| 25 | A | 1167 | G |
| 25 | A | 1185 | U |
| 25 | A | 1194 | A |
| 25 | A | 1196 | A |
| 25 | A | 1197 | C |
| 25 | A | 1199 | G |
| 25 | A | 1200 | G |
| 25 | A | 1202 | A |
| 25 | A | 1207 | C |
| 25 | A | 1208 | A |
| 25 | A | 1217 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | A | 1218 | G |
| 25 | A | 1227 | A |
| 25 | A | 1229 | G |
| 25 | A | 1243 | G |
| 25 | A | 1244 | A |
| 25 | A | 1245 | G |
| 25 | A | 1251 | U |
| 25 | A | 1256 | A |
| 25 | A | 1257 | U |
| 25 | A | 1258 | U |
| 25 | A | 1286 | U |
| 25 | A | 1314 | U |
| 25 | A | 1315 | U |
| 25 | A | 1321 | A |
| 25 | A | 1339 | C |
| 25 | A | 1340 | U |
| 25 | A | 1341 | A |
| 25 | A | 1344 | A |
| 25 | A | 1345 | A |
| 25 | A | 1349 | G |
| 25 | A | 1354 | G |
| 25 | A | 1361 | U |
| 25 | A | 1362 | U |
| 25 | A | 1363 | U |
| 25 | A | 1364 | G |
| 25 | A | 1370 | U |
| 25 | A | 1371 | A |
| 25 | A | 1372 | U |
| 25 | A | 1390 | U |
| 25 | A | 1398 | U |
| 25 | A | 1399 | C |
| 25 | A | 1400 | A |
| 25 | A | 1412 | G |
| 25 | A | 1413 | U |
| 25 | A | 1415 | U |
| 25 | A | 1427 | A |
| 25 | A | 1428 | G |
| 25 | A | 1446 | A |
| 25 | A | 1458 | G |
| 25 | A | 1459 | C |
| 25 | A | 1461 | C |
| 25 | A | 1471 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | A | 1473 | U |
| 25 | A | 1474 | G |
| 25 | A | 1475 | A |
| 25 | A | 1482 | C |
| 25 | A | 1486 | G |
| 25 | A | 1490 | C |
| 25 | A | 1491 | U |
| 25 | A | 1492 | A |
| 25 | A | 1493 | A |
| 25 | A | 1506 | G |
| 25 | A | 1515 | A |
| 25 | A | 1516 | A |
| 25 | A | 1517 | U |
| 25 | A | 1521 | G |
| 25 | A | 1523 | G |
| 25 | A | 1524 | A |
| 25 | A | 1526 | A |
| 25 | A | 1535 | U |
| 25 | A | 1536 | G |
| 25 | A | 1537 | C |
| 25 | A | 1538 | U |
| 25 | A | 1542 | G |
| 25 | A | 1557 | U |
| 25 | A | 1559 | A |
| 25 | A | 1569 | A |
| 25 | A | 1574 | G |
| 25 | A | 1584 | G |
| 25 | A | 1590 | G |
| 25 | A | 1601 | G |
| 25 | A | 1614 | A |
| 25 | A | 1616 | G |
| 25 | A | 1619 | C |
| 25 | A | 1624 | C |
| 25 | A | 1626 | U |
| 25 | A | 1631 | A |
| 25 | A | 1657 | U |
| 25 | A | 1658 | G |
| 25 | A | 1680 | G |
| 25 | A | 1683 | C |
| 25 | A | 1684 | U |
| 25 | A | 1686 | C |
| 25 | A | 1698 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | A | 1699 | G |
| 25 | A | 1700 | C |
| 25 | A | 1701 | A |
| 25 | A | 1702 | A |
| 25 | A | 1703 | C |
| 25 | A | 1711 | C |
| 25 | A | 1712 | A |
| 25 | A | 1713 | G |
| 25 | A | 1731 | A |
| 25 | A | 1750 | A |
| 25 | A | 1760 | G |
| 25 | A | 1762 | A |
| 25 | A | 1766 | A |
| 25 | A | 1769 | U |
| 25 | A | 1780 | G |
| 25 | A | 1782 | A |
| 25 | A | 1783 | C |
| 25 | A | 1792 | G |
| 25 | A | 1793 | G |
| 25 | A | 1794 | A |
| 25 | A | 1795 | U |
| 25 | A | 1796 | C |

All (186) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 65 | A |
| 1 | 1 | 210 | U |
| 1 | 1 | 239 | G |
| 1 | 1 | 282 | G |
| 1 | 1 | 547 | G |
| 1 | 1 | 647 | A |
| 1 | 1 | 763 | G |
| 1 | 1 | 873 | C |
| 1 | 1 | 916 | G |
| 1 | 1 | 979 | U |
| 1 | 1 | 981 | U |
| 1 | 1 | 993 | G |
| 1 | 1 | 1064 | A |
| 1 | 1 | 1094 | U |
| 1 | 1 | 1097 | G |
| 1 | 1 | 1273 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 1307 | G |
| 1 | 1 | 1329 | U |
| 1 | 1 | 1352 | A |
| 1 | 1 | 1355 | A |
| 1 | 1 | 1562 | C |
| 1 | 1 | 1568 | U |
| 1 | 1 | 1716 | U |
| 1 | 1 | 1820 | U |
| 1 | 1 | 2101 | C |
| 1 | 1 | 2112 | U |
| 1 | 1 | 2209 | U |
| 1 | 1 | 2249 | G |
| 1 | 1 | 2372 | A |
| 1 | 1 | 2418 | G |
| 1 | 1 | 2537 | U |
| 1 | 1 | 2541 | U |
| 1 | 1 | 2593 | A |
| 1 | 1 | 2772 | C |
| 1 | 1 | 2801 | A |
| 1 | 1 | 2818 | U |
| 1 | 1 | 3056 | U |
| 1 | 1 | 3078 | U |
| 1 | 1 | 3121 | U |
| 1 | 1 | 3218 | A |
| 1 | 1 | 3228 | C |
| 1 | 1 | 3269 | U |
| 1 | 1 | 3350 | C |
| 1 | 1 | 3351 | U |
| 1 | 1 | 3353 | G |
| 1 | 1 | 3375 | A |
| 3 | 4 | 85 | G |
| 3 | 4 | 125 | U |
| 25 | 6 | 25 | C |
| 25 | 6 | 139 | C |
| 25 | 6 | 145 | A |
| 25 | 6 | 158 | U |
| 25 | 6 | 187 | G |
| 25 | 6 | 192 | U |
| 25 | 6 | 217 | A |
| 25 | 6 | 272 | U |
| 25 | 6 | 417 | A |
| 25 | 6 | 512 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | 6 | 542 | A |
| 25 | 6 | 558 | U |
| 25 | 6 | 678 | A |
| 25 | 6 | 755 | A |
| 25 | 6 | 829 | A |
| 25 | 6 | 834 | G |
| 25 | 6 | 1051 | G |
| 25 | 6 | 1058 | U |
| 25 | 6 | 1081 | A |
| 25 | 6 | 1097 | U |
| 25 | 6 | 1207 | C |
| 25 | 6 | 1244 | A |
| 25 | 6 | 1255 | G |
| 25 | 6 | 1344 | A |
| 25 | 6 | 1481 | C |
| 25 | 6 | 1489 | U |
| 25 | 6 | 1491 | U |
| 25 | 6 | 1535 | U |
| 25 | 6 | 1568 | C |
| 25 | 6 | 1573 | A |
| 25 | 6 | 1620 | C |
| 25 | 6 | 1657 | U |
| 1 | AR | 40 | A |
| 1 | AR | 65 | A |
| 1 | AR | 588 | G |
| 1 | AR | 637 | C |
| 1 | AR | 715 | A |
| 1 | AR | 763 | G |
| 1 | AR | 873 | C |
| 1 | AR | 916 | G |
| 1 | AR | 979 | U |
| 1 | AR | 981 | U |
| 1 | AR | 993 | G |
| 1 | AR | 1064 | A |
| 1 | AR | 1097 | G |
| 1 | AR | 1103 | A |
| 1 | AR | 1238 | C |
| 1 | AR | 1241 | U |
| 1 | AR | 1284 | C |
| 1 | AR | 1307 | G |
| 1 | AR | 1329 | U |
| 1 | AR | 1331 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | AR | 1352 | A |
| 1 | AR | 1355 | A |
| 1 | AR | 1554 | U |
| 1 | AR | 1562 | C |
| 1 | AR | 1589 | A |
| 1 | AR | 1716 | U |
| 1 | AR | 1815 | U |
| 1 | AR | 1816 | A |
| 1 | AR | 1820 | U |
| 1 | AR | 1846 | C |
| 1 | AR | 2101 | C |
| 1 | AR | 2112 | U |
| 1 | AR | 2209 | U |
| 1 | AR | 2252 | A |
| 1 | AR | 2255 | A |
| 1 | AR | 2260 | U |
| 1 | AR | 2269 | U |
| 1 | AR | 2373 | A |
| 1 | AR | 2374 | C |
| 1 | AR | 2404 | A |
| 1 | AR | 2418 | G |
| 1 | AR | 2537 | U |
| 1 | AR | 2541 | U |
| 1 | AR | 2593 | A |
| 1 | AR | 2728 | G |
| 1 | AR | 2801 | A |
| 1 | AR | 2818 | U |
| 1 | AR | 2872 | A |
| 1 | AR | 3078 | U |
| 1 | AR | 3121 | U |
| 1 | AR | 3218 | A |
| 1 | AR | 3228 | C |
| 1 | AR | 3269 | U |
| 1 | AR | 3276 | G |
| 1 | AR | 3316 | A |
| 1 | AR | 3317 | U |
| 1 | AR | 3350 | C |
| 1 | AR | 3375 | A |
| 2 | AS | 52 | G |
| 3 | AT | 82 | U |
| 3 | AT | 85 | G |
| 25 | A | 25 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | A | 45 | U |
| 25 | A | 73 | U |
| 25 | A | 130 | C |
| 25 | A | 131 | C |
| 25 | A | 139 | C |
| 25 | A | 158 | U |
| 25 | A | 187 | G |
| 25 | A | 218 | A |
| 25 | A | 240 | U |
| 25 | A | 278 | U |
| 25 | A | 280 | U |
| 25 | A | 417 | A |
| 25 | A | 497 | G |
| 25 | A | 499 | U |
| 25 | A | 501 | U |
| 25 | A | 503 | G |
| 25 | A | 512 | A |
| 25 | A | 555 | A |
| 25 | A | 685 | A |
| 25 | A | 704 | C |
| 25 | A | 720 | G |
| 25 | A | 721 | U |
| 25 | A | 755 | A |
| 25 | A | 829 | A |
| 25 | A | 1051 | G |
| 25 | A | 1081 | A |
| 25 | A | 1150 | G |
| 25 | A | 1157 | A |
| 25 | A | 1196 | A |
| 25 | A | 1207 | C |
| 25 | A | 1226 | A |
| 25 | A | 1244 | A |
| 25 | A | 1250 | U |
| 25 | A | 1344 | A |
| 25 | A | 1370 | U |
| 25 | A | 1481 | C |
| 25 | A | 1489 | U |
| 25 | A | 1568 | C |
| 25 | A | 1573 | A |
| 25 | A | 1600 | A |
| 25 | A | 1615 | C |
| 25 | A | 1657 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | A | 1698 | G |
| 25 | A | 1761 | U |

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2548 ligands modelled in this entry, 1 is modelled with single atom and 1477 are monoatomic - leaving 1070 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 | $\# Z > 2$ |
| 84 | OHX | 1 | 3634 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1968 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3404 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3559 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1972 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3575 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3733 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3490 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3571 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3461 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3504 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3522 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3575 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1980 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | M | 201 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | 6 | 1985 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3658 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3711 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1963 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3617 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3643 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2024 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3606 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3532 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3594 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3481 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2007 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3655 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 4 | 206 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3478 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3663 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3709 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3552 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3436 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3491 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3540 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3582 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3707 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3448 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1964 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1966 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3589 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3619 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AK | 102 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3603 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1909 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3588 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3703 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3411 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3633 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3608 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AS | 206 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3509 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3663 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1908 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1990 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3579 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3562 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | A | 2031 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 3 | 206 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3460 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 4 | 214 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AT | 211 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3425 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 4 | 202 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3679 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | c8 | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AS | 209 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3713 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1904 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | CG | 302 | - | 0,6,6 | - | - | - | | |
| 87 | GOL | AR | 4262 | 84 | 5,5,5 | 0.26 | 0 | 5,5,5 | 0.53 | 0 |
| 84 | OHX | 1 | 3494 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3417 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3431 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3457 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3653 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3402 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3452 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1903 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3638 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1954 | - | 0,6,6 | - | - | - | | |
| 86 | HN8 | AR | 4263 | - | 24,26,26 | 0.29 | 0 | 36,41,41 | 1.60 | 4 (11%) |
| 84 | OHX | A | 1939 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3480 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3691 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3430 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3585 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3707 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2027 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3673 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | c4 | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1970 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1956 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3651 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 2 | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AT | 217 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3581 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | DH | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3435 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3727 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | 6 | 1923 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | T | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 4 | 209 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1973 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3565 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1963 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3434 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3409 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1943 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3565 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3596 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3508 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | J | 301 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3571 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3525 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1999 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3453 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3418 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3529 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3468 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3406 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3721 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3449 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1925 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3437 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3699 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AS | 203 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3418 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | DD | 101 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1913 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3624 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1953 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | CE | 402 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1946 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3590 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3620 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2001 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 3 | 209 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1910 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1978 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3605 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2050 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3602 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | 6 | 2051 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3424 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1910 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 401 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3433 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2000 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2015 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2045 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3422 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3599 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3647 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3566 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3426 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3577 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1933 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1971 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1947 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3446 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3505 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3462 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3710 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1933 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1924 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1937 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1947 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3401 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1992 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3583 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3517 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3522 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3527 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3641 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AT | 206 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 3 | 202 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3686 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3502 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3650 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3632 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3661 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1950 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3500 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3553 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3674 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | AR | 3593 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3513 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3604 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3592 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3550 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3668 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3719 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3503 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AS | 207 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1928 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1944 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3619 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1961 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3668 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1984 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1913 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3492 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1994 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1915 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3718 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3483 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3498 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2003 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3718 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3499 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2020 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3456 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3524 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3420 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3613 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1920 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1917 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 401 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3618 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3664 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1950 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2010 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3682 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 4 | 208 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3623 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3645 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3419 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3681 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | AR | 3556 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3534 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2001 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3468 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3467 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3428 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1952 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2011 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2017 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3546 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3685 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2009 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 4 | 213 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3445 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3516 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3622 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3715 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3476 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | CP | 501 | - | 0,6,6 | - | - | - | | |
| 87 | GOL | A | 2160 | - | 5,5,5 | 0.10 | 0 | 5,5,5 | 0.29 | 0 |
| 84 | OHX | 1 | 3512 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1934 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2027 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3482 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1982 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3528 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3407 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3677 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1903 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3438 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1934 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1975 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1982 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3676 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3691 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3576 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2006 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3537 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3569 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1989 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2035 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3669 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | O | 201 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | A | 1936 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3555 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3669 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3473 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3432 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3458 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1970 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1997 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1906 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3645 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3741 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2025 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3432 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2039 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3470 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3631 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1905 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3610 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AT | 214 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | y | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1959 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3444 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1941 | - | 0,6,6 | - | - | - | | |
| 87 | GOL | v | 305 | - | 5,5,5 | 0.18 | 0 | 5,5,5 | 0.54 | 0 |
| 84 | OHX | 1 | 3574 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1941 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3637 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3716 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2016 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | CX | 202 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3729 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3511 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3637 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3697 | 84 | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1917 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3461 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3505 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3728 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1901 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3665 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3702 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3626 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3465 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | 6 | 2011 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3621 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3598 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3584 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3654 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3698 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3704 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3472 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3662 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3471 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1988 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3705 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3713 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3413 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3744 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3466 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3442 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3586 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3587 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3722 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3410 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3495 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3525 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3594 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2038 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3586 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3640 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3495 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3513 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3703 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1929 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3625 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | z | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1931 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3558 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1921 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1939 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2052 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | c1 | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1977 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3612 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1919 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3514 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | A | 1909 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3633 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | A | 1958 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3732 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3652 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3523 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3460 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3530 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3415 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | A | 1915 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | c3 | 201 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3424 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | A | 1974 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3591 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | A | 1949 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | e | 101 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3568 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 6 | 1995 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 3 | 201 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 6 | 2040 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3717 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3521 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AM | 101 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 6 | 1964 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3723 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3411 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3539 | 84 | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3529 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3451 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | A | 1930 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3683 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3656 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3658 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3603 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AT | 210 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | CV | 201 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3608 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3676 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3577 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3632 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3739 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | A | 2040 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3651 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | AR | 3481 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3536 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | CF | 401 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3440 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3590 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3588 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2007 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3616 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3646 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1921 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3609 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2006 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3573 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3596 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3582 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3475 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3740 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3447 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3402 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3430 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2034 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1958 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3518 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3694 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3695 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3687 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3431 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3457 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2009 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2039 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | c5 | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 4 | 203 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AH | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3693 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3684 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 3 | 205 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | x | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2037 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1949 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3684 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3720 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3602 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3666 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | AR | 3601 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3642 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3446 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3720 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2035 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | x | 202 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3570 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3517 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1960 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3673 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1930 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3630 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3502 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3672 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1960 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3492 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3508 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | CL | 301 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3476 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3560 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 4 | 215 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3688 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3593 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2030 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3464 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3656 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1981 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3423 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3671 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3688 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1998 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3533 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3563 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1943 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1981 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2043 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3569 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1979 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2019 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3547 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1912 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2017 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2041 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | AS | 205 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3647 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2005 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3543 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3725 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1999 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3678 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AT | 202 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3561 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3648 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AS | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1971 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3690 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 4 | 211 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1923 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2044 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3551 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2003 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3403 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3661 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3489 | 87 | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3510 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3459 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3462 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3599 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3541 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3401 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1940 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1976 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3497 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3709 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1920 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3549 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3743 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2000 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1924 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1911 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3655 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3470 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1987 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3405 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3674 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2028 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | AR | 3675 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AT | 204 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3421 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3600 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2042 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3738 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3427 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3568 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1968 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1987 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1995 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2018 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1977 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1986 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2002 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3450 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3698 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3659 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3485 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | CG | 301 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2002 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3706 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3504 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2036 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3479 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3627 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3615 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1919 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2041 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1940 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3706 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3524 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2028 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3479 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3689 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1918 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3426 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3700 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3561 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1925 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AS | 210 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3519 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3614 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | 1 | 3631 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2026 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1916 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1984 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3648 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3644 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3712 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3626 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3516 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1932 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3443 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2034 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3412 | - | 0,6,6 | - | - | - | | |
| 86 | HN8 | 1 | 4223 | - | 24,26,26 | 0.28 | 0 | 36,41,41 | 1.03 | 2 (5%) |
| 84 | OHX | 6 | 1967 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1975 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3443 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3528 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3685 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3549 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3578 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1935 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3708 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2014 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AG | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3469 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1911 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1938 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3480 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3717 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3745 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2031 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3428 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3467 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3473 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3662 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1992 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2004 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3496 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3660 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3537 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3416 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1994 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | 6 | 1986 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3507 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3507 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3445 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3622 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3491 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3422 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3701 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1991 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3493 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3613 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AP | 502 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | r | 301 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3410 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3562 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3465 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2032 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1991 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1997 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3454 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3629 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2021 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3614 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3427 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3420 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2008 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3548 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1926 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3696 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2016 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3657 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2043 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3559 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 3 | 203 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2012 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3472 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2048 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3499 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3497 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3451 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 4 | 212 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3667 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1998 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | 6 | 1980 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3710 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3471 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3444 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3439 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 6 | 1932 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | A | 1922 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3503 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3486 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3686 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | A | 1965 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3526 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | A | 1948 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3723 | 1 | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3429 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3531 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3670 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3453 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | A | 1914 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3607 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AT | 207 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3567 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3617 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3649 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 6 | 1946 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3640 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3459 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3413 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3490 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | A | 1954 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3692 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3635 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 4 | 204 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | A | 2014 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3506 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3520 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3544 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3636 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3680 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 6 | 2029 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 6 | 1916 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3506 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | A | 1902 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | AT | 203 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | v | 301 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 6 | 1908 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 6 | 1996 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3477 | 84 | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3731 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | A | 2025 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3620 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3639 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3560 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3724 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3478 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3583 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3523 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3667 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3530 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3621 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 6 | 2008 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 3 | 204 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3724 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3554 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3483 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3488 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3554 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3556 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3597 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3570 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3642 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3597 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3531 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3666 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | A | 1978 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3711 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | K | 201 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3693 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3486 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3501 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | A | 1931 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3595 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3652 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3545 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 6 | 1966 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3487 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | 1 | 3498 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3553 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3591 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | Q | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3417 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3475 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3487 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3515 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3532 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3675 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3677 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3474 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1902 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2049 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3604 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3576 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1969 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3699 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3598 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AT | 213 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3489 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3646 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3671 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3694 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3687 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3546 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1904 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1922 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3695 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1973 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3736 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1951 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3452 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3557 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3689 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1912 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3518 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3540 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3425 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3514 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1914 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3441 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3519 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | 1 | 3708 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3579 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3714 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2047 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3665 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3542 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2013 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AS | 208 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3406 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1935 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1956 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3660 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3601 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3630 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3635 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 3 | 208 | - | 0,6,6 | - | - | - | | |
| 87 | GOL | 6 | 2199 | - | 5,5,5 | 0.10 | 0 | 5,5,5 | 0.33 | 0 |
| 84 | OHX | CX | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3442 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3450 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3659 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1937 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3679 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3643 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3606 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | CF | 402 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3609 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3700 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AT | 205 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3580 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1989 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3464 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3735 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 4 | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1969 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3434 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3533 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3409 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3611 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1936 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3572 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3616 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3678 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | A | 2042 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3625 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3737 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3702 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3572 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3605 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3585 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3701 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3414 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2022 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1945 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3543 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3690 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3715 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3509 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3563 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1938 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3403 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3566 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3683 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | DQ | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | h | 401 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3589 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3437 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3712 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1957 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3721 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AT | 212 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1927 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1948 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3412 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3574 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3535 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1957 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AC | 101 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3541 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3440 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3535 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 4 | 207 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3405 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3624 | - | 0,6,6 | - | - | - | | |
| 87 | GOL | AR | 4261 | 1 | 5,5,5 | 0.14 | 0 | 5,5,5 | 0.33 | 0 |
| 84 | OHX | AR | 3421 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | AR | 3600 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3512 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2038 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3634 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1945 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3615 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3628 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3510 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AT | 215 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2033 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1928 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1944 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2023 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3536 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3587 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1926 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2033 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3581 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3627 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2046 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3527 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3408 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 4 | 216 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3580 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3455 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3592 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3650 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3636 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3680 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2020 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3455 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3629 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2013 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AT | 208 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3439 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2010 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3447 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3682 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3521 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3414 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1955 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3644 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | CM | 201 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | AR | 3484 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3429 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3500 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | A | 1906 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3454 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | A | 1972 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3463 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3638 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3494 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 6 | 2024 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3730 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 6 | 1927 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3496 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 6 | 1962 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | CK | 201 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3526 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3734 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3551 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3557 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3469 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | A | 1962 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | A | 1967 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3639 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3704 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | A | 2036 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | k | 401 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3416 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3441 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3493 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3552 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3714 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3578 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3419 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3716 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | A | 1953 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3618 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3555 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | A | 1976 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | d9 | 101 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3544 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3681 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | A | 1952 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 6 | 2004 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | A | 2026 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1993 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3610 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1990 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1959 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1901 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3550 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3742 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3482 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3458 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1983 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3408 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AT | 209 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 3 | 207 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1993 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3548 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3696 | 84 | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1983 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3657 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2005 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3719 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1955 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1918 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3436 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1996 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3404 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3448 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | CE | 401 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2032 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3697 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2022 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1942 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1907 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2021 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3558 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3595 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3664 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3485 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1942 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3515 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1907 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3511 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3567 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | AR | 3623 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3649 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3415 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1979 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3534 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3501 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3477 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3433 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1985 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3547 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3654 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AS | 211 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2012 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3545 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3670 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1988 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3456 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3607 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2015 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3564 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3641 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AS | 202 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1951 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2037 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3584 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3539 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3423 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3564 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AT | 216 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AT | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | s8 | 301 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3542 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3672 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3449 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3474 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3438 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3653 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3520 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 2030 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3692 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3726 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 6 | 1905 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 4 | 205 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | AR | 3628 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 4 | 210 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3705 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 6 | 1961 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3484 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | A | 2023 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3466 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3573 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3611 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3463 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 1 | 3538 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3407 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3488 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3538 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3612 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | A | 2029 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 6 | 1974 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AR | 3435 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | A | 2019 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | 6 | 1965 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | A | 1929 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | A | 2018 | - | 0,6,6 | - | - | - | - | - |
| 84 | OHX | AS | 204 | - | 0,6,6 | - | - | - | - | - |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 86 | HN8 | AR | 4263 | - | - | 0/2/48/48 | 0/6/5/5 |
| 87 | GOL | AR | 4261 | 1 | - | 2/4/4/4 | - |
| 87 | GOL | A | 2160 | - | - | 0/4/4/4 | - |
| 87 | GOL | v | 305 | - | - | 2/4/4/4 | - |
| 87 | GOL | AR | 4262 | 84 | - | 1/4/4/4 | - |
| 86 | HN8 | 1 | 4223 | - | - | 0/2/48/48 | 0/6/5/5 |
| 87 | GOL | 6 | 2199 | - | - | 0/4/4/4 | - |

There are no bond length outliers.

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 86 | AR | 4263 | HN8 | C5-C1-C3 | -5.16 | 100.15 | 106.09 |
| 86 | AR | 4263 | HN8 | C5-C1-C2 | -5.00 | 102.67 | 106.70 |
| 86 | AR | 4263 | HN8 | C5-C1-C7 | 4.00 | 116.29 | 114.53 |
| 86 | 1 | 4223 | HN8 | C5-C1-C7 | 3.71 | 116.17 | 114.53 |
| 86 | AR | 4263 | HN8 | C3-C1-C2 | 2.87 | 107.05 | 102.28 |
| 86 | 1 | 4223 | HN8 | O1-C9-C17 | -2.42 | 102.25 | 109.31 |

There are no chirality outliers.

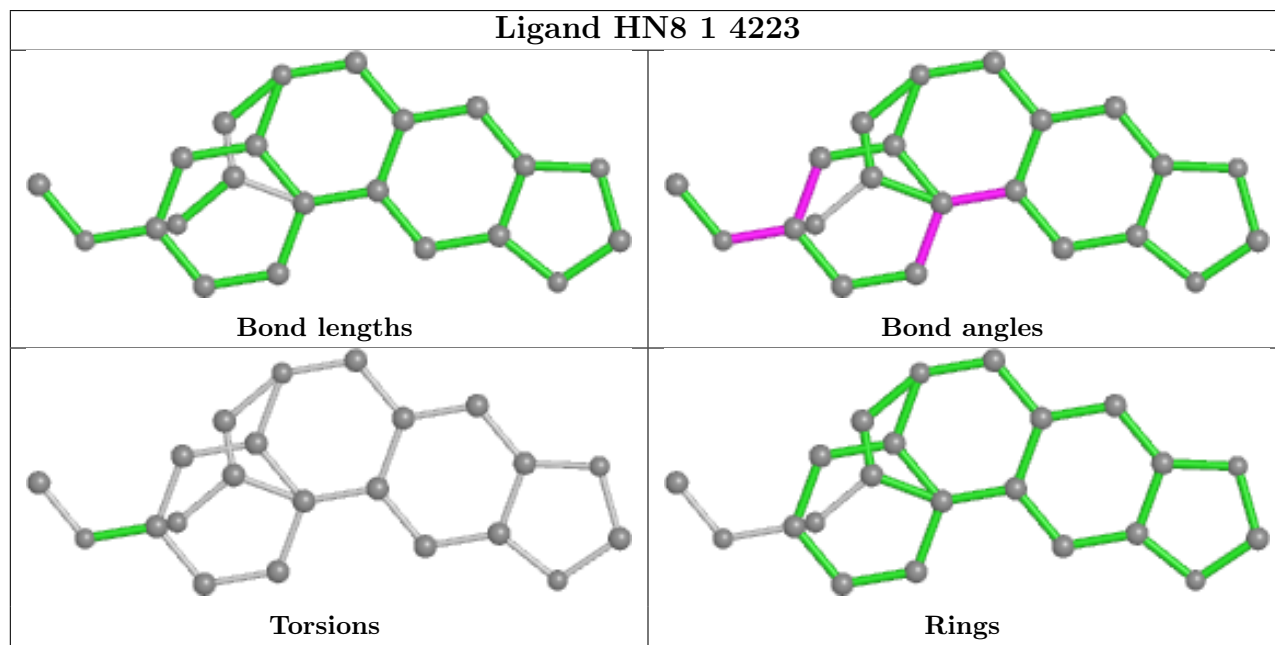
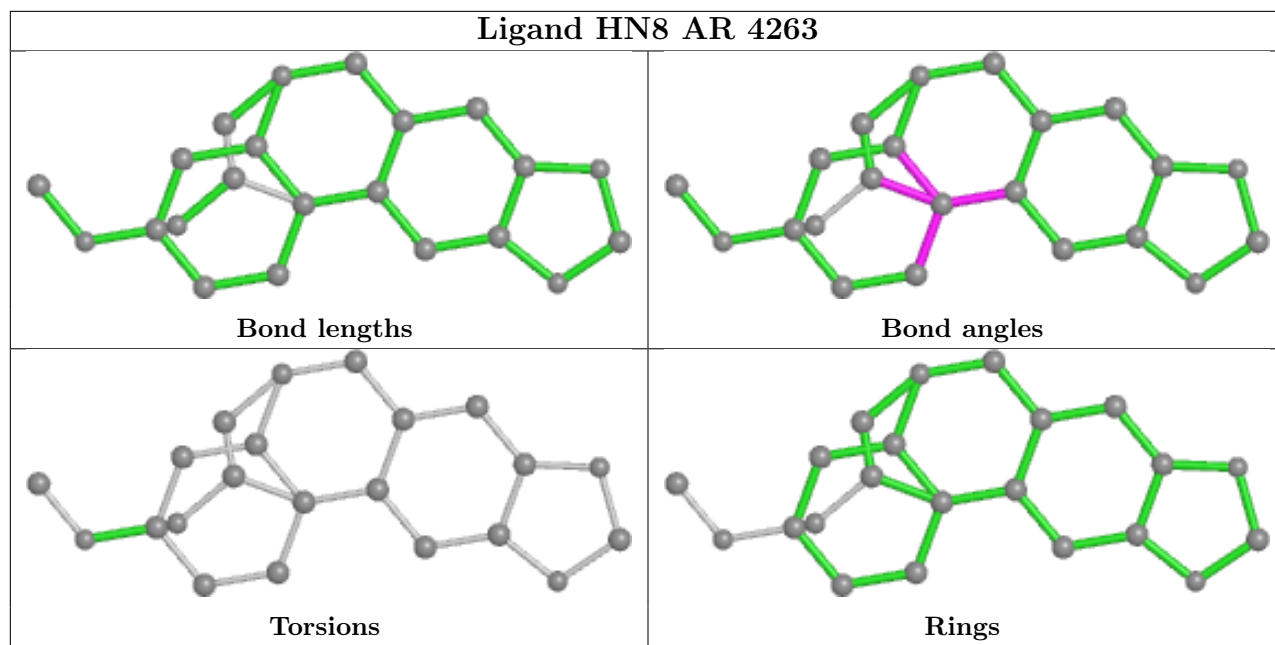
All (5) torsion outliers are listed below:

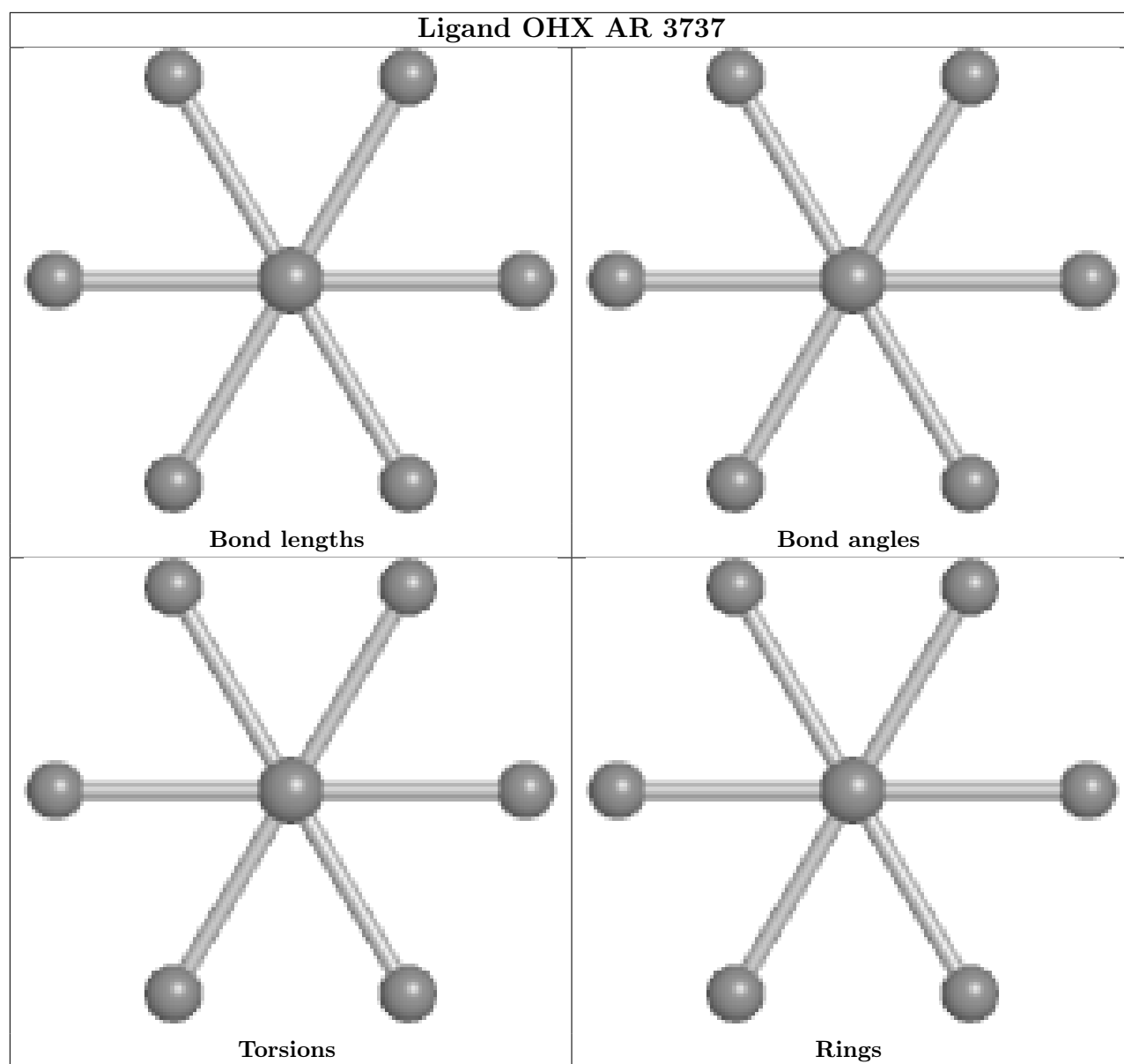
| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-------------|
| 87 | v | 305 | GOL | O1-C1-C2-C3 |
| 87 | AR | 4261 | GOL | C1-C2-C3-O3 |
| 87 | v | 305 | GOL | O1-C1-C2-O2 |
| 87 | AR | 4261 | GOL | O2-C2-C3-O3 |
| 87 | AR | 4262 | GOL | C1-C2-C3-O3 |

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 48 | sM | 2 |
| 25 | A | 1 |
| 47 | m2 | 1 |

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| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 5 | CE | 1 |
| 50 | s0 | 1 |
| 54 | s4 | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | sM | 85:SER | C | 119:UNK | N | 44.14 |
| 1 | sM | 139:UNK | C | 155:UNK | N | 37.59 |
| 1 | A | 1716:C | O3' | 1717:G | P | 4.52 |
| 1 | m2 | 23:UNK | C | 28:UNK | N | 3.62 |
| 1 | CE | 168:LYS | C | 169:THR | N | 1.19 |
| 1 | s0 | 160:ILE | C | 161:PRO | N | 1.19 |
| 1 | s4 | 82:TYR | C | 83:PRO | N | 1.18 |

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1 | 1 | 3149/3396 (92%) | 0.22 | 98 (3%) 49 26 | 26, 47, 129, 223 | 0 |
| 1 | AR | 3149/3396 (92%) | 0.30 | 104 (3%) 46 24 | 27, 49, 123, 225 | 0 |
| 2 | 3 | 121/121 (100%) | -0.11 | 0 100 100 | 35, 63, 75, 82 | 0 |
| 2 | AS | 121/121 (100%) | -0.04 | 1 (0%) 86 72 | 34, 52, 66, 73 | 0 |
| 3 | 4 | 158/158 (100%) | 0.21 | 5 (3%) 47 25 | 34, 51, 91, 138 | 0 |
| 3 | AT | 158/158 (100%) | 0.25 | 6 (3%) 40 20 | 34, 60, 99, 128 | 0 |
| 4 | CD | 252/252 (100%) | 0.04 | 3 (1%) 79 61 | 33, 52, 74, 82 | 0 |
| 4 | j | 252/252 (100%) | 0.04 | 1 (0%) 92 84 | 31, 46, 64, 77 | 0 |
| 5 | CE | 386/386 (100%) | -0.18 | 1 (0%) 94 88 | 25, 41, 55, 95 | 0 |
| 5 | k | 386/386 (100%) | -0.02 | 3 (0%) 86 72 | 25, 48, 62, 80 | 0 |
| 6 | CF | 361/361 (100%) | -0.11 | 1 (0%) 94 88 | 31, 47, 65, 88 | 0 |
| 6 | l | 361/361 (100%) | -0.12 | 1 (0%) 94 88 | 27, 44, 62, 71 | 0 |
| 7 | CG | 296/296 (100%) | 0.15 | 13 (4%) 34 17 | 39, 57, 83, 104 | 0 |
| 7 | m | 296/296 (100%) | 0.48 | 17 (5%) 23 11 | 46, 69, 89, 115 | 0 |
| 8 | CH | 156/175 (89%) | 0.07 | 3 (1%) 66 46 | 37, 46, 68, 84 | 0 |
| 8 | n | 156/175 (89%) | 0.04 | 1 (0%) 89 78 | 36, 43, 66, 86 | 0 |
| 9 | CI | 222/222 (100%) | -0.13 | 3 (1%) 75 56 | 27, 35, 78, 133 | 0 |
| 9 | o | 222/222 (100%) | -0.16 | 4 (1%) 68 47 | 29, 38, 73, 123 | 0 |
| 10 | CJ | 233/233 (100%) | 0.79 | 32 (13%) 3 1 | 70, 82, 123, 144 | 0 |
| 10 | p | 233/233 (100%) | 0.49 | 13 (5%) 24 11 | 56, 70, 105, 116 | 0 |
| 11 | CK | 191/191 (100%) | -0.16 | 3 (1%) 72 51 | 35, 45, 66, 82 | 0 |
| 11 | q | 191/191 (100%) | -0.25 | 0 100 100 | 42, 53, 66, 86 | 0 |
| 12 | CL | 211/220 (95%) | 0.45 | 13 (6%) 20 9 | 39, 59, 80, 93 | 0 |
| 12 | r | 211/220 (95%) | -0.04 | 2 (0%) 84 69 | 33, 46, 81, 96 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13 | CM | 169/169 (100%) | -0.19 | 1 (0%) 89 78 | 40, 61, 75, 83 | 0 |
| 13 | s | 169/169 (100%) | 0.09 | 4 (2%) 59 37 | 55, 77, 90, 96 | 0 |
| 14 | CN | 193/193 (100%) | 0.54 | 15 (7%) 13 5 | 41, 62, 101, 119 | 0 |
| 14 | t | 193/193 (100%) | -0.05 | 0 100 100 | 33, 53, 95, 125 | 0 |
| 15 | CO | 136/136 (100%) | -0.34 | 1 (0%) 87 75 | 34, 40, 63, 71 | 0 |
| 15 | u | 136/136 (100%) | -0.29 | 3 (2%) 62 41 | 37, 43, 60, 68 | 0 |
| 16 | CP | 203/203 (100%) | -0.11 | 0 100 100 | 38, 55, 67, 71 | 0 |
| 16 | v | 203/203 (100%) | -0.17 | 0 100 100 | 33, 44, 57, 64 | 0 |
| 17 | CQ | 197/197 (100%) | -0.20 | 3 (1%) 73 54 | 25, 30, 60, 66 | 0 |
| 17 | w | 197/197 (100%) | -0.27 | 0 100 100 | 28, 34, 55, 60 | 0 |
| 18 | CR | 183/183 (100%) | 1.33 | 29 (15%) 2 1 | 31, 39, 137, 167 | 0 |
| 18 | x | 183/183 (100%) | 0.53 | 21 (11%) 4 2 | 32, 40, 105, 140 | 0 |
| 19 | CS | 185/185 (100%) | -0.16 | 0 100 100 | 32, 45, 56, 60 | 0 |
| 19 | y | 185/185 (100%) | -0.14 | 0 100 100 | 33, 43, 63, 87 | 0 |
| 20 | CT | 188/188 (100%) | 0.12 | 9 (4%) 30 14 | 48, 63, 158, 169 | 0 |
| 20 | z | 188/188 (100%) | 0.16 | 7 (3%) 41 21 | 48, 64, 150, 167 | 0 |
| 21 | 0 | 172/172 (100%) | -0.19 | 1 (0%) 89 78 | 35, 41, 55, 65 | 0 |
| 21 | CU | 172/172 (100%) | -0.35 | 0 100 100 | 30, 37, 50, 57 | 0 |
| 22 | 2 | 159/159 (100%) | -0.07 | 2 (1%) 77 59 | 34, 45, 87, 97 | 0 |
| 22 | CV | 159/159 (100%) | -0.21 | 0 100 100 | 31, 41, 74, 84 | 0 |
| 23 | 5 | 100/100 (100%) | 0.81 | 12 (12%) 4 2 | 79, 93, 105, 123 | 0 |
| 23 | CW | 100/100 (100%) | 1.11 | 21 (21%) 1 0 | 77, 87, 98, 119 | 0 |
| 24 | CX | 136/136 (100%) | 0.14 | 1 (0%) 87 75 | 29, 38, 57, 59 | 0 |
| 24 | IR | 136/136 (100%) | 0.04 | 4 (2%) 51 28 | 31, 43, 56, 62 | 0 |
| 25 | 6 | 1783/1800 (99%) | 0.43 | 115 (6%) 19 8 | 41, 78, 169, 233 | 0 |
| 25 | A | 1781/1800 (98%) | 0.51 | 128 (7%) 15 6 | 49, 87, 186, 250 | 0 |
| 26 | 7 | 98/98 (100%) | 1.75 | 29 (29%) 0 0 | 43, 59, 150, 157 | 0 |
| 26 | CY | 98/98 (100%) | 0.41 | 11 (11%) 5 2 | 38, 53, 145, 177 | 0 |
| 27 | 8 | 121/121 (100%) | -0.03 | 1 (0%) 86 72 | 44, 57, 77, 117 | 0 |
| 27 | CZ | 121/121 (100%) | 0.05 | 4 (3%) 46 24 | 48, 64, 85, 100 | 0 |
| 28 | 9 | 126/126 (100%) | 0.67 | 6 (4%) 30 14 | 40, 55, 64, 73 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 28 | DA | 126/126 (100%) | 0.69 | 7 (5%) 24 11 | 40, 57, 73, 82 | 0 |
| 29 | AA | 135/135 (100%) | 1.73 | 47 (34%) 0 0 | 69, 83, 94, 104 | 0 |
| 29 | DB | 135/135 (100%) | 0.90 | 16 (11%) 4 2 | 81, 95, 110, 120 | 0 |
| 30 | AB | 148/148 (100%) | -0.08 | 0 100 100 | 27, 46, 73, 86 | 0 |
| 30 | DC | 148/148 (100%) | 0.02 | 1 (0%) 87 75 | 30, 51, 71, 77 | 0 |
| 31 | AC | 58/58 (100%) | -0.07 | 0 100 100 | 32, 52, 102, 122 | 0 |
| 31 | DD | 58/58 (100%) | -0.06 | 0 100 100 | 38, 51, 80, 88 | 0 |
| 32 | AD | 97/97 (100%) | 0.38 | 6 (6%) 20 9 | 67, 77, 99, 110 | 0 |
| 32 | DE | 97/97 (100%) | -0.29 | 0 100 100 | 71, 83, 105, 109 | 0 |
| 33 | AE | 109/109 (100%) | 0.20 | 2 (1%) 68 47 | 42, 56, 95, 106 | 0 |
| 33 | DF | 109/109 (100%) | 0.18 | 3 (2%) 53 30 | 41, 52, 92, 111 | 0 |
| 34 | AF | 127/127 (100%) | 0.01 | 3 (2%) 59 37 | 25, 40, 52, 69 | 0 |
| 34 | DG | 127/127 (100%) | 0.06 | 2 (1%) 72 51 | 24, 43, 55, 77 | 0 |
| 35 | AG | 106/106 (100%) | -0.15 | 1 (0%) 84 69 | 31, 36, 61, 72 | 0 |
| 35 | DH | 106/106 (100%) | -0.13 | 1 (0%) 84 69 | 28, 35, 64, 87 | 0 |
| 36 | AH | 112/112 (100%) | 0.26 | 6 (5%) 25 12 | 43, 63, 104, 114 | 0 |
| 36 | DI | 112/112 (100%) | 0.29 | 1 (0%) 84 69 | 46, 68, 113, 125 | 0 |
| 37 | AI | 119/119 (100%) | 0.27 | 6 (5%) 28 13 | 46, 61, 70, 77 | 0 |
| 37 | DJ | 119/119 (100%) | 0.27 | 6 (5%) 28 13 | 51, 67, 81, 88 | 0 |
| 38 | AJ | 99/99 (100%) | 0.24 | 3 (3%) 50 27 | 52, 61, 93, 113 | 0 |
| 38 | DK | 99/99 (100%) | 0.26 | 4 (4%) 38 19 | 59, 70, 92, 110 | 0 |
| 39 | AK | 87/87 (100%) | 0.10 | 3 (3%) 45 24 | 32, 36, 63, 86 | 0 |
| 39 | DL | 87/87 (100%) | 0.24 | 3 (3%) 45 24 | 36, 42, 77, 113 | 0 |
| 40 | AL | 77/77 (100%) | 0.19 | 2 (2%) 56 33 | 67, 79, 101, 108 | 0 |
| 40 | DM | 77/77 (100%) | 1.93 | 30 (38%) 0 0 | 76, 88, 107, 115 | 0 |
| 41 | AM | 50/50 (100%) | -0.07 | 0 100 100 | 42, 45, 52, 62 | 0 |
| 41 | DN | 50/50 (100%) | -0.04 | 0 100 100 | 45, 49, 59, 70 | 0 |
| 42 | AN | 52/52 (100%) | 0.61 | 5 (9%) 8 2 | 37, 43, 61, 69 | 0 |
| 42 | DO | 52/52 (100%) | 0.02 | 1 (1%) 66 46 | 32, 35, 48, 62 | 0 |
| 43 | AO | 25/25 (100%) | -0.14 | 0 100 100 | 52, 54, 59, 59 | 0 |
| 43 | DP | 25/25 (100%) | -0.20 | 0 100 100 | 43, 46, 59, 63 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 44 | AP | 105/105 (100%) | 0.66 | 9 (8%) 10 4 | 34, 50, 74, 103 | 0 |
| 44 | DQ | 105/105 (100%) | 0.25 | 0 100 100 | 37, 50, 65, 97 | 0 |
| 45 | AQ | 91/91 (100%) | -0.22 | 0 100 100 | 40, 50, 67, 80 | 0 |
| 45 | DR | 91/91 (100%) | -0.24 | 0 100 100 | 39, 53, 69, 79 | 0 |
| 46 | i | 159/272 (58%) | 0.57 | 19 (11%) 4 2 | 70, 90, 143, 148 | 0 |
| 47 | m2 | 0/150 | - | - | - | - |
| 48 | sM | 63/104 (60%) | 0.77 | 6 (9%) 8 2 | 62, 91, 108, 114 | 0 |
| 49 | p0 | 143/311 (45%) | 1.60 | 53 (37%) 0 0 | 89, 108, 172, 179 | 0 |
| 50 | B | 206/206 (100%) | 0.86 | 27 (13%) 3 1 | 93, 110, 125, 146 | 0 |
| 50 | s0 | 206/206 (100%) | 0.32 | 8 (3%) 39 20 | 77, 97, 115, 120 | 0 |
| 51 | C | 214/216 (99%) | 1.64 | 78 (36%) 0 0 | 93, 121, 142, 150 | 0 |
| 51 | s1 | 216/216 (100%) | 0.53 | 13 (6%) 21 10 | 68, 83, 110, 129 | 0 |
| 52 | D | 217/217 (100%) | 0.03 | 2 (0%) 84 69 | 68, 87, 108, 125 | 0 |
| 52 | s2 | 217/217 (100%) | 0.07 | 2 (0%) 84 69 | 57, 76, 92, 106 | 0 |
| 53 | E | 223/223 (100%) | 0.65 | 19 (8%) 10 4 | 74, 91, 118, 137 | 0 |
| 53 | s3 | 223/223 (100%) | 0.70 | 27 (12%) 4 1 | 75, 103, 134, 148 | 0 |
| 54 | F | 260/260 (100%) | 0.62 | 22 (8%) 10 4 | 63, 87, 97, 121 | 0 |
| 54 | s4 | 260/260 (100%) | 0.16 | 7 (2%) 54 31 | 53, 84, 98, 128 | 0 |
| 55 | G | 206/206 (100%) | 0.77 | 22 (10%) 6 2 | 92, 112, 131, 141 | 0 |
| 55 | s5 | 206/206 (100%) | 0.95 | 34 (16%) 1 1 | 74, 95, 114, 122 | 0 |
| 56 | H | 226/226 (100%) | 0.87 | 39 (17%) 1 0 | 61, 94, 116, 143 | 0 |
| 56 | s6 | 218/226 (96%) | 0.63 | 26 (11%) 4 2 | 52, 83, 111, 124 | 0 |
| 57 | I | 184/186 (98%) | 1.03 | 29 (15%) 2 1 | 87, 119, 148, 156 | 0 |
| 57 | s7 | 186/186 (100%) | 1.00 | 32 (17%) 1 0 | 77, 112, 147, 152 | 0 |
| 58 | J | 188/199 (94%) | 0.29 | 9 (4%) 30 14 | 53, 70, 111, 126 | 0 |
| 58 | s8 | 188/199 (94%) | 0.57 | 14 (7%) 14 5 | 49, 73, 124, 140 | 0 |
| 59 | K | 185/185 (100%) | 1.06 | 34 (18%) 1 0 | 77, 95, 129, 158 | 0 |
| 59 | s9 | 185/185 (100%) | 0.68 | 15 (8%) 12 5 | 67, 85, 116, 151 | 0 |
| 60 | L | 96/105 (91%) | 1.12 | 16 (16%) 1 1 | 81, 102, 129, 139 | 0 |
| 60 | c0 | 96/105 (91%) | 2.34 | 55 (57%) 0 0 | 96, 126, 139, 147 | 0 |
| 61 | M | 155/155 (100%) | 0.82 | 16 (10%) 6 2 | 56, 70, 126, 137 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 61 | c1 | 146/155 (94%) | 0.46 | 8 (5%) 25 11 | 55, 70, 104, 131 | 0 |
| 62 | N | 124/124 (100%) | 1.99 | 64 (51%) 0 0 | 133, 140, 152, 160 | 0 |
| 62 | c2 | 124/124 (100%) | 3.01 | 87 (70%) 0 0 | 161, 169, 184, 190 | 0 |
| 63 | O | 150/150 (100%) | 0.41 | 9 (6%) 21 10 | 64, 85, 100, 104 | 0 |
| 63 | c3 | 150/150 (100%) | 0.16 | 4 (2%) 54 31 | 59, 78, 96, 111 | 0 |
| 64 | P | 127/128 (99%) | 1.40 | 36 (28%) 0 0 | 66, 119, 135, 138 | 0 |
| 64 | c4 | 128/128 (100%) | 0.63 | 11 (8%) 10 4 | 57, 81, 91, 94 | 0 |
| 65 | Q | 124/141 (87%) | 0.49 | 7 (5%) 24 11 | 75, 89, 126, 146 | 0 |
| 65 | c5 | 135/141 (95%) | 0.80 | 16 (11%) 4 2 | 82, 97, 118, 131 | 0 |
| 66 | R | 141/142 (99%) | 1.05 | 25 (17%) 1 0 | 81, 107, 115, 120 | 0 |
| 66 | c6 | 142/142 (100%) | 0.69 | 15 (10%) 6 2 | 67, 91, 106, 127 | 0 |
| 67 | S | 120/125 (96%) | 0.56 | 14 (11%) 4 2 | 90, 109, 134, 138 | 0 |
| 67 | c7 | 117/125 (93%) | 0.13 | 6 (5%) 28 13 | 78, 97, 122, 130 | 0 |
| 68 | T | 145/145 (100%) | 0.79 | 17 (11%) 4 2 | 71, 99, 129, 140 | 0 |
| 68 | c8 | 145/145 (100%) | 0.71 | 16 (11%) 5 2 | 79, 91, 116, 127 | 0 |
| 69 | U | 143/143 (100%) | 1.00 | 22 (15%) 2 1 | 84, 102, 119, 133 | 0 |
| 69 | c9 | 143/143 (100%) | 1.11 | 30 (20%) 1 0 | 71, 86, 106, 119 | 0 |
| 70 | V | 107/110 (97%) | 0.14 | 2 (1%) 66 46 | 73, 109, 141, 145 | 0 |
| 70 | d0 | 110/110 (100%) | 0.46 | 12 (10%) 5 2 | 70, 111, 154, 172 | 0 |
| 71 | W | 87/87 (100%) | 0.61 | 8 (9%) 9 3 | 90, 96, 115, 124 | 0 |
| 71 | d1 | 87/87 (100%) | 0.14 | 4 (4%) 32 16 | 75, 83, 110, 121 | 0 |
| 72 | X | 129/129 (100%) | 0.15 | 2 (1%) 72 51 | 68, 81, 88, 101 | 0 |
| 72 | d2 | 129/129 (100%) | 0.05 | 1 (0%) 86 72 | 57, 70, 81, 97 | 0 |
| 73 | Y | 144/144 (100%) | 0.22 | 3 (2%) 63 43 | 57, 62, 73, 88 | 0 |
| 73 | d3 | 144/144 (100%) | -0.08 | 0 100 100 | 46, 52, 66, 78 | 0 |
| 74 | Z | 134/134 (100%) | 0.47 | 15 (11%) 5 2 | 69, 97, 114, 125 | 0 |
| 74 | d4 | 134/134 (100%) | 0.23 | 11 (8%) 11 4 | 62, 88, 103, 122 | 0 |
| 75 | a | 70/70 (100%) | 2.04 | 28 (40%) 0 0 | 111, 123, 138, 139 | 0 |
| 75 | d5 | 69/70 (98%) | 1.43 | 22 (31%) 0 0 | 93, 113, 124, 127 | 0 |
| 76 | b | 97/97 (100%) | 0.42 | 5 (5%) 27 12 | 67, 83, 135, 138 | 0 |
| 76 | d6 | 97/97 (100%) | 0.14 | 1 (1%) 82 67 | 51, 63, 95, 101 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 77 | c | 81/81 (100%) | 1.03 | 15 (18%) 1 0 | 82, 95, 127, 134 | 0 |
| 77 | d7 | 81/81 (100%) | 1.14 | 15 (18%) 1 0 | 72, 87, 126, 132 | 0 |
| 78 | d | 63/63 (100%) | 0.96 | 7 (11%) 5 2 | 104, 121, 132, 134 | 0 |
| 78 | d8 | 63/63 (100%) | 1.97 | 34 (53%) 0 0 | 91, 107, 121, 125 | 0 |
| 79 | d9 | 53/53 (100%) | 1.20 | 10 (18%) 1 0 | 71, 82, 120, 128 | 0 |
| 79 | e | 53/53 (100%) | 0.69 | 4 (7%) 14 5 | 75, 80, 96, 104 | 0 |
| 80 | e0 | 62/62 (100%) | 0.97 | 9 (14%) 2 1 | 59, 83, 113, 125 | 0 |
| 80 | f | 60/62 (96%) | 1.14 | 11 (18%) 1 0 | 63, 92, 131, 134 | 0 |
| 81 | g | 71/71 (100%) | 1.75 | 29 (40%) 0 0 | 105, 124, 144, 150 | 0 |
| 82 | h | 318/318 (100%) | 1.11 | 70 (22%) 0 0 | 97, 115, 135, 147 | 0 |
| 82 | sR | 318/318 (100%) | 0.61 | 32 (10%) 7 2 | 99, 121, 140, 157 | 0 |
| 83 | e1 | 51/51 (100%) | 2.31 | 23 (45%) 0 0 | 145, 157, 165, 167 | 0 |
| All | All | 33004/34167 (96%) | 0.39 | 2308 (6%) 16 7 | 24, 66, 132, 250 | 0 |

All (2308) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 18 | CR | 161 | ALA | 24.1 |
| 18 | CR | 162 | GLU | 20.5 |
| 26 | 7 | 76 | VAL | 18.1 |
| 18 | CR | 160 | ALA | 16.2 |
| 26 | 7 | 75 | THR | 15.8 |
| 18 | CR | 159 | LYS | 15.5 |
| 18 | CR | 179 | GLN | 14.3 |
| 18 | x | 162 | GLU | 13.0 |
| 18 | CR | 178 | ALA | 12.4 |
| 18 | CR | 158 | ALA | 12.1 |
| 55 | G | 152 | GLY | 11.8 |
| 75 | a | 36 | ALA | 11.2 |
| 28 | DA | 127 | GLU | 10.9 |
| 25 | A | 1702 | A | 10.6 |
| 26 | 7 | 84 | GLY | 10.4 |
| 1 | AR | 1569 | U | 10.1 |
| 18 | x | 161 | ALA | 10.0 |
| 61 | M | 147 | GLY | 9.9 |
| 25 | A | 1709 | C | 9.7 |
| 25 | A | 1708 | U | 9.6 |
| 61 | c1 | 3 | THR | 9.6 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 62 | c2 | 105 | LYS | 9.2 |
| 18 | CR | 165 | VAL | 9.1 |
| 26 | 7 | 88 | ASP | 8.8 |
| 51 | C | 100 | PHE | 8.7 |
| 25 | A | 913 | G | 8.7 |
| 61 | M | 145 | ALA | 8.6 |
| 61 | M | 146 | ALA | 8.5 |
| 25 | A | 1694 | A | 8.4 |
| 18 | x | 163 | LYS | 8.4 |
| 1 | AR | 2445 | A | 8.4 |
| 18 | CR | 168 | LEU | 8.3 |
| 18 | x | 184 | ALA | 8.2 |
| 26 | 7 | 81 | PRO | 8.2 |
| 18 | CR | 167 | ARG | 8.0 |
| 18 | CR | 176 | ILE | 8.0 |
| 80 | e0 | 62 | VAL | 7.9 |
| 62 | c2 | 63 | VAL | 7.8 |
| 49 | p0 | 192 | ASP | 7.7 |
| 18 | CR | 174 | GLY | 7.7 |
| 77 | c | 38 | PRO | 7.7 |
| 26 | 7 | 86 | SER | 7.7 |
| 55 | G | 151 | GLY | 7.6 |
| 18 | CR | 163 | LYS | 7.6 |
| 25 | A | 1703 | C | 7.6 |
| 10 | CJ | 254 | ASP | 7.5 |
| 23 | CW | 9 | GLN | 7.5 |
| 44 | AP | 106 | PHE | 7.5 |
| 61 | M | 2 | SER | 7.5 |
| 18 | CR | 175 | ARG | 7.5 |
| 25 | A | 1698 | G | 7.5 |
| 1 | 1 | 1569 | U | 7.4 |
| 25 | A | 1699 | G | 7.4 |
| 74 | d4 | 134 | ALA | 7.4 |
| 25 | A | 194 | U | 7.3 |
| 25 | A | 1704 | U | 7.3 |
| 20 | CT | 182 | ASP | 7.3 |
| 61 | M | 152 | GLN | 7.3 |
| 59 | K | 181 | ALA | 7.3 |
| 25 | A | 1711 | C | 7.2 |
| 60 | c0 | 79 | TYR | 7.2 |
| 25 | A | 1696 | G | 7.2 |
| 18 | CR | 180 | LYS | 7.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 61 | M | 150 | ASN | 7.2 |
| 18 | x | 160 | ALA | 7.1 |
| 26 | CY | 81 | PRO | 7.1 |
| 18 | CR | 170 | SER | 7.1 |
| 1 | 1 | 1568 | U | 7.1 |
| 65 | c5 | 4 | ALA | 7.0 |
| 74 | d4 | 135 | ASP | 7.0 |
| 25 | A | 1693 | A | 7.0 |
| 1 | AR | 2502 | A | 7.0 |
| 1 | 1 | 1570 | U | 7.0 |
| 18 | CR | 164 | LYS | 6.9 |
| 1 | AR | 252 | U | 6.9 |
| 82 | h | 4 | ASN | 6.8 |
| 83 | e1 | 102 | VAL | 6.8 |
| 25 | A | 134 | U | 6.8 |
| 1 | AR | 2535 | A | 6.8 |
| 61 | M | 153 | PHE | 6.7 |
| 26 | CY | 95 | SER | 6.7 |
| 1 | 1 | 2539 | C | 6.7 |
| 62 | c2 | 64 | SER | 6.6 |
| 64 | P | 16 | VAL | 6.6 |
| 26 | 7 | 85 | ALA | 6.6 |
| 25 | A | 1059 | U | 6.6 |
| 25 | A | 1697 | G | 6.6 |
| 55 | G | 153 | GLY | 6.6 |
| 66 | R | 92 | TYR | 6.5 |
| 62 | N | 62 | LEU | 6.5 |
| 18 | x | 159 | LYS | 6.5 |
| 18 | x | 164 | LYS | 6.5 |
| 25 | A | 1700 | C | 6.5 |
| 25 | A | 135 | A | 6.5 |
| 46 | i | 16 | ASP | 6.5 |
| 46 | i | 85 | SER | 6.5 |
| 82 | h | 52 | GLN | 6.5 |
| 82 | h | 3 | SER | 6.4 |
| 18 | CR | 184 | ALA | 6.4 |
| 25 | A | 1705 | C | 6.4 |
| 18 | CR | 157 | VAL | 6.4 |
| 26 | 7 | 82 | ILE | 6.4 |
| 64 | P | 15 | GLY | 6.4 |
| 79 | d9 | 4 | GLU | 6.3 |
| 25 | 6 | 718 | U | 6.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 46 | i | 88 | ARG | 6.2 |
| 77 | d7 | 59 | CYS | 6.2 |
| 25 | 6 | 1694 | A | 6.2 |
| 26 | 7 | 77 | LYS | 6.2 |
| 62 | c2 | 47 | GLU | 6.2 |
| 26 | 7 | 74 | LYS | 6.2 |
| 82 | h | 212 | ALA | 6.2 |
| 66 | R | 66 | ARG | 6.1 |
| 1 | 1 | 1955 | U | 6.1 |
| 1 | AR | 2504 | U | 6.1 |
| 1 | AR | 1567 | U | 6.1 |
| 10 | CJ | 253 | SER | 6.0 |
| 25 | A | 238 | U | 6.0 |
| 83 | e1 | 113 | LYS | 6.0 |
| 51 | C | 98 | THR | 6.0 |
| 62 | c2 | 43 | ARG | 6.0 |
| 79 | d9 | 5 | ASN | 6.0 |
| 51 | C | 230 | ALA | 6.0 |
| 1 | AR | 2539 | C | 6.0 |
| 62 | c2 | 121 | VAL | 5.9 |
| 60 | c0 | 67 | THR | 5.9 |
| 62 | c2 | 123 | VAL | 5.9 |
| 3 | AT | 81 | U | 5.9 |
| 1 | 1 | 1952 | G | 5.9 |
| 18 | CR | 183 | ALA | 5.9 |
| 25 | 6 | 658 | C | 5.9 |
| 25 | A | 1692 | G | 5.8 |
| 82 | h | 2 | ALA | 5.8 |
| 26 | 7 | 87 | LEU | 5.8 |
| 40 | DM | 34 | ALA | 5.8 |
| 61 | M | 155 | LYS | 5.8 |
| 28 | 9 | 127 | GLU | 5.8 |
| 66 | R | 21 | HIS | 5.8 |
| 26 | 7 | 90 | ILE | 5.8 |
| 61 | c1 | 2 | SER | 5.8 |
| 66 | R | 20 | ALA | 5.7 |
| 80 | f | 60 | PRO | 5.7 |
| 51 | C | 20 | VAL | 5.7 |
| 25 | 6 | 225 | A | 5.7 |
| 55 | s5 | 152 | GLY | 5.7 |
| 25 | 6 | 194 | U | 5.7 |
| 62 | c2 | 28 | LEU | 5.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | AR | 1570 | U | 5.6 |
| 26 | CY | 96 | LEU | 5.6 |
| 25 | A | 656 | G | 5.6 |
| 39 | DL | 88 | ALA | 5.6 |
| 1 | AR | 2503 | G | 5.6 |
| 62 | c2 | 65 | SER | 5.6 |
| 25 | 6 | 1228 | G | 5.5 |
| 7 | CG | 295 | GLY | 5.5 |
| 83 | e1 | 112 | GLY | 5.5 |
| 51 | C | 96 | LEU | 5.5 |
| 55 | s5 | 37 | GLN | 5.5 |
| 55 | G | 154 | ALA | 5.5 |
| 25 | 6 | 1256 | A | 5.4 |
| 25 | A | 1707 | A | 5.4 |
| 62 | c2 | 75 | VAL | 5.4 |
| 1 | AR | 1571 | A | 5.4 |
| 61 | M | 3 | THR | 5.4 |
| 25 | 6 | 239 | C | 5.4 |
| 80 | e0 | 63 | GLN | 5.4 |
| 66 | R | 5 | PRO | 5.4 |
| 64 | P | 75 | GLY | 5.4 |
| 1 | 1 | 1349 | G | 5.4 |
| 82 | h | 79 | TYR | 5.4 |
| 1 | 1 | 2205 | U | 5.4 |
| 1 | AR | 2506 | U | 5.3 |
| 60 | c0 | 48 | SER | 5.3 |
| 25 | 6 | 656 | G | 5.3 |
| 53 | s3 | 145 | ALA | 5.3 |
| 82 | h | 7 | LEU | 5.3 |
| 1 | AR | 3154 | C | 5.3 |
| 25 | A | 719 | U | 5.3 |
| 62 | c2 | 92 | ALA | 5.3 |
| 1 | AR | 1581 | C | 5.3 |
| 25 | 6 | 1695 | G | 5.3 |
| 10 | CJ | 121 | SER | 5.3 |
| 62 | c2 | 74 | LEU | 5.3 |
| 75 | a | 67 | ASP | 5.2 |
| 10 | CJ | 118 | GLU | 5.2 |
| 60 | c0 | 64 | TYR | 5.2 |
| 1 | AR | 2537 | U | 5.2 |
| 39 | DL | 87 | SER | 5.2 |
| 1 | AR | 3275 | U | 5.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | AR | 1572 | U | 5.2 |
| 56 | s6 | 169 | TYR | 5.2 |
| 26 | 7 | 69 | LYS | 5.2 |
| 65 | c5 | 50 | THR | 5.2 |
| 1 | AR | 1351 | U | 5.1 |
| 44 | AP | 104 | LEU | 5.1 |
| 60 | c0 | 76 | LEU | 5.1 |
| 80 | f | 53 | LYS | 5.1 |
| 1 | AR | 2505 | U | 5.1 |
| 61 | M | 149 | ALA | 5.1 |
| 25 | 6 | 506 | A | 5.1 |
| 23 | CW | 11 | ILE | 5.1 |
| 51 | C | 95 | ASN | 5.1 |
| 75 | a | 97 | LYS | 5.0 |
| 53 | s3 | 176 | LEU | 5.0 |
| 74 | Z | 2 | SER | 5.0 |
| 83 | e1 | 146 | SER | 5.0 |
| 50 | B | 28 | ASN | 5.0 |
| 25 | A | 132 | U | 5.0 |
| 55 | G | 222 | LYS | 5.0 |
| 18 | CR | 169 | THR | 5.0 |
| 62 | c2 | 103 | LEU | 5.0 |
| 1 | AR | 1566 | A | 5.0 |
| 25 | 6 | 229 | U | 5.0 |
| 25 | A | 1695 | G | 5.0 |
| 25 | A | 261 | U | 5.0 |
| 57 | I | 74 | GLN | 5.0 |
| 51 | C | 231 | LEU | 5.0 |
| 18 | x | 158 | ALA | 5.0 |
| 65 | Q | 51 | SER | 5.0 |
| 10 | CJ | 107 | GLU | 4.9 |
| 62 | c2 | 30 | VAL | 4.9 |
| 25 | 6 | 676 | G | 4.9 |
| 82 | sR | 319 | ASN | 4.9 |
| 81 | g | 146 | SER | 4.9 |
| 1 | 1 | 1571 | A | 4.9 |
| 25 | A | 914 | G | 4.9 |
| 25 | A | 1686 | C | 4.9 |
| 75 | d5 | 37 | GLN | 4.9 |
| 1 | AR | 1025 | A | 4.9 |
| 25 | 6 | 1227 | A | 4.9 |
| 34 | AF | 128 | LEU | 4.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 65 | c5 | 5 | VAL | 4.9 |
| 82 | h | 6 | VAL | 4.9 |
| 26 | CY | 97 | LYS | 4.9 |
| 51 | C | 86 | LEU | 4.8 |
| 18 | CR | 177 | ALA | 4.8 |
| 55 | G | 155 | ALA | 4.8 |
| 1 | AR | 1574 | C | 4.8 |
| 26 | 7 | 68 | ALA | 4.8 |
| 62 | c2 | 45 | LEU | 4.8 |
| 26 | 7 | 80 | ARG | 4.8 |
| 1 | AR | 3156 | U | 4.8 |
| 7 | CG | 290 | ILE | 4.8 |
| 7 | CG | 296 | GLN | 4.8 |
| 55 | s5 | 151 | GLY | 4.8 |
| 26 | 7 | 95 | SER | 4.8 |
| 40 | DM | 32 | ASN | 4.8 |
| 1 | 1 | 1243 | G | 4.8 |
| 62 | c2 | 59 | LEU | 4.8 |
| 60 | c0 | 98 | THR | 4.8 |
| 1 | AR | 2507 | C | 4.7 |
| 25 | 6 | 1707 | A | 4.7 |
| 51 | C | 101 | HIS | 4.7 |
| 25 | 6 | 678 | A | 4.7 |
| 62 | c2 | 104 | GLY | 4.7 |
| 40 | DM | 31 | LEU | 4.7 |
| 26 | CY | 67 | VAL | 4.7 |
| 75 | a | 69 | LEU | 4.7 |
| 77 | c | 33 | LEU | 4.7 |
| 62 | c2 | 34 | THR | 4.7 |
| 1 | AR | 2444 | C | 4.7 |
| 57 | I | 87 | ASP | 4.7 |
| 75 | a | 48 | ASP | 4.7 |
| 25 | 6 | 1229 | G | 4.7 |
| 62 | c2 | 60 | VAL | 4.7 |
| 69 | c9 | 4 | VAL | 4.7 |
| 62 | N | 67 | THR | 4.6 |
| 46 | i | 89 | ARG | 4.6 |
| 65 | c5 | 10 | ARG | 4.6 |
| 69 | c9 | 2 | PRO | 4.6 |
| 62 | c2 | 107 | ASP | 4.6 |
| 80 | e0 | 49 | LEU | 4.6 |
| 57 | I | 32 | PRO | 4.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 82 | sR | 121 | MET | 4.6 |
| 62 | c2 | 80 | ASN | 4.6 |
| 78 | d8 | 65 | ARG | 4.6 |
| 65 | Q | 50 | THR | 4.6 |
| 1 | 1 | 1236 | G | 4.6 |
| 1 | 1 | 1268 | G | 4.6 |
| 25 | A | 133 | U | 4.6 |
| 62 | c2 | 112 | ALA | 4.6 |
| 1 | 1 | 1350 | A | 4.6 |
| 25 | A | 1701 | A | 4.6 |
| 61 | M | 4 | GLU | 4.6 |
| 64 | P | 40 | ALA | 4.6 |
| 18 | x | 174 | GLY | 4.6 |
| 25 | 6 | 721 | U | 4.6 |
| 39 | AK | 87 | SER | 4.6 |
| 60 | c0 | 50 | THR | 4.6 |
| 83 | e1 | 115 | THR | 4.6 |
| 83 | e1 | 104 | SER | 4.6 |
| 3 | AT | 80 | A | 4.6 |
| 25 | A | 718 | U | 4.5 |
| 25 | A | 1687 | U | 4.5 |
| 1 | 1 | 1266 | G | 4.5 |
| 18 | x | 179 | GLN | 4.5 |
| 55 | s5 | 155 | ALA | 4.5 |
| 59 | K | 138 | LYS | 4.5 |
| 61 | M | 154 | ALA | 4.5 |
| 56 | s6 | 217 | SER | 4.5 |
| 1 | 1 | 1242 | G | 4.5 |
| 60 | c0 | 57 | THR | 4.5 |
| 40 | DM | 11 | PHE | 4.5 |
| 55 | s5 | 156 | ARG | 4.5 |
| 26 | 7 | 83 | THR | 4.5 |
| 69 | U | 71 | VAL | 4.5 |
| 62 | N | 49 | THR | 4.5 |
| 25 | A | 658 | C | 4.5 |
| 68 | T | 2 | SER | 4.5 |
| 25 | A | 241 | U | 4.5 |
| 29 | AA | 95 | VAL | 4.5 |
| 1 | 1 | 1352 | A | 4.5 |
| 26 | 7 | 96 | LEU | 4.4 |
| 60 | c0 | 65 | TYR | 4.4 |
| 1 | AR | 2536 | A | 4.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 29 | AA | 5 | LEU | 4.4 |
| 1 | 1 | 1762 | C | 4.4 |
| 64 | P | 29 | HIS | 4.4 |
| 26 | 7 | 70 | LYS | 4.4 |
| 10 | CJ | 115 | ALA | 4.4 |
| 25 | A | 715 | U | 4.4 |
| 40 | DM | 71 | PRO | 4.4 |
| 1 | AR | 1579 | C | 4.4 |
| 7 | CG | 297 | GLN | 4.4 |
| 18 | CR | 172 | GLN | 4.4 |
| 37 | DJ | 120 | ALA | 4.4 |
| 25 | A | 239 | C | 4.4 |
| 62 | N | 50 | LYS | 4.4 |
| 62 | N | 64 | SER | 4.4 |
| 51 | C | 47 | LEU | 4.4 |
| 75 | a | 65 | LEU | 4.4 |
| 25 | A | 1710 | U | 4.4 |
| 23 | 5 | 89 | LEU | 4.4 |
| 60 | c0 | 69 | THR | 4.4 |
| 65 | c5 | 52 | LYS | 4.4 |
| 26 | CY | 68 | ALA | 4.3 |
| 57 | I | 38 | LEU | 4.3 |
| 62 | c2 | 71 | ILE | 4.3 |
| 51 | C | 226 | GLY | 4.3 |
| 25 | A | 1706 | C | 4.3 |
| 10 | CJ | 106 | LYS | 4.3 |
| 29 | AA | 99 | GLU | 4.3 |
| 58 | s8 | 67 | TRP | 4.3 |
| 46 | i | 87 | THR | 4.3 |
| 62 | c2 | 115 | VAL | 4.3 |
| 68 | T | 13 | HIS | 4.3 |
| 62 | N | 111 | ASN | 4.3 |
| 79 | e | 4 | GLU | 4.3 |
| 29 | AA | 72 | ILE | 4.3 |
| 51 | C | 84 | ILE | 4.3 |
| 1 | AR | 2501 | U | 4.3 |
| 51 | C | 99 | ASN | 4.3 |
| 62 | c2 | 116 | VAL | 4.3 |
| 18 | CR | 166 | VAL | 4.3 |
| 22 | 2 | 121 | ALA | 4.3 |
| 33 | DF | 82 | GLU | 4.3 |
| 40 | DM | 30 | LYS | 4.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 53 | E | 217 | ILE | 4.3 |
| 54 | F | 167 | GLY | 4.3 |
| 62 | c2 | 114 | LYS | 4.3 |
| 83 | e1 | 145 | HIS | 4.3 |
| 53 | s3 | 174 | HIS | 4.3 |
| 1 | 1 | 1567 | U | 4.2 |
| 62 | c2 | 56 | GLU | 4.2 |
| 51 | C | 55 | LYS | 4.2 |
| 62 | c2 | 76 | GLU | 4.2 |
| 25 | 6 | 226 | A | 4.2 |
| 56 | s6 | 166 | GLU | 4.2 |
| 25 | 6 | 240 | U | 4.2 |
| 61 | M | 148 | LYS | 4.2 |
| 61 | M | 151 | LYS | 4.2 |
| 25 | A | 136 | C | 4.2 |
| 60 | c0 | 68 | LEU | 4.2 |
| 1 | 1 | 1265 | U | 4.2 |
| 51 | C | 41 | ARG | 4.2 |
| 55 | G | 41 | LYS | 4.2 |
| 62 | c2 | 119 | SER | 4.2 |
| 61 | M | 156 | PHE | 4.2 |
| 1 | AR | 3276 | G | 4.2 |
| 59 | K | 186 | GLU | 4.2 |
| 63 | O | 151 | ASN | 4.2 |
| 78 | d8 | 13 | ILE | 4.2 |
| 78 | d8 | 43 | ASN | 4.2 |
| 25 | A | 183 | U | 4.2 |
| 62 | c2 | 91 | VAL | 4.2 |
| 28 | 9 | 120 | GLN | 4.2 |
| 81 | g | 104 | SER | 4.2 |
| 33 | AE | 82 | GLU | 4.2 |
| 82 | sR | 51 | ASP | 4.2 |
| 62 | c2 | 113 | ARG | 4.2 |
| 70 | d0 | 121 | ASN | 4.2 |
| 82 | h | 253 | ALA | 4.2 |
| 75 | a | 73 | GLY | 4.2 |
| 1 | 1 | 1351 | U | 4.1 |
| 10 | CJ | 252 | ASN | 4.1 |
| 26 | 7 | 89 | LEU | 4.1 |
| 60 | c0 | 70 | GLU | 4.1 |
| 77 | d7 | 33 | LEU | 4.1 |
| 83 | e1 | 107 | LYS | 4.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 9 | CI | 26 | VAL | 4.1 |
| 62 | N | 41 | LEU | 4.1 |
| 29 | AA | 107 | ARG | 4.1 |
| 82 | sR | 46 | LYS | 4.1 |
| 1 | AR | 1815 | U | 4.1 |
| 25 | A | 820 | U | 4.1 |
| 62 | c2 | 61 | VAL | 4.1 |
| 7 | CG | 287 | ALA | 4.1 |
| 25 | 6 | 679 | U | 4.1 |
| 49 | p0 | 197 | PHE | 4.1 |
| 46 | i | 18 | VAL | 4.1 |
| 60 | c0 | 9 | ASN | 4.1 |
| 83 | e1 | 114 | VAL | 4.1 |
| 49 | p0 | 25 | LEU | 4.1 |
| 10 | CJ | 117 | ALA | 4.1 |
| 60 | c0 | 3 | MET | 4.1 |
| 10 | CJ | 111 | LYS | 4.1 |
| 38 | AJ | 99 | ARG | 4.1 |
| 77 | c | 41 | LEU | 4.1 |
| 60 | c0 | 37 | THR | 4.0 |
| 1 | 1 | 2207 | A | 4.0 |
| 25 | A | 1690 | G | 4.0 |
| 26 | 7 | 72 | SER | 4.0 |
| 65 | c5 | 6 | ASN | 4.0 |
| 12 | CL | 112 | GLN | 4.0 |
| 51 | C | 91 | VAL | 4.0 |
| 62 | c2 | 125 | ASN | 4.0 |
| 68 | T | 8 | GLN | 4.0 |
| 75 | a | 71 | ILE | 4.0 |
| 1 | 1 | 1267 | U | 4.0 |
| 48 | sM | 84 | LYS | 4.0 |
| 62 | c2 | 29 | LYS | 4.0 |
| 1 | 1 | 1278 | A | 4.0 |
| 25 | 6 | 214 | G | 4.0 |
| 23 | CW | 10 | LYS | 4.0 |
| 62 | c2 | 93 | ASP | 4.0 |
| 55 | s5 | 153 | GLY | 4.0 |
| 57 | s7 | 93 | LEU | 4.0 |
| 25 | A | 131 | C | 4.0 |
| 64 | P | 27 | PHE | 4.0 |
| 62 | c2 | 46 | ARG | 4.0 |
| 25 | A | 506 | A | 4.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 60 | c0 | 55 | VAL | 4.0 |
| 40 | DM | 33 | LYS | 4.0 |
| 82 | h | 115 | ILE | 4.0 |
| 67 | S | 126 | ALA | 4.0 |
| 60 | c0 | 95 | ARG | 3.9 |
| 39 | AK | 84 | SER | 3.9 |
| 55 | G | 150 | GLY | 3.9 |
| 62 | c2 | 111 | ASN | 3.9 |
| 75 | a | 60 | VAL | 3.9 |
| 26 | 7 | 79 | GLN | 3.9 |
| 62 | N | 110 | GLY | 3.9 |
| 82 | h | 262 | VAL | 3.9 |
| 51 | C | 38 | PHE | 3.9 |
| 77 | d7 | 62 | ILE | 3.9 |
| 1 | AR | 2441 | A | 3.9 |
| 40 | DM | 72 | THR | 3.9 |
| 51 | C | 25 | THR | 3.9 |
| 69 | c9 | 19 | ALA | 3.9 |
| 46 | i | 17 | VAL | 3.9 |
| 25 | 6 | 487 | G | 3.9 |
| 70 | d0 | 17 | GLN | 3.9 |
| 60 | c0 | 49 | LEU | 3.9 |
| 21 | 0 | 1 | MET | 3.9 |
| 1 | AR | 1580 | A | 3.9 |
| 25 | 6 | 1255 | G | 3.9 |
| 25 | 6 | 712 | G | 3.9 |
| 25 | 6 | 1700 | C | 3.9 |
| 54 | s4 | 261 | LEU | 3.9 |
| 82 | h | 315 | VAL | 3.9 |
| 71 | d1 | 43 | GLY | 3.9 |
| 55 | G | 181 | GLU | 3.9 |
| 60 | c0 | 42 | VAL | 3.8 |
| 67 | S | 86 | PRO | 3.8 |
| 62 | N | 78 | LEU | 3.8 |
| 25 | A | 195 | G | 3.8 |
| 18 | x | 181 | ARG | 3.8 |
| 70 | d0 | 18 | GLN | 3.8 |
| 10 | CJ | 250 | ALA | 3.8 |
| 55 | s5 | 154 | ALA | 3.8 |
| 1 | 1 | 1271 | A | 3.8 |
| 82 | h | 263 | PHE | 3.8 |
| 49 | p0 | 292 | GLU | 3.8 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 65 | c5 | 134 | THR | 3.8 |
| 62 | N | 28 | LEU | 3.8 |
| 64 | P | 41 | ARG | 3.8 |
| 20 | CT | 175 | GLN | 3.8 |
| 29 | AA | 106 | GLN | 3.8 |
| 62 | N | 20 | ALA | 3.8 |
| 66 | c6 | 4 | VAL | 3.8 |
| 83 | e1 | 106 | TYR | 3.8 |
| 54 | F | 143 | ASP | 3.8 |
| 62 | N | 63 | VAL | 3.8 |
| 56 | s6 | 164 | LYS | 3.8 |
| 68 | c8 | 18 | LEU | 3.8 |
| 25 | A | 228 | G | 3.8 |
| 46 | i | 273 | THR | 3.8 |
| 59 | K | 182 | GLU | 3.8 |
| 69 | U | 5 | SER | 3.8 |
| 10 | CJ | 122 | LYS | 3.8 |
| 25 | 6 | 75 | U | 3.8 |
| 25 | 6 | 1710 | U | 3.8 |
| 51 | C | 59 | ASP | 3.8 |
| 55 | G | 210 | ALA | 3.8 |
| 1 | 1 | 3154 | C | 3.8 |
| 20 | CT | 183 | ALA | 3.8 |
| 25 | A | 899 | G | 3.8 |
| 62 | c2 | 72 | ILE | 3.8 |
| 7 | m | 124 | GLU | 3.7 |
| 49 | p0 | 284 | ALA | 3.7 |
| 62 | c2 | 102 | GLY | 3.7 |
| 23 | 5 | 108 | TYR | 3.7 |
| 62 | c2 | 62 | LEU | 3.7 |
| 10 | CJ | 249 | ARG | 3.7 |
| 55 | s5 | 61 | TYR | 3.7 |
| 60 | L | 12 | HIS | 3.7 |
| 1 | AR | 546 | C | 3.7 |
| 62 | N | 32 | LEU | 3.7 |
| 48 | sM | 85 | SER | 3.7 |
| 1 | AR | 2538 | U | 3.7 |
| 26 | 7 | 67 | VAL | 3.7 |
| 10 | p | 121 | SER | 3.7 |
| 51 | C | 130 | SER | 3.7 |
| 53 | s3 | 44 | THR | 3.7 |
| 68 | c8 | 17 | LEU | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 57 | s7 | 90 | VAL | 3.7 |
| 60 | c0 | 73 | VAL | 3.7 |
| 1 | AR | 1568 | U | 3.7 |
| 25 | 6 | 1692 | G | 3.7 |
| 62 | c2 | 124 | LYS | 3.7 |
| 68 | T | 44 | ASN | 3.7 |
| 23 | CW | 97 | SER | 3.7 |
| 62 | c2 | 23 | THR | 3.7 |
| 81 | g | 87 | THR | 3.7 |
| 51 | C | 29 | TRP | 3.7 |
| 1 | AR | 1352 | A | 3.7 |
| 1 | 1 | 1576 | G | 3.7 |
| 68 | T | 6 | GLN | 3.7 |
| 81 | g | 105 | TYR | 3.7 |
| 1 | 1 | 1259 | A | 3.7 |
| 25 | 6 | 1693 | A | 3.7 |
| 53 | E | 179 | GLN | 3.7 |
| 55 | G | 37 | GLN | 3.7 |
| 62 | c2 | 122 | VAL | 3.7 |
| 46 | i | 15 | ALA | 3.7 |
| 57 | s7 | 3 | ALA | 3.7 |
| 61 | c1 | 145 | ALA | 3.7 |
| 62 | N | 85 | LYS | 3.7 |
| 25 | 6 | 675 | U | 3.7 |
| 20 | z | 187 | GLU | 3.7 |
| 7 | m | 131 | LEU | 3.7 |
| 82 | sR | 191 | ASP | 3.7 |
| 14 | CN | 131 | LYS | 3.7 |
| 51 | C | 94 | LYS | 3.7 |
| 25 | 6 | 1699 | G | 3.7 |
| 60 | c0 | 54 | TYR | 3.7 |
| 62 | N | 91 | VAL | 3.7 |
| 75 | a | 38 | HIS | 3.7 |
| 7 | m | 297 | GLN | 3.7 |
| 56 | H | 217 | SER | 3.7 |
| 63 | O | 61 | THR | 3.7 |
| 62 | c2 | 120 | VAL | 3.7 |
| 68 | T | 22 | VAL | 3.7 |
| 25 | 6 | 727 | U | 3.6 |
| 10 | p | 115 | ALA | 3.6 |
| 59 | K | 184 | SER | 3.6 |
| 77 | c | 32 | PHE | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | AR | 1016 | C | 3.6 |
| 7 | m | 295 | GLY | 3.6 |
| 25 | 6 | 1059 | U | 3.6 |
| 78 | d8 | 31 | GLU | 3.6 |
| 1 | AR | 1562 | C | 3.6 |
| 1 | AR | 2546 | C | 3.6 |
| 51 | C | 207 | LEU | 3.6 |
| 56 | H | 147 | LEU | 3.6 |
| 39 | AK | 86 | ALA | 3.6 |
| 25 | 6 | 1257 | U | 3.6 |
| 1 | AR | 2442 | G | 3.6 |
| 18 | x | 180 | LYS | 3.6 |
| 29 | AA | 109 | GLU | 3.6 |
| 25 | A | 1060 | U | 3.6 |
| 53 | E | 88 | ALA | 3.6 |
| 29 | AA | 94 | SER | 3.6 |
| 62 | N | 66 | VAL | 3.6 |
| 14 | CN | 129 | ASN | 3.6 |
| 1 | 1 | 1566 | A | 3.6 |
| 62 | N | 52 | LEU | 3.6 |
| 26 | 7 | 78 | ALA | 3.6 |
| 29 | AA | 2 | ALA | 3.6 |
| 25 | A | 182 | A | 3.6 |
| 25 | A | 488 | G | 3.6 |
| 53 | s3 | 175 | VAL | 3.6 |
| 62 | N | 112 | ALA | 3.6 |
| 49 | p0 | 50 | VAL | 3.6 |
| 49 | p0 | 293 | GLU | 3.6 |
| 50 | B | 198 | MET | 3.6 |
| 57 | s7 | 2 | SER | 3.6 |
| 81 | g | 93 | HIS | 3.6 |
| 25 | A | 232 | U | 3.6 |
| 25 | A | 196 | G | 3.6 |
| 75 | a | 42 | LEU | 3.6 |
| 11 | CK | 189 | GLU | 3.6 |
| 18 | x | 176 | ILE | 3.6 |
| 62 | c2 | 94 | ALA | 3.6 |
| 67 | S | 125 | SER | 3.6 |
| 56 | s6 | 165 | GLY | 3.6 |
| 80 | f | 49 | LEU | 3.6 |
| 1 | AR | 2545 | C | 3.6 |
| 25 | 6 | 710 | U | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | 1 | 1577 | G | 3.6 |
| 1 | AR | 1349 | G | 3.6 |
| 1 | AR | 2440 | G | 3.6 |
| 14 | CN | 93 | ILE | 3.6 |
| 25 | A | 201 | G | 3.6 |
| 50 | B | 39 | ASN | 3.6 |
| 67 | c7 | 104 | ASN | 3.6 |
| 77 | d7 | 57 | GLU | 3.6 |
| 80 | e0 | 50 | VAL | 3.6 |
| 50 | B | 196 | SER | 3.6 |
| 83 | e1 | 111 | GLU | 3.5 |
| 53 | E | 218 | LEU | 3.5 |
| 82 | h | 296 | ALA | 3.5 |
| 25 | 6 | 493 | U | 3.5 |
| 62 | c2 | 117 | GLY | 3.5 |
| 62 | N | 109 | GLU | 3.5 |
| 56 | s6 | 215 | ARG | 3.5 |
| 14 | CN | 95 | ILE | 3.5 |
| 53 | s3 | 71 | LEU | 3.5 |
| 81 | g | 129 | GLY | 3.5 |
| 7 | m | 117 | GLU | 3.5 |
| 51 | C | 31 | ASP | 3.5 |
| 10 | p | 116 | VAL | 3.5 |
| 58 | s8 | 123 | LYS | 3.5 |
| 82 | h | 314 | GLN | 3.5 |
| 66 | R | 3 | ALA | 3.5 |
| 76 | d6 | 45 | VAL | 3.5 |
| 59 | K | 178 | ALA | 3.5 |
| 69 | U | 50 | ALA | 3.5 |
| 18 | x | 166 | VAL | 3.5 |
| 51 | s1 | 89 | ASP | 3.5 |
| 23 | CW | 14 | THR | 3.5 |
| 29 | AA | 100 | THR | 3.5 |
| 75 | a | 44 | GLN | 3.5 |
| 49 | p0 | 191 | TYR | 3.5 |
| 79 | d9 | 23 | VAL | 3.5 |
| 64 | P | 80 | HIS | 3.5 |
| 29 | AA | 92 | PHE | 3.5 |
| 50 | B | 97 | PRO | 3.5 |
| 82 | h | 261 | LYS | 3.5 |
| 1 | AR | 544 | C | 3.5 |
| 23 | 5 | 27 | VAL | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 68 | T | 5 | VAL | 3.5 |
| 1 | 1 | 1572 | U | 3.5 |
| 60 | c0 | 78 | GLU | 3.5 |
| 64 | P | 79 | VAL | 3.5 |
| 46 | i | 274 | LYS | 3.5 |
| 1 | 1 | 1764 | U | 3.5 |
| 1 | 1 | 2570 | U | 3.5 |
| 1 | AR | 2443 | A | 3.5 |
| 61 | M | 144 | ALA | 3.5 |
| 56 | H | 12 | SER | 3.5 |
| 62 | N | 68 | GLU | 3.5 |
| 51 | C | 32 | ILE | 3.5 |
| 54 | F | 261 | LEU | 3.5 |
| 68 | c8 | 14 | ILE | 3.5 |
| 10 | CJ | 255 | SER | 3.4 |
| 57 | I | 78 | THR | 3.4 |
| 64 | P | 14 | PHE | 3.4 |
| 56 | H | 41 | VAL | 3.4 |
| 81 | g | 109 | ASP | 3.4 |
| 40 | DM | 74 | LYS | 3.4 |
| 62 | c2 | 85 | LYS | 3.4 |
| 64 | P | 33 | LEU | 3.4 |
| 77 | d7 | 82 | LYS | 3.4 |
| 77 | d7 | 58 | SER | 3.4 |
| 20 | z | 188 | ASP | 3.4 |
| 50 | B | 199 | PRO | 3.4 |
| 53 | s3 | 42 | THR | 3.4 |
| 77 | c | 45 | THR | 3.4 |
| 58 | s8 | 200 | LYS | 3.4 |
| 59 | s9 | 93 | LEU | 3.4 |
| 65 | c5 | 136 | SER | 3.4 |
| 51 | C | 97 | LEU | 3.4 |
| 60 | c0 | 46 | LEU | 3.4 |
| 50 | B | 166 | GLY | 3.4 |
| 55 | s5 | 92 | ARG | 3.4 |
| 51 | C | 217 | LEU | 3.4 |
| 60 | L | 66 | TYR | 3.4 |
| 18 | CR | 181 | ARG | 3.4 |
| 56 | H | 50 | PHE | 3.4 |
| 25 | A | 1691 | A | 3.4 |
| 62 | c2 | 79 | ALA | 3.4 |
| 74 | Z | 34 | ASN | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 29 | AA | 105 | SER | 3.4 |
| 32 | AD | 35 | ARG | 3.4 |
| 25 | A | 192 | U | 3.4 |
| 25 | 6 | 228 | G | 3.4 |
| 1 | 1 | 1248 | C | 3.4 |
| 60 | c0 | 1 | MET | 3.4 |
| 83 | e1 | 109 | ASP | 3.4 |
| 78 | d | 44 | VAL | 3.4 |
| 65 | c5 | 51 | SER | 3.4 |
| 74 | d4 | 2 | SER | 3.4 |
| 25 | A | 1058 | U | 3.4 |
| 58 | s8 | 199 | LYS | 3.4 |
| 83 | e1 | 143 | LYS | 3.4 |
| 23 | CW | 44 | GLU | 3.4 |
| 23 | 5 | 10 | LYS | 3.4 |
| 3 | 4 | 82 | U | 3.4 |
| 25 | A | 240 | U | 3.4 |
| 29 | AA | 70 | PRO | 3.4 |
| 51 | s1 | 54 | LEU | 3.4 |
| 52 | s2 | 92 | ALA | 3.4 |
| 62 | c2 | 27 | ALA | 3.4 |
| 66 | c6 | 142 | TYR | 3.4 |
| 81 | g | 85 | TYR | 3.4 |
| 75 | d5 | 86 | GLU | 3.4 |
| 62 | c2 | 86 | VAL | 3.3 |
| 69 | U | 108 | LEU | 3.3 |
| 82 | h | 221 | MET | 3.4 |
| 82 | h | 252 | LEU | 3.3 |
| 18 | x | 177 | ALA | 3.3 |
| 37 | DJ | 2 | ALA | 3.3 |
| 55 | s5 | 35 | GLN | 3.3 |
| 51 | s1 | 97 | LEU | 3.3 |
| 62 | N | 71 | ILE | 3.3 |
| 62 | c2 | 89 | ILE | 3.3 |
| 82 | h | 313 | TRP | 3.3 |
| 1 | 1 | 1269 | U | 3.3 |
| 74 | Z | 133 | ASN | 3.3 |
| 18 | x | 165 | VAL | 3.3 |
| 71 | d1 | 39 | VAL | 3.3 |
| 53 | E | 183 | GLY | 3.3 |
| 28 | DA | 126 | LEU | 3.3 |
| 64 | P | 11 | SER | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 26 | 7 | 71 | ARG | 3.3 |
| 12 | CL | 186 | GLU | 3.3 |
| 77 | d7 | 38 | PRO | 3.3 |
| 82 | sR | 314 | GLN | 3.3 |
| 51 | C | 42 | ASN | 3.3 |
| 1 | AR | 1350 | A | 3.3 |
| 25 | 6 | 719 | U | 3.3 |
| 25 | A | 912 | U | 3.3 |
| 82 | h | 248 | ASN | 3.3 |
| 25 | 6 | 1221 | A | 3.3 |
| 25 | A | 713 | A | 3.3 |
| 59 | K | 180 | LYS | 3.3 |
| 25 | 6 | 484 | C | 3.3 |
| 25 | 6 | 495 | C | 3.3 |
| 25 | A | 231 | U | 3.3 |
| 29 | AA | 108 | GLU | 3.3 |
| 51 | C | 40 | ASN | 3.3 |
| 82 | h | 254 | ALA | 3.3 |
| 74 | Z | 67 | GLY | 3.3 |
| 78 | d8 | 66 | LEU | 3.3 |
| 20 | z | 177 | VAL | 3.3 |
| 62 | N | 94 | ALA | 3.3 |
| 1 | AR | 250 | U | 3.3 |
| 81 | g | 143 | LYS | 3.3 |
| 62 | c2 | 126 | TRP | 3.3 |
| 83 | e1 | 108 | VAL | 3.3 |
| 25 | 6 | 483 | A | 3.3 |
| 25 | A | 1712 | A | 3.3 |
| 25 | 6 | 655 | G | 3.3 |
| 68 | c8 | 15 | LEU | 3.3 |
| 66 | c6 | 19 | VAL | 3.3 |
| 81 | g | 124 | PRO | 3.3 |
| 49 | p0 | 280 | ALA | 3.3 |
| 69 | c9 | 55 | TYR | 3.3 |
| 57 | I | 89 | HIS | 3.3 |
| 1 | AR | 3157 | U | 3.3 |
| 37 | AI | 13 | SER | 3.3 |
| 66 | R | 26 | LYS | 3.3 |
| 51 | C | 26 | ARG | 3.3 |
| 9 | o | 27 | ALA | 3.3 |
| 57 | I | 52 | ALA | 3.3 |
| 62 | N | 40 | GLY | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 51 | C | 45 | LYS | 3.3 |
| 1 | 1 | 1270 | A | 3.2 |
| 7 | m | 126 | GLU | 3.2 |
| 60 | c0 | 74 | GLU | 3.2 |
| 75 | d5 | 89 | ILE | 3.2 |
| 25 | A | 730 | G | 3.2 |
| 65 | c5 | 133 | ALA | 3.2 |
| 62 | N | 74 | LEU | 3.2 |
| 82 | h | 71 | CYS | 3.2 |
| 32 | AD | 83 | LYS | 3.2 |
| 81 | g | 107 | LYS | 3.2 |
| 25 | 6 | 241 | U | 3.2 |
| 25 | 6 | 1226 | A | 3.2 |
| 26 | 7 | 91 | LYS | 3.2 |
| 27 | CZ | 22 | LYS | 3.2 |
| 60 | c0 | 41 | TYR | 3.2 |
| 62 | N | 73 | LYS | 3.2 |
| 25 | 6 | 224 | C | 3.2 |
| 55 | s5 | 30 | PRO | 3.2 |
| 58 | J | 136 | SER | 3.2 |
| 58 | s8 | 148 | ALA | 3.2 |
| 64 | P | 78 | ALA | 3.2 |
| 29 | AA | 18 | TYR | 3.2 |
| 25 | A | 1681 | A | 3.2 |
| 55 | G | 161 | ASP | 3.2 |
| 55 | s5 | 145 | ASP | 3.2 |
| 67 | c7 | 87 | GLU | 3.2 |
| 60 | c0 | 44 | LYS | 3.2 |
| 62 | c2 | 96 | GLN | 3.2 |
| 71 | W | 34 | ILE | 3.2 |
| 49 | p0 | 296 | ALA | 3.2 |
| 67 | S | 123 | ASN | 3.2 |
| 18 | x | 157 | VAL | 3.2 |
| 77 | d7 | 77 | THR | 3.2 |
| 25 | 6 | 1231 | U | 3.2 |
| 25 | 6 | 1708 | U | 3.2 |
| 68 | T | 17 | LEU | 3.2 |
| 82 | h | 81 | LEU | 3.2 |
| 59 | K | 141 | VAL | 3.2 |
| 78 | d | 7 | VAL | 3.2 |
| 29 | DB | 56 | LYS | 3.2 |
| 57 | I | 108 | GLN | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 65 | Q | 12 | PHE | 3.2 |
| 82 | sR | 303 | ALA | 3.2 |
| 25 | 6 | 490 | C | 3.2 |
| 56 | s6 | 218 | GLU | 3.2 |
| 1 | AR | 245 | U | 3.2 |
| 1 | AR | 2571 | U | 3.2 |
| 25 | A | 193 | U | 3.2 |
| 51 | C | 233 | GLY | 3.2 |
| 61 | c1 | 147 | GLY | 3.2 |
| 10 | CJ | 114 | ALA | 3.2 |
| 64 | P | 13 | VAL | 3.2 |
| 64 | P | 20 | TYR | 3.2 |
| 81 | g | 102 | VAL | 3.2 |
| 80 | e0 | 61 | SER | 3.2 |
| 8 | CH | 130 | ILE | 3.2 |
| 51 | C | 37 | THR | 3.2 |
| 66 | R | 57 | LEU | 3.2 |
| 71 | W | 69 | LEU | 3.2 |
| 11 | CK | 190 | ASP | 3.2 |
| 50 | B | 175 | TYR | 3.2 |
| 1 | 1 | 1237 | G | 3.2 |
| 18 | CR | 173 | ARG | 3.2 |
| 25 | 6 | 1712 | A | 3.2 |
| 50 | s0 | 24 | LEU | 3.2 |
| 59 | s9 | 128 | LEU | 3.2 |
| 62 | c2 | 38 | HIS | 3.2 |
| 68 | T | 23 | ASP | 3.2 |
| 7 | m | 123 | GLU | 3.2 |
| 17 | CQ | 182 | ASN | 3.2 |
| 25 | 6 | 1696 | G | 3.2 |
| 4 | CD | 252 | THR | 3.2 |
| 10 | CJ | 116 | VAL | 3.2 |
| 53 | s3 | 177 | MET | 3.2 |
| 56 | H | 156 | PHE | 3.2 |
| 66 | c6 | 46 | PHE | 3.2 |
| 9 | CI | 25 | GLN | 3.2 |
| 49 | p0 | 285 | SER | 3.2 |
| 62 | c2 | 143 | GLN | 3.2 |
| 69 | c9 | 5 | SER | 3.2 |
| 51 | C | 85 | LYS | 3.1 |
| 53 | s3 | 217 | ILE | 3.1 |
| 65 | Q | 10 | ARG | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 50 | B | 50 | VAL | 3.1 |
| 64 | P | 42 | VAL | 3.1 |
| 67 | c7 | 88 | VAL | 3.1 |
| 51 | C | 56 | SER | 3.1 |
| 75 | a | 98 | GLN | 3.1 |
| 57 | s7 | 58 | LEU | 3.1 |
| 25 | 6 | 238 | U | 3.1 |
| 25 | A | 1370 | U | 3.1 |
| 60 | c0 | 20 | VAL | 3.1 |
| 60 | c0 | 94 | GLU | 3.1 |
| 23 | CW | 52 | ASN | 3.1 |
| 62 | c2 | 44 | GLY | 3.1 |
| 8 | CH | 129 | GLU | 3.1 |
| 1 | AR | 251 | G | 3.1 |
| 69 | c9 | 66 | TYR | 3.1 |
| 10 | CJ | 256 | ALA | 3.1 |
| 49 | p0 | 288 | ALA | 3.1 |
| 1 | AR | 246 | U | 3.1 |
| 5 | k | 387 | LEU | 3.1 |
| 25 | A | 230 | C | 3.1 |
| 56 | s6 | 212 | LEU | 3.1 |
| 39 | DL | 86 | ALA | 3.1 |
| 66 | R | 29 | ILE | 3.1 |
| 66 | c6 | 36 | ILE | 3.1 |
| 59 | s9 | 184 | SER | 3.1 |
| 74 | d4 | 133 | ASN | 3.1 |
| 1 | 1 | 439 | C | 3.1 |
| 1 | 1 | 1574 | C | 3.1 |
| 1 | AR | 1563 | C | 3.1 |
| 1 | AR | 2572 | C | 3.1 |
| 81 | g | 145 | HIS | 3.1 |
| 51 | C | 221 | PRO | 3.1 |
| 62 | c2 | 132 | GLU | 3.1 |
| 82 | h | 74 | THR | 3.1 |
| 25 | A | 729 | G | 3.1 |
| 55 | s5 | 36 | ALA | 3.1 |
| 7 | CG | 5 | LYS | 3.1 |
| 82 | sR | 52 | GLN | 3.1 |
| 57 | s7 | 60 | ILE | 3.1 |
| 26 | CY | 98 | PRO | 3.1 |
| 62 | N | 48 | SER | 3.1 |
| 54 | F | 168 | LYS | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 56 | H | 221 | ALA | 3.1 |
| 57 | s7 | 72 | LYS | 3.1 |
| 62 | c2 | 73 | LYS | 3.1 |
| 9 | o | 25 | GLN | 3.1 |
| 54 | F | 252 | ARG | 3.1 |
| 7 | CG | 291 | ALA | 3.1 |
| 40 | DM | 29 | LYS | 3.1 |
| 51 | C | 227 | ALA | 3.1 |
| 1 | 1 | 1761 | C | 3.1 |
| 25 | A | 188 | A | 3.1 |
| 54 | F | 255 | ARG | 3.1 |
| 64 | P | 83 | ILE | 3.1 |
| 75 | a | 41 | ILE | 3.1 |
| 51 | C | 28 | GLU | 3.1 |
| 53 | s3 | 148 | LYS | 3.1 |
| 62 | c2 | 90 | LYS | 3.1 |
| 81 | g | 151 | ASN | 3.1 |
| 20 | CT | 176 | ARG | 3.1 |
| 82 | h | 294 | TRP | 3.1 |
| 60 | c0 | 47 | GLN | 3.1 |
| 62 | N | 89 | ILE | 3.1 |
| 74 | d4 | 67 | GLY | 3.1 |
| 29 | AA | 96 | VAL | 3.1 |
| 10 | p | 152 | LEU | 3.1 |
| 29 | AA | 91 | ALA | 3.1 |
| 82 | h | 33 | LEU | 3.1 |
| 83 | e1 | 110 | ALA | 3.1 |
| 50 | B | 54 | TRP | 3.1 |
| 64 | P | 43 | THR | 3.1 |
| 69 | c9 | 112 | GLY | 3.1 |
| 77 | c | 44 | THR | 3.1 |
| 29 | AA | 114 | VAL | 3.1 |
| 59 | K | 87 | SER | 3.0 |
| 83 | e1 | 134 | ASN | 3.0 |
| 10 | p | 202 | GLU | 3.0 |
| 56 | s6 | 162 | VAL | 3.0 |
| 64 | P | 102 | LEU | 3.0 |
| 59 | K | 164 | PHE | 3.0 |
| 62 | c2 | 128 | ALA | 3.0 |
| 63 | O | 15 | ALA | 3.0 |
| 82 | h | 36 | ALA | 3.0 |
| 1 | 1 | 1272 | C | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 25 | 6 | 489 | C | 3.0 |
| 62 | N | 119 | SER | 3.0 |
| 25 | 6 | 1491 | U | 3.0 |
| 29 | DB | 75 | VAL | 3.0 |
| 58 | s8 | 141 | ARG | 3.0 |
| 68 | c8 | 32 | LEU | 3.0 |
| 51 | C | 223 | PHE | 3.0 |
| 54 | F | 133 | LYS | 3.0 |
| 69 | U | 21 | PHE | 3.0 |
| 68 | c8 | 53 | ASP | 3.0 |
| 23 | CW | 68 | THR | 3.0 |
| 42 | AN | 108 | THR | 3.0 |
| 50 | B | 24 | LEU | 3.0 |
| 56 | s6 | 168 | THR | 3.0 |
| 71 | W | 53 | TYR | 3.0 |
| 25 | A | 845 | G | 3.0 |
| 40 | DM | 73 | LEU | 3.0 |
| 1 | 1 | 1580 | A | 3.0 |
| 69 | U | 6 | VAL | 3.0 |
| 64 | P | 99 | GLN | 3.0 |
| 82 | h | 283 | LYS | 3.0 |
| 62 | c2 | 39 | ASP | 3.0 |
| 1 | 1 | 1277 | C | 3.0 |
| 1 | AR | 1354 | G | 3.0 |
| 25 | 6 | 227 | U | 3.0 |
| 29 | DB | 74 | VAL | 3.0 |
| 69 | c9 | 131 | ASP | 3.0 |
| 9 | CI | 27 | ALA | 3.0 |
| 55 | s5 | 68 | ILE | 3.0 |
| 1 | 1 | 2538 | U | 3.0 |
| 1 | AR | 545 | U | 3.0 |
| 25 | A | 191 | C | 3.0 |
| 28 | DA | 120 | GLN | 3.0 |
| 56 | s6 | 216 | LEU | 3.0 |
| 82 | sR | 252 | LEU | 3.0 |
| 56 | H | 27 | PHE | 3.0 |
| 29 | AA | 93 | LYS | 3.0 |
| 55 | G | 36 | ALA | 3.0 |
| 82 | h | 295 | SER | 3.0 |
| 66 | R | 96 | TYR | 3.0 |
| 64 | P | 93 | THR | 3.0 |
| 4 | CD | 253 | GLN | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | AR | 1816 | A | 3.0 |
| 25 | 6 | 1223 | A | 3.0 |
| 1 | 1 | 547 | G | 3.0 |
| 23 | CW | 53 | ALA | 3.0 |
| 25 | A | 1229 | G | 3.0 |
| 27 | CZ | 23 | ALA | 3.0 |
| 64 | c4 | 45 | GLY | 3.0 |
| 54 | F | 138 | TYR | 3.0 |
| 55 | s5 | 78 | ALA | 3.0 |
| 66 | c6 | 64 | ASP | 3.0 |
| 68 | c8 | 5 | VAL | 3.0 |
| 23 | 5 | 80 | THR | 3.0 |
| 1 | 1 | 1815 | U | 3.0 |
| 3 | 4 | 158 | U | 3.0 |
| 7 | m | 119 | TYR | 3.0 |
| 57 | s7 | 162 | ILE | 3.0 |
| 40 | DM | 45 | VAL | 3.0 |
| 49 | p0 | 190 | VAL | 3.0 |
| 68 | c8 | 22 | VAL | 3.0 |
| 25 | A | 1713 | G | 3.0 |
| 51 | C | 39 | GLU | 3.0 |
| 66 | R | 56 | GLY | 3.0 |
| 55 | s5 | 148 | ARG | 3.0 |
| 1 | 1 | 1260 | A | 3.0 |
| 51 | C | 36 | SER | 3.0 |
| 51 | C | 74 | GLN | 3.0 |
| 75 | d5 | 44 | GLN | 3.0 |
| 1 | 1 | 1261 | G | 2.9 |
| 51 | C | 44 | GLY | 2.9 |
| 29 | AA | 26 | VAL | 2.9 |
| 46 | i | 19 | VAL | 2.9 |
| 10 | CJ | 245 | LYS | 2.9 |
| 61 | c1 | 5 | LEU | 2.9 |
| 62 | c2 | 133 | LEU | 2.9 |
| 12 | r | 209 | ASN | 2.9 |
| 12 | CL | 209 | ASN | 2.9 |
| 25 | A | 189 | C | 2.9 |
| 57 | s7 | 52 | ALA | 2.9 |
| 81 | g | 100 | LEU | 2.9 |
| 82 | h | 32 | LEU | 2.9 |
| 12 | CL | 213 | PHE | 2.9 |
| 36 | AH | 73 | SER | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 56 | H | 80 | ASN | 2.9 |
| 3 | AT | 83 | C | 2.9 |
| 25 | A | 696 | C | 2.9 |
| 83 | e1 | 135 | HIS | 2.9 |
| 1 | 1 | 1240 | A | 2.9 |
| 58 | s8 | 139 | ALA | 2.9 |
| 82 | h | 78 | ALA | 2.9 |
| 78 | d8 | 64 | ARG | 2.9 |
| 1 | AR | 547 | G | 2.9 |
| 25 | 6 | 677 | G | 2.9 |
| 75 | d5 | 52 | LYS | 2.9 |
| 25 | 6 | 726 | C | 2.9 |
| 34 | AF | 2 | ALA | 2.9 |
| 65 | c5 | 128 | HIS | 2.9 |
| 71 | W | 54 | ALA | 2.9 |
| 74 | Z | 129 | VAL | 2.9 |
| 75 | a | 82 | HIS | 2.9 |
| 25 | 6 | 1285 | U | 2.9 |
| 78 | d | 26 | THR | 2.9 |
| 80 | f | 54 | ARG | 2.9 |
| 1 | AR | 543 | C | 2.9 |
| 25 | 6 | 1220 | C | 2.9 |
| 69 | U | 72 | GLY | 2.9 |
| 1 | AR | 249 | U | 2.9 |
| 29 | AA | 42 | LEU | 2.9 |
| 50 | B | 9 | LEU | 2.9 |
| 38 | DK | 27 | SER | 2.9 |
| 60 | c0 | 51 | SER | 2.9 |
| 66 | R | 143 | ARG | 2.9 |
| 69 | c9 | 18 | TYR | 2.9 |
| 60 | c0 | 56 | LYS | 2.9 |
| 62 | N | 47 | GLU | 2.9 |
| 1 | 1 | 1759 | C | 2.9 |
| 51 | s1 | 53 | GLY | 2.9 |
| 29 | AA | 80 | LEU | 2.9 |
| 32 | AD | 24 | THR | 2.9 |
| 14 | CN | 182 | ILE | 2.9 |
| 23 | CW | 105 | LEU | 2.9 |
| 62 | N | 88 | LEU | 2.9 |
| 67 | S | 85 | VAL | 2.9 |
| 53 | s3 | 151 | LYS | 2.9 |
| 54 | F | 134 | LYS | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 54 | s4 | 134 | LYS | 2.9 |
| 1 | 1 | 1256 | G | 2.9 |
| 25 | 6 | 1217 | A | 2.9 |
| 78 | d | 43 | ASN | 2.9 |
| 81 | g | 134 | ASN | 2.9 |
| 49 | p0 | 64 | ARG | 2.9 |
| 50 | B | 41 | ARG | 2.9 |
| 62 | c2 | 77 | GLY | 2.9 |
| 66 | c6 | 114 | ARG | 2.9 |
| 78 | d8 | 8 | THR | 2.9 |
| 56 | H | 212 | LEU | 2.9 |
| 75 | d5 | 50 | ILE | 2.9 |
| 53 | s3 | 107 | PHE | 2.9 |
| 58 | J | 148 | ALA | 2.9 |
| 1 | AR | 1028 | U | 2.9 |
| 59 | s9 | 185 | GLY | 2.9 |
| 53 | s3 | 184 | ILE | 2.9 |
| 56 | H | 153 | VAL | 2.9 |
| 66 | R | 63 | ILE | 2.9 |
| 78 | d8 | 9 | LEU | 2.9 |
| 62 | c2 | 101 | ALA | 2.9 |
| 70 | d0 | 14 | GLN | 2.9 |
| 51 | C | 89 | ASP | 2.9 |
| 25 | A | 184 | C | 2.9 |
| 64 | P | 34 | SER | 2.9 |
| 25 | 6 | 192 | U | 2.9 |
| 25 | A | 137 | U | 2.9 |
| 42 | DO | 77 | ILE | 2.9 |
| 62 | N | 86 | VAL | 2.9 |
| 77 | d7 | 37 | CYS | 2.9 |
| 49 | p0 | 290 | PRO | 2.9 |
| 82 | sR | 301 | LEU | 2.9 |
| 24 | lR | 4 | ASN | 2.8 |
| 1 | 1 | 1763 | U | 2.8 |
| 18 | CR | 156 | ALA | 2.8 |
| 53 | E | 148 | LYS | 2.8 |
| 83 | e1 | 105 | TYR | 2.8 |
| 49 | p0 | 287 | ASP | 2.8 |
| 20 | CT | 185 | LEU | 2.8 |
| 25 | 6 | 722 | G | 2.8 |
| 25 | 6 | 829 | A | 2.8 |
| 54 | s4 | 131 | LEU | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 57 | I | 77 | LEU | 2.8 |
| 59 | K | 116 | LEU | 2.8 |
| 82 | sR | 49 | GLY | 2.8 |
| 51 | C | 35 | PRO | 2.8 |
| 68 | T | 58 | ALA | 2.8 |
| 1 | AR | 3153 | U | 2.8 |
| 25 | A | 921 | U | 2.8 |
| 40 | DM | 69 | LEU | 2.8 |
| 75 | d5 | 87 | GLY | 2.8 |
| 51 | C | 66 | VAL | 2.8 |
| 12 | r | 217 | PHE | 2.8 |
| 29 | AA | 69 | LYS | 2.8 |
| 55 | s5 | 20 | PHE | 2.8 |
| 60 | c0 | 45 | ALA | 2.8 |
| 1 | AR | 3155 | U | 2.8 |
| 50 | B | 18 | LEU | 2.8 |
| 53 | s3 | 150 | MET | 2.8 |
| 68 | T | 11 | PHE | 2.8 |
| 7 | CG | 294 | ALA | 2.8 |
| 23 | CW | 106 | ALA | 2.8 |
| 29 | AA | 35 | SER | 2.8 |
| 65 | Q | 101 | ALA | 2.8 |
| 82 | h | 319 | ASN | 2.8 |
| 7 | m | 236 | LEU | 2.8 |
| 57 | I | 165 | LYS | 2.8 |
| 67 | S | 110 | VAL | 2.8 |
| 24 | CX | 4 | ASN | 2.8 |
| 69 | c9 | 127 | ASN | 2.8 |
| 82 | h | 34 | LEU | 2.8 |
| 49 | p0 | 196 | VAL | 2.8 |
| 53 | s3 | 152 | PHE | 2.8 |
| 82 | h | 211 | ILE | 2.8 |
| 1 | 1 | 2095 | G | 2.8 |
| 3 | AT | 158 | U | 2.8 |
| 38 | DK | 100 | HIS | 2.8 |
| 57 | I | 80 | GLU | 2.8 |
| 34 | DG | 2 | ALA | 2.8 |
| 77 | c | 37 | CYS | 2.8 |
| 78 | d8 | 24 | GLY | 2.8 |
| 75 | d5 | 60 | VAL | 2.8 |
| 1 | AR | 1814 | A | 2.8 |
| 25 | 6 | 1058 | U | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 25 | A | 657 | U | 2.8 |
| 62 | c2 | 57 | ALA | 2.8 |
| 69 | c9 | 130 | ARG | 2.8 |
| 34 | DG | 128 | LEU | 2.8 |
| 53 | s3 | 182 | LEU | 2.8 |
| 54 | F | 123 | LEU | 2.8 |
| 82 | h | 305 | TYR | 2.8 |
| 1 | 1 | 1234 | G | 2.8 |
| 57 | I | 86 | GLN | 2.8 |
| 18 | x | 182 | ILE | 2.8 |
| 23 | 5 | 11 | ILE | 2.8 |
| 25 | A | 491 | C | 2.8 |
| 40 | AL | 5 | ILE | 2.8 |
| 59 | s9 | 148 | VAL | 2.8 |
| 60 | c0 | 22 | VAL | 2.8 |
| 75 | d5 | 51 | LEU | 2.8 |
| 51 | C | 220 | GLN | 2.8 |
| 66 | R | 22 | VAL | 2.8 |
| 81 | g | 130 | VAL | 2.8 |
| 69 | c9 | 113 | ILE | 2.8 |
| 26 | CY | 66 | GLU | 2.8 |
| 37 | DJ | 24 | LEU | 2.8 |
| 62 | N | 36 | LEU | 2.8 |
| 82 | sR | 244 | ALA | 2.8 |
| 1 | 1 | 2569 | A | 2.8 |
| 1 | AR | 2540 | A | 2.8 |
| 25 | 6 | 1701 | A | 2.8 |
| 25 | A | 197 | A | 2.8 |
| 54 | F | 129 | VAL | 2.8 |
| 54 | F | 256 | ARG | 2.8 |
| 60 | c0 | 35 | ILE | 2.8 |
| 83 | e1 | 131 | PHE | 2.8 |
| 62 | N | 43 | ARG | 2.8 |
| 64 | P | 18 | ARG | 2.8 |
| 32 | AD | 95 | ALA | 2.8 |
| 33 | DF | 112 | ASP | 2.8 |
| 59 | K | 185 | GLY | 2.8 |
| 49 | p0 | 26 | PHE | 2.8 |
| 62 | N | 113 | ARG | 2.8 |
| 69 | U | 25 | GLN | 2.8 |
| 75 | a | 40 | VAL | 2.8 |
| 51 | C | 67 | GLU | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 80 | f | 56 | MET | 2.8 |
| 79 | d9 | 17 | GLY | 2.8 |
| 46 | i | 84 | LYS | 2.8 |
| 81 | g | 83 | LYS | 2.8 |
| 44 | AP | 105 | GLN | 2.7 |
| 81 | g | 137 | ASP | 2.8 |
| 1 | 1 | 1765 | U | 2.7 |
| 1 | AR | 1564 | U | 2.7 |
| 3 | 4 | 81 | U | 2.7 |
| 56 | H | 1 | MET | 2.7 |
| 60 | L | 49 | LEU | 2.7 |
| 57 | s7 | 92 | PHE | 2.7 |
| 58 | J | 8 | ARG | 2.7 |
| 79 | d9 | 6 | VAL | 2.7 |
| 29 | AA | 102 | GLU | 2.7 |
| 54 | F | 163 | ASP | 2.7 |
| 23 | CW | 13 | LYS | 2.7 |
| 66 | c6 | 38 | LEU | 2.7 |
| 1 | AR | 1954 | G | 2.7 |
| 25 | 6 | 837 | G | 2.7 |
| 28 | 9 | 71 | SER | 2.7 |
| 63 | O | 59 | GLY | 2.7 |
| 68 | T | 10 | SER | 2.7 |
| 3 | AT | 79 | A | 2.7 |
| 33 | AE | 79 | ARG | 2.7 |
| 73 | Y | 57 | LEU | 2.7 |
| 1 | AR | 3277 | U | 2.7 |
| 25 | 6 | 657 | U | 2.7 |
| 25 | 6 | 1052 | U | 2.7 |
| 29 | AA | 11 | ALA | 2.7 |
| 32 | AD | 23 | TYR | 2.7 |
| 60 | c0 | 23 | ALA | 2.7 |
| 82 | sR | 24 | ALA | 2.7 |
| 10 | p | 89 | GLU | 2.7 |
| 53 | E | 139 | SER | 2.7 |
| 57 | s7 | 31 | SER | 2.7 |
| 1 | AR | 2573 | G | 2.7 |
| 50 | s0 | 46 | HIS | 2.7 |
| 1 | 1 | 1244 | A | 2.7 |
| 28 | 9 | 85 | VAL | 2.7 |
| 50 | B | 189 | VAL | 2.7 |
| 59 | K | 104 | PHE | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 62 | c2 | 37 | VAL | 2.7 |
| 3 | AT | 84 | C | 2.7 |
| 25 | A | 716 | C | 2.7 |
| 25 | A | 911 | U | 2.7 |
| 75 | d5 | 88 | ILE | 2.7 |
| 42 | AN | 106 | ARG | 2.7 |
| 53 | E | 143 | ARG | 2.7 |
| 7 | m | 293 | LEU | 2.7 |
| 59 | K | 118 | LEU | 2.7 |
| 56 | H | 152 | ASP | 2.7 |
| 29 | AA | 71 | PHE | 2.7 |
| 62 | N | 117 | GLY | 2.7 |
| 78 | d8 | 32 | PHE | 2.7 |
| 37 | AI | 2 | ALA | 2.7 |
| 49 | p0 | 28 | VAL | 2.7 |
| 48 | sM | 83 | LYS | 2.7 |
| 62 | N | 108 | ARG | 2.7 |
| 52 | s2 | 105 | GLY | 2.7 |
| 59 | K | 183 | ALA | 2.7 |
| 40 | DM | 5 | ILE | 2.7 |
| 82 | h | 310 | ILE | 2.7 |
| 1 | AR | 1573 | G | 2.7 |
| 1 | AR | 1576 | G | 2.7 |
| 25 | 6 | 496 | G | 2.7 |
| 25 | A | 714 | G | 2.7 |
| 67 | S | 74 | GLN | 2.7 |
| 68 | c8 | 10 | SER | 2.7 |
| 78 | d8 | 6 | PRO | 2.7 |
| 82 | sR | 235 | SER | 2.7 |
| 25 | 6 | 320 | U | 2.7 |
| 25 | A | 794 | U | 2.7 |
| 10 | CJ | 119 | GLY | 2.7 |
| 10 | CJ | 251 | LYS | 2.7 |
| 49 | p0 | 88 | PHE | 2.7 |
| 77 | d7 | 46 | VAL | 2.7 |
| 23 | CW | 108 | TYR | 2.7 |
| 58 | J | 72 | ILE | 2.7 |
| 25 | A | 200 | A | 2.7 |
| 59 | K | 54 | ARG | 2.7 |
| 64 | c4 | 47 | LYS | 2.7 |
| 82 | sR | 309 | VAL | 2.7 |
| 51 | C | 60 | ALA | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 62 | c2 | 52 | LEU | 2.7 |
| 78 | d8 | 54 | LEU | 2.7 |
| 37 | DJ | 119 | LYS | 2.7 |
| 57 | s7 | 24 | PHE | 2.7 |
| 75 | a | 37 | GLN | 2.7 |
| 53 | s3 | 221 | SER | 2.7 |
| 55 | G | 24 | VAL | 2.7 |
| 14 | CN | 132 | ALA | 2.7 |
| 49 | p0 | 295 | ALA | 2.7 |
| 59 | s9 | 183 | ALA | 2.7 |
| 60 | L | 41 | TYR | 2.7 |
| 60 | c0 | 66 | TYR | 2.7 |
| 74 | d4 | 26 | ASP | 2.7 |
| 1 | AR | 1577 | G | 2.7 |
| 25 | A | 1255 | G | 2.7 |
| 53 | E | 54 | ARG | 2.7 |
| 50 | B | 32 | HIS | 2.7 |
| 12 | CL | 218 | ALA | 2.7 |
| 51 | s1 | 56 | SER | 2.7 |
| 54 | F | 24 | SER | 2.7 |
| 69 | c9 | 125 | SER | 2.7 |
| 1 | AR | 601 | U | 2.7 |
| 40 | DM | 54 | LEU | 2.7 |
| 25 | 6 | 1703 | C | 2.7 |
| 37 | AI | 8 | GLU | 2.7 |
| 29 | DB | 116 | LYS | 2.6 |
| 51 | C | 133 | TYR | 2.6 |
| 56 | H | 175 | ILE | 2.7 |
| 57 | I | 55 | LYS | 2.6 |
| 60 | c0 | 14 | TYR | 2.6 |
| 63 | c3 | 22 | ALA | 2.7 |
| 66 | c6 | 29 | ILE | 2.7 |
| 78 | d8 | 56 | LEU | 2.6 |
| 25 | 6 | 1232 | U | 2.6 |
| 7 | m | 127 | GLY | 2.6 |
| 68 | c8 | 6 | GLN | 2.6 |
| 77 | d7 | 35 | VAL | 2.6 |
| 1 | 1 | 1228 | C | 2.6 |
| 1 | 1 | 1238 | C | 2.6 |
| 1 | 1 | 1581 | C | 2.6 |
| 29 | AA | 46 | ILE | 2.6 |
| 35 | AG | 2 | ALA | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 25 | 6 | 488 | G | 2.6 |
| 49 | p0 | 24 | SER | 2.6 |
| 58 | J | 143 | TRP | 2.6 |
| 40 | DM | 43 | PHE | 2.6 |
| 79 | e | 5 | ASN | 2.6 |
| 25 | A | 917 | U | 2.6 |
| 49 | p0 | 47 | GLY | 2.6 |
| 49 | p0 | 80 | VAL | 2.6 |
| 62 | N | 127 | GLY | 2.6 |
| 60 | c0 | 71 | GLU | 2.6 |
| 60 | c0 | 93 | GLN | 2.6 |
| 38 | DK | 98 | ARG | 2.6 |
| 51 | C | 182 | ALA | 2.6 |
| 60 | L | 23 | ALA | 2.6 |
| 64 | P | 110 | LEU | 2.6 |
| 64 | c4 | 60 | ALA | 2.6 |
| 68 | T | 102 | ALA | 2.6 |
| 75 | a | 80 | LEU | 2.6 |
| 82 | sR | 172 | ALA | 2.6 |
| 82 | sR | 226 | ALA | 2.6 |
| 1 | 1 | 2772 | C | 2.6 |
| 1 | AR | 247 | C | 2.6 |
| 1 | AR | 439 | C | 2.6 |
| 50 | B | 203 | PHE | 2.6 |
| 52 | D | 144 | TRP | 2.6 |
| 1 | AR | 1565 | G | 2.6 |
| 25 | 6 | 1698 | G | 2.6 |
| 59 | K | 142 | ASN | 2.6 |
| 62 | c2 | 40 | GLY | 2.6 |
| 40 | DM | 16 | ARG | 2.6 |
| 49 | p0 | 60 | ARG | 2.6 |
| 75 | a | 53 | GLU | 2.6 |
| 1 | AR | 2543 | U | 2.6 |
| 38 | DK | 58 | ILE | 2.6 |
| 48 | sM | 66 | ALA | 2.6 |
| 63 | O | 16 | ILE | 2.6 |
| 82 | h | 23 | LEU | 2.6 |
| 1 | AR | 621 | A | 2.6 |
| 82 | h | 251 | TRP | 2.6 |
| 75 | a | 68 | ARG | 2.6 |
| 70 | d0 | 15 | GLN | 2.6 |
| 26 | CY | 82 | ILE | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 59 | K | 76 | LEU | 2.6 |
| 1 | 1 | 2522 | G | 2.6 |
| 1 | 1 | 3319 | U | 2.6 |
| 25 | A | 178 | U | 2.6 |
| 49 | p0 | 86 | PHE | 2.6 |
| 17 | CQ | 187 | GLU | 2.6 |
| 29 | AA | 47 | GLU | 2.6 |
| 66 | c6 | 141 | SER | 2.6 |
| 78 | d8 | 44 | VAL | 2.6 |
| 1 | AR | 1582 | C | 2.6 |
| 51 | C | 92 | GLN | 2.6 |
| 10 | CJ | 109 | LEU | 2.6 |
| 60 | c0 | 11 | ILE | 2.6 |
| 63 | c3 | 66 | ILE | 2.6 |
| 75 | a | 51 | LEU | 2.6 |
| 78 | d | 54 | LEU | 2.6 |
| 53 | s3 | 223 | LYS | 2.6 |
| 25 | 6 | 725 | U | 2.6 |
| 25 | 6 | 1254 | U | 2.6 |
| 25 | A | 918 | U | 2.6 |
| 57 | I | 63 | PRO | 2.6 |
| 1 | 1 | 1954 | G | 2.6 |
| 1 | 1 | 2206 | G | 2.6 |
| 10 | CJ | 161 | GLU | 2.6 |
| 29 | AA | 45 | GLY | 2.6 |
| 62 | c2 | 127 | GLY | 2.6 |
| 83 | e1 | 127 | GLY | 2.6 |
| 57 | I | 31 | SER | 2.6 |
| 10 | CJ | 26 | LEU | 2.6 |
| 18 | x | 168 | LEU | 2.6 |
| 25 | 6 | 1230 | A | 2.6 |
| 40 | DM | 36 | LYS | 2.6 |
| 62 | c2 | 97 | LEU | 2.6 |
| 72 | X | 55 | ASP | 2.6 |
| 1 | 1 | 1275 | C | 2.6 |
| 51 | C | 46 | THR | 2.6 |
| 1 | AR | 1765 | U | 2.6 |
| 25 | 6 | 1704 | U | 2.6 |
| 26 | 7 | 92 | GLU | 2.6 |
| 29 | DB | 102 | GLU | 2.6 |
| 29 | AA | 111 | LYS | 2.6 |
| 60 | L | 68 | LEU | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 75 | a | 88 | ILE | 2.6 |
| 79 | d9 | 20 | GLN | 2.6 |
| 10 | p | 97 | TYR | 2.6 |
| 25 | 6 | 729 | G | 2.6 |
| 25 | A | 142 | G | 2.6 |
| 26 | 7 | 73 | ARG | 2.6 |
| 37 | AI | 120 | ALA | 2.6 |
| 77 | c | 79 | PHE | 2.6 |
| 25 | A | 541 | A | 2.6 |
| 49 | p0 | 29 | GLY | 2.6 |
| 49 | p0 | 188 | VAL | 2.6 |
| 51 | C | 229 | MET | 2.6 |
| 64 | c4 | 125 | SER | 2.6 |
| 14 | CN | 112 | ASN | 2.6 |
| 23 | CW | 56 | VAL | 2.6 |
| 25 | A | 235 | G | 2.6 |
| 55 | G | 70 | VAL | 2.6 |
| 57 | s7 | 7 | LYS | 2.6 |
| 60 | L | 67 | THR | 2.6 |
| 76 | b | 60 | PRO | 2.6 |
| 81 | g | 115 | THR | 2.6 |
| 1 | AR | 3319 | U | 2.6 |
| 25 | 6 | 1687 | U | 2.6 |
| 57 | s7 | 49 | ILE | 2.6 |
| 15 | CO | 138 | ALA | 2.6 |
| 23 | CW | 15 | PHE | 2.6 |
| 49 | p0 | 286 | GLY | 2.6 |
| 58 | J | 181 | GLY | 2.6 |
| 62 | N | 75 | VAL | 2.6 |
| 62 | N | 121 | VAL | 2.6 |
| 62 | N | 53 | THR | 2.6 |
| 66 | c6 | 115 | THR | 2.6 |
| 75 | d5 | 105 | THR | 2.6 |
| 29 | DB | 36 | HIS | 2.6 |
| 18 | x | 183 | ALA | 2.6 |
| 59 | s9 | 139 | GLN | 2.6 |
| 29 | AA | 113 | VAL | 2.6 |
| 51 | C | 43 | VAL | 2.6 |
| 53 | s3 | 142 | LEU | 2.6 |
| 29 | DB | 72 | ILE | 2.6 |
| 51 | C | 232 | HIS | 2.6 |
| 70 | d0 | 78 | THR | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 10 | CJ | 120 | LYS | 2.5 |
| 34 | AF | 127 | ALA | 2.5 |
| 57 | I | 76 | LYS | 2.5 |
| 58 | s8 | 162 | ALA | 2.5 |
| 65 | c5 | 7 | ALA | 2.5 |
| 65 | c5 | 9 | LYS | 2.5 |
| 1 | 1 | 252 | U | 2.5 |
| 1 | 1 | 2208 | A | 2.5 |
| 25 | A | 181 | A | 2.5 |
| 25 | 6 | 1690 | G | 2.5 |
| 27 | CZ | 33 | ARG | 2.5 |
| 82 | h | 213 | SER | 2.5 |
| 28 | 9 | 126 | LEU | 2.5 |
| 56 | s6 | 173 | PRO | 2.5 |
| 60 | c0 | 97 | PRO | 2.5 |
| 29 | AA | 101 | PHE | 2.5 |
| 80 | f | 48 | THR | 2.5 |
| 35 | DH | 60 | ARG | 2.5 |
| 57 | s7 | 57 | ALA | 2.5 |
| 70 | d0 | 98 | GLN | 2.5 |
| 62 | N | 120 | VAL | 2.5 |
| 25 | A | 910 | C | 2.5 |
| 50 | B | 194 | PRO | 2.5 |
| 51 | C | 23 | PRO | 2.5 |
| 56 | H | 173 | PRO | 2.5 |
| 57 | s7 | 157 | LYS | 2.5 |
| 62 | c2 | 136 | ILE | 2.5 |
| 74 | d4 | 34 | ASN | 2.5 |
| 10 | CJ | 110 | THR | 2.5 |
| 82 | h | 318 | ALA | 2.5 |
| 69 | c9 | 114 | VAL | 2.5 |
| 58 | s8 | 137 | LYS | 2.5 |
| 55 | s5 | 55 | ASP | 2.5 |
| 75 | a | 93 | SER | 2.5 |
| 82 | h | 264 | SER | 2.5 |
| 55 | s5 | 129 | PRO | 2.5 |
| 64 | P | 94 | PRO | 2.5 |
| 36 | AH | 71 | THR | 2.5 |
| 50 | s0 | 20 | ALA | 2.5 |
| 55 | s5 | 79 | ASN | 2.5 |
| 64 | P | 101 | ALA | 2.5 |
| 25 | 6 | 1265 | G | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 25 | 6 | 1697 | G | 2.5 |
| 58 | J | 71 | GLY | 2.5 |
| 64 | P | 28 | VAL | 2.5 |
| 57 | I | 81 | LEU | 2.5 |
| 77 | d7 | 36 | LYS | 2.5 |
| 61 | c1 | 20 | PHE | 2.5 |
| 82 | sR | 316 | MET | 2.5 |
| 55 | G | 96 | SER | 2.5 |
| 55 | G | 223 | SER | 2.5 |
| 46 | i | 137 | GLU | 2.5 |
| 44 | AP | 11 | TYR | 2.5 |
| 1 | 1 | 1239 | C | 2.5 |
| 13 | CM | 174 | LYS | 2.5 |
| 25 | 6 | 1219 | A | 2.5 |
| 40 | DM | 6 | THR | 2.5 |
| 49 | p0 | 89 | THR | 2.5 |
| 50 | B | 139 | VAL | 2.5 |
| 59 | K | 95 | TYR | 2.5 |
| 62 | N | 116 | VAL | 2.5 |
| 62 | N | 124 | LYS | 2.5 |
| 64 | c4 | 97 | GLY | 2.5 |
| 74 | Z | 29 | HIS | 2.5 |
| 59 | K | 3 | ARG | 2.5 |
| 51 | s1 | 90 | GLU | 2.5 |
| 77 | c | 28 | PRO | 2.5 |
| 7 | m | 122 | VAL | 2.5 |
| 25 | 6 | 494 | U | 2.5 |
| 44 | AP | 102 | GLN | 2.5 |
| 53 | s3 | 222 | VAL | 2.5 |
| 60 | c0 | 13 | GLN | 2.5 |
| 66 | R | 90 | VAL | 2.5 |
| 71 | W | 32 | VAL | 2.5 |
| 82 | h | 309 | VAL | 2.5 |
| 57 | I | 29 | ASN | 2.5 |
| 38 | AJ | 98 | ARG | 2.5 |
| 1 | 1 | 1103 | A | 2.5 |
| 1 | AR | 2569 | A | 2.5 |
| 27 | CZ | 142 | ILE | 2.5 |
| 69 | U | 35 | ASP | 2.5 |
| 69 | U | 103 | LYS | 2.5 |
| 12 | CL | 188 | GLY | 2.5 |
| 57 | I | 90 | VAL | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 61 | c1 | 146 | ALA | 2.5 |
| 81 | g | 88 | PRO | 2.5 |
| 25 | A | 499 | U | 2.5 |
| 50 | B | 201 | LEU | 2.5 |
| 66 | R | 114 | ARG | 2.5 |
| 42 | AN | 119 | ASN | 2.5 |
| 49 | p0 | 81 | LYS | 2.5 |
| 9 | o | 23 | ALA | 2.5 |
| 18 | x | 178 | ALA | 2.5 |
| 26 | CY | 85 | ALA | 2.5 |
| 51 | C | 131 | ASP | 2.5 |
| 51 | C | 190 | PRO | 2.5 |
| 55 | G | 182 | ALA | 2.5 |
| 57 | s7 | 123 | ASP | 2.5 |
| 62 | c2 | 42 | ALA | 2.5 |
| 75 | a | 61 | SER | 2.5 |
| 78 | d8 | 59 | SER | 2.5 |
| 55 | s5 | 130 | ILE | 2.5 |
| 62 | N | 100 | TRP | 2.5 |
| 62 | c2 | 100 | TRP | 2.5 |
| 25 | 6 | 142 | G | 2.5 |
| 70 | d0 | 72 | ASN | 2.5 |
| 82 | sR | 168 | THR | 2.5 |
| 82 | sR | 177 | MET | 2.5 |
| 62 | N | 122 | VAL | 2.5 |
| 66 | R | 55 | VAL | 2.5 |
| 74 | Z | 61 | ARG | 2.5 |
| 20 | z | 185 | LEU | 2.5 |
| 69 | U | 132 | LEU | 2.5 |
| 56 | H | 45 | PHE | 2.5 |
| 25 | A | 507 | U | 2.5 |
| 55 | s5 | 224 | ASN | 2.5 |
| 65 | c5 | 89 | MET | 2.5 |
| 10 | CJ | 113 | ALA | 2.5 |
| 25 | 6 | 720 | G | 2.5 |
| 49 | p0 | 87 | VAL | 2.5 |
| 53 | E | 142 | LEU | 2.5 |
| 23 | 5 | 9 | GLN | 2.5 |
| 63 | O | 17 | PRO | 2.5 |
| 1 | 1 | 1025 | A | 2.5 |
| 3 | 4 | 79 | A | 2.5 |
| 60 | c0 | 34 | GLU | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 62 | c2 | 106 | ILE | 2.5 |
| 75 | a | 89 | ILE | 2.5 |
| 25 | 6 | 711 | U | 2.5 |
| 56 | H | 66 | GLY | 2.5 |
| 63 | O | 60 | VAL | 2.5 |
| 74 | Z | 6 | THR | 2.5 |
| 78 | d8 | 41 | VAL | 2.5 |
| 46 | i | 105 | LYS | 2.5 |
| 66 | R | 60 | PHE | 2.5 |
| 26 | CY | 94 | ARG | 2.5 |
| 68 | c8 | 144 | ARG | 2.5 |
| 82 | h | 5 | GLU | 2.5 |
| 2 | AS | 73 | C | 2.4 |
| 82 | sR | 313 | TRP | 2.4 |
| 82 | h | 271 | VAL | 2.4 |
| 25 | 6 | 1361 | U | 2.4 |
| 25 | A | 920 | U | 2.4 |
| 80 | f | 55 | ARG | 2.4 |
| 56 | H | 218 | GLU | 2.4 |
| 59 | K | 162 | SER | 2.4 |
| 51 | C | 225 | VAL | 2.4 |
| 1 | 1 | 1232 | C | 2.4 |
| 49 | p0 | 79 | PHE | 2.4 |
| 82 | sR | 227 | ALA | 2.4 |
| 55 | s5 | 157 | ARG | 2.4 |
| 64 | P | 114 | ARG | 2.4 |
| 78 | d8 | 27 | GLN | 2.4 |
| 5 | CE | 386 | ASP | 2.4 |
| 51 | C | 215 | VAL | 2.4 |
| 67 | S | 124 | VAL | 2.4 |
| 69 | c9 | 128 | GLY | 2.4 |
| 74 | Z | 35 | VAL | 2.4 |
| 49 | p0 | 283 | ALA | 2.4 |
| 1 | AR | 1353 | U | 2.4 |
| 1 | AR | 2544 | U | 2.4 |
| 10 | p | 122 | LYS | 2.4 |
| 25 | A | 227 | U | 2.4 |
| 56 | H | 226 | ILE | 2.4 |
| 14 | CN | 94 | GLY | 2.4 |
| 49 | p0 | 76 | LEU | 2.4 |
| 50 | B | 23 | HIS | 2.4 |
| 54 | F | 76 | VAL | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 60 | L | 48 | SER | 2.4 |
| 56 | s6 | 213 | ALA | 2.4 |
| 62 | c2 | 69 | ALA | 2.4 |
| 69 | U | 107 | ALA | 2.4 |
| 78 | d8 | 63 | ALA | 2.4 |
| 53 | E | 213 | GLU | 2.4 |
| 40 | DM | 10 | GLN | 2.4 |
| 68 | T | 14 | ILE | 2.4 |
| 80 | e0 | 48 | THR | 2.4 |
| 25 | A | 894 | U | 2.4 |
| 56 | H | 177 | ARG | 2.4 |
| 69 | c9 | 9 | VAL | 2.4 |
| 75 | d5 | 42 | LEU | 2.4 |
| 78 | d8 | 48 | VAL | 2.4 |
| 78 | d8 | 57 | MET | 2.4 |
| 25 | 6 | 714 | G | 2.4 |
| 51 | C | 132 | ASP | 2.4 |
| 59 | s9 | 146 | PHE | 2.4 |
| 56 | H | 148 | SER | 2.4 |
| 67 | S | 107 | SER | 2.4 |
| 37 | AI | 64 | GLU | 2.4 |
| 50 | s0 | 173 | ILE | 2.4 |
| 49 | p0 | 104 | ARG | 2.4 |
| 51 | C | 183 | GLN | 2.4 |
| 64 | P | 12 | GLN | 2.4 |
| 81 | g | 117 | LEU | 2.4 |
| 7 | m | 201 | GLY | 2.4 |
| 37 | AI | 3 | GLY | 2.4 |
| 57 | s7 | 69 | GLY | 2.4 |
| 12 | CL | 217 | PHE | 2.4 |
| 57 | s7 | 158 | ASP | 2.4 |
| 60 | c0 | 75 | TYR | 2.4 |
| 11 | CK | 191 | LEU | 2.4 |
| 29 | AA | 103 | GLN | 2.4 |
| 55 | s5 | 165 | LEU | 2.4 |
| 58 | s8 | 111 | GLN | 2.4 |
| 67 | c7 | 105 | GLN | 2.4 |
| 75 | d5 | 68 | ARG | 2.4 |
| 10 | CJ | 35 | GLY | 2.4 |
| 36 | AH | 72 | VAL | 2.4 |
| 60 | L | 3 | MET | 2.4 |
| 66 | R | 11 | GLY | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 70 | d0 | 36 | ASN | 2.4 |
| 77 | c | 39 | GLY | 2.4 |
| 78 | d8 | 5 | THR | 2.4 |
| 78 | d8 | 45 | LYS | 2.4 |
| 78 | d | 35 | ASP | 2.4 |
| 80 | f | 2 | ALA | 2.4 |
| 1 | AR | 1628 | C | 2.4 |
| 18 | CR | 182 | ILE | 2.4 |
| 25 | 6 | 1706 | C | 2.4 |
| 50 | s0 | 185 | ARG | 2.4 |
| 28 | DA | 90 | VAL | 2.4 |
| 44 | AP | 99 | GLN | 2.4 |
| 51 | C | 73 | LEU | 2.4 |
| 55 | s5 | 150 | GLY | 2.4 |
| 40 | DM | 37 | PRO | 2.4 |
| 53 | s3 | 65 | ARG | 2.4 |
| 63 | c3 | 15 | ALA | 2.4 |
| 69 | U | 51 | GLU | 2.4 |
| 1 | 1 | 3155 | U | 2.4 |
| 57 | s7 | 73 | VAL | 2.4 |
| 59 | K | 148 | VAL | 2.4 |
| 62 | N | 105 | LYS | 2.4 |
| 68 | T | 43 | SER | 2.4 |
| 10 | CJ | 182 | GLY | 2.4 |
| 25 | A | 793 | A | 2.4 |
| 29 | AA | 38 | PHE | 2.4 |
| 55 | s5 | 43 | PHE | 2.4 |
| 23 | CW | 98 | THR | 2.4 |
| 62 | N | 51 | ALA | 2.4 |
| 1 | 1 | 1229 | G | 2.4 |
| 40 | DM | 27 | ILE | 2.4 |
| 60 | c0 | 26 | ASP | 2.4 |
| 24 | lR | 5 | GLY | 2.4 |
| 51 | C | 93 | GLY | 2.4 |
| 1 | AR | 1762 | C | 2.4 |
| 25 | 6 | 1709 | C | 2.4 |
| 25 | A | 233 | C | 2.4 |
| 26 | 7 | 93 | ARG | 2.4 |
| 55 | s5 | 225 | ARG | 2.4 |
| 78 | d8 | 67 | ARG | 2.4 |
| 1 | 1 | 440 | A | 2.4 |
| 68 | c8 | 19 | ASN | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 77 | d7 | 53 | ALA | 2.4 |
| 78 | d8 | 39 | THR | 2.4 |
| 25 | 6 | 794 | U | 2.4 |
| 29 | DB | 58 | GLY | 2.4 |
| 50 | B | 29 | VAL | 2.4 |
| 57 | I | 56 | LYS | 2.4 |
| 53 | E | 184 | ILE | 2.4 |
| 54 | F | 162 | ILE | 2.4 |
| 62 | N | 128 | ALA | 2.4 |
| 62 | c2 | 84 | ASN | 2.4 |
| 69 | c9 | 136 | ALA | 2.4 |
| 82 | sR | 317 | THR | 2.4 |
| 29 | DB | 95 | VAL | 2.3 |
| 36 | AH | 77 | GLY | 2.3 |
| 56 | H | 36 | VAL | 2.3 |
| 53 | s3 | 25 | PHE | 2.3 |
| 56 | H | 190 | GLN | 2.3 |
| 57 | I | 101 | LYS | 2.3 |
| 10 | p | 129 | PRO | 2.3 |
| 69 | c9 | 111 | ILE | 2.3 |
| 76 | b | 65 | PRO | 2.3 |
| 62 | c2 | 32 | LEU | 2.3 |
| 74 | Z | 125 | LEU | 2.3 |
| 29 | AA | 74 | VAL | 2.3 |
| 82 | h | 25 | THR | 2.3 |
| 72 | X | 73 | GLY | 2.3 |
| 28 | DA | 113 | LYS | 2.3 |
| 25 | 6 | 705 | U | 2.3 |
| 49 | p0 | 18 | TYR | 2.3 |
| 56 | H | 169 | TYR | 2.3 |
| 60 | c0 | 43 | ILE | 2.3 |
| 12 | CL | 185 | ARG | 2.3 |
| 29 | DB | 10 | VAL | 2.3 |
| 1 | AR | 1024 | G | 2.3 |
| 51 | C | 50 | LYS | 2.3 |
| 56 | H | 16 | PHE | 2.3 |
| 62 | N | 80 | ASN | 2.3 |
| 65 | c5 | 135 | THR | 2.3 |
| 82 | h | 99 | THR | 2.3 |
| 55 | s5 | 31 | GLU | 2.3 |
| 57 | I | 150 | GLN | 2.3 |
| 7 | m | 192 | PRO | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 10 | p | 109 | LEU | 2.3 |
| 25 | A | 919 | A | 2.3 |
| 53 | E | 178 | ARG | 2.3 |
| 54 | s4 | 149 | TYR | 2.3 |
| 55 | s5 | 77 | TYR | 2.3 |
| 62 | c2 | 48 | SER | 2.3 |
| 82 | h | 301 | LEU | 2.3 |
| 68 | T | 56 | LYS | 2.3 |
| 29 | AA | 90 | GLU | 2.3 |
| 79 | d9 | 45 | GLU | 2.3 |
| 50 | B | 43 | ASP | 2.3 |
| 51 | C | 224 | ASP | 2.3 |
| 1 | AR | 1031 | C | 2.3 |
| 78 | d8 | 42 | ARG | 2.3 |
| 15 | u | 9 | ALA | 2.3 |
| 51 | C | 54 | LEU | 2.3 |
| 58 | s8 | 115 | ALA | 2.3 |
| 59 | K | 156 | ILE | 2.3 |
| 7 | m | 125 | VAL | 2.3 |
| 29 | AA | 61 | LYS | 2.3 |
| 59 | s9 | 177 | ALA | 2.3 |
| 51 | C | 21 | VAL | 2.3 |
| 55 | s5 | 168 | VAL | 2.3 |
| 75 | d5 | 70 | LYS | 2.3 |
| 1 | AR | 1103 | A | 2.3 |
| 25 | A | 728 | U | 2.3 |
| 54 | F | 25 | GLY | 2.3 |
| 59 | K | 111 | THR | 2.3 |
| 75 | d5 | 102 | THR | 2.3 |
| 40 | DM | 7 | ASP | 2.3 |
| 17 | CQ | 183 | ALA | 2.3 |
| 29 | AA | 25 | ILE | 2.3 |
| 62 | N | 42 | ALA | 2.3 |
| 62 | N | 59 | LEU | 2.3 |
| 69 | U | 28 | LEU | 2.3 |
| 69 | c9 | 17 | ALA | 2.3 |
| 75 | d5 | 46 | LYS | 2.3 |
| 1 | AR | 3278 | C | 2.3 |
| 49 | p0 | 27 | VAL | 2.3 |
| 12 | CL | 194 | GLY | 2.3 |
| 25 | 6 | 234 | G | 2.3 |
| 46 | i | 98 | GLY | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 49 | p0 | 282 | SER | 2.3 |
| 51 | C | 24 | PHE | 2.3 |
| 62 | N | 55 | GLY | 2.3 |
| 67 | c7 | 86 | PRO | 2.3 |
| 14 | CN | 136 | GLU | 2.3 |
| 25 | 6 | 242 | U | 2.3 |
| 78 | d8 | 29 | ARG | 2.3 |
| 15 | u | 137 | LYS | 2.3 |
| 29 | DB | 21 | LYS | 2.3 |
| 38 | AJ | 29 | LYS | 2.3 |
| 42 | AN | 121 | LEU | 2.3 |
| 60 | L | 5 | LYS | 2.3 |
| 62 | c2 | 41 | LEU | 2.3 |
| 65 | Q | 78 | THR | 2.3 |
| 49 | p0 | 73 | PHE | 2.3 |
| 64 | P | 74 | VAL | 2.3 |
| 82 | h | 54 | PHE | 2.3 |
| 20 | CT | 170 | ARG | 2.3 |
| 57 | s7 | 32 | PRO | 2.3 |
| 59 | s9 | 186 | GLU | 2.3 |
| 62 | c2 | 25 | GLU | 2.3 |
| 71 | W | 18 | SER | 2.3 |
| 82 | h | 246 | SER | 2.3 |
| 56 | s6 | 171 | LYS | 2.3 |
| 1 | 1 | 1353 | U | 2.3 |
| 25 | A | 486 | G | 2.3 |
| 57 | s7 | 89 | HIS | 2.3 |
| 59 | K | 105 | LEU | 2.3 |
| 76 | b | 44 | ILE | 2.3 |
| 82 | h | 182 | ASN | 2.3 |
| 13 | s | 11 | ASP | 2.3 |
| 56 | s6 | 156 | PHE | 2.3 |
| 82 | h | 77 | GLY | 2.3 |
| 29 | DB | 73 | LYS | 2.3 |
| 60 | L | 4 | PRO | 2.3 |
| 82 | h | 206 | PRO | 2.3 |
| 56 | s6 | 148 | SER | 2.3 |
| 25 | 6 | 189 | C | 2.3 |
| 69 | c9 | 22 | LEU | 2.3 |
| 74 | Z | 63 | GLN | 2.3 |
| 10 | p | 130 | TYR | 2.3 |
| 53 | E | 25 | PHE | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 53 | E | 27 | ARG | 2.3 |
| 53 | s3 | 40 | ARG | 2.3 |
| 66 | R | 7 | VAL | 2.3 |
| 1 | 1 | 1635 | G | 2.3 |
| 62 | c2 | 98 | GLY | 2.3 |
| 62 | c2 | 68 | GLU | 2.3 |
| 69 | U | 38 | LYS | 2.3 |
| 10 | p | 99 | PRO | 2.3 |
| 70 | d0 | 105 | GLN | 2.3 |
| 56 | H | 186 | ARG | 2.3 |
| 79 | e | 23 | VAL | 2.3 |
| 81 | g | 106 | TYR | 2.3 |
| 82 | h | 8 | VAL | 2.3 |
| 23 | 5 | 52 | ASN | 2.3 |
| 55 | G | 186 | ASN | 2.3 |
| 64 | P | 31 | THR | 2.3 |
| 64 | P | 38 | THR | 2.3 |
| 66 | R | 62 | ASN | 2.3 |
| 82 | h | 146 | GLY | 2.3 |
| 37 | DJ | 8 | GLU | 2.3 |
| 66 | R | 105 | LEU | 2.3 |
| 60 | L | 11 | ILE | 2.3 |
| 56 | s6 | 167 | LYS | 2.3 |
| 71 | W | 37 | ALA | 2.3 |
| 75 | d5 | 104 | ALA | 2.3 |
| 51 | C | 102 | GLY | 2.3 |
| 56 | H | 165 | GLY | 2.3 |
| 74 | Z | 46 | GLU | 2.3 |
| 80 | f | 52 | GLY | 2.3 |
| 25 | A | 490 | C | 2.3 |
| 25 | A | 558 | U | 2.3 |
| 53 | E | 111 | ASN | 2.3 |
| 82 | sR | 224 | ASN | 2.3 |
| 53 | s3 | 178 | ARG | 2.3 |
| 65 | c5 | 109 | PRO | 2.3 |
| 82 | h | 247 | PRO | 2.3 |
| 14 | CN | 145 | PHE | 2.3 |
| 59 | s9 | 141 | VAL | 2.3 |
| 64 | P | 17 | ALA | 2.3 |
| 78 | d8 | 55 | VAL | 2.3 |
| 1 | 1 | 3351 | U | 2.2 |
| 49 | p0 | 31 | ASP | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 51 | s1 | 98 | THR | 2.2 |
| 62 | c2 | 58 | LEU | 2.2 |
| 78 | d8 | 61 | ARG | 2.2 |
| 82 | h | 202 | LEU | 2.2 |
| 1 | 1 | 1582 | C | 2.2 |
| 54 | F | 127 | LYS | 2.2 |
| 69 | U | 124 | ILE | 2.2 |
| 51 | s1 | 91 | VAL | 2.2 |
| 56 | H | 210 | GLN | 2.2 |
| 60 | L | 22 | VAL | 2.2 |
| 20 | z | 178 | ALA | 2.2 |
| 44 | AP | 90 | HIS | 2.2 |
| 59 | s9 | 182 | GLU | 2.2 |
| 75 | d5 | 38 | HIS | 2.2 |
| 81 | g | 110 | ALA | 2.2 |
| 25 | 6 | 188 | A | 2.2 |
| 57 | I | 79 | ARG | 2.2 |
| 74 | d4 | 32 | ARG | 2.2 |
| 62 | N | 84 | ASN | 2.2 |
| 56 | H | 5 | ILE | 2.2 |
| 57 | s7 | 177 | THR | 2.2 |
| 69 | U | 101 | ASN | 2.2 |
| 82 | sR | 165 | ASP | 2.2 |
| 1 | 1 | 3352 | U | 2.2 |
| 24 | lR | 137 | VAL | 2.2 |
| 29 | DB | 96 | VAL | 2.2 |
| 14 | CN | 114 | GLN | 2.2 |
| 40 | DM | 60 | GLY | 2.2 |
| 57 | s7 | 11 | GLN | 2.2 |
| 23 | 5 | 94 | ARG | 2.2 |
| 25 | A | 898 | A | 2.2 |
| 54 | F | 171 | ASP | 2.2 |
| 62 | c2 | 70 | ASN | 2.2 |
| 74 | d4 | 3 | ASP | 2.2 |
| 82 | h | 317 | THR | 2.2 |
| 1 | 1 | 1262 | G | 2.2 |
| 1 | 1 | 2209 | U | 2.2 |
| 1 | 1 | 2501 | U | 2.2 |
| 20 | CT | 178 | ALA | 2.2 |
| 49 | p0 | 62 | ALA | 2.2 |
| 54 | s4 | 258 | GLN | 2.2 |
| 71 | d1 | 44 | ARG | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 76 | b | 62 | TYR | 2.2 |
| 82 | h | 27 | ALA | 2.2 |
| 1 | AR | 1759 | C | 2.2 |
| 25 | 6 | 1711 | C | 2.2 |
| 29 | AA | 33 | SER | 2.2 |
| 66 | c6 | 89 | LEU | 2.2 |
| 29 | DB | 118 | PHE | 2.2 |
| 82 | h | 312 | VAL | 2.2 |
| 1 | 1 | 1245 | A | 2.2 |
| 18 | CR | 171 | ARG | 2.2 |
| 7 | m | 100 | ALA | 2.2 |
| 9 | o | 28 | ALA | 2.2 |
| 55 | s5 | 28 | PRO | 2.2 |
| 13 | s | 90 | GLN | 2.2 |
| 62 | c2 | 20 | ALA | 2.2 |
| 71 | d1 | 42 | GLU | 2.2 |
| 25 | 6 | 1258 | U | 2.2 |
| 14 | CN | 116 | LEU | 2.2 |
| 56 | H | 178 | LEU | 2.2 |
| 69 | U | 40 | SER | 2.2 |
| 50 | s0 | 41 | ARG | 2.2 |
| 62 | N | 33 | ARG | 2.2 |
| 23 | 5 | 22 | PRO | 2.2 |
| 53 | E | 93 | ASP | 2.2 |
| 53 | s3 | 34 | TYR | 2.2 |
| 64 | c4 | 70 | LYS | 2.2 |
| 81 | g | 94 | LYS | 2.2 |
| 59 | s9 | 112 | GLN | 2.2 |
| 62 | N | 69 | ALA | 2.2 |
| 67 | c7 | 25 | THR | 2.2 |
| 76 | b | 48 | ALA | 2.2 |
| 82 | h | 180 | ALA | 2.2 |
| 1 | AR | 2508 | U | 2.2 |
| 25 | 6 | 232 | U | 2.2 |
| 25 | 6 | 501 | U | 2.2 |
| 25 | 6 | 1702 | A | 2.2 |
| 25 | A | 280 | U | 2.2 |
| 25 | A | 1688 | U | 2.2 |
| 63 | c3 | 25 | TRP | 2.2 |
| 23 | 5 | 38 | ILE | 2.2 |
| 49 | p0 | 187 | VAL | 2.2 |
| 51 | C | 65 | VAL | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 56 | s6 | 175 | ILE | 2.2 |
| 67 | S | 88 | VAL | 2.2 |
| 25 | 6 | 1233 | G | 2.2 |
| 25 | A | 682 | C | 2.2 |
| 51 | C | 90 | GLU | 2.2 |
| 51 | s1 | 228 | LEU | 2.2 |
| 55 | G | 198 | LEU | 2.2 |
| 23 | 5 | 28 | PHE | 2.2 |
| 25 | 6 | 754 | A | 2.2 |
| 25 | 6 | 1224 | A | 2.2 |
| 51 | s1 | 20 | VAL | 2.2 |
| 64 | c4 | 83 | ILE | 2.2 |
| 70 | V | 120 | SER | 2.2 |
| 77 | c | 30 | SER | 2.2 |
| 78 | d8 | 28 | VAL | 2.2 |
| 75 | d5 | 72 | GLY | 2.2 |
| 62 | N | 79 | ALA | 2.2 |
| 62 | N | 101 | ALA | 2.2 |
| 60 | L | 46 | LEU | 2.2 |
| 82 | h | 267 | PRO | 2.2 |
| 1 | 1 | 1246 | G | 2.2 |
| 1 | 1 | 1573 | G | 2.2 |
| 5 | k | 287 | LYS | 2.2 |
| 46 | i | 86 | ASN | 2.2 |
| 48 | sM | 82 | THR | 2.2 |
| 60 | c0 | 10 | LYS | 2.2 |
| 75 | a | 56 | THR | 2.2 |
| 74 | d4 | 27 | VAL | 2.2 |
| 25 | A | 493 | U | 2.2 |
| 53 | E | 87 | TYR | 2.2 |
| 58 | s8 | 117 | TYR | 2.2 |
| 74 | Z | 69 | SER | 2.2 |
| 56 | H | 124 | LEU | 2.2 |
| 59 | K | 119 | ALA | 2.2 |
| 83 | e1 | 140 | TYR | 2.2 |
| 28 | DA | 83 | ASP | 2.2 |
| 68 | c8 | 12 | GLN | 2.2 |
| 69 | c9 | 35 | ASP | 2.2 |
| 60 | c0 | 96 | ASN | 2.2 |
| 69 | c9 | 14 | PHE | 2.2 |
| 25 | 6 | 1235 | C | 2.2 |
| 50 | B | 48 | ILE | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 81 | g | 86 | THR | 2.2 |
| 14 | CN | 130 | GLY | 2.2 |
| 25 | A | 720 | G | 2.2 |
| 7 | CG | 293 | LEU | 2.2 |
| 20 | CT | 181 | ARG | 2.2 |
| 40 | DM | 26 | LYS | 2.2 |
| 74 | Z | 132 | ARG | 2.2 |
| 25 | 6 | 579 | A | 2.2 |
| 55 | s5 | 158 | GLN | 2.2 |
| 57 | s7 | 22 | GLN | 2.2 |
| 71 | W | 40 | ASP | 2.2 |
| 49 | p0 | 59 | VAL | 2.2 |
| 56 | s6 | 36 | VAL | 2.2 |
| 57 | I | 51 | VAL | 2.2 |
| 59 | K | 113 | VAL | 2.2 |
| 82 | h | 43 | ILE | 2.2 |
| 1 | 1 | 2572 | C | 2.2 |
| 60 | L | 44 | LYS | 2.2 |
| 68 | T | 3 | LEU | 2.2 |
| 1 | 1 | 2571 | U | 2.2 |
| 1 | 1 | 1953 | G | 2.2 |
| 25 | 6 | 1050 | G | 2.2 |
| 60 | c0 | 36 | ASP | 2.2 |
| 82 | sR | 30 | PRO | 2.2 |
| 62 | N | 106 | ILE | 2.2 |
| 12 | CL | 204 | GLY | 2.2 |
| 29 | AA | 79 | HIS | 2.2 |
| 57 | s7 | 126 | LEU | 2.1 |
| 59 | K | 60 | LEU | 2.1 |
| 59 | K | 86 | LEU | 2.1 |
| 1 | 1 | 1255 | C | 2.1 |
| 1 | 1 | 2507 | C | 2.1 |
| 6 | CF | 218 | ALA | 2.1 |
| 15 | u | 138 | ALA | 2.1 |
| 40 | AL | 34 | ALA | 2.1 |
| 75 | a | 47 | TYR | 2.1 |
| 12 | CL | 205 | SER | 2.1 |
| 1 | AR | 1630 | U | 2.1 |
| 1 | AR | 1763 | U | 2.1 |
| 33 | DF | 110 | GLU | 2.1 |
| 36 | AH | 110 | GLU | 2.1 |
| 40 | DM | 70 | PRO | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 80 | e0 | 45 | VAL | 2.1 |
| 82 | sR | 315 | VAL | 2.1 |
| 1 | 1 | 1230 | G | 2.1 |
| 1 | AR | 1561 | G | 2.1 |
| 49 | p0 | 82 | GLY | 2.1 |
| 54 | F | 144 | GLY | 2.1 |
| 55 | G | 75 | GLY | 2.1 |
| 60 | c0 | 19 | GLY | 2.1 |
| 69 | c9 | 32 | GLY | 2.1 |
| 23 | CW | 57 | THR | 2.1 |
| 51 | s1 | 61 | LEU | 2.1 |
| 51 | s1 | 217 | LEU | 2.1 |
| 55 | G | 175 | LEU | 2.1 |
| 60 | c0 | 28 | ASN | 2.1 |
| 63 | O | 138 | ASN | 2.1 |
| 83 | e1 | 123 | ASN | 2.1 |
| 49 | p0 | 289 | ALA | 2.1 |
| 73 | Y | 85 | ALA | 2.1 |
| 6 | l | 2 | SER | 2.1 |
| 49 | p0 | 48 | ARG | 2.1 |
| 62 | c2 | 82 | PRO | 2.1 |
| 69 | U | 126 | GLU | 2.1 |
| 70 | d0 | 102 | ARG | 2.1 |
| 77 | c | 36 | LYS | 2.1 |
| 63 | O | 53 | LEU | 2.1 |
| 66 | R | 52 | LEU | 2.1 |
| 69 | U | 80 | TYR | 2.1 |
| 69 | c9 | 16 | ASN | 2.1 |
| 69 | c9 | 43 | ASN | 2.1 |
| 75 | a | 101 | TYR | 2.1 |
| 79 | d9 | 27 | HIS | 2.1 |
| 82 | h | 306 | THR | 2.1 |
| 12 | CL | 183 | LYS | 2.1 |
| 40 | DM | 56 | ILE | 2.1 |
| 51 | C | 68 | VAL | 2.1 |
| 58 | s8 | 152 | ILE | 2.1 |
| 62 | N | 21 | GLU | 2.1 |
| 77 | d7 | 54 | VAL | 2.1 |
| 51 | C | 103 | MET | 2.1 |
| 1 | AR | 2542 | U | 2.1 |
| 25 | A | 237 | C | 2.1 |
| 25 | A | 717 | C | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 49 | p0 | 46 | ARG | 2.1 |
| 50 | B | 147 | THR | 2.1 |
| 66 | R | 23 | LYS | 2.1 |
| 66 | c6 | 143 | ARG | 2.1 |
| 64 | P | 39 | ILE | 2.1 |
| 64 | c4 | 48 | VAL | 2.1 |
| 78 | d8 | 58 | GLU | 2.1 |
| 7 | CG | 9 | SER | 2.1 |
| 25 | A | 505 | A | 2.1 |
| 80 | f | 6 | GLY | 2.1 |
| 83 | e1 | 122 | SER | 2.1 |
| 4 | CD | 34 | TYR | 2.1 |
| 57 | I | 43 | PHE | 2.1 |
| 59 | K | 120 | LYS | 2.1 |
| 69 | c9 | 119 | LYS | 2.1 |
| 80 | e0 | 55 | ARG | 2.1 |
| 82 | sR | 214 | ALA | 2.1 |
| 7 | m | 221 | GLU | 2.1 |
| 10 | CJ | 123 | GLN | 2.1 |
| 14 | CN | 57 | VAL | 2.1 |
| 56 | H | 162 | VAL | 2.1 |
| 57 | s7 | 29 | ASN | 2.1 |
| 68 | c8 | 20 | THR | 2.1 |
| 75 | d5 | 41 | ILE | 2.1 |
| 77 | d7 | 40 | CYS | 2.1 |
| 57 | s7 | 154 | LEU | 2.1 |
| 69 | U | 105 | LEU | 2.1 |
| 32 | AD | 22 | LYS | 2.1 |
| 56 | H | 149 | LYS | 2.1 |
| 77 | c | 80 | ARG | 2.1 |
| 23 | CW | 33 | TYR | 2.1 |
| 79 | d9 | 43 | PHE | 2.1 |
| 23 | CW | 34 | ALA | 2.1 |
| 56 | s6 | 205 | ALA | 2.1 |
| 29 | AA | 40 | HIS | 2.1 |
| 44 | AP | 92 | GLU | 2.1 |
| 46 | i | 116 | GLU | 2.1 |
| 23 | CW | 100 | THR | 2.1 |
| 64 | P | 97 | GLY | 2.1 |
| 64 | c4 | 44 | GLY | 2.1 |
| 64 | c4 | 65 | GLN | 2.1 |
| 79 | d9 | 31 | ILE | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 60 | L | 59 | PHE | 2.1 |
| 60 | c0 | 16 | PHE | 2.1 |
| 80 | e0 | 27 | PRO | 2.1 |
| 82 | sR | 26 | SER | 2.1 |
| 5 | k | 386 | ASP | 2.1 |
| 20 | z | 189 | ALA | 2.1 |
| 50 | s0 | 40 | ALA | 2.1 |
| 65 | Q | 54 | ALA | 2.1 |
| 67 | S | 87 | GLU | 2.1 |
| 69 | c9 | 29 | GLU | 2.1 |
| 25 | A | 1227 | A | 2.1 |
| 72 | d2 | 56 | HIS | 2.1 |
| 82 | h | 113 | VAL | 2.1 |
| 10 | p | 201 | THR | 2.1 |
| 20 | z | 181 | ARG | 2.1 |
| 25 | A | 1237 | G | 2.1 |
| 56 | H | 180 | THR | 2.1 |
| 70 | V | 67 | THR | 2.1 |
| 79 | e | 30 | LEU | 2.1 |
| 82 | h | 137 | LYS | 2.1 |
| 51 | s1 | 23 | PRO | 2.1 |
| 27 | 8 | 23 | ALA | 2.1 |
| 53 | s3 | 144 | ALA | 2.1 |
| 69 | c9 | 51 | GLU | 2.1 |
| 51 | C | 72 | ASP | 2.1 |
| 54 | F | 254 | ARG | 2.1 |
| 69 | U | 24 | ARG | 2.1 |
| 25 | 6 | 138 | A | 2.1 |
| 25 | A | 830 | U | 2.1 |
| 25 | A | 1240 | U | 2.1 |
| 29 | AA | 118 | PHE | 2.1 |
| 57 | s7 | 131 | PHE | 2.1 |
| 78 | d8 | 19 | THR | 2.1 |
| 1 | 1 | 1233 | G | 2.1 |
| 25 | A | 1716 | C | 2.1 |
| 29 | AA | 117 | ALA | 2.1 |
| 30 | DC | 97 | GLU | 2.1 |
| 49 | p0 | 44 | GLU | 2.1 |
| 8 | CH | 15 | VAL | 2.1 |
| 24 | lR | 2 | SER | 2.1 |
| 29 | DB | 69 | LYS | 2.1 |
| 60 | c0 | 52 | LYS | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 54 | s4 | 253 | ASP | 2.1 |
| 56 | H | 18 | ILE | 2.1 |
| 62 | N | 46 | ARG | 2.1 |
| 77 | c | 35 | VAL | 2.1 |
| 81 | g | 149 | LYS | 2.1 |
| 54 | F | 259 | GLN | 2.1 |
| 57 | I | 11 | GLN | 2.1 |
| 62 | N | 126 | TRP | 2.1 |
| 1 | AR | 1356 | U | 2.1 |
| 1 | AR | 1764 | U | 2.1 |
| 1 | AR | 2565 | U | 2.1 |
| 4 | j | 252 | THR | 2.1 |
| 25 | 6 | 231 | U | 2.1 |
| 25 | A | 725 | U | 2.1 |
| 1 | 1 | 1231 | A | 2.1 |
| 3 | 4 | 80 | A | 2.1 |
| 7 | CG | 263 | GLU | 2.1 |
| 13 | s | 167 | TYR | 2.1 |
| 56 | s6 | 177 | ARG | 2.1 |
| 56 | s6 | 209 | ALA | 2.1 |
| 57 | I | 17 | GLU | 2.1 |
| 68 | c8 | 146 | ALA | 2.1 |
| 69 | c9 | 137 | ALA | 2.1 |
| 74 | d4 | 4 | ALA | 2.1 |
| 78 | d8 | 10 | ALA | 2.1 |
| 82 | sR | 318 | ALA | 2.1 |
| 55 | s5 | 96 | SER | 2.1 |
| 59 | K | 63 | ASP | 2.1 |
| 62 | c2 | 78 | LEU | 2.1 |
| 82 | sR | 205 | SER | 2.1 |
| 1 | AR | 1268 | G | 2.1 |
| 29 | DB | 57 | HIS | 2.1 |
| 10 | CJ | 137 | ASN | 2.1 |
| 28 | 9 | 98 | ASN | 2.1 |
| 29 | AA | 3 | LYS | 2.1 |
| 37 | DJ | 102 | GLU | 2.1 |
| 50 | B | 21 | ASN | 2.1 |
| 59 | K | 6 | ARG | 2.1 |
| 75 | d5 | 103 | ARG | 2.1 |
| 7 | CG | 288 | ALA | 2.1 |
| 49 | p0 | 51 | VAL | 2.1 |
| 49 | p0 | 277 | ALA | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 56 | s6 | 206 | ALA | 2.1 |
| 1 | 1 | 1263 | A | 2.1 |
| 1 | AR | 1575 | A | 2.1 |
| 82 | h | 73 | LEU | 2.1 |
| 57 | s7 | 66 | SER | 2.1 |
| 58 | s8 | 149 | SER | 2.1 |
| 29 | AA | 130 | PHE | 2.0 |
| 44 | AP | 22 | GLN | 2.0 |
| 54 | s4 | 133 | LYS | 2.0 |
| 68 | c8 | 11 | PHE | 2.0 |
| 56 | H | 225 | GLU | 2.0 |
| 56 | s6 | 160 | ARG | 2.0 |
| 81 | g | 116 | LYS | 2.0 |
| 1 | AR | 243 | G | 2.0 |
| 20 | CT | 179 | GLU | 2.0 |
| 10 | CJ | 45 | ASN | 2.0 |
| 36 | AH | 112 | ALA | 2.0 |
| 36 | DI | 59 | PRO | 2.0 |
| 56 | H | 49 | VAL | 2.0 |
| 56 | s6 | 163 | THR | 2.0 |
| 59 | K | 4 | ALA | 2.0 |
| 66 | c6 | 39 | VAL | 2.0 |
| 70 | d0 | 107 | THR | 2.0 |
| 82 | h | 83 | ALA | 2.0 |
| 40 | DM | 35 | GLY | 2.0 |
| 50 | B | 188 | LEU | 2.0 |
| 56 | s6 | 147 | LEU | 2.0 |
| 66 | R | 65 | ILE | 2.0 |
| 78 | d | 56 | LEU | 2.0 |
| 1 | AR | 253 | A | 2.0 |
| 49 | p0 | 195 | GLN | 2.0 |
| 57 | I | 85 | PHE | 2.0 |
| 57 | s7 | 161 | GLN | 2.0 |
| 58 | J | 141 | ARG | 2.0 |
| 82 | h | 59 | ARG | 2.0 |
| 40 | DM | 2 | ALA | 2.0 |
| 51 | C | 34 | ALA | 2.0 |
| 59 | s9 | 181 | ALA | 2.0 |
| 80 | f | 45 | VAL | 2.0 |
| 8 | n | 97 | ASN | 2.0 |
| 28 | DA | 91 | ASN | 2.0 |
| 1 | 1 | 250 | U | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 50 | s0 | 166 | GLY | 2.0 |
| 60 | c0 | 53 | GLY | 2.0 |
| 62 | N | 125 | ASN | 2.0 |
| 51 | C | 30 | PHE | 2.0 |
| 53 | s3 | 51 | ARG | 2.0 |
| 69 | c9 | 122 | ARG | 2.0 |
| 75 | d5 | 58 | ARG | 2.0 |
| 82 | h | 231 | MET | 2.0 |
| 25 | A | 733 | A | 2.0 |
| 10 | CJ | 67 | ILE | 2.0 |
| 29 | AA | 6 | LYS | 2.0 |
| 49 | p0 | 43 | LYS | 2.0 |
| 59 | s9 | 180 | LYS | 2.0 |
| 82 | sR | 47 | LEU | 2.0 |
| 13 | s | 60 | ARG | 2.0 |
| 14 | CN | 133 | PRO | 2.0 |
| 62 | N | 102 | GLY | 2.0 |
| 73 | Y | 2 | GLY | 2.0 |
| 1 | 1 | 545 | U | 2.0 |
| 25 | 6 | 74 | U | 2.0 |
| 25 | A | 187 | G | 2.0 |
| 53 | E | 214 | GLU | 2.0 |
| 55 | s5 | 39 | GLU | 2.0 |
| 67 | S | 70 | SER | 2.0 |
| 66 | c6 | 28 | LEU | 2.0 |
| 81 | g | 152 | ALA | 2.0 |
| 25 | 6 | 491 | C | 2.0 |
| 48 | sM | 50 | ASN | 2.0 |
| 77 | c | 42 | ASN | 2.0 |
| 40 | DM | 4 | GLU | 2.0 |
| 1 | 1 | 1241 | U | 2.0 |
| 1 | 1 | 1348 | U | 2.0 |
| 1 | AR | 2541 | U | 2.0 |
| 22 | 2 | 120 | LYS | 2.0 |
| 23 | CW | 70 | LYS | 2.0 |
| 25 | A | 1682 | U | 2.0 |
| 42 | AN | 120 | GLN | 2.0 |
| 59 | K | 112 | GLN | 2.0 |
| 57 | s7 | 175 | LYS | 2.0 |
| 61 | c1 | 117 | VAL | 2.0 |
| 67 | S | 53 | TYR | 2.0 |
| 78 | d8 | 30 | VAL | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 46 | i | 255 | ALA | 2.0 |
| 58 | J | 147 | ALA | 2.0 |
| 64 | c4 | 62 | LEU | 2.0 |
| 7 | CG | 3 | PHE | 2.0 |
| 25 | A | 895 | G | 2.0 |
| 52 | D | 145 | GLY | 2.0 |
| 56 | H | 33 | GLY | 2.0 |
| 74 | Z | 66 | GLY | 2.0 |
| 78 | d8 | 53 | ILE | 2.0 |
| 25 | A | 217 | A | 2.0 |
| 64 | P | 37 | GLU | 2.0 |
| 67 | S | 101 | ASN | 2.0 |
| 82 | h | 316 | MET | 2.0 |
| 25 | A | 500 | C | 2.0 |
| 46 | i | 83 | LYS | 2.0 |
| 12 | CL | 181 | TYR | 2.0 |
| 56 | H | 216 | LEU | 2.0 |
| 57 | I | 34 | LEU | 2.0 |
| 62 | N | 60 | VAL | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 85 | MG | 6 | 2176 | 1/1 | 0.31 | 0.68 | 93,93,93,93 | 0 |
| 85 | MG | 1 | 3951 | 1/1 | 0.45 | 0.33 | 69,69,69,69 | 0 |
| 85 | MG | 6 | 2158 | 1/1 | 0.46 | 0.75 | 74,74,74,74 | 0 |
| 85 | MG | 1 | 4140 | 1/1 | 0.46 | 0.29 | 187,187,187,187 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85 | MG | A | 2130 | 1/1 | 0.46 | 0.62 | 74,74,74,74 | 0 |
| 85 | MG | 1 | 3813 | 1/1 | 0.48 | 0.37 | 61,61,61,61 | 0 |
| 85 | MG | 1 | 3958 | 1/1 | 0.49 | 0.38 | 44,44,44,44 | 0 |
| 85 | MG | 1 | 4053 | 1/1 | 0.49 | 0.41 | 74,74,74,74 | 0 |
| 85 | MG | 1 | 3965 | 1/1 | 0.51 | 0.57 | 94,94,94,94 | 0 |
| 85 | MG | A | 2121 | 1/1 | 0.52 | 0.31 | 62,62,62,62 | 0 |
| 85 | MG | 1 | 3948 | 1/1 | 0.55 | 0.23 | 73,73,73,73 | 0 |
| 85 | MG | AR | 4196 | 1/1 | 0.55 | 0.43 | 43,43,43,43 | 0 |
| 85 | MG | 4 | 229 | 1/1 | 0.56 | 0.41 | 54,54,54,54 | 0 |
| 85 | MG | AS | 228 | 1/1 | 0.56 | 0.42 | 84,84,84,84 | 0 |
| 85 | MG | AR | 4102 | 1/1 | 0.57 | 0.98 | 30,30,30,30 | 0 |
| 85 | MG | AR | 4104 | 1/1 | 0.57 | 0.39 | 66,66,66,66 | 0 |
| 85 | MG | 1 | 4150 | 1/1 | 0.57 | 0.26 | 49,49,49,49 | 0 |
| 85 | MG | A | 2150 | 1/1 | 0.57 | 0.16 | 86,86,86,86 | 0 |
| 85 | MG | 1 | 4152 | 1/1 | 0.59 | 0.80 | 111,111,111,111 | 0 |
| 85 | MG | AR | 4122 | 1/1 | 0.60 | 0.25 | 68,68,68,68 | 0 |
| 85 | MG | 1 | 4104 | 1/1 | 0.60 | 0.45 | 53,53,53,53 | 0 |
| 85 | MG | AR | 3890 | 1/1 | 0.60 | 0.42 | 29,29,29,29 | 0 |
| 85 | MG | AR | 4013 | 1/1 | 0.60 | 0.29 | 65,65,65,65 | 0 |
| 85 | MG | 1 | 3989 | 1/1 | 0.60 | 0.26 | 55,55,55,55 | 0 |
| 85 | MG | 6 | 2168 | 1/1 | 0.60 | 0.31 | 132,132,132,132 | 0 |
| 85 | MG | 1 | 3772 | 1/1 | 0.61 | 0.20 | 35,35,35,35 | 0 |
| 85 | MG | 6 | 2180 | 1/1 | 0.61 | 0.60 | 64,64,64,64 | 0 |
| 85 | MG | A | 2124 | 1/1 | 0.61 | 0.30 | 68,68,68,68 | 0 |
| 85 | MG | 6 | 2185 | 1/1 | 0.61 | 0.46 | 89,89,89,89 | 0 |
| 85 | MG | AR | 4254 | 1/1 | 0.61 | 0.38 | 56,56,56,56 | 0 |
| 85 | MG | A | 2155 | 1/1 | 0.61 | 0.46 | 75,75,75,75 | 0 |
| 85 | MG | 6 | 2194 | 1/1 | 0.62 | 0.15 | 108,108,108,108 | 0 |
| 85 | MG | 6 | 2160 | 1/1 | 0.62 | 0.38 | 85,85,85,85 | 0 |
| 85 | MG | 4 | 221 | 1/1 | 0.63 | 0.54 | 51,51,51,51 | 0 |
| 85 | MG | 1 | 4004 | 1/1 | 0.64 | 0.26 | 44,44,44,44 | 0 |
| 85 | MG | AR | 4125 | 1/1 | 0.64 | 0.29 | 82,82,82,82 | 0 |
| 85 | MG | AS | 220 | 1/1 | 0.64 | 0.36 | 68,68,68,68 | 0 |
| 85 | MG | AR | 3950 | 1/1 | 0.65 | 0.27 | 47,47,47,47 | 0 |
| 85 | MG | 1 | 3823 | 1/1 | 0.65 | 0.27 | 41,41,41,41 | 0 |
| 85 | MG | 6 | 2191 | 1/1 | 0.65 | 0.44 | 87,87,87,87 | 0 |
| 85 | MG | AR | 3955 | 1/1 | 0.66 | 0.17 | 34,34,34,34 | 0 |
| 85 | MG | AR | 4255 | 1/1 | 0.67 | 0.64 | 57,57,57,57 | 0 |
| 85 | MG | 1 | 4124 | 1/1 | 0.68 | 0.22 | 48,48,48,48 | 0 |
| 85 | MG | t | 202 | 1/1 | 0.68 | 0.26 | 101,101,101,101 | 0 |
| 85 | MG | AR | 4219 | 1/1 | 0.68 | 0.17 | 67,67,67,67 | 0 |
| 85 | MG | AR | 4074 | 1/1 | 0.68 | 0.23 | 77,77,77,77 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85 | MG | AR | 4174 | 1/1 | 0.69 | 0.42 | 39,39,39,39 | 0 |
| 85 | MG | AT | 218 | 1/1 | 0.69 | 0.34 | 30,30,30,30 | 0 |
| 85 | MG | A | 2099 | 1/1 | 0.69 | 0.69 | 71,71,71,71 | 0 |
| 85 | MG | A | 2103 | 1/1 | 0.69 | 0.55 | 73,73,73,73 | 0 |
| 85 | MG | AR | 3833 | 1/1 | 0.69 | 0.30 | 49,49,49,49 | 0 |
| 85 | MG | 1 | 3930 | 1/1 | 0.69 | 0.57 | 40,40,40,40 | 0 |
| 85 | MG | 1 | 3952 | 1/1 | 0.69 | 0.24 | 77,77,77,77 | 0 |
| 85 | MG | 1 | 3820 | 1/1 | 0.69 | 0.60 | 65,65,65,65 | 0 |
| 85 | MG | 6 | 2086 | 1/1 | 0.69 | 0.25 | 82,82,82,82 | 0 |
| 85 | MG | A | 2117 | 1/1 | 0.70 | 0.19 | 71,71,71,71 | 0 |
| 85 | MG | 6 | 2133 | 1/1 | 0.70 | 0.66 | 61,61,61,61 | 0 |
| 85 | MG | A | 2085 | 1/1 | 0.70 | 0.40 | 63,63,63,63 | 0 |
| 85 | MG | AR | 4170 | 1/1 | 0.70 | 0.27 | 32,32,32,32 | 0 |
| 85 | MG | A | 2139 | 1/1 | 0.70 | 0.36 | 64,64,64,64 | 0 |
| 85 | MG | 6 | 2174 | 1/1 | 0.70 | 0.44 | 58,58,58,58 | 0 |
| 85 | MG | A | 2151 | 1/1 | 0.70 | 0.69 | 52,52,52,52 | 0 |
| 85 | MG | A | 2112 | 1/1 | 0.70 | 0.37 | 86,86,86,86 | 0 |
| 85 | MG | Y | 201 | 1/1 | 0.70 | 0.20 | 61,61,61,61 | 0 |
| 85 | MG | 6 | 2154 | 1/1 | 0.71 | 0.41 | 54,54,54,54 | 0 |
| 85 | MG | 1 | 403 | 1/1 | 0.71 | 0.47 | 37,37,37,37 | 0 |
| 85 | MG | 1 | 4061 | 1/1 | 0.71 | 0.31 | 54,54,54,54 | 0 |
| 85 | MG | AR | 4119 | 1/1 | 0.71 | 0.39 | 91,91,91,91 | 0 |
| 84 | OHX | AR | 3737 | 7/7 | 0.71 | 0.46 | 158,158,158,159 | 0 |
| 85 | MG | 4 | 233 | 1/1 | 0.71 | 0.20 | 48,48,48,48 | 0 |
| 85 | MG | AR | 4037 | 1/1 | 0.71 | 0.34 | 70,70,70,70 | 0 |
| 85 | MG | AR | 4003 | 1/1 | 0.72 | 0.43 | 45,45,45,45 | 0 |
| 85 | MG | AR | 4222 | 1/1 | 0.72 | 0.39 | 58,58,58,58 | 0 |
| 85 | MG | 1 | 3814 | 1/1 | 0.72 | 0.22 | 77,77,77,77 | 0 |
| 85 | MG | AR | 4030 | 1/1 | 0.72 | 0.57 | 59,59,59,59 | 0 |
| 85 | MG | s | 300 | 1/1 | 0.72 | 0.27 | 70,70,70,70 | 0 |
| 85 | MG | AR | 4049 | 1/1 | 0.72 | 0.19 | 50,50,50,50 | 0 |
| 85 | MG | 1 | 4101 | 1/1 | 0.72 | 0.51 | 38,38,38,38 | 0 |
| 85 | MG | A | 2046 | 1/1 | 0.72 | 0.29 | 67,67,67,67 | 0 |
| 85 | MG | A | 2062 | 1/1 | 0.72 | 0.71 | 65,65,65,65 | 0 |
| 85 | MG | AR | 4181 | 1/1 | 0.72 | 0.24 | 50,50,50,50 | 0 |
| 85 | MG | AR | 3817 | 1/1 | 0.72 | 0.24 | 112,112,112,112 | 0 |
| 85 | MG | AR | 4034 | 1/1 | 0.73 | 0.45 | 60,60,60,60 | 0 |
| 85 | MG | AR | 4214 | 1/1 | 0.73 | 0.24 | 55,55,55,55 | 0 |
| 85 | MG | AT | 224 | 1/1 | 0.73 | 0.23 | 68,68,68,68 | 0 |
| 85 | MG | CD | 302 | 1/1 | 0.73 | 0.49 | 36,36,36,36 | 0 |
| 85 | MG | A | 2128 | 1/1 | 0.73 | 0.50 | 78,78,78,78 | 0 |
| 85 | MG | DC | 203 | 1/1 | 0.73 | 0.31 | 47,47,47,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85 | MG | 6 | 2124 | 1/1 | 0.73 | 0.28 | 66,66,66,66 | 0 |
| 85 | MG | A | 2146 | 1/1 | 0.73 | 0.16 | 120,120,120,120 | 0 |
| 85 | MG | 1 | 4161 | 1/1 | 0.73 | 0.25 | 69,69,69,69 | 0 |
| 85 | MG | AR | 4011 | 1/1 | 0.73 | 0.39 | 58,58,58,58 | 0 |
| 85 | MG | 1 | 4190 | 1/1 | 0.73 | 0.56 | 25,25,25,25 | 0 |
| 85 | MG | 1 | 3988 | 1/1 | 0.73 | 0.37 | 34,34,34,34 | 0 |
| 85 | MG | AR | 4024 | 1/1 | 0.74 | 0.78 | 53,53,53,53 | 0 |
| 85 | MG | AS | 225 | 1/1 | 0.74 | 0.35 | 58,58,58,58 | 0 |
| 85 | MG | AR | 4161 | 1/1 | 0.74 | 0.27 | 39,39,39,39 | 0 |
| 85 | MG | AR | 3783 | 1/1 | 0.74 | 0.32 | 44,44,44,44 | 0 |
| 85 | MG | 1 | 3983 | 1/1 | 0.74 | 0.52 | 55,55,55,55 | 0 |
| 85 | MG | 1 | 4151 | 1/1 | 0.74 | 0.28 | 41,41,41,41 | 0 |
| 85 | MG | A | 2131 | 1/1 | 0.74 | 0.43 | 64,64,64,64 | 0 |
| 85 | MG | A | 2135 | 1/1 | 0.74 | 0.56 | 55,55,55,55 | 0 |
| 85 | MG | 1 | 4081 | 1/1 | 0.74 | 0.39 | 29,29,29,29 | 0 |
| 85 | MG | 1 | 4129 | 1/1 | 0.74 | 0.43 | 33,33,33,33 | 0 |
| 85 | MG | 1 | 4131 | 1/1 | 0.74 | 0.32 | 48,48,48,48 | 0 |
| 85 | MG | 6 | 2192 | 1/1 | 0.74 | 0.67 | 74,74,74,74 | 0 |
| 85 | MG | 1 | 4056 | 1/1 | 0.74 | 0.30 | 51,51,51,51 | 0 |
| 85 | MG | AR | 3782 | 1/1 | 0.74 | 0.35 | 36,36,36,36 | 0 |
| 85 | MG | A | 2118 | 1/1 | 0.75 | 0.92 | 80,80,80,80 | 0 |
| 85 | MG | AR | 4215 | 1/1 | 0.75 | 0.28 | 70,70,70,70 | 0 |
| 85 | MG | AR | 3995 | 1/1 | 0.75 | 0.34 | 65,65,65,65 | 0 |
| 85 | MG | AR | 3827 | 1/1 | 0.75 | 0.35 | 58,58,58,58 | 0 |
| 85 | MG | A | 2045 | 1/1 | 0.75 | 0.79 | 58,58,58,58 | 0 |
| 85 | MG | 1 | 4158 | 1/1 | 0.75 | 0.46 | 47,47,47,47 | 0 |
| 85 | MG | A | 2054 | 1/1 | 0.75 | 0.23 | 66,66,66,66 | 0 |
| 85 | MG | A | 2136 | 1/1 | 0.75 | 0.71 | 74,74,74,74 | 0 |
| 85 | MG | 6 | 2083 | 1/1 | 0.75 | 0.46 | 63,63,63,63 | 0 |
| 85 | MG | AR | 4022 | 1/1 | 0.75 | 0.44 | 30,30,30,30 | 0 |
| 85 | MG | 1 | 3816 | 1/1 | 0.75 | 0.34 | 44,44,44,44 | 0 |
| 85 | MG | AR | 4117 | 1/1 | 0.75 | 0.31 | 64,64,64,64 | 0 |
| 85 | MG | 6 | 2117 | 1/1 | 0.75 | 0.28 | 65,65,65,65 | 0 |
| 85 | MG | AT | 222 | 1/1 | 0.75 | 0.34 | 43,43,43,43 | 0 |
| 85 | MG | 4 | 235 | 1/1 | 0.76 | 0.50 | 70,70,70,70 | 0 |
| 85 | MG | CM | 202 | 1/1 | 0.76 | 0.15 | 62,62,62,62 | 0 |
| 85 | MG | 1 | 3790 | 1/1 | 0.76 | 0.12 | 43,43,43,43 | 0 |
| 85 | MG | 1 | 3857 | 1/1 | 0.76 | 0.25 | 56,56,56,56 | 0 |
| 85 | MG | 1 | 4093 | 1/1 | 0.76 | 0.37 | 57,57,57,57 | 0 |
| 85 | MG | 6 | 2188 | 1/1 | 0.76 | 0.54 | 66,66,66,66 | 0 |
| 85 | MG | AR | 4257 | 1/1 | 0.76 | 0.32 | 51,51,51,51 | 0 |
| 85 | MG | 6 | 2189 | 1/1 | 0.76 | 0.34 | 63,63,63,63 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85 | MG | 1 | 4155 | 1/1 | 0.76 | 0.23 | 53,53,53,53 | 0 |
| 85 | MG | 1 | 4148 | 1/1 | 0.76 | 0.18 | 53,53,53,53 | 0 |
| 85 | MG | 6 | 2088 | 1/1 | 0.76 | 0.35 | 82,82,82,82 | 0 |
| 85 | MG | AR | 4087 | 1/1 | 0.76 | 0.36 | 63,63,63,63 | 0 |
| 85 | MG | AR | 3776 | 1/1 | 0.76 | 0.33 | 76,76,76,76 | 0 |
| 85 | MG | AS | 219 | 1/1 | 0.77 | 0.24 | 58,58,58,58 | 0 |
| 85 | MG | 6 | 2162 | 1/1 | 0.77 | 0.26 | 60,60,60,60 | 0 |
| 85 | MG | 6 | 2163 | 1/1 | 0.77 | 0.42 | 48,48,48,48 | 0 |
| 85 | MG | AR | 4171 | 1/1 | 0.77 | 0.17 | 88,88,88,88 | 0 |
| 85 | MG | AR | 4085 | 1/1 | 0.77 | 0.46 | 35,35,35,35 | 0 |
| 85 | MG | 6 | 2081 | 1/1 | 0.77 | 0.25 | 55,55,55,55 | 0 |
| 84 | OHX | 1 | 3691 | 7/7 | 0.77 | 0.31 | 201,201,201,201 | 0 |
| 85 | MG | 1 | 3744 | 1/1 | 0.77 | 0.42 | 83,83,83,83 | 0 |
| 85 | MG | AR | 3921 | 1/1 | 0.77 | 0.31 | 38,38,38,38 | 0 |
| 85 | MG | 1 | 3801 | 1/1 | 0.77 | 0.54 | 37,37,37,37 | 0 |
| 85 | MG | 6 | 2074 | 1/1 | 0.77 | 0.37 | 62,62,62,62 | 0 |
| 85 | MG | AR | 4225 | 1/1 | 0.77 | 0.35 | 34,34,34,34 | 0 |
| 85 | MG | AR | 4244 | 1/1 | 0.77 | 0.40 | 45,45,45,45 | 0 |
| 85 | MG | AR | 3976 | 1/1 | 0.77 | 0.44 | 81,81,81,81 | 0 |
| 85 | MG | A | 2084 | 1/1 | 0.77 | 0.22 | 72,72,72,72 | 0 |
| 85 | MG | AR | 4156 | 1/1 | 0.77 | 1.08 | 72,72,72,72 | 0 |
| 85 | MG | V | 201 | 1/1 | 0.77 | 0.50 | 70,70,70,70 | 0 |
| 85 | MG | AR | 4160 | 1/1 | 0.77 | 0.26 | 78,78,78,78 | 0 |
| 85 | MG | b | 101 | 1/1 | 0.77 | 0.45 | 65,65,65,65 | 0 |
| 85 | MG | 1 | 3811 | 1/1 | 0.78 | 0.30 | 44,44,44,44 | 0 |
| 85 | MG | 6 | 2197 | 1/1 | 0.78 | 0.57 | 56,56,56,56 | 0 |
| 85 | MG | AF | 202 | 1/1 | 0.78 | 0.27 | 28,28,28,28 | 0 |
| 85 | MG | AR | 4123 | 1/1 | 0.78 | 0.36 | 57,57,57,57 | 0 |
| 85 | MG | AR | 4005 | 1/1 | 0.78 | 0.62 | 40,40,40,40 | 0 |
| 85 | MG | AR | 4141 | 1/1 | 0.78 | 0.36 | 37,37,37,37 | 0 |
| 85 | MG | 1 | 3976 | 1/1 | 0.78 | 0.14 | 61,61,61,61 | 0 |
| 85 | MG | 1 | 3941 | 1/1 | 0.78 | 0.41 | 78,78,78,78 | 0 |
| 85 | MG | 1 | 4012 | 1/1 | 0.78 | 0.44 | 50,50,50,50 | 0 |
| 85 | MG | AR | 3803 | 1/1 | 0.78 | 0.51 | 35,35,35,35 | 0 |
| 85 | MG | 1 | 4087 | 1/1 | 0.78 | 0.23 | 59,59,59,59 | 0 |
| 85 | MG | 1 | 4092 | 1/1 | 0.78 | 0.64 | 54,54,54,54 | 0 |
| 85 | MG | 1 | 4187 | 1/1 | 0.78 | 0.35 | 43,43,43,43 | 0 |
| 85 | MG | x | 206 | 1/1 | 0.78 | 0.58 | 35,35,35,35 | 0 |
| 85 | MG | 6 | 2157 | 1/1 | 0.78 | 0.28 | 56,56,56,56 | 0 |
| 85 | MG | 1 | 4046 | 1/1 | 0.78 | 0.34 | 37,37,37,37 | 0 |
| 85 | MG | 6 | 2076 | 1/1 | 0.78 | 0.58 | 105,105,105,105 | 0 |
| 85 | MG | AR | 4220 | 1/1 | 0.78 | 0.39 | 44,44,44,44 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 85 | MG | AR | 3968 | 1/1 | 0.78 | 0.32 | 30,30,30,30 | 0 |
| 85 | MG | AR | 3971 | 1/1 | 0.78 | 0.42 | 57,57,57,57 | 0 |
| 87 | GOL | AR | 4261 | 6/6 | 0.78 | 0.34 | 48,48,48,48 | 0 |
| 85 | MG | 6 | 2183 | 1/1 | 0.79 | 0.58 | 71,71,71,71 | 0 |
| 85 | MG | AR | 4097 | 1/1 | 0.79 | 0.58 | 40,40,40,40 | 0 |
| 85 | MG | 4 | 236 | 1/1 | 0.79 | 0.19 | 50,50,50,50 | 0 |
| 85 | MG | 4 | 238 | 1/1 | 0.79 | 0.26 | 35,35,35,35 | 0 |
| 85 | MG | AR | 4110 | 1/1 | 0.79 | 0.50 | 46,46,46,46 | 0 |
| 85 | MG | 1 | 3751 | 1/1 | 0.79 | 0.35 | 40,40,40,40 | 0 |
| 85 | MG | 1 | 3800 | 1/1 | 0.79 | 0.61 | 45,45,45,45 | 0 |
| 85 | MG | DI | 202 | 1/1 | 0.79 | 0.36 | 56,56,56,56 | 0 |
| 85 | MG | 6 | 2092 | 1/1 | 0.79 | 0.58 | 93,93,93,93 | 0 |
| 85 | MG | 6 | 2193 | 1/1 | 0.79 | 0.45 | 55,55,55,55 | 0 |
| 85 | MG | 6 | 2167 | 1/1 | 0.79 | 0.50 | 53,53,53,53 | 0 |
| 85 | MG | 1 | 4023 | 1/1 | 0.79 | 0.48 | 57,57,57,57 | 0 |
| 85 | MG | AR | 3964 | 1/1 | 0.79 | 0.29 | 35,35,35,35 | 0 |
| 85 | MG | 1 | 3750 | 1/1 | 0.79 | 0.18 | 55,55,55,55 | 0 |
| 85 | MG | AR | 4063 | 1/1 | 0.79 | 0.12 | 54,54,54,54 | 0 |
| 85 | MG | 1 | 3994 | 1/1 | 0.79 | 0.27 | 47,47,47,47 | 0 |
| 85 | MG | 1 | 4001 | 1/1 | 0.79 | 0.45 | 47,47,47,47 | 0 |
| 87 | GOL | 6 | 2199 | 6/6 | 0.79 | 0.44 | 49,49,49,49 | 0 |
| 85 | MG | A | 2116 | 1/1 | 0.79 | 0.61 | 67,67,67,67 | 0 |
| 88 | ZN | d7 | 101 | 1/1 | 0.79 | 0.47 | 143,143,143,143 | 0 |
| 85 | MG | AT | 231 | 1/1 | 0.80 | 0.83 | 52,52,52,52 | 0 |
| 85 | MG | 1 | 3807 | 1/1 | 0.80 | 0.18 | 41,41,41,41 | 0 |
| 85 | MG | 1 | 4040 | 1/1 | 0.80 | 0.30 | 74,74,74,74 | 0 |
| 85 | MG | AR | 3986 | 1/1 | 0.80 | 0.21 | 56,56,56,56 | 0 |
| 85 | MG | AR | 4223 | 1/1 | 0.80 | 0.30 | 61,61,61,61 | 0 |
| 85 | MG | 1 | 4074 | 1/1 | 0.80 | 0.24 | 37,37,37,37 | 0 |
| 85 | MG | AR | 3998 | 1/1 | 0.80 | 0.45 | 40,40,40,40 | 0 |
| 85 | MG | 1 | 4044 | 1/1 | 0.80 | 0.32 | 47,47,47,47 | 0 |
| 85 | MG | 1 | 4127 | 1/1 | 0.80 | 0.26 | 45,45,45,45 | 0 |
| 85 | MG | 6 | 2130 | 1/1 | 0.80 | 0.31 | 66,66,66,66 | 0 |
| 85 | MG | 4 | 232 | 1/1 | 0.80 | 0.28 | 37,37,37,37 | 0 |
| 85 | MG | A | 2091 | 1/1 | 0.80 | 0.43 | 71,71,71,71 | 0 |
| 85 | MG | 1 | 3852 | 1/1 | 0.80 | 0.33 | 38,38,38,38 | 0 |
| 85 | MG | AR | 4194 | 1/1 | 0.80 | 0.27 | 53,53,53,53 | 0 |
| 85 | MG | 1 | 4014 | 1/1 | 0.80 | 0.37 | 57,57,57,57 | 0 |
| 85 | MG | AR | 4198 | 1/1 | 0.80 | 0.59 | 51,51,51,51 | 0 |
| 85 | MG | AR | 3779 | 1/1 | 0.80 | 0.38 | 73,73,73,73 | 0 |
| 87 | GOL | AR | 4262 | 6/6 | 0.80 | 0.34 | 48,48,48,48 | 0 |
| 85 | MG | 1 | 4159 | 1/1 | 0.80 | 0.39 | 43,43,43,43 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 85 | MG | A | 2083 | 1/1 | 0.81 | 0.18 | 68,68,68,68 | 0 |
| 85 | MG | 6 | 2146 | 1/1 | 0.81 | 1.00 | 80,80,80,80 | 0 |
| 84 | OHX | 1 | 3668 | 7/7 | 0.81 | 0.45 | 124,124,124,124 | 0 |
| 85 | MG | AR | 4128 | 1/1 | 0.81 | 0.21 | 55,55,55,55 | 0 |
| 85 | MG | 1 | 4027 | 1/1 | 0.81 | 0.39 | 35,35,35,35 | 0 |
| 85 | MG | AR | 4155 | 1/1 | 0.81 | 0.45 | 34,34,34,34 | 0 |
| 85 | MG | 1 | 4203 | 1/1 | 0.81 | 0.24 | 31,31,31,31 | 0 |
| 85 | MG | A | 2114 | 1/1 | 0.81 | 0.39 | 76,76,76,76 | 0 |
| 85 | MG | 1 | 4088 | 1/1 | 0.81 | 0.25 | 44,44,44,44 | 0 |
| 85 | MG | AS | 217 | 1/1 | 0.81 | 0.47 | 44,44,44,44 | 0 |
| 85 | MG | 1 | 3963 | 1/1 | 0.81 | 0.25 | 45,45,45,45 | 0 |
| 85 | MG | AR | 4169 | 1/1 | 0.81 | 0.29 | 46,46,46,46 | 0 |
| 85 | MG | 1 | 3840 | 1/1 | 0.81 | 0.31 | 78,78,78,78 | 0 |
| 85 | MG | 1 | 3998 | 1/1 | 0.81 | 0.34 | 36,36,36,36 | 0 |
| 85 | MG | AR | 3760 | 1/1 | 0.81 | 0.14 | 53,53,53,53 | 0 |
| 85 | MG | AR | 3761 | 1/1 | 0.81 | 0.33 | 31,31,31,31 | 0 |
| 85 | MG | AR | 4182 | 1/1 | 0.81 | 0.37 | 79,79,79,79 | 0 |
| 85 | MG | 1 | 3966 | 1/1 | 0.81 | 0.18 | 69,69,69,69 | 0 |
| 84 | OHX | 1 | 3717 | 7/7 | 0.81 | 0.54 | 144,144,144,145 | 0 |
| 85 | MG | CE | 407 | 1/1 | 0.81 | 0.59 | 41,41,41,41 | 0 |
| 85 | MG | CG | 304 | 1/1 | 0.81 | 0.25 | 56,56,56,56 | 0 |
| 85 | MG | CJ | 301 | 1/1 | 0.81 | 0.22 | 78,78,78,78 | 0 |
| 85 | MG | A | 2152 | 1/1 | 0.81 | 0.70 | 43,43,43,43 | 0 |
| 85 | MG | AR | 3780 | 1/1 | 0.81 | 0.17 | 88,88,88,88 | 0 |
| 85 | MG | AR | 4200 | 1/1 | 0.81 | 0.25 | 48,48,48,48 | 0 |
| 85 | MG | DE | 201 | 1/1 | 0.81 | 0.28 | 72,72,72,72 | 0 |
| 85 | MG | AR | 4206 | 1/1 | 0.81 | 0.28 | 33,33,33,33 | 0 |
| 85 | MG | 1 | 3954 | 1/1 | 0.81 | 0.15 | 46,46,46,46 | 0 |
| 85 | MG | j | 302 | 1/1 | 0.81 | 0.25 | 35,35,35,35 | 0 |
| 85 | MG | 1 | 3987 | 1/1 | 0.81 | 0.68 | 65,65,65,65 | 0 |
| 85 | MG | 1 | 4170 | 1/1 | 0.81 | 0.49 | 41,41,41,41 | 0 |
| 85 | MG | AR | 4039 | 1/1 | 0.82 | 0.38 | 56,56,56,56 | 0 |
| 85 | MG | 6 | 2152 | 1/1 | 0.82 | 0.43 | 62,62,62,62 | 0 |
| 85 | MG | AR | 4056 | 1/1 | 0.82 | 0.38 | 44,44,44,44 | 0 |
| 85 | MG | AR | 4060 | 1/1 | 0.82 | 0.27 | 70,70,70,70 | 0 |
| 85 | MG | AR | 3836 | 1/1 | 0.82 | 0.45 | 48,48,48,48 | 0 |
| 85 | MG | 1 | 3985 | 1/1 | 0.82 | 0.60 | 50,50,50,50 | 0 |
| 85 | MG | AR | 3903 | 1/1 | 0.82 | 0.69 | 39,39,39,39 | 0 |
| 85 | MG | 6 | 2072 | 1/1 | 0.82 | 0.70 | 40,40,40,40 | 0 |
| 85 | MG | AR | 3944 | 1/1 | 0.82 | 0.17 | 38,38,38,38 | 0 |
| 85 | MG | A | 2098 | 1/1 | 0.82 | 0.48 | 65,65,65,65 | 0 |
| 85 | MG | AR | 4101 | 1/1 | 0.82 | 0.25 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85 | MG | AR | 4224 | 1/1 | 0.82 | 0.49 | 47,47,47,47 | 0 |
| 85 | MG | A | 2107 | 1/1 | 0.82 | 0.31 | 80,80,80,80 | 0 |
| 85 | MG | AR | 3945 | 1/1 | 0.82 | 0.15 | 40,40,40,40 | 0 |
| 85 | MG | AR | 4239 | 1/1 | 0.82 | 0.42 | 39,39,39,39 | 0 |
| 85 | MG | 1 | 4045 | 1/1 | 0.82 | 0.34 | 39,39,39,39 | 0 |
| 85 | MG | 1 | 3925 | 1/1 | 0.82 | 0.13 | 46,46,46,46 | 0 |
| 85 | MG | 1 | 3855 | 1/1 | 0.82 | 0.32 | 44,44,44,44 | 0 |
| 85 | MG | AR | 3749 | 1/1 | 0.82 | 0.19 | 42,42,42,42 | 0 |
| 85 | MG | AR | 3751 | 1/1 | 0.82 | 0.36 | 36,36,36,36 | 0 |
| 85 | MG | AR | 3756 | 1/1 | 0.82 | 0.36 | 36,36,36,36 | 0 |
| 85 | MG | AR | 3984 | 1/1 | 0.82 | 0.65 | 50,50,50,50 | 0 |
| 85 | MG | 1 | 4013 | 1/1 | 0.82 | 0.33 | 52,52,52,52 | 0 |
| 85 | MG | 1 | 4119 | 1/1 | 0.82 | 0.28 | 35,35,35,35 | 0 |
| 85 | MG | 1 | 4060 | 1/1 | 0.82 | 0.36 | 44,44,44,44 | 0 |
| 85 | MG | AT | 221 | 1/1 | 0.82 | 0.76 | 52,52,52,52 | 0 |
| 85 | MG | A | 2140 | 1/1 | 0.82 | 0.82 | 82,82,82,82 | 0 |
| 85 | MG | 1 | 3863 | 1/1 | 0.82 | 0.20 | 55,55,55,55 | 0 |
| 85 | MG | 6 | 2099 | 1/1 | 0.82 | 0.39 | 51,51,51,51 | 0 |
| 85 | MG | AT | 228 | 1/1 | 0.82 | 0.37 | 47,47,47,47 | 0 |
| 85 | MG | 1 | 4165 | 1/1 | 0.82 | 0.40 | 24,24,24,24 | 0 |
| 85 | MG | 1 | 3955 | 1/1 | 0.82 | 0.43 | 51,51,51,51 | 0 |
| 85 | MG | CE | 403 | 1/1 | 0.82 | 0.32 | 22,22,22,22 | 0 |
| 85 | MG | AR | 4014 | 1/1 | 0.82 | 0.39 | 57,57,57,57 | 0 |
| 85 | MG | AR | 3794 | 1/1 | 0.82 | 0.24 | 34,34,34,34 | 0 |
| 85 | MG | c6 | 201 | 1/1 | 0.82 | 0.22 | 89,89,89,89 | 0 |
| 85 | MG | c9 | 201 | 1/1 | 0.82 | 0.10 | 79,79,79,79 | 0 |
| 85 | MG | 1 | 3997 | 1/1 | 0.82 | 0.17 | 54,54,54,54 | 0 |
| 85 | MG | AR | 3811 | 1/1 | 0.82 | 0.20 | 50,50,50,50 | 0 |
| 85 | MG | 1 | 3866 | 1/1 | 0.82 | 0.39 | 34,34,34,34 | 0 |
| 87 | GOL | A | 2160 | 6/6 | 0.82 | 0.35 | 60,60,60,60 | 0 |
| 85 | MG | x | 203 | 1/1 | 0.82 | 0.39 | 63,63,63,63 | 0 |
| 85 | MG | 1 | 3761 | 1/1 | 0.83 | 0.30 | 41,41,41,41 | 0 |
| 85 | MG | 6 | 2178 | 1/1 | 0.83 | 0.36 | 57,57,57,57 | 0 |
| 85 | MG | AR | 3812 | 1/1 | 0.83 | 0.42 | 32,32,32,32 | 0 |
| 85 | MG | AR | 3816 | 1/1 | 0.83 | 0.24 | 39,39,39,39 | 0 |
| 85 | MG | A | 2048 | 1/1 | 0.83 | 0.33 | 52,52,52,52 | 0 |
| 84 | OHX | A | 2034 | 7/7 | 0.83 | 0.20 | 231,232,232,232 | 0 |
| 85 | MG | 4 | 234 | 1/1 | 0.83 | 0.43 | 44,44,44,44 | 0 |
| 85 | MG | A | 2081 | 1/1 | 0.83 | 0.31 | 66,66,66,66 | 0 |
| 85 | MG | 1 | 3779 | 1/1 | 0.83 | 0.48 | 55,55,55,55 | 0 |
| 85 | MG | 6 | 2186 | 1/1 | 0.83 | 0.31 | 107,107,107,107 | 0 |
| 85 | MG | 1 | 3739 | 1/1 | 0.83 | 0.32 | 51,51,51,51 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 85 | MG | 6 | 2111 | 1/1 | 0.83 | 0.42 | 61,61,61,61 | 0 |
| 85 | MG | A | 2094 | 1/1 | 0.83 | 0.38 | 110,110,110,110 | 0 |
| 85 | MG | AR | 3911 | 1/1 | 0.83 | 0.42 | 40,40,40,40 | 0 |
| 85 | MG | AR | 4075 | 1/1 | 0.83 | 0.31 | 36,36,36,36 | 0 |
| 85 | MG | AR | 4221 | 1/1 | 0.83 | 0.28 | 35,35,35,35 | 0 |
| 85 | MG | AR | 4076 | 1/1 | 0.83 | 0.32 | 48,48,48,48 | 0 |
| 85 | MG | 1 | 3993 | 1/1 | 0.83 | 0.62 | 42,42,42,42 | 0 |
| 85 | MG | 1 | 4098 | 1/1 | 0.83 | 0.27 | 47,47,47,47 | 0 |
| 85 | MG | AR | 4089 | 1/1 | 0.83 | 0.10 | 62,62,62,62 | 0 |
| 85 | MG | AR | 4232 | 1/1 | 0.83 | 0.43 | 28,28,28,28 | 0 |
| 85 | MG | AR | 4090 | 1/1 | 0.83 | 0.49 | 57,57,57,57 | 0 |
| 85 | MG | AR | 4240 | 1/1 | 0.83 | 0.55 | 70,70,70,70 | 0 |
| 85 | MG | AR | 4094 | 1/1 | 0.83 | 0.31 | 43,43,43,43 | 0 |
| 85 | MG | A | 2127 | 1/1 | 0.83 | 0.29 | 83,83,83,83 | 0 |
| 85 | MG | AR | 4245 | 1/1 | 0.83 | 0.22 | 26,26,26,26 | 0 |
| 85 | MG | 1 | 3819 | 1/1 | 0.83 | 0.40 | 27,27,27,27 | 0 |
| 85 | MG | 1 | 3870 | 1/1 | 0.83 | 0.28 | 47,47,47,47 | 0 |
| 85 | MG | 6 | 2138 | 1/1 | 0.83 | 0.30 | 73,73,73,73 | 0 |
| 85 | MG | 6 | 2140 | 1/1 | 0.83 | 0.40 | 69,69,69,69 | 0 |
| 85 | MG | 1 | 4118 | 1/1 | 0.83 | 0.34 | 43,43,43,43 | 0 |
| 85 | MG | AR | 4116 | 1/1 | 0.83 | 0.30 | 99,99,99,99 | 0 |
| 85 | MG | v | 303 | 1/1 | 0.83 | 0.24 | 44,44,44,44 | 0 |
| 85 | MG | AR | 3973 | 1/1 | 0.83 | 0.23 | 40,40,40,40 | 0 |
| 85 | MG | AR | 3975 | 1/1 | 0.83 | 0.27 | 31,31,31,31 | 0 |
| 85 | MG | AR | 3752 | 1/1 | 0.83 | 0.21 | 37,37,37,37 | 0 |
| 85 | MG | 1 | 4050 | 1/1 | 0.83 | 0.36 | 31,31,31,31 | 0 |
| 84 | OHX | AR | 3664 | 7/7 | 0.83 | 0.43 | 180,180,181,181 | 0 |
| 85 | MG | AR | 3994 | 1/1 | 0.83 | 0.32 | 25,25,25,25 | 0 |
| 85 | MG | 6 | 2064 | 1/1 | 0.83 | 0.68 | 53,53,53,53 | 0 |
| 85 | MG | 6 | 2068 | 1/1 | 0.83 | 0.46 | 61,61,61,61 | 0 |
| 85 | MG | 6 | 2070 | 1/1 | 0.83 | 0.39 | 73,73,73,73 | 0 |
| 84 | OHX | AR | 3686 | 7/7 | 0.83 | 0.38 | 156,156,156,157 | 0 |
| 85 | MG | 1 | 3972 | 1/1 | 0.83 | 0.85 | 45,45,45,45 | 0 |
| 84 | OHX | 6 | 2045 | 7/7 | 0.83 | 0.34 | 141,141,142,142 | 0 |
| 85 | MG | 1 | 3843 | 1/1 | 0.83 | 0.41 | 24,24,24,24 | 0 |
| 85 | MG | AR | 4173 | 1/1 | 0.83 | 0.31 | 53,53,53,53 | 0 |
| 85 | MG | AR | 3841 | 1/1 | 0.84 | 0.29 | 54,54,54,54 | 0 |
| 85 | MG | 1 | 4145 | 1/1 | 0.84 | 0.33 | 42,42,42,42 | 0 |
| 85 | MG | 1 | 4070 | 1/1 | 0.84 | 0.20 | 68,68,68,68 | 0 |
| 85 | MG | 1 | 3853 | 1/1 | 0.84 | 0.55 | 48,48,48,48 | 0 |
| 85 | MG | AR | 4086 | 1/1 | 0.84 | 0.40 | 42,42,42,42 | 0 |
| 85 | MG | 1 | 4202 | 1/1 | 0.84 | 0.56 | 19,19,19,19 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85 | MG | 1 | 4003 | 1/1 | 0.84 | 0.35 | 79,79,79,79 | 0 |
| 85 | MG | AR | 4188 | 1/1 | 0.84 | 1.10 | 31,31,31,31 | 0 |
| 84 | OHX | AR | 3719 | 7/7 | 0.84 | 0.42 | 133,133,133,133 | 0 |
| 85 | MG | 1 | 4006 | 1/1 | 0.84 | 0.57 | 47,47,47,47 | 0 |
| 85 | MG | AR | 4019 | 1/1 | 0.84 | 0.27 | 45,45,45,45 | 0 |
| 85 | MG | AT | 226 | 1/1 | 0.84 | 0.30 | 63,63,63,63 | 0 |
| 85 | MG | AR | 4021 | 1/1 | 0.84 | 0.17 | 82,82,82,82 | 0 |
| 85 | MG | 1 | 4091 | 1/1 | 0.84 | 0.32 | 47,47,47,47 | 0 |
| 85 | MG | AR | 3960 | 1/1 | 0.84 | 0.21 | 41,41,41,41 | 0 |
| 85 | MG | 6 | 2118 | 1/1 | 0.84 | 0.14 | 93,93,93,93 | 0 |
| 85 | MG | AR | 4113 | 1/1 | 0.84 | 0.58 | 37,37,37,37 | 0 |
| 85 | MG | AR | 4032 | 1/1 | 0.84 | 0.37 | 48,48,48,48 | 0 |
| 85 | MG | 1 | 3931 | 1/1 | 0.84 | 0.53 | 32,32,32,32 | 0 |
| 85 | MG | AR | 4035 | 1/1 | 0.84 | 0.38 | 43,43,43,43 | 0 |
| 85 | MG | CP | 502 | 1/1 | 0.84 | 0.42 | 45,45,45,45 | 0 |
| 85 | MG | CQ | 204 | 1/1 | 0.84 | 0.41 | 30,30,30,30 | 0 |
| 85 | MG | CR | 202 | 1/1 | 0.84 | 0.28 | 29,29,29,29 | 0 |
| 85 | MG | AB | 207 | 1/1 | 0.84 | 0.24 | 34,34,34,34 | 0 |
| 85 | MG | 6 | 2173 | 1/1 | 0.84 | 0.73 | 48,48,48,48 | 0 |
| 85 | MG | AR | 4044 | 1/1 | 0.84 | 0.56 | 60,60,60,60 | 0 |
| 85 | MG | AR | 4045 | 1/1 | 0.84 | 0.30 | 55,55,55,55 | 0 |
| 85 | MG | A | 2159 | 1/1 | 0.84 | 0.93 | 64,64,64,64 | 0 |
| 85 | MG | AR | 4234 | 1/1 | 0.84 | 0.45 | 32,32,32,32 | 0 |
| 85 | MG | A | 2047 | 1/1 | 0.84 | 0.65 | 55,55,55,55 | 0 |
| 85 | MG | AR | 4046 | 1/1 | 0.84 | 0.26 | 46,46,46,46 | 0 |
| 85 | MG | 1 | 4160 | 1/1 | 0.84 | 0.32 | 34,34,34,34 | 0 |
| 84 | OHX | AR | 3717 | 7/7 | 0.84 | 0.42 | 144,144,144,144 | 0 |
| 85 | MG | A | 2068 | 1/1 | 0.84 | 0.56 | 84,84,84,84 | 0 |
| 85 | MG | A | 2069 | 1/1 | 0.84 | 0.49 | 58,58,58,58 | 0 |
| 85 | MG | 1 | 4163 | 1/1 | 0.84 | 0.24 | 44,44,44,44 | 0 |
| 85 | MG | AR | 4253 | 1/1 | 0.84 | 0.17 | 41,41,41,41 | 0 |
| 85 | MG | 1 | 4065 | 1/1 | 0.84 | 0.31 | 48,48,48,48 | 0 |
| 85 | MG | 1 | 3940 | 1/1 | 0.85 | 0.37 | 43,43,43,43 | 0 |
| 85 | MG | A | 2089 | 1/1 | 0.85 | 0.19 | 90,90,90,90 | 0 |
| 85 | MG | 1 | 3967 | 1/1 | 0.85 | 0.20 | 38,38,38,38 | 0 |
| 85 | MG | 1 | 3799 | 1/1 | 0.85 | 0.41 | 37,37,37,37 | 0 |
| 85 | MG | A | 2095 | 1/1 | 0.85 | 0.25 | 96,96,96,96 | 0 |
| 85 | MG | 1 | 3754 | 1/1 | 0.85 | 0.52 | 37,37,37,37 | 0 |
| 85 | MG | 1 | 4111 | 1/1 | 0.85 | 0.55 | 44,44,44,44 | 0 |
| 85 | MG | A | 2101 | 1/1 | 0.85 | 0.38 | 64,64,64,64 | 0 |
| 85 | MG | AS | 226 | 1/1 | 0.85 | 0.21 | 67,67,67,67 | 0 |
| 84 | OHX | AR | 3705 | 7/7 | 0.85 | 0.36 | 141,142,142,142 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85 | MG | AR | 3988 | 1/1 | 0.85 | 0.81 | 50,50,50,50 | 0 |
| 85 | MG | 1 | 3984 | 1/1 | 0.85 | 0.27 | 70,70,70,70 | 0 |
| 85 | MG | 6 | 2145 | 1/1 | 0.85 | 0.20 | 59,59,59,59 | 0 |
| 85 | MG | 1 | 4064 | 1/1 | 0.85 | 0.30 | 58,58,58,58 | 0 |
| 85 | MG | AR | 4183 | 1/1 | 0.85 | 0.23 | 55,55,55,55 | 0 |
| 85 | MG | 1 | 3805 | 1/1 | 0.85 | 0.20 | 29,29,29,29 | 0 |
| 84 | OHX | A | 1971 | 7/7 | 0.85 | 0.23 | 149,150,151,151 | 0 |
| 85 | MG | 1 | 3874 | 1/1 | 0.85 | 0.55 | 49,49,49,49 | 0 |
| 85 | MG | AR | 4093 | 1/1 | 0.85 | 0.37 | 46,46,46,46 | 0 |
| 85 | MG | AR | 3862 | 1/1 | 0.85 | 0.21 | 56,56,56,56 | 0 |
| 85 | MG | AR | 4096 | 1/1 | 0.85 | 0.32 | 54,54,54,54 | 0 |
| 85 | MG | AR | 3873 | 1/1 | 0.85 | 0.46 | 31,31,31,31 | 0 |
| 85 | MG | AR | 4017 | 1/1 | 0.85 | 0.31 | 95,95,95,95 | 0 |
| 85 | MG | 4 | 220 | 1/1 | 0.85 | 0.34 | 64,64,64,64 | 0 |
| 85 | MG | AR | 4103 | 1/1 | 0.85 | 0.19 | 47,47,47,47 | 0 |
| 85 | MG | A | 2142 | 1/1 | 0.85 | 0.13 | 80,80,80,80 | 0 |
| 85 | MG | 1 | 4135 | 1/1 | 0.85 | 0.48 | 51,51,51,51 | 0 |
| 85 | MG | 1 | 4077 | 1/1 | 0.85 | 0.27 | 33,33,33,33 | 0 |
| 84 | OHX | AR | 3728 | 7/7 | 0.85 | 0.42 | 151,152,152,152 | 0 |
| 85 | MG | AR | 4025 | 1/1 | 0.85 | 0.25 | 31,31,31,31 | 0 |
| 85 | MG | 1 | 4082 | 1/1 | 0.85 | 0.30 | 35,35,35,35 | 0 |
| 85 | MG | AR | 3759 | 1/1 | 0.85 | 0.62 | 34,34,34,34 | 0 |
| 85 | MG | 1 | 3959 | 1/1 | 0.85 | 0.27 | 66,66,66,66 | 0 |
| 85 | MG | AR | 4238 | 1/1 | 0.85 | 0.38 | 36,36,36,36 | 0 |
| 85 | MG | A | 2050 | 1/1 | 0.85 | 0.39 | 67,67,67,67 | 0 |
| 85 | MG | 1 | 4042 | 1/1 | 0.85 | 0.41 | 48,48,48,48 | 0 |
| 85 | MG | AR | 3958 | 1/1 | 0.85 | 0.56 | 38,38,38,38 | 0 |
| 85 | MG | 1 | 3731 | 1/1 | 0.85 | 0.49 | 36,36,36,36 | 0 |
| 85 | MG | AR | 4140 | 1/1 | 0.85 | 0.49 | 44,44,44,44 | 0 |
| 85 | MG | 6 | 2110 | 1/1 | 0.85 | 0.54 | 54,54,54,54 | 0 |
| 85 | MG | AR | 4142 | 1/1 | 0.85 | 0.31 | 46,46,46,46 | 0 |
| 85 | MG | 1 | 3797 | 1/1 | 0.85 | 0.18 | 79,79,79,79 | 0 |
| 85 | MG | DC | 202 | 1/1 | 0.86 | 0.30 | 48,48,48,48 | 0 |
| 85 | MG | 6 | 2066 | 1/1 | 0.86 | 0.35 | 74,74,74,74 | 0 |
| 85 | MG | AR | 3954 | 1/1 | 0.86 | 0.30 | 44,44,44,44 | 0 |
| 85 | MG | 1 | 4038 | 1/1 | 0.86 | 0.72 | 41,41,41,41 | 0 |
| 85 | MG | DQ | 203 | 1/1 | 0.86 | 0.22 | 45,45,45,45 | 0 |
| 85 | MG | AR | 4187 | 1/1 | 0.86 | 0.43 | 36,36,36,36 | 0 |
| 85 | MG | AR | 3957 | 1/1 | 0.86 | 0.13 | 55,55,55,55 | 0 |
| 85 | MG | AR | 4071 | 1/1 | 0.86 | 0.27 | 39,39,39,39 | 0 |
| 85 | MG | 3 | 216 | 1/1 | 0.86 | 0.40 | 58,58,58,58 | 0 |
| 85 | MG | 1 | 3759 | 1/1 | 0.86 | 0.12 | 41,41,41,41 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85 | MG | 1 | 3926 | 1/1 | 0.86 | 0.16 | 37,37,37,37 | 0 |
| 84 | OHX | 1 | 3709 | 7/7 | 0.86 | 0.35 | 157,158,158,158 | 0 |
| 85 | MG | 6 | 2161 | 1/1 | 0.86 | 0.49 | 58,58,58,58 | 0 |
| 84 | OHX | 6 | 2046 | 7/7 | 0.86 | 0.36 | 151,152,152,152 | 0 |
| 85 | MG | A | 2075 | 1/1 | 0.86 | 0.43 | 74,74,74,74 | 0 |
| 85 | MG | 1 | 3936 | 1/1 | 0.86 | 0.54 | 61,61,61,61 | 0 |
| 84 | OHX | 1 | 3714 | 7/7 | 0.86 | 0.51 | 146,147,147,148 | 0 |
| 85 | MG | AR | 4092 | 1/1 | 0.86 | 0.32 | 47,47,47,47 | 0 |
| 85 | MG | AR | 3982 | 1/1 | 0.86 | 0.24 | 53,53,53,53 | 0 |
| 85 | MG | 6 | 2087 | 1/1 | 0.86 | 0.30 | 56,56,56,56 | 0 |
| 84 | OHX | AR | 3734 | 7/7 | 0.86 | 0.55 | 148,148,148,149 | 0 |
| 85 | MG | A | 2092 | 1/1 | 0.86 | 0.27 | 91,91,91,91 | 0 |
| 85 | MG | 6 | 2090 | 1/1 | 0.86 | 0.31 | 49,49,49,49 | 0 |
| 85 | MG | AR | 3991 | 1/1 | 0.86 | 0.14 | 98,98,98,98 | 0 |
| 84 | OHX | 1 | 3702 | 7/7 | 0.86 | 0.22 | 219,219,219,219 | 0 |
| 85 | MG | 1 | 3981 | 1/1 | 0.86 | 0.50 | 50,50,50,50 | 0 |
| 85 | MG | 6 | 2105 | 1/1 | 0.86 | 0.48 | 64,64,64,64 | 0 |
| 85 | MG | AR | 3814 | 1/1 | 0.86 | 0.31 | 105,105,105,105 | 0 |
| 85 | MG | 1 | 4007 | 1/1 | 0.86 | 0.42 | 29,29,29,29 | 0 |
| 85 | MG | A | 2109 | 1/1 | 0.86 | 0.41 | 60,60,60,60 | 0 |
| 85 | MG | A | 2110 | 1/1 | 0.86 | 0.67 | 116,116,116,116 | 0 |
| 85 | MG | 1 | 4009 | 1/1 | 0.86 | 0.66 | 42,42,42,42 | 0 |
| 85 | MG | AR | 4248 | 1/1 | 0.86 | 0.94 | 45,45,45,45 | 0 |
| 85 | MG | 6 | 2115 | 1/1 | 0.86 | 0.41 | 85,85,85,85 | 0 |
| 85 | MG | AR | 4118 | 1/1 | 0.86 | 0.41 | 31,31,31,31 | 0 |
| 85 | MG | AR | 3829 | 1/1 | 0.86 | 0.66 | 66,66,66,66 | 0 |
| 85 | MG | AR | 4120 | 1/1 | 0.86 | 0.27 | 31,31,31,31 | 0 |
| 84 | OHX | A | 1946 | 7/7 | 0.86 | 0.22 | 165,166,166,167 | 0 |
| 85 | MG | 1 | 3752 | 1/1 | 0.86 | 0.42 | 57,57,57,57 | 0 |
| 85 | MG | AR | 3840 | 1/1 | 0.86 | 0.31 | 47,47,47,47 | 0 |
| 85 | MG | AR | 4127 | 1/1 | 0.86 | 0.17 | 77,77,77,77 | 0 |
| 85 | MG | 6 | 2122 | 1/1 | 0.86 | 0.48 | 61,61,61,61 | 0 |
| 85 | MG | AR | 3852 | 1/1 | 0.86 | 0.24 | 37,37,37,37 | 0 |
| 85 | MG | 1 | 4183 | 1/1 | 0.86 | 0.17 | 44,44,44,44 | 0 |
| 85 | MG | AR | 4029 | 1/1 | 0.86 | 0.22 | 42,42,42,42 | 0 |
| 85 | MG | AR | 4145 | 1/1 | 0.86 | 0.20 | 70,70,70,70 | 0 |
| 85 | MG | AR | 4146 | 1/1 | 0.86 | 0.19 | 34,34,34,34 | 0 |
| 85 | MG | AT | 225 | 1/1 | 0.86 | 0.91 | 53,53,53,53 | 0 |
| 85 | MG | v | 304 | 1/1 | 0.86 | 0.62 | 52,52,52,52 | 0 |
| 85 | MG | AT | 227 | 1/1 | 0.86 | 0.89 | 79,79,79,79 | 0 |
| 85 | MG | 1 | 3953 | 1/1 | 0.86 | 0.20 | 46,46,46,46 | 0 |
| 85 | MG | AR | 4157 | 1/1 | 0.86 | 0.28 | 75,75,75,75 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85 | MG | A | 2156 | 1/1 | 0.86 | 0.62 | 45,45,45,45 | 0 |
| 85 | MG | AR | 4159 | 1/1 | 0.86 | 0.38 | 36,36,36,36 | 0 |
| 85 | MG | T | 202 | 1/1 | 0.86 | 0.09 | 97,97,97,97 | 0 |
| 85 | MG | U | 201 | 1/1 | 0.86 | 0.42 | 76,76,76,76 | 0 |
| 85 | MG | AR | 3894 | 1/1 | 0.86 | 0.53 | 45,45,45,45 | 0 |
| 85 | MG | 6 | 2195 | 1/1 | 0.86 | 0.65 | 35,35,35,35 | 0 |
| 85 | MG | AR | 4164 | 1/1 | 0.86 | 0.23 | 41,41,41,41 | 0 |
| 84 | OHX | 1 | 3724 | 7/7 | 0.86 | 0.22 | 113,113,113,113 | 0 |
| 85 | MG | AB | 202 | 1/1 | 0.86 | 0.31 | 29,29,29,29 | 0 |
| 87 | GOL | v | 305 | 6/6 | 0.86 | 0.26 | 38,38,38,38 | 0 |
| 85 | MG | AR | 3935 | 1/1 | 0.86 | 0.62 | 49,49,49,49 | 0 |
| 85 | MG | 6 | 2059 | 1/1 | 0.86 | 0.43 | 70,70,70,70 | 0 |
| 85 | MG | 1 | 3832 | 1/1 | 0.86 | 0.41 | 26,26,26,26 | 0 |
| 85 | MG | CR | 203 | 1/1 | 0.86 | 0.15 | 95,95,95,95 | 0 |
| 85 | MG | CR | 204 | 1/1 | 0.86 | 0.21 | 46,46,46,46 | 0 |
| 85 | MG | 1 | 3908 | 1/1 | 0.87 | 0.50 | 62,62,62,62 | 0 |
| 85 | MG | 1 | 3961 | 1/1 | 0.87 | 0.19 | 40,40,40,40 | 0 |
| 85 | MG | A | 2088 | 1/1 | 0.87 | 0.53 | 59,59,59,59 | 0 |
| 85 | MG | 1 | 4000 | 1/1 | 0.87 | 0.23 | 43,43,43,43 | 0 |
| 84 | OHX | AR | 3741 | 7/7 | 0.87 | 0.38 | 207,208,208,208 | 0 |
| 85 | MG | 1 | 4193 | 1/1 | 0.87 | 0.37 | 23,23,23,23 | 0 |
| 84 | OHX | 1 | 3708 | 7/7 | 0.87 | 0.39 | 134,134,134,134 | 0 |
| 85 | MG | 1 | 4128 | 1/1 | 0.87 | 0.45 | 51,51,51,51 | 0 |
| 85 | MG | 1 | 4210 | 1/1 | 0.87 | 0.30 | 24,24,24,24 | 0 |
| 85 | MG | 6 | 2079 | 1/1 | 0.87 | 0.24 | 45,45,45,45 | 0 |
| 85 | MG | 6 | 2164 | 1/1 | 0.87 | 0.35 | 53,53,53,53 | 0 |
| 85 | MG | AR | 4080 | 1/1 | 0.87 | 0.51 | 32,32,32,32 | 0 |
| 85 | MG | 1 | 4211 | 1/1 | 0.87 | 0.63 | 42,42,42,42 | 0 |
| 84 | OHX | z | 201 | 7/7 | 0.87 | 0.39 | 155,156,157,157 | 0 |
| 85 | MG | 6 | 2169 | 1/1 | 0.87 | 0.63 | 49,49,49,49 | 0 |
| 84 | OHX | A | 2007 | 7/7 | 0.87 | 0.26 | 200,200,201,201 | 0 |
| 85 | MG | 1 | 3971 | 1/1 | 0.87 | 0.46 | 35,35,35,35 | 0 |
| 85 | MG | 1 | 4138 | 1/1 | 0.87 | 0.28 | 33,33,33,33 | 0 |
| 85 | MG | 1 | 3845 | 1/1 | 0.87 | 0.40 | 18,18,18,18 | 0 |
| 84 | OHX | A | 2025 | 7/7 | 0.87 | 0.48 | 173,173,173,173 | 0 |
| 84 | OHX | AR | 3640 | 7/7 | 0.87 | 0.32 | 126,126,126,126 | 0 |
| 85 | MG | CF | 403 | 1/1 | 0.87 | 0.40 | 34,34,34,34 | 0 |
| 85 | MG | 1 | 3944 | 1/1 | 0.87 | 0.48 | 32,32,32,32 | 0 |
| 85 | MG | 1 | 3767 | 1/1 | 0.87 | 0.12 | 60,60,60,60 | 0 |
| 85 | MG | A | 2129 | 1/1 | 0.87 | 0.30 | 57,57,57,57 | 0 |
| 85 | MG | CL | 302 | 1/1 | 0.87 | 0.36 | 68,68,68,68 | 0 |
| 84 | OHX | AR | 3652 | 7/7 | 0.87 | 0.44 | 112,112,113,113 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 85 | MG | A | 2134 | 1/1 | 0.87 | 0.35 | 70,70,70,70 | 0 |
| 85 | MG | AR | 4207 | 1/1 | 0.87 | 0.50 | 48,48,48,48 | 0 |
| 85 | MG | 1 | 4154 | 1/1 | 0.87 | 0.21 | 46,46,46,46 | 0 |
| 85 | MG | AR | 3842 | 1/1 | 0.87 | 0.16 | 47,47,47,47 | 0 |
| 85 | MG | AR | 3845 | 1/1 | 0.87 | 0.41 | 23,23,23,23 | 0 |
| 85 | MG | AR | 3851 | 1/1 | 0.87 | 0.29 | 38,38,38,38 | 0 |
| 85 | MG | CU | 201 | 1/1 | 0.87 | 0.40 | 38,38,38,38 | 0 |
| 85 | MG | DA | 201 | 1/1 | 0.87 | 0.28 | 48,48,48,48 | 0 |
| 85 | MG | 1 | 3778 | 1/1 | 0.87 | 0.46 | 49,49,49,49 | 0 |
| 85 | MG | AR | 4020 | 1/1 | 0.87 | 0.23 | 41,41,41,41 | 0 |
| 85 | MG | n | 201 | 1/1 | 0.87 | 0.26 | 43,43,43,43 | 0 |
| 85 | MG | 6 | 2120 | 1/1 | 0.87 | 0.42 | 69,69,69,69 | 0 |
| 84 | OHX | 6 | 1960 | 7/7 | 0.87 | 0.22 | 118,118,118,118 | 0 |
| 85 | MG | 1 | 3786 | 1/1 | 0.87 | 0.20 | 40,40,40,40 | 0 |
| 84 | OHX | 6 | 2040 | 7/7 | 0.87 | 0.29 | 184,184,185,185 | 0 |
| 85 | MG | AR | 4124 | 1/1 | 0.87 | 0.18 | 39,39,39,39 | 0 |
| 85 | MG | 1 | 3892 | 1/1 | 0.87 | 0.41 | 23,23,23,23 | 0 |
| 85 | MG | AR | 3913 | 1/1 | 0.87 | 0.43 | 26,26,26,26 | 0 |
| 85 | MG | s6 | 301 | 1/1 | 0.87 | 0.29 | 77,77,77,77 | 0 |
| 85 | MG | A | 2053 | 1/1 | 0.87 | 0.72 | 57,57,57,57 | 0 |
| 85 | MG | 1 | 3996 | 1/1 | 0.87 | 0.44 | 64,64,64,64 | 0 |
| 85 | MG | d4 | 201 | 1/1 | 0.87 | 0.38 | 53,53,53,53 | 0 |
| 85 | MG | 1 | 4108 | 1/1 | 0.87 | 0.21 | 42,42,42,42 | 0 |
| 85 | MG | AR | 4246 | 1/1 | 0.87 | 0.41 | 22,22,22,22 | 0 |
| 85 | MG | 6 | 2141 | 1/1 | 0.87 | 0.32 | 52,52,52,52 | 0 |
| 85 | MG | AR | 4250 | 1/1 | 0.87 | 0.80 | 59,59,59,59 | 0 |
| 85 | MG | x | 209 | 1/1 | 0.87 | 0.66 | 39,39,39,39 | 0 |
| 85 | MG | AR | 3947 | 1/1 | 0.87 | 0.50 | 44,44,44,44 | 0 |
| 85 | MG | AS | 215 | 1/1 | 0.88 | 0.36 | 58,58,58,58 | 0 |
| 85 | MG | 3 | 220 | 1/1 | 0.88 | 0.17 | 68,68,68,68 | 0 |
| 85 | MG | A | 2087 | 1/1 | 0.88 | 0.50 | 78,78,78,78 | 0 |
| 85 | MG | AR | 4051 | 1/1 | 0.88 | 0.38 | 40,40,40,40 | 0 |
| 85 | MG | 1 | 3803 | 1/1 | 0.88 | 0.42 | 41,41,41,41 | 0 |
| 85 | MG | AS | 223 | 1/1 | 0.88 | 0.28 | 41,41,41,41 | 0 |
| 85 | MG | AS | 224 | 1/1 | 0.88 | 0.24 | 55,55,55,55 | 0 |
| 85 | MG | A | 2093 | 1/1 | 0.88 | 0.14 | 100,100,100,100 | 0 |
| 85 | MG | 1 | 4137 | 1/1 | 0.88 | 0.17 | 55,55,55,55 | 0 |
| 85 | MG | 6 | 2171 | 1/1 | 0.88 | 0.25 | 56,56,56,56 | 0 |
| 85 | MG | 4 | 222 | 1/1 | 0.88 | 0.28 | 33,33,33,33 | 0 |
| 85 | MG | 1 | 3939 | 1/1 | 0.88 | 0.29 | 39,39,39,39 | 0 |
| 84 | OHX | A | 2036 | 7/7 | 0.88 | 0.15 | 252,253,253,253 | 0 |
| 84 | OHX | A | 2041 | 7/7 | 0.88 | 0.46 | 139,139,140,140 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85 | MG | 6 | 2103 | 1/1 | 0.88 | 0.33 | 69,69,69,69 | 0 |
| 85 | MG | 1 | 4084 | 1/1 | 0.88 | 0.27 | 32,32,32,32 | 0 |
| 84 | OHX | 1 | 3687 | 7/7 | 0.88 | 0.42 | 149,149,150,150 | 0 |
| 85 | MG | AR | 4175 | 1/1 | 0.88 | 0.25 | 35,35,35,35 | 0 |
| 85 | MG | 1 | 3945 | 1/1 | 0.88 | 0.29 | 57,57,57,57 | 0 |
| 85 | MG | AR | 3838 | 1/1 | 0.88 | 0.37 | 27,27,27,27 | 0 |
| 85 | MG | 1 | 4033 | 1/1 | 0.88 | 0.21 | 58,58,58,58 | 0 |
| 84 | OHX | AR | 3707 | 7/7 | 0.88 | 0.25 | 129,129,130,130 | 0 |
| 85 | MG | CE | 404 | 1/1 | 0.88 | 0.29 | 27,27,27,27 | 0 |
| 84 | OHX | AR | 3517 | 7/7 | 0.88 | 0.16 | 145,146,146,146 | 0 |
| 85 | MG | AR | 3999 | 1/1 | 0.88 | 0.30 | 44,44,44,44 | 0 |
| 85 | MG | 1 | 3785 | 1/1 | 0.88 | 0.45 | 25,25,25,25 | 0 |
| 84 | OHX | 6 | 2018 | 7/7 | 0.88 | 0.23 | 189,189,189,189 | 0 |
| 85 | MG | 1 | 3787 | 1/1 | 0.88 | 0.46 | 46,46,46,46 | 0 |
| 85 | MG | AR | 3861 | 1/1 | 0.88 | 0.37 | 30,30,30,30 | 0 |
| 85 | MG | A | 2133 | 1/1 | 0.88 | 0.20 | 72,72,72,72 | 0 |
| 85 | MG | 1 | 3897 | 1/1 | 0.88 | 0.21 | 46,46,46,46 | 0 |
| 85 | MG | AR | 3868 | 1/1 | 0.88 | 0.46 | 25,25,25,25 | 0 |
| 85 | MG | 1 | 4162 | 1/1 | 0.88 | 0.25 | 40,40,40,40 | 0 |
| 85 | MG | 1 | 4110 | 1/1 | 0.88 | 0.24 | 30,30,30,30 | 0 |
| 84 | OHX | AR | 3720 | 7/7 | 0.88 | 0.33 | 152,152,152,152 | 0 |
| 85 | MG | x | 208 | 1/1 | 0.88 | 0.33 | 46,46,46,46 | 0 |
| 85 | MG | AR | 4023 | 1/1 | 0.88 | 0.23 | 31,31,31,31 | 0 |
| 85 | MG | AR | 3907 | 1/1 | 0.88 | 0.63 | 25,25,25,25 | 0 |
| 85 | MG | 1 | 4113 | 1/1 | 0.88 | 0.26 | 57,57,57,57 | 0 |
| 85 | MG | 1 | 4115 | 1/1 | 0.88 | 0.23 | 36,36,36,36 | 0 |
| 84 | OHX | AR | 3722 | 7/7 | 0.88 | 0.31 | 140,141,141,141 | 0 |
| 85 | MG | DL | 102 | 1/1 | 0.88 | 0.50 | 39,39,39,39 | 0 |
| 84 | OHX | AR | 3726 | 7/7 | 0.88 | 0.42 | 118,118,118,118 | 0 |
| 85 | MG | 1 | 3927 | 1/1 | 0.88 | 0.24 | 42,42,42,42 | 0 |
| 85 | MG | AR | 4126 | 1/1 | 0.88 | 0.69 | 83,83,83,83 | 0 |
| 85 | MG | 1 | 4125 | 1/1 | 0.88 | 0.38 | 23,23,23,23 | 0 |
| 85 | MG | 1 | 3758 | 1/1 | 0.88 | 0.50 | 32,32,32,32 | 0 |
| 85 | MG | AR | 4130 | 1/1 | 0.88 | 0.15 | 31,31,31,31 | 0 |
| 84 | OHX | AR | 3690 | 7/7 | 0.88 | 0.47 | 117,118,118,118 | 0 |
| 85 | MG | 1 | 3933 | 1/1 | 0.88 | 0.11 | 49,49,49,49 | 0 |
| 85 | MG | 3 | 212 | 1/1 | 0.88 | 0.44 | 62,62,62,62 | 0 |
| 85 | MG | AR | 4251 | 1/1 | 0.88 | 0.41 | 59,59,59,59 | 0 |
| 85 | MG | 1 | 3934 | 1/1 | 0.88 | 0.44 | 54,54,54,54 | 0 |
| 85 | MG | A | 2070 | 1/1 | 0.88 | 0.53 | 79,79,79,79 | 0 |
| 85 | MG | AR | 4047 | 1/1 | 0.88 | 0.14 | 54,54,54,54 | 0 |
| 85 | MG | A | 2080 | 1/1 | 0.88 | 0.39 | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 85 | MG | AR | 4149 | 1/1 | 0.88 | 0.38 | 66,66,66,66 | 0 |
| 85 | MG | AR | 4150 | 1/1 | 0.88 | 0.18 | 44,44,44,44 | 0 |
| 85 | MG | DI | 201 | 1/1 | 0.89 | 0.22 | 68,68,68,68 | 0 |
| 85 | MG | AR | 4050 | 1/1 | 0.89 | 0.31 | 91,91,91,91 | 0 |
| 85 | MG | 3 | 211 | 1/1 | 0.89 | 0.35 | 38,38,38,38 | 0 |
| 85 | MG | AR | 4186 | 1/1 | 0.89 | 0.21 | 33,33,33,33 | 0 |
| 85 | MG | 1 | 3873 | 1/1 | 0.89 | 0.23 | 48,48,48,48 | 0 |
| 85 | MG | AR | 4059 | 1/1 | 0.89 | 0.20 | 47,47,47,47 | 0 |
| 85 | MG | 1 | 3777 | 1/1 | 0.89 | 0.17 | 30,30,30,30 | 0 |
| 85 | MG | 6 | 2190 | 1/1 | 0.89 | 0.48 | 66,66,66,66 | 0 |
| 85 | MG | AR | 4067 | 1/1 | 0.89 | 0.34 | 34,34,34,34 | 0 |
| 85 | MG | AR | 4069 | 1/1 | 0.89 | 0.23 | 26,26,26,26 | 0 |
| 85 | MG | 1 | 3881 | 1/1 | 0.89 | 0.55 | 31,31,31,31 | 0 |
| 85 | MG | AR | 4073 | 1/1 | 0.89 | 0.39 | 40,40,40,40 | 0 |
| 85 | MG | AR | 4210 | 1/1 | 0.89 | 0.72 | 54,54,54,54 | 0 |
| 85 | MG | 3 | 221 | 1/1 | 0.89 | 0.47 | 34,34,34,34 | 0 |
| 85 | MG | AR | 3943 | 1/1 | 0.89 | 0.10 | 41,41,41,41 | 0 |
| 85 | MG | 1 | 3886 | 1/1 | 0.89 | 0.41 | 21,21,21,21 | 0 |
| 85 | MG | 1 | 4130 | 1/1 | 0.89 | 0.27 | 45,45,45,45 | 0 |
| 85 | MG | AR | 4083 | 1/1 | 0.89 | 0.28 | 31,31,31,31 | 0 |
| 85 | MG | 1 | 3995 | 1/1 | 0.89 | 0.31 | 34,34,34,34 | 0 |
| 85 | MG | 4 | 228 | 1/1 | 0.89 | 0.26 | 54,54,54,54 | 0 |
| 84 | OHX | AR | 3733 | 7/7 | 0.89 | 0.33 | 187,188,188,188 | 0 |
| 84 | OHX | c4 | 201 | 7/7 | 0.89 | 0.53 | 152,152,153,153 | 0 |
| 85 | MG | 1 | 3726 | 1/1 | 0.89 | 0.84 | 54,54,54,54 | 0 |
| 85 | MG | 1 | 3999 | 1/1 | 0.89 | 0.33 | 41,41,41,41 | 0 |
| 85 | MG | 1 | 4073 | 1/1 | 0.89 | 0.38 | 40,40,40,40 | 0 |
| 85 | MG | 1 | 3956 | 1/1 | 0.89 | 0.54 | 34,34,34,34 | 0 |
| 85 | MG | AR | 3967 | 1/1 | 0.89 | 0.55 | 42,42,42,42 | 0 |
| 85 | MG | 6 | 2123 | 1/1 | 0.89 | 0.24 | 69,69,69,69 | 0 |
| 85 | MG | AR | 4099 | 1/1 | 0.89 | 0.16 | 41,41,41,41 | 0 |
| 85 | MG | 4 | 237 | 1/1 | 0.89 | 0.20 | 38,38,38,38 | 0 |
| 85 | MG | 1 | 3915 | 1/1 | 0.89 | 0.12 | 36,36,36,36 | 0 |
| 85 | MG | 4 | 240 | 1/1 | 0.89 | 0.57 | 32,32,32,32 | 0 |
| 85 | MG | AR | 3764 | 1/1 | 0.89 | 0.34 | 33,33,33,33 | 0 |
| 85 | MG | 6 | 2134 | 1/1 | 0.89 | 0.22 | 80,80,80,80 | 0 |
| 85 | MG | AR | 3777 | 1/1 | 0.89 | 0.31 | 37,37,37,37 | 0 |
| 85 | MG | 1 | 4080 | 1/1 | 0.89 | 0.22 | 35,35,35,35 | 0 |
| 84 | OHX | 6 | 2051 | 7/7 | 0.89 | 0.29 | 172,172,172,173 | 0 |
| 85 | MG | 1 | 3960 | 1/1 | 0.89 | 0.21 | 33,33,33,33 | 0 |
| 85 | MG | 6 | 2144 | 1/1 | 0.89 | 0.38 | 74,74,74,74 | 0 |
| 85 | MG | r | 302 | 1/1 | 0.89 | 0.22 | 37,37,37,37 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 85 | MG | 1 | 4005 | 1/1 | 0.89 | 0.35 | 36,36,36,36 | 0 |
| 85 | MG | 6 | 2149 | 1/1 | 0.89 | 0.32 | 46,46,46,46 | 0 |
| 85 | MG | 6 | 2150 | 1/1 | 0.89 | 0.13 | 77,77,77,77 | 0 |
| 85 | MG | A | 2125 | 1/1 | 0.89 | 0.85 | 56,56,56,56 | 0 |
| 84 | OHX | 6 | 1975 | 7/7 | 0.89 | 0.43 | 120,120,120,120 | 0 |
| 84 | OHX | AR | 3602 | 7/7 | 0.89 | 0.18 | 143,143,144,144 | 0 |
| 85 | MG | 1 | 3928 | 1/1 | 0.89 | 0.27 | 34,34,34,34 | 0 |
| 84 | OHX | CF | 401 | 7/7 | 0.89 | 0.31 | 146,146,147,147 | 0 |
| 84 | OHX | 6 | 2006 | 7/7 | 0.89 | 0.29 | 151,151,152,152 | 0 |
| 85 | MG | AR | 4135 | 1/1 | 0.89 | 0.18 | 62,62,62,62 | 0 |
| 85 | MG | x | 207 | 1/1 | 0.89 | 0.31 | 33,33,33,33 | 0 |
| 85 | MG | AR | 3834 | 1/1 | 0.89 | 0.47 | 33,33,33,33 | 0 |
| 85 | MG | 1 | 3932 | 1/1 | 0.89 | 0.19 | 55,55,55,55 | 0 |
| 84 | OHX | 1 | 3723 | 7/7 | 0.89 | 0.35 | 113,113,113,113 | 0 |
| 84 | OHX | A | 1985 | 7/7 | 0.89 | 0.31 | 140,140,141,141 | 0 |
| 85 | MG | AT | 229 | 1/1 | 0.89 | 0.42 | 55,55,55,55 | 0 |
| 85 | MG | AR | 4148 | 1/1 | 0.89 | 0.28 | 43,43,43,43 | 0 |
| 85 | MG | A | 2149 | 1/1 | 0.89 | 0.25 | 60,60,60,60 | 0 |
| 85 | MG | 1 | 4029 | 1/1 | 0.89 | 0.11 | 47,47,47,47 | 0 |
| 85 | MG | 1 | 4184 | 1/1 | 0.89 | 0.26 | 36,36,36,36 | 0 |
| 85 | MG | AR | 4153 | 1/1 | 0.89 | 0.19 | 88,88,88,88 | 0 |
| 85 | MG | AR | 4154 | 1/1 | 0.89 | 0.32 | 39,39,39,39 | 0 |
| 85 | MG | AR | 4028 | 1/1 | 0.89 | 0.19 | 41,41,41,41 | 0 |
| 84 | OHX | 1 | 3620 | 7/7 | 0.89 | 0.35 | 118,118,118,118 | 0 |
| 85 | MG | D | 301 | 1/1 | 0.89 | 0.58 | 58,58,58,58 | 0 |
| 85 | MG | 1 | 4036 | 1/1 | 0.89 | 0.42 | 70,70,70,70 | 0 |
| 85 | MG | 1 | 3982 | 1/1 | 0.89 | 0.37 | 32,32,32,32 | 0 |
| 84 | OHX | A | 2015 | 7/7 | 0.89 | 0.41 | 169,170,171,172 | 0 |
| 84 | OHX | 1 | 3712 | 7/7 | 0.89 | 0.34 | 133,133,133,133 | 0 |
| 85 | MG | AR | 4163 | 1/1 | 0.89 | 0.23 | 62,62,62,62 | 0 |
| 84 | OHX | 1 | 3721 | 7/7 | 0.89 | 0.35 | 127,127,127,128 | 0 |
| 84 | OHX | AR | 3729 | 7/7 | 0.89 | 0.46 | 120,120,120,121 | 0 |
| 85 | MG | AR | 4043 | 1/1 | 0.89 | 0.38 | 37,37,37,37 | 0 |
| 85 | MG | CR | 205 | 1/1 | 0.89 | 0.40 | 31,31,31,31 | 0 |
| 85 | MG | d5 | 201 | 1/1 | 0.89 | 0.09 | 71,71,71,71 | 0 |
| 85 | MG | AR | 3882 | 1/1 | 0.89 | 0.14 | 47,47,47,47 | 0 |
| 85 | MG | 1 | 4219 | 1/1 | 0.89 | 0.26 | 98,98,98,98 | 0 |
| 85 | MG | DC | 201 | 1/1 | 0.89 | 0.45 | 30,30,30,30 | 0 |
| 85 | MG | AR | 3891 | 1/1 | 0.89 | 0.27 | 69,69,69,69 | 0 |
| 85 | MG | 6 | 2085 | 1/1 | 0.89 | 0.47 | 75,75,75,75 | 0 |
| 85 | MG | AR | 3899 | 1/1 | 0.89 | 0.60 | 45,45,45,45 | 0 |
| 85 | MG | AR | 3765 | 1/1 | 0.90 | 0.39 | 71,71,71,71 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 85 | MG | AR | 3773 | 1/1 | 0.90 | 0.29 | 41,41,41,41 | 0 |
| 84 | OHX | A | 2042 | 7/7 | 0.90 | 0.21 | 172,173,173,174 | 0 |
| 84 | OHX | A | 2043 | 7/7 | 0.90 | 0.19 | 155,156,156,157 | 0 |
| 85 | MG | 1 | 4102 | 1/1 | 0.90 | 0.37 | 57,57,57,57 | 0 |
| 84 | OHX | AR | 3692 | 7/7 | 0.90 | 0.31 | 170,171,171,171 | 0 |
| 84 | OHX | 1 | 3656 | 7/7 | 0.90 | 0.50 | 143,143,143,144 | 0 |
| 85 | MG | 1 | 3818 | 1/1 | 0.90 | 0.43 | 39,39,39,39 | 0 |
| 84 | OHX | 6 | 2001 | 7/7 | 0.90 | 0.28 | 119,120,120,120 | 0 |
| 85 | MG | 1 | 3737 | 1/1 | 0.90 | 0.93 | 57,57,57,57 | 0 |
| 85 | MG | AR | 3807 | 1/1 | 0.90 | 0.38 | 25,25,25,25 | 0 |
| 84 | OHX | 1 | 3710 | 7/7 | 0.90 | 0.33 | 136,137,137,137 | 0 |
| 85 | MG | AR | 4166 | 1/1 | 0.90 | 0.16 | 38,38,38,38 | 0 |
| 85 | MG | 1 | 4116 | 1/1 | 0.90 | 0.52 | 44,44,44,44 | 0 |
| 85 | MG | 4 | 231 | 1/1 | 0.90 | 0.23 | 58,58,58,58 | 0 |
| 85 | MG | 6 | 2139 | 1/1 | 0.90 | 0.22 | 45,45,45,45 | 0 |
| 85 | MG | AR | 4033 | 1/1 | 0.90 | 0.26 | 40,40,40,40 | 0 |
| 85 | MG | 1 | 4117 | 1/1 | 0.90 | 0.31 | 41,41,41,41 | 0 |
| 85 | MG | AR | 3821 | 1/1 | 0.90 | 0.21 | 42,42,42,42 | 0 |
| 85 | MG | A | 2051 | 1/1 | 0.90 | 0.47 | 67,67,67,67 | 0 |
| 85 | MG | 1 | 3830 | 1/1 | 0.90 | 0.22 | 44,44,44,44 | 0 |
| 84 | OHX | 1 | 3501 | 7/7 | 0.90 | 0.17 | 126,126,127,127 | 0 |
| 85 | MG | AR | 4040 | 1/1 | 0.90 | 0.26 | 43,43,43,43 | 0 |
| 85 | MG | A | 2065 | 1/1 | 0.90 | 0.73 | 57,57,57,57 | 0 |
| 85 | MG | AR | 4042 | 1/1 | 0.90 | 0.12 | 57,57,57,57 | 0 |
| 85 | MG | 1 | 4015 | 1/1 | 0.90 | 0.37 | 67,67,67,67 | 0 |
| 85 | MG | 1 | 4020 | 1/1 | 0.90 | 0.39 | 34,34,34,34 | 0 |
| 84 | OHX | 6 | 2021 | 7/7 | 0.90 | 0.25 | 181,181,182,182 | 0 |
| 84 | OHX | 6 | 2039 | 7/7 | 0.90 | 0.62 | 132,133,133,134 | 0 |
| 85 | MG | AR | 4197 | 1/1 | 0.90 | 0.27 | 35,35,35,35 | 0 |
| 85 | MG | 1 | 4028 | 1/1 | 0.90 | 0.16 | 46,46,46,46 | 0 |
| 84 | OHX | 1 | 3626 | 7/7 | 0.90 | 0.35 | 124,124,124,124 | 0 |
| 85 | MG | 1 | 3851 | 1/1 | 0.90 | 0.36 | 34,34,34,34 | 0 |
| 84 | OHX | 6 | 2041 | 7/7 | 0.90 | 0.34 | 143,144,145,145 | 0 |
| 84 | OHX | 1 | 3642 | 7/7 | 0.90 | 0.45 | 135,135,136,136 | 0 |
| 84 | OHX | 1 | 3718 | 7/7 | 0.90 | 0.39 | 149,149,149,149 | 0 |
| 85 | MG | t | 201 | 1/1 | 0.90 | 0.17 | 51,51,51,51 | 0 |
| 85 | MG | 1 | 3962 | 1/1 | 0.90 | 0.41 | 39,39,39,39 | 0 |
| 85 | MG | AR | 4064 | 1/1 | 0.90 | 0.24 | 38,38,38,38 | 0 |
| 84 | OHX | 1 | 3719 | 7/7 | 0.90 | 0.52 | 120,120,121,121 | 0 |
| 85 | MG | 6 | 2166 | 1/1 | 0.90 | 0.49 | 53,53,53,53 | 0 |
| 85 | MG | AR | 4070 | 1/1 | 0.90 | 0.19 | 50,50,50,50 | 0 |
| 85 | MG | 1 | 4147 | 1/1 | 0.90 | 0.21 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 85 | MG | 1 | 3762 | 1/1 | 0.90 | 0.56 | 30,30,30,30 | 0 |
| 85 | MG | A | 2102 | 1/1 | 0.90 | 0.49 | 58,58,58,58 | 0 |
| 85 | MG | x | 205 | 1/1 | 0.90 | 0.66 | 33,33,33,33 | 0 |
| 85 | MG | A | 2106 | 1/1 | 0.90 | 0.50 | 58,58,58,58 | 0 |
| 85 | MG | 1 | 3766 | 1/1 | 0.90 | 0.16 | 73,73,73,73 | 0 |
| 85 | MG | 1 | 3869 | 1/1 | 0.90 | 0.49 | 34,34,34,34 | 0 |
| 84 | OHX | 6 | 2052 | 7/7 | 0.90 | 0.33 | 143,144,144,144 | 0 |
| 85 | MG | 1 | 4055 | 1/1 | 0.90 | 0.17 | 33,33,33,33 | 0 |
| 85 | MG | A | 2113 | 1/1 | 0.90 | 0.48 | 73,73,73,73 | 0 |
| 85 | MG | AR | 4084 | 1/1 | 0.90 | 0.22 | 34,34,34,34 | 0 |
| 85 | MG | 1 | 3771 | 1/1 | 0.90 | 0.42 | 33,33,33,33 | 0 |
| 85 | MG | 1 | 4156 | 1/1 | 0.90 | 0.19 | 44,44,44,44 | 0 |
| 85 | MG | AR | 3914 | 1/1 | 0.90 | 0.43 | 32,32,32,32 | 0 |
| 84 | OHX | AR | 3738 | 7/7 | 0.90 | 0.15 | 141,142,142,142 | 0 |
| 85 | MG | A | 2122 | 1/1 | 0.90 | 0.17 | 86,86,86,86 | 0 |
| 84 | OHX | AM | 101 | 7/7 | 0.90 | 0.43 | 121,121,121,121 | 0 |
| 85 | MG | AR | 4252 | 1/1 | 0.90 | 0.37 | 50,50,50,50 | 0 |
| 84 | OHX | 1 | 3696 | 7/7 | 0.90 | 0.39 | 146,146,147,147 | 0 |
| 84 | OHX | 1 | 3700 | 7/7 | 0.90 | 0.36 | 148,148,149,149 | 0 |
| 84 | OHX | AR | 3604 | 7/7 | 0.90 | 0.19 | 158,159,159,159 | 0 |
| 85 | MG | AR | 3946 | 1/1 | 0.90 | 0.30 | 59,59,59,59 | 0 |
| 85 | MG | AS | 213 | 1/1 | 0.90 | 0.45 | 26,26,26,26 | 0 |
| 85 | MG | A | 2132 | 1/1 | 0.90 | 0.26 | 98,98,98,98 | 0 |
| 85 | MG | 1 | 3898 | 1/1 | 0.90 | 0.46 | 33,33,33,33 | 0 |
| 85 | MG | AR | 4098 | 1/1 | 0.90 | 0.20 | 46,46,46,46 | 0 |
| 85 | MG | AS | 218 | 1/1 | 0.90 | 0.30 | 33,33,33,33 | 0 |
| 85 | MG | AR | 3948 | 1/1 | 0.90 | 0.54 | 40,40,40,40 | 0 |
| 85 | MG | 6 | 2078 | 1/1 | 0.90 | 0.45 | 42,42,42,42 | 0 |
| 84 | OHX | AR | 3631 | 7/7 | 0.90 | 0.18 | 175,176,177,177 | 0 |
| 85 | MG | 6 | 2080 | 1/1 | 0.90 | 0.64 | 69,69,69,69 | 0 |
| 85 | MG | AR | 3956 | 1/1 | 0.90 | 0.22 | 29,29,29,29 | 0 |
| 84 | OHX | 1 | 3644 | 7/7 | 0.90 | 0.25 | 166,167,167,167 | 0 |
| 85 | MG | 6 | 2082 | 1/1 | 0.90 | 0.48 | 54,54,54,54 | 0 |
| 84 | OHX | AR | 3646 | 7/7 | 0.90 | 0.37 | 108,108,108,108 | 0 |
| 85 | MG | 6 | 2198 | 1/1 | 0.90 | 0.56 | 49,49,49,49 | 0 |
| 85 | MG | 1 | 3793 | 1/1 | 0.90 | 0.30 | 37,37,37,37 | 0 |
| 85 | MG | AB | 204 | 1/1 | 0.90 | 0.29 | 52,52,52,52 | 0 |
| 84 | OHX | 3 | 209 | 7/7 | 0.90 | 0.28 | 152,152,152,152 | 0 |
| 84 | OHX | A | 2026 | 7/7 | 0.90 | 0.40 | 123,123,124,124 | 0 |
| 85 | MG | AG | 202 | 1/1 | 0.90 | 0.20 | 43,43,43,43 | 0 |
| 85 | MG | AH | 202 | 1/1 | 0.90 | 0.15 | 58,58,58,58 | 0 |
| 85 | MG | 1 | 4085 | 1/1 | 0.90 | 0.39 | 51,51,51,51 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85 | MG | AR | 3750 | 1/1 | 0.90 | 0.41 | 27,27,27,27 | 0 |
| 85 | MG | CD | 301 | 1/1 | 0.90 | 0.36 | 34,34,34,34 | 0 |
| 85 | MG | s4 | 301 | 1/1 | 0.90 | 0.23 | 59,59,59,59 | 0 |
| 85 | MG | 1 | 4198 | 1/1 | 0.90 | 0.60 | 43,43,43,43 | 0 |
| 84 | OHX | A | 2029 | 7/7 | 0.90 | 0.20 | 184,184,184,184 | 0 |
| 85 | MG | AR | 3753 | 1/1 | 0.90 | 0.33 | 26,26,26,26 | 0 |
| 85 | MG | AR | 4134 | 1/1 | 0.90 | 0.27 | 44,44,44,44 | 0 |
| 85 | MG | AR | 3755 | 1/1 | 0.90 | 0.18 | 56,56,56,56 | 0 |
| 84 | OHX | A | 2030 | 7/7 | 0.90 | 0.47 | 142,143,143,144 | 0 |
| 85 | MG | 1 | 4209 | 1/1 | 0.90 | 0.67 | 48,48,48,48 | 0 |
| 84 | OHX | x | 201 | 7/7 | 0.90 | 0.39 | 110,110,110,110 | 0 |
| 84 | OHX | 1 | 3707 | 7/7 | 0.90 | 0.40 | 125,125,126,126 | 0 |
| 84 | OHX | 1 | 3653 | 7/7 | 0.90 | 0.29 | 133,133,133,133 | 0 |
| 85 | MG | AR | 4009 | 1/1 | 0.90 | 0.34 | 37,37,37,37 | 0 |
| 85 | MG | 1 | 4035 | 1/1 | 0.91 | 0.60 | 47,47,47,47 | 0 |
| 85 | MG | 1 | 3746 | 1/1 | 0.91 | 0.41 | 26,26,26,26 | 0 |
| 85 | MG | 1 | 4037 | 1/1 | 0.91 | 0.30 | 30,30,30,30 | 0 |
| 85 | MG | 6 | 2196 | 1/1 | 0.91 | 0.76 | 48,48,48,48 | 0 |
| 84 | OHX | AR | 3665 | 7/7 | 0.91 | 0.39 | 133,133,133,133 | 0 |
| 84 | OHX | AR | 3745 | 7/7 | 0.91 | 0.34 | 128,128,128,128 | 0 |
| 85 | MG | AB | 201 | 1/1 | 0.91 | 0.28 | 34,34,34,34 | 0 |
| 84 | OHX | AS | 211 | 7/7 | 0.91 | 0.29 | 141,141,142,142 | 0 |
| 85 | MG | AB | 203 | 1/1 | 0.91 | 0.34 | 32,32,32,32 | 0 |
| 84 | OHX | AT | 213 | 7/7 | 0.91 | 0.25 | 137,137,137,137 | 0 |
| 85 | MG | AB | 205 | 1/1 | 0.91 | 0.22 | 40,40,40,40 | 0 |
| 85 | MG | AR | 4136 | 1/1 | 0.91 | 0.27 | 36,36,36,36 | 0 |
| 85 | MG | AR | 4137 | 1/1 | 0.91 | 0.48 | 79,79,79,79 | 0 |
| 85 | MG | AR | 4139 | 1/1 | 0.91 | 0.35 | 46,46,46,46 | 0 |
| 85 | MG | 1 | 3847 | 1/1 | 0.91 | 0.54 | 28,28,28,28 | 0 |
| 85 | MG | 1 | 3848 | 1/1 | 0.91 | 0.40 | 60,60,60,60 | 0 |
| 85 | MG | CX | 204 | 1/1 | 0.91 | 0.21 | 46,46,46,46 | 0 |
| 85 | MG | AR | 3979 | 1/1 | 0.91 | 0.57 | 41,41,41,41 | 0 |
| 85 | MG | 1 | 3849 | 1/1 | 0.91 | 0.44 | 23,23,23,23 | 0 |
| 84 | OHX | AR | 3677 | 7/7 | 0.91 | 0.38 | 110,111,111,111 | 0 |
| 85 | MG | AR | 4147 | 1/1 | 0.91 | 0.23 | 31,31,31,31 | 0 |
| 84 | OHX | 4 | 215 | 7/7 | 0.91 | 0.28 | 137,138,138,138 | 0 |
| 84 | OHX | A | 1970 | 7/7 | 0.91 | 0.35 | 132,132,133,133 | 0 |
| 85 | MG | 1 | 4174 | 1/1 | 0.91 | 0.83 | 55,55,55,55 | 0 |
| 85 | MG | 1 | 4058 | 1/1 | 0.91 | 0.31 | 51,51,51,51 | 0 |
| 84 | OHX | 1 | 3596 | 7/7 | 0.91 | 0.49 | 143,144,144,144 | 0 |
| 85 | MG | DQ | 204 | 1/1 | 0.91 | 0.35 | 32,32,32,32 | 0 |
| 85 | MG | 1 | 3765 | 1/1 | 0.91 | 0.49 | 21,21,21,21 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85 | MG | 1 | 3861 | 1/1 | 0.91 | 0.24 | 34,34,34,34 | 0 |
| 84 | OHX | 1 | 3695 | 7/7 | 0.91 | 0.61 | 154,154,155,155 | 0 |
| 85 | MG | 1 | 3865 | 1/1 | 0.91 | 0.32 | 45,45,45,45 | 0 |
| 85 | MG | 6 | 2109 | 1/1 | 0.91 | 0.42 | 56,56,56,56 | 0 |
| 84 | OHX | A | 1993 | 7/7 | 0.91 | 0.38 | 151,151,152,152 | 0 |
| 84 | OHX | AR | 3695 | 7/7 | 0.91 | 0.30 | 122,122,123,123 | 0 |
| 85 | MG | AR | 3770 | 1/1 | 0.91 | 0.44 | 32,32,32,32 | 0 |
| 85 | MG | A | 2056 | 1/1 | 0.91 | 0.34 | 65,65,65,65 | 0 |
| 85 | MG | AR | 3771 | 1/1 | 0.91 | 0.36 | 42,42,42,42 | 0 |
| 85 | MG | 1 | 3979 | 1/1 | 0.91 | 0.31 | 39,39,39,39 | 0 |
| 85 | MG | A | 2067 | 1/1 | 0.91 | 0.81 | 64,64,64,64 | 0 |
| 84 | OHX | 6 | 2048 | 7/7 | 0.91 | 0.35 | 173,174,174,174 | 0 |
| 84 | OHX | A | 2021 | 7/7 | 0.91 | 0.43 | 133,133,134,134 | 0 |
| 85 | MG | AR | 3778 | 1/1 | 0.91 | 0.26 | 42,42,42,42 | 0 |
| 85 | MG | 1 | 4213 | 1/1 | 0.91 | 0.64 | 50,50,50,50 | 0 |
| 84 | OHX | A | 2023 | 7/7 | 0.91 | 0.26 | 144,145,145,145 | 0 |
| 85 | MG | AR | 4176 | 1/1 | 0.91 | 0.23 | 33,33,33,33 | 0 |
| 85 | MG | AR | 4177 | 1/1 | 0.91 | 0.30 | 32,32,32,32 | 0 |
| 85 | MG | AR | 4180 | 1/1 | 0.91 | 0.39 | 48,48,48,48 | 0 |
| 84 | OHX | 1 | 3673 | 7/7 | 0.91 | 0.56 | 133,133,133,133 | 0 |
| 85 | MG | A | 2086 | 1/1 | 0.91 | 0.24 | 66,66,66,66 | 0 |
| 85 | MG | AR | 4026 | 1/1 | 0.91 | 0.33 | 60,60,60,60 | 0 |
| 85 | MG | 1 | 3884 | 1/1 | 0.91 | 0.34 | 29,29,29,29 | 0 |
| 85 | MG | AR | 4184 | 1/1 | 0.91 | 0.16 | 69,69,69,69 | 0 |
| 85 | MG | AR | 3789 | 1/1 | 0.91 | 0.39 | 36,36,36,36 | 0 |
| 85 | MG | 6 | 2127 | 1/1 | 0.91 | 0.47 | 54,54,54,54 | 0 |
| 85 | MG | AR | 3796 | 1/1 | 0.91 | 0.41 | 64,64,64,64 | 0 |
| 85 | MG | 6 | 2129 | 1/1 | 0.91 | 0.38 | 62,62,62,62 | 0 |
| 85 | MG | 1 | 3782 | 1/1 | 0.91 | 0.45 | 58,58,58,58 | 0 |
| 85 | MG | 3 | 217 | 1/1 | 0.91 | 0.36 | 40,40,40,40 | 0 |
| 84 | OHX | 1 | 3720 | 7/7 | 0.91 | 0.28 | 128,128,129,129 | 0 |
| 84 | OHX | AR | 3718 | 7/7 | 0.91 | 0.47 | 166,167,167,167 | 0 |
| 85 | MG | AR | 4205 | 1/1 | 0.91 | 0.24 | 59,59,59,59 | 0 |
| 85 | MG | AR | 3815 | 1/1 | 0.91 | 0.24 | 32,32,32,32 | 0 |
| 85 | MG | 1 | 3992 | 1/1 | 0.91 | 0.24 | 40,40,40,40 | 0 |
| 84 | OHX | 1 | 3676 | 7/7 | 0.91 | 0.30 | 149,150,150,150 | 0 |
| 85 | MG | 1 | 3899 | 1/1 | 0.91 | 0.35 | 39,39,39,39 | 0 |
| 85 | MG | AR | 3824 | 1/1 | 0.91 | 0.13 | 77,77,77,77 | 0 |
| 85 | MG | AR | 4216 | 1/1 | 0.91 | 0.20 | 44,44,44,44 | 0 |
| 85 | MG | 6 | 2142 | 1/1 | 0.91 | 0.24 | 83,83,83,83 | 0 |
| 85 | MG | 6 | 2143 | 1/1 | 0.91 | 0.31 | 75,75,75,75 | 0 |
| 85 | MG | AR | 3832 | 1/1 | 0.91 | 0.53 | 30,30,30,30 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85 | MG | 4 | 227 | 1/1 | 0.91 | 0.40 | 52,52,52,52 | 0 |
| 85 | MG | 1 | 4100 | 1/1 | 0.91 | 0.27 | 53,53,53,53 | 0 |
| 85 | MG | 1 | 3901 | 1/1 | 0.91 | 0.49 | 39,39,39,39 | 0 |
| 85 | MG | 1 | 3789 | 1/1 | 0.91 | 0.17 | 42,42,42,42 | 0 |
| 85 | MG | AR | 4231 | 1/1 | 0.91 | 0.35 | 32,32,32,32 | 0 |
| 85 | MG | 1 | 3913 | 1/1 | 0.91 | 0.59 | 28,28,28,28 | 0 |
| 84 | OHX | 6 | 2002 | 7/7 | 0.91 | 0.27 | 132,133,133,134 | 0 |
| 85 | MG | AR | 4236 | 1/1 | 0.91 | 0.42 | 23,23,23,23 | 0 |
| 85 | MG | 1 | 4109 | 1/1 | 0.91 | 0.14 | 66,66,66,66 | 0 |
| 85 | MG | 1 | 3917 | 1/1 | 0.91 | 0.26 | 30,30,30,30 | 0 |
| 85 | MG | AR | 4068 | 1/1 | 0.91 | 0.12 | 99,99,99,99 | 0 |
| 85 | MG | 1 | 3920 | 1/1 | 0.91 | 0.10 | 41,41,41,41 | 0 |
| 84 | OHX | A | 2035 | 7/7 | 0.91 | 0.48 | 130,131,131,131 | 0 |
| 84 | OHX | 6 | 2004 | 7/7 | 0.91 | 0.40 | 157,157,158,158 | 0 |
| 84 | OHX | A | 2038 | 7/7 | 0.91 | 0.34 | 146,147,147,147 | 0 |
| 84 | OHX | A | 2039 | 7/7 | 0.91 | 0.41 | 166,167,168,168 | 0 |
| 85 | MG | k | 402 | 1/1 | 0.91 | 0.37 | 37,37,37,37 | 0 |
| 85 | MG | 6 | 2165 | 1/1 | 0.91 | 0.35 | 51,51,51,51 | 0 |
| 85 | MG | AR | 3889 | 1/1 | 0.91 | 0.36 | 35,35,35,35 | 0 |
| 85 | MG | 1 | 3929 | 1/1 | 0.91 | 0.30 | 34,34,34,34 | 0 |
| 84 | OHX | 1 | 3701 | 7/7 | 0.91 | 0.31 | 139,139,140,140 | 0 |
| 85 | MG | AR | 4256 | 1/1 | 0.91 | 0.43 | 49,49,49,49 | 0 |
| 85 | MG | AR | 3892 | 1/1 | 0.91 | 0.48 | 31,31,31,31 | 0 |
| 84 | OHX | AR | 3727 | 7/7 | 0.91 | 0.23 | 187,188,188,188 | 0 |
| 85 | MG | AR | 3896 | 1/1 | 0.91 | 0.55 | 36,36,36,36 | 0 |
| 85 | MG | AR | 3897 | 1/1 | 0.91 | 0.44 | 51,51,51,51 | 0 |
| 85 | MG | 1 | 4011 | 1/1 | 0.91 | 0.37 | 44,44,44,44 | 0 |
| 84 | OHX | 6 | 2008 | 7/7 | 0.91 | 0.18 | 136,136,136,136 | 0 |
| 85 | MG | H | 301 | 1/1 | 0.91 | 0.10 | 83,83,83,83 | 0 |
| 84 | OHX | s8 | 301 | 7/7 | 0.91 | 0.32 | 167,167,168,168 | 0 |
| 84 | OHX | c3 | 201 | 7/7 | 0.91 | 0.24 | 155,156,156,157 | 0 |
| 84 | OHX | AR | 3639 | 7/7 | 0.91 | 0.22 | 138,139,139,139 | 0 |
| 85 | MG | w | 202 | 1/1 | 0.91 | 0.32 | 31,31,31,31 | 0 |
| 84 | OHX | AR | 3730 | 7/7 | 0.91 | 0.33 | 176,176,176,176 | 0 |
| 85 | MG | AR | 3922 | 1/1 | 0.91 | 0.49 | 31,31,31,31 | 0 |
| 85 | MG | AR | 4100 | 1/1 | 0.91 | 0.28 | 57,57,57,57 | 0 |
| 85 | MG | AR | 3929 | 1/1 | 0.91 | 0.37 | 25,25,25,25 | 0 |
| 85 | MG | c8 | 202 | 1/1 | 0.91 | 0.33 | 79,79,79,79 | 0 |
| 85 | MG | AR | 3934 | 1/1 | 0.91 | 0.31 | 32,32,32,32 | 0 |
| 85 | MG | 1 | 4021 | 1/1 | 0.91 | 0.15 | 44,44,44,44 | 0 |
| 85 | MG | 1 | 4022 | 1/1 | 0.91 | 0.59 | 53,53,53,53 | 0 |
| 85 | MG | d6 | 101 | 1/1 | 0.91 | 0.34 | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84 | OHX | 1 | 3659 | 7/7 | 0.91 | 0.32 | 140,140,140,141 | 0 |
| 85 | MG | 1 | 3732 | 1/1 | 0.91 | 0.44 | 26,26,26,26 | 0 |
| 84 | OHX | 3 | 205 | 7/7 | 0.91 | 0.21 | 127,128,128,128 | 0 |
| 84 | OHX | 1 | 3716 | 7/7 | 0.91 | 0.45 | 138,138,139,139 | 0 |
| 85 | MG | 1 | 4030 | 1/1 | 0.91 | 0.73 | 72,72,72,72 | 0 |
| 84 | OHX | 4 | 213 | 7/7 | 0.91 | 0.31 | 117,117,117,117 | 0 |
| 84 | OHX | CF | 402 | 7/7 | 0.92 | 0.34 | 145,146,146,146 | 0 |
| 85 | MG | AT | 220 | 1/1 | 0.92 | 0.47 | 53,53,53,53 | 0 |
| 84 | OHX | CG | 302 | 7/7 | 0.92 | 0.38 | 147,147,147,148 | 0 |
| 85 | MG | 1 | 3755 | 1/1 | 0.92 | 0.42 | 36,36,36,36 | 0 |
| 85 | MG | 1 | 4079 | 1/1 | 0.92 | 0.21 | 97,97,97,97 | 0 |
| 85 | MG | 1 | 3969 | 1/1 | 0.92 | 0.21 | 41,41,41,41 | 0 |
| 85 | MG | 1 | 3970 | 1/1 | 0.92 | 0.30 | 31,31,31,31 | 0 |
| 85 | MG | 4 | 225 | 1/1 | 0.92 | 0.32 | 25,25,25,25 | 0 |
| 84 | OHX | AR | 3668 | 7/7 | 0.92 | 0.37 | 131,132,132,132 | 0 |
| 85 | MG | 1 | 3862 | 1/1 | 0.92 | 0.46 | 52,52,52,52 | 0 |
| 85 | MG | 1 | 3974 | 1/1 | 0.92 | 0.22 | 28,28,28,28 | 0 |
| 85 | MG | AR | 3902 | 1/1 | 0.92 | 0.57 | 42,42,42,42 | 0 |
| 84 | OHX | 6 | 2033 | 7/7 | 0.92 | 0.39 | 150,151,151,152 | 0 |
| 85 | MG | 1 | 3864 | 1/1 | 0.92 | 0.25 | 38,38,38,38 | 0 |
| 85 | MG | 1 | 4089 | 1/1 | 0.92 | 0.21 | 42,42,42,42 | 0 |
| 84 | OHX | 1 | 3627 | 7/7 | 0.92 | 0.28 | 141,142,142,143 | 0 |
| 84 | OHX | A | 1981 | 7/7 | 0.92 | 0.16 | 194,195,195,195 | 0 |
| 85 | MG | 1 | 3764 | 1/1 | 0.92 | 0.58 | 41,41,41,41 | 0 |
| 84 | OHX | 1 | 3692 | 7/7 | 0.92 | 0.29 | 113,113,113,113 | 0 |
| 85 | MG | AR | 3924 | 1/1 | 0.92 | 0.49 | 27,27,27,27 | 0 |
| 85 | MG | AR | 3927 | 1/1 | 0.92 | 0.45 | 35,35,35,35 | 0 |
| 85 | MG | 1 | 4099 | 1/1 | 0.92 | 0.23 | 44,44,44,44 | 0 |
| 85 | MG | 1 | 3871 | 1/1 | 0.92 | 0.47 | 30,30,30,30 | 0 |
| 84 | OHX | l | 401 | 7/7 | 0.92 | 0.41 | 143,143,144,144 | 0 |
| 84 | OHX | A | 2006 | 7/7 | 0.92 | 0.31 | 149,150,150,150 | 0 |
| 85 | MG | l | 402 | 1/1 | 0.92 | 0.33 | 57,57,57,57 | 0 |
| 85 | MG | 1 | 3877 | 1/1 | 0.92 | 0.71 | 36,36,36,36 | 0 |
| 85 | MG | 1 | 4107 | 1/1 | 0.92 | 0.16 | 40,40,40,40 | 0 |
| 85 | MG | o | 302 | 1/1 | 0.92 | 0.21 | 39,39,39,39 | 0 |
| 85 | MG | 1 | 3990 | 1/1 | 0.92 | 0.30 | 24,24,24,24 | 0 |
| 85 | MG | DA | 202 | 1/1 | 0.92 | 0.20 | 45,45,45,45 | 0 |
| 84 | OHX | AR | 3694 | 7/7 | 0.92 | 0.33 | 146,147,147,147 | 0 |
| 84 | OHX | A | 2011 | 7/7 | 0.92 | 0.23 | 149,149,150,150 | 0 |
| 84 | OHX | A | 2012 | 7/7 | 0.92 | 0.37 | 139,140,140,140 | 0 |
| 85 | MG | t | 203 | 1/1 | 0.92 | 0.42 | 29,29,29,29 | 0 |
| 84 | OHX | 1 | 3665 | 7/7 | 0.92 | 0.36 | 129,129,129,129 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 84 | OHX | A | 2017 | 7/7 | 0.92 | 0.31 | 158,159,160,160 | 0 |
| 84 | OHX | A | 2019 | 7/7 | 0.92 | 0.29 | 176,176,176,176 | 0 |
| 85 | MG | AR | 3961 | 1/1 | 0.92 | 0.53 | 43,43,43,43 | 0 |
| 84 | OHX | 1 | 3666 | 7/7 | 0.92 | 0.42 | 117,118,118,118 | 0 |
| 85 | MG | x | 204 | 1/1 | 0.92 | 0.35 | 28,28,28,28 | 0 |
| 84 | OHX | 1 | 3698 | 7/7 | 0.92 | 0.30 | 162,163,163,163 | 0 |
| 85 | MG | 1 | 3905 | 1/1 | 0.92 | 0.47 | 38,38,38,38 | 0 |
| 84 | OHX | AR | 3709 | 7/7 | 0.92 | 0.28 | 110,111,111,111 | 0 |
| 85 | MG | 1 | 4002 | 1/1 | 0.92 | 0.56 | 37,37,37,37 | 0 |
| 84 | OHX | AR | 3716 | 7/7 | 0.92 | 0.37 | 143,143,143,143 | 0 |
| 85 | MG | AR | 3977 | 1/1 | 0.92 | 0.41 | 41,41,41,41 | 0 |
| 85 | MG | 6 | 2056 | 1/1 | 0.92 | 0.22 | 77,77,77,77 | 0 |
| 85 | MG | AR | 3980 | 1/1 | 0.92 | 0.86 | 40,40,40,40 | 0 |
| 85 | MG | A | 2057 | 1/1 | 0.92 | 0.46 | 70,70,70,70 | 0 |
| 85 | MG | A | 2061 | 1/1 | 0.92 | 0.50 | 59,59,59,59 | 0 |
| 84 | OHX | 6 | 2050 | 7/7 | 0.92 | 0.47 | 159,159,160,160 | 0 |
| 85 | MG | 6 | 2060 | 1/1 | 0.92 | 0.34 | 47,47,47,47 | 0 |
| 84 | OHX | 1 | 3651 | 7/7 | 0.92 | 0.26 | 130,130,131,131 | 0 |
| 84 | OHX | 6 | 1977 | 7/7 | 0.92 | 0.25 | 150,151,151,152 | 0 |
| 85 | MG | AR | 3747 | 1/1 | 0.92 | 0.30 | 23,23,23,23 | 0 |
| 85 | MG | AR | 3992 | 1/1 | 0.92 | 0.64 | 67,67,67,67 | 0 |
| 85 | MG | AR | 4165 | 1/1 | 0.92 | 0.21 | 43,43,43,43 | 0 |
| 84 | OHX | 1 | 3672 | 7/7 | 0.92 | 0.41 | 147,147,147,148 | 0 |
| 85 | MG | 1 | 4008 | 1/1 | 0.92 | 0.29 | 37,37,37,37 | 0 |
| 85 | MG | AR | 3996 | 1/1 | 0.92 | 0.33 | 56,56,56,56 | 0 |
| 84 | OHX | AR | 3721 | 7/7 | 0.92 | 0.38 | 139,139,140,140 | 0 |
| 84 | OHX | A | 2037 | 7/7 | 0.92 | 0.44 | 153,154,154,155 | 0 |
| 85 | MG | 1 | 3802 | 1/1 | 0.92 | 0.18 | 86,86,86,86 | 0 |
| 85 | MG | 6 | 2077 | 1/1 | 0.92 | 0.54 | 39,39,39,39 | 0 |
| 84 | OHX | AR | 3506 | 7/7 | 0.92 | 0.21 | 112,112,112,112 | 0 |
| 85 | MG | 1 | 4146 | 1/1 | 0.92 | 0.17 | 48,48,48,48 | 0 |
| 85 | MG | AR | 4178 | 1/1 | 0.92 | 0.19 | 24,24,24,24 | 0 |
| 84 | OHX | 1 | 3652 | 7/7 | 0.92 | 0.33 | 110,110,110,110 | 0 |
| 84 | OHX | AR | 3599 | 7/7 | 0.92 | 0.24 | 136,136,136,136 | 0 |
| 84 | OHX | 1 | 3722 | 1/7 | 0.92 | 0.12 | 136,136,136,136 | 0 |
| 85 | MG | AR | 4018 | 1/1 | 0.92 | 0.21 | 36,36,36,36 | 0 |
| 84 | OHX | 6 | 2005 | 7/7 | 0.92 | 0.42 | 126,126,127,127 | 0 |
| 84 | OHX | 1 | 3488 | 7/7 | 0.92 | 0.17 | 109,109,109,110 | 0 |
| 85 | MG | A | 2100 | 1/1 | 0.92 | 0.44 | 92,92,92,92 | 0 |
| 84 | OHX | AR | 3732 | 7/7 | 0.92 | 0.52 | 146,146,147,147 | 0 |
| 85 | MG | 1 | 4026 | 1/1 | 0.92 | 0.41 | 65,65,65,65 | 0 |
| 85 | MG | AR | 4189 | 1/1 | 0.92 | 1.14 | 32,32,32,32 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 85 | MG | AR | 4192 | 1/1 | 0.92 | 0.19 | 29,29,29,29 | 0 |
| 85 | MG | 1 | 3937 | 1/1 | 0.92 | 0.12 | 68,68,68,68 | 0 |
| 85 | MG | 1 | 3938 | 1/1 | 0.92 | 0.21 | 34,34,34,34 | 0 |
| 85 | MG | 6 | 2091 | 1/1 | 0.92 | 0.41 | 61,61,61,61 | 0 |
| 84 | OHX | 6 | 2007 | 7/7 | 0.92 | 0.28 | 145,146,146,146 | 0 |
| 85 | MG | AR | 4027 | 1/1 | 0.92 | 0.23 | 76,76,76,76 | 0 |
| 85 | MG | 6 | 2095 | 1/1 | 0.92 | 0.43 | 41,41,41,41 | 0 |
| 85 | MG | A | 2115 | 1/1 | 0.92 | 0.38 | 83,83,83,83 | 0 |
| 84 | OHX | c5 | 201 | 7/7 | 0.92 | 0.19 | 161,161,161,161 | 0 |
| 85 | MG | 6 | 2100 | 1/1 | 0.92 | 0.51 | 36,36,36,36 | 0 |
| 85 | MG | AR | 4209 | 1/1 | 0.92 | 0.40 | 74,74,74,74 | 0 |
| 85 | MG | AR | 4031 | 1/1 | 0.92 | 0.20 | 39,39,39,39 | 0 |
| 85 | MG | AR | 3785 | 1/1 | 0.92 | 0.47 | 57,57,57,57 | 0 |
| 84 | OHX | d9 | 101 | 7/7 | 0.92 | 0.48 | 153,153,154,154 | 0 |
| 85 | MG | AR | 3792 | 1/1 | 0.92 | 0.51 | 43,43,43,43 | 0 |
| 85 | MG | A | 2126 | 1/1 | 0.92 | 0.68 | 64,64,64,64 | 0 |
| 85 | MG | 1 | 3942 | 1/1 | 0.92 | 0.26 | 32,32,32,32 | 0 |
| 85 | MG | 6 | 2106 | 1/1 | 0.92 | 0.39 | 50,50,50,50 | 0 |
| 85 | MG | AR | 4038 | 1/1 | 0.92 | 0.23 | 35,35,35,35 | 0 |
| 85 | MG | 1 | 3943 | 1/1 | 0.92 | 0.54 | 37,37,37,37 | 0 |
| 85 | MG | AR | 3804 | 1/1 | 0.92 | 0.45 | 27,27,27,27 | 0 |
| 85 | MG | 1 | 3821 | 1/1 | 0.92 | 0.52 | 66,66,66,66 | 0 |
| 85 | MG | AR | 3808 | 1/1 | 0.92 | 0.34 | 28,28,28,28 | 0 |
| 85 | MG | AR | 4226 | 1/1 | 0.92 | 0.41 | 24,24,24,24 | 0 |
| 85 | MG | AR | 4230 | 1/1 | 0.92 | 0.55 | 18,18,18,18 | 0 |
| 84 | OHX | 1 | 3643 | 7/7 | 0.92 | 0.39 | 114,114,114,114 | 0 |
| 85 | MG | 1 | 4039 | 1/1 | 0.92 | 0.48 | 40,40,40,40 | 0 |
| 85 | MG | AR | 4233 | 1/1 | 0.92 | 0.33 | 31,31,31,31 | 0 |
| 85 | MG | 1 | 3947 | 1/1 | 0.92 | 0.21 | 26,26,26,26 | 0 |
| 85 | MG | A | 2143 | 1/1 | 0.92 | 0.38 | 106,106,106,106 | 0 |
| 85 | MG | 1 | 3728 | 1/1 | 0.92 | 0.61 | 52,52,52,52 | 0 |
| 85 | MG | 1 | 3949 | 1/1 | 0.92 | 0.47 | 44,44,44,44 | 0 |
| 85 | MG | 6 | 2121 | 1/1 | 0.92 | 0.28 | 41,41,41,41 | 0 |
| 85 | MG | AR | 3820 | 1/1 | 0.92 | 0.26 | 43,43,43,43 | 0 |
| 85 | MG | AR | 4055 | 1/1 | 0.92 | 0.17 | 40,40,40,40 | 0 |
| 84 | OHX | AR | 3644 | 7/7 | 0.92 | 0.31 | 126,127,127,127 | 0 |
| 85 | MG | 1 | 3833 | 1/1 | 0.92 | 0.70 | 24,24,24,24 | 0 |
| 85 | MG | A | 2157 | 1/1 | 0.92 | 0.79 | 75,75,75,75 | 0 |
| 85 | MG | 1 | 3834 | 1/1 | 0.92 | 0.51 | 22,22,22,22 | 0 |
| 85 | MG | AR | 4061 | 1/1 | 0.92 | 0.53 | 50,50,50,50 | 0 |
| 85 | MG | F | 301 | 1/1 | 0.92 | 0.33 | 64,64,64,64 | 0 |
| 84 | OHX | 1 | 3688 | 7/7 | 0.92 | 0.25 | 129,130,130,130 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85 | MG | 1 | 4054 | 1/1 | 0.92 | 0.21 | 56,56,56,56 | 0 |
| 84 | OHX | AR | 3647 | 7/7 | 0.92 | 0.29 | 126,126,127,127 | 0 |
| 85 | MG | 6 | 2132 | 1/1 | 0.92 | 0.35 | 42,42,42,42 | 0 |
| 85 | MG | AR | 3835 | 1/1 | 0.92 | 0.41 | 45,45,45,45 | 0 |
| 84 | OHX | 1 | 3690 | 7/7 | 0.92 | 0.41 | 122,123,123,123 | 0 |
| 85 | MG | 1 | 3740 | 1/1 | 0.92 | 0.36 | 30,30,30,30 | 0 |
| 85 | MG | AR | 4072 | 1/1 | 0.92 | 0.25 | 70,70,70,70 | 0 |
| 85 | MG | AS | 214 | 1/1 | 0.92 | 0.30 | 52,52,52,52 | 0 |
| 84 | OHX | AS | 210 | 7/7 | 0.92 | 0.24 | 115,115,116,116 | 0 |
| 85 | MG | 1 | 4214 | 1/1 | 0.92 | 0.39 | 43,43,43,43 | 0 |
| 85 | MG | 1 | 4218 | 1/1 | 0.92 | 0.14 | 32,32,32,32 | 0 |
| 84 | OHX | AR | 3657 | 7/7 | 0.92 | 0.39 | 114,114,115,115 | 0 |
| 85 | MG | 3 | 210 | 1/1 | 0.92 | 0.39 | 59,59,59,59 | 0 |
| 85 | MG | 1 | 3850 | 1/1 | 0.92 | 0.48 | 31,31,31,31 | 0 |
| 84 | OHX | 6 | 2023 | 7/7 | 0.92 | 0.38 | 161,161,162,162 | 0 |
| 85 | MG | 3 | 214 | 1/1 | 0.92 | 0.52 | 34,34,34,34 | 0 |
| 85 | MG | AR | 3864 | 1/1 | 0.92 | 0.29 | 40,40,40,40 | 0 |
| 85 | MG | AS | 227 | 1/1 | 0.92 | 0.32 | 45,45,45,45 | 0 |
| 84 | OHX | 6 | 2030 | 7/7 | 0.92 | 0.29 | 118,118,118,119 | 0 |
| 85 | MG | AR | 4058 | 1/1 | 0.93 | 0.53 | 61,61,61,61 | 0 |
| 85 | MG | 1 | 4017 | 1/1 | 0.93 | 0.21 | 101,101,101,101 | 0 |
| 85 | MG | 1 | 4018 | 1/1 | 0.93 | 0.33 | 38,38,38,38 | 0 |
| 84 | OHX | AR | 3739 | 7/7 | 0.93 | 0.51 | 148,149,149,150 | 0 |
| 85 | MG | 6 | 2112 | 1/1 | 0.93 | 0.53 | 46,46,46,46 | 0 |
| 85 | MG | AR | 3823 | 1/1 | 0.93 | 0.51 | 39,39,39,39 | 0 |
| 84 | OHX | AR | 3740 | 7/7 | 0.93 | 0.25 | 161,161,161,162 | 0 |
| 85 | MG | 6 | 2116 | 1/1 | 0.93 | 0.21 | 62,62,62,62 | 0 |
| 84 | OHX | 1 | 3614 | 7/7 | 0.93 | 0.28 | 133,133,133,134 | 0 |
| 84 | OHX | 1 | 3618 | 7/7 | 0.93 | 0.19 | 190,190,190,190 | 0 |
| 85 | MG | 1 | 4178 | 1/1 | 0.93 | 0.40 | 28,28,28,28 | 0 |
| 85 | MG | 1 | 4025 | 1/1 | 0.93 | 0.48 | 32,32,32,32 | 0 |
| 85 | MG | 1 | 3921 | 1/1 | 0.93 | 0.12 | 57,57,57,57 | 0 |
| 84 | OHX | AS | 209 | 7/7 | 0.93 | 0.31 | 140,140,140,140 | 0 |
| 85 | MG | 1 | 4189 | 1/1 | 0.93 | 0.36 | 27,27,27,27 | 0 |
| 85 | MG | AR | 3839 | 1/1 | 0.93 | 0.43 | 33,33,33,33 | 0 |
| 85 | MG | AR | 4077 | 1/1 | 0.93 | 0.32 | 40,40,40,40 | 0 |
| 85 | MG | AR | 4078 | 1/1 | 0.93 | 0.52 | 60,60,60,60 | 0 |
| 85 | MG | AT | 223 | 1/1 | 0.93 | 0.79 | 45,45,45,45 | 0 |
| 85 | MG | 6 | 2125 | 1/1 | 0.93 | 0.32 | 75,75,75,75 | 0 |
| 84 | OHX | AR | 3606 | 7/7 | 0.93 | 0.31 | 113,113,114,114 | 0 |
| 84 | OHX | 1 | 3552 | 7/7 | 0.93 | 0.10 | 150,150,151,151 | 0 |
| 85 | MG | 1 | 3773 | 1/1 | 0.93 | 0.21 | 38,38,38,38 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 85 | MG | AR | 3847 | 1/1 | 0.93 | 0.16 | 38,38,38,38 | 0 |
| 84 | OHX | AR | 3635 | 7/7 | 0.93 | 0.22 | 137,138,138,138 | 0 |
| 84 | OHX | AT | 217 | 7/7 | 0.93 | 0.37 | 128,128,128,128 | 0 |
| 84 | OHX | CE | 402 | 7/7 | 0.93 | 0.38 | 138,139,139,139 | 0 |
| 85 | MG | 6 | 2137 | 1/1 | 0.93 | 0.12 | 82,82,82,82 | 0 |
| 84 | OHX | AR | 3636 | 7/7 | 0.93 | 0.48 | 133,133,134,134 | 0 |
| 84 | OHX | 1 | 3556 | 7/7 | 0.93 | 0.27 | 117,117,117,117 | 0 |
| 84 | OHX | 1 | 3704 | 7/7 | 0.93 | 0.33 | 116,117,117,117 | 0 |
| 84 | OHX | A | 1918 | 7/7 | 0.93 | 0.23 | 128,129,129,129 | 0 |
| 85 | MG | CG | 303 | 1/1 | 0.93 | 0.13 | 62,62,62,62 | 0 |
| 85 | MG | 1 | 4217 | 1/1 | 0.93 | 0.92 | 58,58,58,58 | 0 |
| 85 | MG | 1 | 4041 | 1/1 | 0.93 | 0.16 | 45,45,45,45 | 0 |
| 84 | OHX | AR | 3641 | 7/7 | 0.93 | 0.48 | 133,133,133,133 | 0 |
| 84 | OHX | A | 1966 | 7/7 | 0.93 | 0.19 | 131,131,132,132 | 0 |
| 84 | OHX | 1 | 3686 | 7/7 | 0.93 | 0.58 | 156,156,157,157 | 0 |
| 85 | MG | CQ | 201 | 1/1 | 0.93 | 0.38 | 34,34,34,34 | 0 |
| 84 | OHX | 1 | 3655 | 7/7 | 0.93 | 0.37 | 138,138,138,139 | 0 |
| 84 | OHX | 6 | 2013 | 7/7 | 0.93 | 0.32 | 121,122,122,122 | 0 |
| 85 | MG | AR | 4109 | 1/1 | 0.93 | 0.16 | 39,39,39,39 | 0 |
| 84 | OHX | AR | 3649 | 7/7 | 0.93 | 0.50 | 144,144,144,144 | 0 |
| 84 | OHX | AR | 3650 | 7/7 | 0.93 | 0.44 | 118,118,118,118 | 0 |
| 84 | OHX | A | 1996 | 7/7 | 0.93 | 0.32 | 139,140,140,141 | 0 |
| 85 | MG | AR | 3905 | 1/1 | 0.93 | 0.48 | 29,29,29,29 | 0 |
| 84 | OHX | 1 | 3563 | 7/7 | 0.93 | 0.24 | 114,114,115,115 | 0 |
| 85 | MG | 3 | 222 | 1/1 | 0.93 | 0.38 | 52,52,52,52 | 0 |
| 85 | MG | 4 | 217 | 1/1 | 0.93 | 0.56 | 52,52,52,52 | 0 |
| 85 | MG | 1 | 3946 | 1/1 | 0.93 | 0.28 | 34,34,34,34 | 0 |
| 85 | MG | AR | 3920 | 1/1 | 0.93 | 0.50 | 27,27,27,27 | 0 |
| 85 | MG | 1 | 3804 | 1/1 | 0.93 | 0.50 | 35,35,35,35 | 0 |
| 84 | OHX | 1 | 3636 | 7/7 | 0.93 | 0.32 | 126,126,126,126 | 0 |
| 85 | MG | 1 | 4062 | 1/1 | 0.93 | 0.16 | 45,45,45,45 | 0 |
| 85 | MG | AR | 3925 | 1/1 | 0.93 | 0.41 | 34,34,34,34 | 0 |
| 85 | MG | DO | 202 | 1/1 | 0.93 | 0.25 | 42,42,42,42 | 0 |
| 84 | OHX | AR | 3663 | 7/7 | 0.93 | 0.29 | 147,148,148,148 | 0 |
| 85 | MG | AR | 3928 | 1/1 | 0.93 | 0.46 | 39,39,39,39 | 0 |
| 85 | MG | sM | 201 | 1/1 | 0.93 | 0.12 | 41,41,41,41 | 0 |
| 85 | MG | A | 2044 | 1/1 | 0.93 | 0.80 | 50,50,50,50 | 0 |
| 84 | OHX | 6 | 2022 | 7/7 | 0.93 | 0.29 | 153,154,154,155 | 0 |
| 85 | MG | 1 | 4068 | 1/1 | 0.93 | 0.46 | 42,42,42,42 | 0 |
| 85 | MG | 4 | 230 | 1/1 | 0.93 | 0.34 | 35,35,35,35 | 0 |
| 84 | OHX | 1 | 3711 | 7/7 | 0.93 | 0.59 | 119,120,120,120 | 0 |
| 84 | OHX | 6 | 2024 | 7/7 | 0.93 | 0.35 | 151,152,152,153 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 84 | OHX | AR | 3670 | 7/7 | 0.93 | 0.19 | 143,143,144,144 | 0 |
| 85 | MG | A | 2052 | 1/1 | 0.93 | 0.42 | 53,53,53,53 | 0 |
| 84 | OHX | A | 2020 | 7/7 | 0.93 | 0.23 | 147,148,148,148 | 0 |
| 84 | OHX | AR | 3674 | 7/7 | 0.93 | 0.46 | 130,130,130,131 | 0 |
| 85 | MG | A | 2055 | 1/1 | 0.93 | 0.47 | 71,71,71,71 | 0 |
| 85 | MG | AR | 4143 | 1/1 | 0.93 | 0.26 | 34,34,34,34 | 0 |
| 85 | MG | AR | 4144 | 1/1 | 0.93 | 0.33 | 41,41,41,41 | 0 |
| 85 | MG | A | 2060 | 1/1 | 0.93 | 0.62 | 55,55,55,55 | 0 |
| 84 | OHX | AR | 3675 | 7/7 | 0.93 | 0.33 | 138,139,139,139 | 0 |
| 84 | OHX | 4 | 216 | 7/7 | 0.93 | 0.26 | 126,126,126,126 | 0 |
| 84 | OHX | AR | 3678 | 7/7 | 0.93 | 0.42 | 137,137,137,138 | 0 |
| 85 | MG | 1 | 3826 | 1/1 | 0.93 | 0.25 | 33,33,33,33 | 0 |
| 85 | MG | j | 301 | 1/1 | 0.93 | 0.21 | 29,29,29,29 | 0 |
| 85 | MG | 1 | 3828 | 1/1 | 0.93 | 0.55 | 30,30,30,30 | 0 |
| 85 | MG | AR | 4152 | 1/1 | 0.93 | 0.23 | 38,38,38,38 | 0 |
| 85 | MG | A | 2072 | 1/1 | 0.93 | 0.39 | 66,66,66,66 | 0 |
| 85 | MG | 1 | 4086 | 1/1 | 0.93 | 0.29 | 32,32,32,32 | 0 |
| 85 | MG | A | 2076 | 1/1 | 0.93 | 0.35 | 51,51,51,51 | 0 |
| 85 | MG | A | 2078 | 1/1 | 0.93 | 0.68 | 54,54,54,54 | 0 |
| 84 | OHX | 6 | 2032 | 7/7 | 0.93 | 0.50 | 131,131,132,132 | 0 |
| 85 | MG | 1 | 3964 | 1/1 | 0.93 | 0.47 | 68,68,68,68 | 0 |
| 85 | MG | AR | 3962 | 1/1 | 0.93 | 0.19 | 93,93,93,93 | 0 |
| 84 | OHX | 1 | 3661 | 7/7 | 0.93 | 0.32 | 119,120,120,120 | 0 |
| 85 | MG | AR | 4158 | 1/1 | 0.93 | 0.20 | 29,29,29,29 | 0 |
| 85 | MG | AR | 3965 | 1/1 | 0.93 | 0.25 | 50,50,50,50 | 0 |
| 85 | MG | AR | 3966 | 1/1 | 0.93 | 0.45 | 38,38,38,38 | 0 |
| 85 | MG | o | 301 | 1/1 | 0.93 | 0.19 | 34,34,34,34 | 0 |
| 84 | OHX | 6 | 2035 | 7/7 | 0.93 | 0.36 | 142,142,143,143 | 0 |
| 85 | MG | A | 2090 | 1/1 | 0.93 | 0.20 | 57,57,57,57 | 0 |
| 84 | OHX | 6 | 2036 | 7/7 | 0.93 | 0.40 | 135,135,136,136 | 0 |
| 85 | MG | 1 | 3837 | 1/1 | 0.93 | 0.33 | 26,26,26,26 | 0 |
| 84 | OHX | 6 | 2037 | 7/7 | 0.93 | 0.40 | 137,137,138,138 | 0 |
| 85 | MG | AR | 4167 | 1/1 | 0.93 | 0.25 | 71,71,71,71 | 0 |
| 84 | OHX | AR | 3701 | 7/7 | 0.93 | 0.29 | 128,128,128,128 | 0 |
| 84 | OHX | AR | 3704 | 7/7 | 0.93 | 0.38 | 133,133,133,133 | 0 |
| 85 | MG | 1 | 3973 | 1/1 | 0.93 | 0.47 | 37,37,37,37 | 0 |
| 84 | OHX | 6 | 2038 | 7/7 | 0.93 | 0.41 | 148,148,148,148 | 0 |
| 85 | MG | 1 | 3975 | 1/1 | 0.93 | 0.33 | 42,42,42,42 | 0 |
| 84 | OHX | A | 2040 | 7/7 | 0.93 | 0.37 | 162,162,162,162 | 0 |
| 85 | MG | AF | 201 | 1/1 | 0.93 | 0.30 | 41,41,41,41 | 0 |
| 85 | MG | A | 2104 | 1/1 | 0.93 | 0.15 | 137,137,137,137 | 0 |
| 85 | MG | A | 2105 | 1/1 | 0.93 | 0.43 | 94,94,94,94 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 84 | OHX | AR | 3706 | 7/7 | 0.93 | 0.34 | 155,155,155,156 | 0 |
| 84 | OHX | 1 | 3713 | 7/7 | 0.93 | 0.26 | 138,138,138,139 | 0 |
| 84 | OHX | AR | 3708 | 7/7 | 0.93 | 0.26 | 138,138,139,139 | 0 |
| 84 | OHX | K | 201 | 7/7 | 0.93 | 0.51 | 137,137,138,138 | 0 |
| 85 | MG | AR | 3748 | 1/1 | 0.93 | 0.38 | 44,44,44,44 | 0 |
| 84 | OHX | x | 202 | 7/7 | 0.93 | 0.36 | 144,144,145,145 | 0 |
| 84 | OHX | AR | 3711 | 7/7 | 0.93 | 0.37 | 144,144,145,145 | 0 |
| 85 | MG | AR | 4185 | 1/1 | 0.93 | 0.37 | 38,38,38,38 | 0 |
| 84 | OHX | 1 | 3664 | 7/7 | 0.93 | 0.35 | 124,124,124,124 | 0 |
| 85 | MG | AR | 4002 | 1/1 | 0.93 | 0.50 | 28,28,28,28 | 0 |
| 84 | OHX | 6 | 2043 | 7/7 | 0.93 | 0.31 | 145,145,146,146 | 0 |
| 84 | OHX | 6 | 1932 | 7/7 | 0.93 | 0.23 | 132,132,133,133 | 0 |
| 85 | MG | AR | 3754 | 1/1 | 0.93 | 0.31 | 40,40,40,40 | 0 |
| 85 | MG | A | 2123 | 1/1 | 0.93 | 0.51 | 55,55,55,55 | 0 |
| 85 | MG | AR | 4193 | 1/1 | 0.93 | 0.32 | 38,38,38,38 | 0 |
| 84 | OHX | 6 | 1950 | 7/7 | 0.93 | 0.21 | 135,135,136,136 | 0 |
| 85 | MG | 6 | 2065 | 1/1 | 0.93 | 0.58 | 40,40,40,40 | 0 |
| 85 | MG | AR | 3757 | 1/1 | 0.93 | 0.41 | 31,31,31,31 | 0 |
| 85 | MG | AR | 4015 | 1/1 | 0.93 | 0.16 | 45,45,45,45 | 0 |
| 85 | MG | AR | 4016 | 1/1 | 0.93 | 0.36 | 33,33,33,33 | 0 |
| 85 | MG | AR | 4201 | 1/1 | 0.93 | 0.27 | 35,35,35,35 | 0 |
| 85 | MG | AR | 4204 | 1/1 | 0.93 | 0.30 | 38,38,38,38 | 0 |
| 85 | MG | AR | 3758 | 1/1 | 0.93 | 0.30 | 37,37,37,37 | 0 |
| 84 | OHX | 1 | 3694 | 7/7 | 0.93 | 0.41 | 116,116,117,117 | 0 |
| 85 | MG | 6 | 2067 | 1/1 | 0.93 | 0.30 | 45,45,45,45 | 0 |
| 85 | MG | 1 | 3729 | 1/1 | 0.93 | 0.32 | 90,90,90,90 | 0 |
| 84 | OHX | 6 | 2049 | 7/7 | 0.93 | 0.33 | 170,171,171,171 | 0 |
| 85 | MG | AR | 4211 | 1/1 | 0.93 | 0.14 | 73,73,73,73 | 0 |
| 85 | MG | 1 | 3868 | 1/1 | 0.93 | 0.42 | 29,29,29,29 | 0 |
| 85 | MG | AR | 3767 | 1/1 | 0.93 | 0.58 | 35,35,35,35 | 0 |
| 85 | MG | AR | 3769 | 1/1 | 0.93 | 0.26 | 59,59,59,59 | 0 |
| 85 | MG | AR | 4218 | 1/1 | 0.93 | 0.27 | 54,54,54,54 | 0 |
| 85 | MG | A | 2147 | 1/1 | 0.93 | 0.26 | 79,79,79,79 | 0 |
| 84 | OHX | 6 | 1961 | 7/7 | 0.93 | 0.19 | 128,129,129,130 | 0 |
| 85 | MG | 1 | 3734 | 1/1 | 0.93 | 0.34 | 43,43,43,43 | 0 |
| 84 | OHX | AR | 3723 | 7/7 | 0.93 | 0.28 | 146,146,147,147 | 0 |
| 84 | OHX | AR | 3725 | 7/7 | 0.93 | 0.20 | 165,165,165,165 | 0 |
| 85 | MG | 1 | 4136 | 1/1 | 0.93 | 0.27 | 40,40,40,40 | 0 |
| 84 | OHX | 1 | 3485 | 7/7 | 0.93 | 0.16 | 120,121,121,121 | 0 |
| 84 | OHX | 1 | 3609 | 7/7 | 0.93 | 0.40 | 119,120,120,120 | 0 |
| 85 | MG | A | 2158 | 1/1 | 0.93 | 0.34 | 67,67,67,67 | 0 |
| 84 | OHX | 6 | 1986 | 7/7 | 0.93 | 0.32 | 147,148,148,148 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 84 | OHX | 6 | 1987 | 7/7 | 0.93 | 0.28 | 137,137,138,138 | 0 |
| 84 | OHX | 6 | 1989 | 7/7 | 0.93 | 0.43 | 143,144,144,145 | 0 |
| 84 | OHX | AR | 3527 | 7/7 | 0.93 | 0.20 | 112,112,112,112 | 0 |
| 85 | MG | AR | 3788 | 1/1 | 0.93 | 0.50 | 28,28,28,28 | 0 |
| 85 | MG | 1 | 3896 | 1/1 | 0.93 | 0.30 | 36,36,36,36 | 0 |
| 84 | OHX | AR | 3571 | 7/7 | 0.93 | 0.18 | 125,125,125,125 | 0 |
| 84 | OHX | AR | 3596 | 7/7 | 0.93 | 0.24 | 121,121,122,122 | 0 |
| 85 | MG | AR | 4041 | 1/1 | 0.93 | 0.36 | 34,34,34,34 | 0 |
| 85 | MG | 1 | 3756 | 1/1 | 0.93 | 0.42 | 32,32,32,32 | 0 |
| 85 | MG | AR | 4242 | 1/1 | 0.93 | 0.46 | 35,35,35,35 | 0 |
| 85 | MG | c1 | 202 | 1/1 | 0.93 | 0.41 | 67,67,67,67 | 0 |
| 85 | MG | AR | 4243 | 1/1 | 0.93 | 0.59 | 30,30,30,30 | 0 |
| 85 | MG | AR | 3798 | 1/1 | 0.93 | 0.33 | 33,33,33,33 | 0 |
| 85 | MG | 1 | 4153 | 1/1 | 0.93 | 0.18 | 39,39,39,39 | 0 |
| 85 | MG | 6 | 2094 | 1/1 | 0.93 | 0.22 | 37,37,37,37 | 0 |
| 85 | MG | AR | 3805 | 1/1 | 0.93 | 0.44 | 36,36,36,36 | 0 |
| 84 | OHX | AR | 3736 | 7/7 | 0.93 | 0.28 | 132,132,132,133 | 0 |
| 84 | OHX | AR | 3597 | 7/7 | 0.93 | 0.30 | 150,151,151,151 | 0 |
| 85 | MG | 1 | 3906 | 1/1 | 0.93 | 0.36 | 42,42,42,42 | 0 |
| 84 | OHX | 6 | 1992 | 7/7 | 0.93 | 0.23 | 137,137,138,138 | 0 |
| 85 | MG | 1 | 3912 | 1/1 | 0.93 | 0.59 | 22,22,22,22 | 0 |
| 85 | MG | 1 | 4016 | 1/1 | 0.93 | 0.18 | 39,39,39,39 | 0 |
| 88 | ZN | c | 101 | 1/1 | 0.93 | 0.34 | 145,145,145,145 | 0 |
| 85 | MG | AR | 4057 | 1/1 | 0.93 | 0.39 | 41,41,41,41 | 0 |
| 85 | MG | AR | 4227 | 1/1 | 0.94 | 0.33 | 22,22,22,22 | 0 |
| 84 | OHX | AR | 3685 | 7/7 | 0.94 | 0.33 | 120,121,121,121 | 0 |
| 84 | OHX | A | 2032 | 7/7 | 0.94 | 0.20 | 154,154,155,155 | 0 |
| 84 | OHX | A | 2033 | 7/7 | 0.94 | 0.25 | 146,146,147,147 | 0 |
| 85 | MG | AR | 3997 | 1/1 | 0.94 | 0.12 | 44,44,44,44 | 0 |
| 84 | OHX | 6 | 1940 | 7/7 | 0.94 | 0.13 | 149,150,151,151 | 0 |
| 84 | OHX | AR | 3689 | 7/7 | 0.94 | 0.34 | 118,118,119,119 | 0 |
| 85 | MG | AR | 4001 | 1/1 | 0.94 | 0.22 | 38,38,38,38 | 0 |
| 84 | OHX | 1 | 3641 | 7/7 | 0.94 | 0.36 | 141,141,141,141 | 0 |
| 84 | OHX | AR | 3691 | 7/7 | 0.94 | 0.41 | 116,116,116,117 | 0 |
| 85 | MG | AR | 4004 | 1/1 | 0.94 | 0.16 | 32,32,32,32 | 0 |
| 84 | OHX | 6 | 2042 | 7/7 | 0.94 | 0.34 | 151,151,151,151 | 0 |
| 85 | MG | AR | 4006 | 1/1 | 0.94 | 0.55 | 47,47,47,47 | 0 |
| 85 | MG | AR | 4008 | 1/1 | 0.94 | 0.25 | 26,26,26,26 | 0 |
| 84 | OHX | 1 | 3498 | 7/7 | 0.94 | 0.21 | 115,116,116,116 | 0 |
| 85 | MG | AR | 4010 | 1/1 | 0.94 | 0.30 | 30,30,30,30 | 0 |
| 84 | OHX | 1 | 3675 | 7/7 | 0.94 | 0.30 | 140,141,141,141 | 0 |
| 84 | OHX | AR | 3698 | 7/7 | 0.94 | 0.41 | 123,123,123,124 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 84 | OHX | 6 | 1962 | 7/7 | 0.94 | 0.30 | 136,137,137,137 | 0 |
| 84 | OHX | AR | 3702 | 7/7 | 0.94 | 0.40 | 139,139,140,140 | 0 |
| 85 | MG | 4 | 223 | 1/1 | 0.94 | 0.59 | 27,27,27,27 | 0 |
| 85 | MG | 1 | 3880 | 1/1 | 0.94 | 0.59 | 31,31,31,31 | 0 |
| 85 | MG | AB | 206 | 1/1 | 0.94 | 0.27 | 26,26,26,26 | 0 |
| 84 | OHX | 6 | 2047 | 7/7 | 0.94 | 0.32 | 161,162,162,162 | 0 |
| 84 | OHX | Q | 201 | 7/7 | 0.94 | 0.26 | 165,165,165,165 | 0 |
| 84 | OHX | 6 | 1969 | 7/7 | 0.94 | 0.15 | 127,127,128,128 | 0 |
| 85 | MG | 1 | 3890 | 1/1 | 0.94 | 0.47 | 34,34,34,34 | 0 |
| 84 | OHX | 6 | 1971 | 7/7 | 0.94 | 0.24 | 136,136,136,137 | 0 |
| 84 | OHX | 1 | 3610 | 7/7 | 0.94 | 0.23 | 130,130,131,131 | 0 |
| 84 | OHX | 1 | 3679 | 7/7 | 0.94 | 0.30 | 131,131,132,132 | 0 |
| 84 | OHX | 6 | 1979 | 7/7 | 0.94 | 0.46 | 135,135,136,136 | 0 |
| 84 | OHX | AR | 3710 | 7/7 | 0.94 | 0.34 | 137,137,137,138 | 0 |
| 85 | MG | 1 | 3727 | 1/1 | 0.94 | 0.28 | 37,37,37,37 | 0 |
| 84 | OHX | 1 | 3462 | 7/7 | 0.94 | 0.21 | 119,120,120,120 | 0 |
| 85 | MG | 1 | 4049 | 1/1 | 0.94 | 0.25 | 32,32,32,32 | 0 |
| 84 | OHX | AR | 3712 | 7/7 | 0.94 | 0.27 | 109,109,109,109 | 0 |
| 85 | MG | 4 | 241 | 1/1 | 0.94 | 0.58 | 45,45,45,45 | 0 |
| 85 | MG | AS | 230 | 1/1 | 0.94 | 0.42 | 36,36,36,36 | 0 |
| 85 | MG | 1 | 3730 | 1/1 | 0.94 | 0.35 | 36,36,36,36 | 0 |
| 84 | OHX | AR | 3713 | 7/7 | 0.94 | 0.24 | 178,178,179,179 | 0 |
| 84 | OHX | 1 | 3648 | 7/7 | 0.94 | 0.25 | 119,120,120,120 | 0 |
| 85 | MG | AR | 4036 | 1/1 | 0.94 | 0.27 | 41,41,41,41 | 0 |
| 85 | MG | k | 403 | 1/1 | 0.94 | 0.20 | 30,30,30,30 | 0 |
| 84 | OHX | 1 | 3650 | 7/7 | 0.94 | 0.27 | 128,128,128,128 | 0 |
| 85 | MG | 1 | 4057 | 1/1 | 0.94 | 0.23 | 26,26,26,26 | 0 |
| 85 | MG | 1 | 3735 | 1/1 | 0.94 | 0.35 | 24,24,24,24 | 0 |
| 84 | OHX | AR | 3524 | 7/7 | 0.94 | 0.29 | 118,119,119,119 | 0 |
| 85 | MG | 1 | 3738 | 1/1 | 0.94 | 0.35 | 28,28,28,28 | 0 |
| 85 | MG | AR | 3768 | 1/1 | 0.94 | 0.18 | 39,39,39,39 | 0 |
| 85 | MG | 1 | 3922 | 1/1 | 0.94 | 0.45 | 45,45,45,45 | 0 |
| 85 | MG | 1 | 3923 | 1/1 | 0.94 | 0.39 | 51,51,51,51 | 0 |
| 84 | OHX | 1 | 3689 | 7/7 | 0.94 | 0.52 | 140,140,141,141 | 0 |
| 85 | MG | 1 | 4066 | 1/1 | 0.94 | 0.27 | 20,20,20,20 | 0 |
| 84 | OHX | AR | 3528 | 7/7 | 0.94 | 0.21 | 108,108,108,108 | 0 |
| 85 | MG | CE | 406 | 1/1 | 0.94 | 0.19 | 25,25,25,25 | 0 |
| 85 | MG | 1 | 3742 | 1/1 | 0.94 | 0.47 | 38,38,38,38 | 0 |
| 84 | OHX | AR | 3531 | 7/7 | 0.94 | 0.19 | 115,115,115,115 | 0 |
| 84 | OHX | AR | 3552 | 7/7 | 0.94 | 0.28 | 114,114,114,114 | 0 |
| 85 | MG | 1 | 3747 | 1/1 | 0.94 | 0.34 | 37,37,37,37 | 0 |
| 85 | MG | CI | 301 | 1/1 | 0.94 | 0.26 | 33,33,33,33 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 84 | OHX | AR | 3563 | 7/7 | 0.94 | 0.17 | 122,122,123,123 | 0 |
| 84 | OHX | AR | 3564 | 7/7 | 0.94 | 0.14 | 155,155,155,155 | 0 |
| 85 | MG | AR | 3784 | 1/1 | 0.94 | 0.24 | 51,51,51,51 | 0 |
| 84 | OHX | 6 | 1993 | 7/7 | 0.94 | 0.28 | 134,135,135,135 | 0 |
| 85 | MG | 1 | 3753 | 1/1 | 0.94 | 0.54 | 35,35,35,35 | 0 |
| 85 | MG | CQ | 202 | 1/1 | 0.94 | 0.33 | 32,32,32,32 | 0 |
| 85 | MG | 1 | 4083 | 1/1 | 0.94 | 0.29 | 41,41,41,41 | 0 |
| 85 | MG | CR | 201 | 1/1 | 0.94 | 0.65 | 29,29,29,29 | 0 |
| 85 | MG | AR | 3791 | 1/1 | 0.94 | 0.26 | 34,34,34,34 | 0 |
| 84 | OHX | AR | 3590 | 7/7 | 0.94 | 0.37 | 113,113,113,113 | 0 |
| 85 | MG | 6 | 2054 | 1/1 | 0.94 | 0.39 | 49,49,49,49 | 0 |
| 84 | OHX | AR | 3593 | 7/7 | 0.94 | 0.23 | 113,114,114,114 | 0 |
| 84 | OHX | 6 | 1999 | 7/7 | 0.94 | 0.26 | 138,139,139,140 | 0 |
| 85 | MG | AR | 3800 | 1/1 | 0.94 | 0.65 | 33,33,33,33 | 0 |
| 85 | MG | AR | 3801 | 1/1 | 0.94 | 0.38 | 32,32,32,32 | 0 |
| 84 | OHX | 1 | 3615 | 7/7 | 0.94 | 0.38 | 133,133,133,134 | 0 |
| 84 | OHX | 1 | 3514 | 7/7 | 0.94 | 0.18 | 112,112,112,112 | 0 |
| 84 | OHX | AR | 3600 | 7/7 | 0.94 | 0.33 | 119,119,119,119 | 0 |
| 85 | MG | 1 | 4090 | 1/1 | 0.94 | 0.21 | 42,42,42,42 | 0 |
| 85 | MG | DC | 204 | 1/1 | 0.94 | 0.14 | 35,35,35,35 | 0 |
| 84 | OHX | 1 | 3619 | 7/7 | 0.94 | 0.22 | 127,127,127,127 | 0 |
| 85 | MG | AR | 3809 | 1/1 | 0.94 | 0.65 | 37,37,37,37 | 0 |
| 85 | MG | 1 | 3763 | 1/1 | 0.94 | 0.65 | 29,29,29,29 | 0 |
| 85 | MG | AR | 4082 | 1/1 | 0.94 | 0.34 | 24,24,24,24 | 0 |
| 85 | MG | 6 | 2069 | 1/1 | 0.94 | 0.35 | 65,65,65,65 | 0 |
| 85 | MG | AR | 3813 | 1/1 | 0.94 | 0.16 | 55,55,55,55 | 0 |
| 84 | OHX | AR | 3735 | 7/7 | 0.94 | 0.30 | 129,129,129,129 | 0 |
| 84 | OHX | 1 | 3591 | 7/7 | 0.94 | 0.28 | 109,109,109,109 | 0 |
| 85 | MG | sM | 202 | 1/1 | 0.94 | 0.54 | 42,42,42,42 | 0 |
| 84 | OHX | 1 | 3594 | 7/7 | 0.94 | 0.20 | 131,131,132,132 | 0 |
| 84 | OHX | AR | 3607 | 7/7 | 0.94 | 0.30 | 113,113,113,113 | 0 |
| 85 | MG | 1 | 3768 | 1/1 | 0.94 | 0.41 | 36,36,36,36 | 0 |
| 85 | MG | 1 | 3770 | 1/1 | 0.94 | 0.25 | 29,29,29,29 | 0 |
| 85 | MG | 1 | 3950 | 1/1 | 0.94 | 0.14 | 38,38,38,38 | 0 |
| 85 | MG | A | 2049 | 1/1 | 0.94 | 0.50 | 54,54,54,54 | 0 |
| 84 | OHX | AR | 3608 | 7/7 | 0.94 | 0.34 | 131,131,132,132 | 0 |
| 85 | MG | AR | 3825 | 1/1 | 0.94 | 0.27 | 33,33,33,33 | 0 |
| 84 | OHX | AR | 3611 | 7/7 | 0.94 | 0.23 | 126,126,126,126 | 0 |
| 84 | OHX | AR | 3615 | 7/7 | 0.94 | 0.36 | 132,133,133,133 | 0 |
| 85 | MG | AR | 3831 | 1/1 | 0.94 | 0.23 | 44,44,44,44 | 0 |
| 84 | OHX | AR | 3742 | 7/7 | 0.94 | 0.25 | 128,129,129,129 | 0 |
| 84 | OHX | AR | 3622 | 7/7 | 0.94 | 0.24 | 130,131,131,131 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 84 | OHX | 1 | 3540 | 7/7 | 0.94 | 0.18 | 111,111,111,111 | 0 |
| 85 | MG | 1 | 3957 | 1/1 | 0.94 | 0.39 | 37,37,37,37 | 0 |
| 84 | OHX | AR | 3634 | 7/7 | 0.94 | 0.26 | 112,112,113,113 | 0 |
| 85 | MG | AR | 4107 | 1/1 | 0.94 | 0.13 | 78,78,78,78 | 0 |
| 85 | MG | AR | 4108 | 1/1 | 0.94 | 0.19 | 36,36,36,36 | 0 |
| 84 | OHX | 3 | 206 | 7/7 | 0.94 | 0.20 | 127,127,128,128 | 0 |
| 84 | OHX | AT | 212 | 7/7 | 0.94 | 0.30 | 128,128,128,128 | 0 |
| 84 | OHX | 6 | 2010 | 7/7 | 0.94 | 0.33 | 154,155,155,155 | 0 |
| 85 | MG | AR | 4114 | 1/1 | 0.94 | 0.28 | 40,40,40,40 | 0 |
| 85 | MG | A | 2071 | 1/1 | 0.94 | 0.33 | 64,64,64,64 | 0 |
| 85 | MG | 1 | 4123 | 1/1 | 0.94 | 0.22 | 51,51,51,51 | 0 |
| 84 | OHX | AT | 215 | 7/7 | 0.94 | 0.20 | 137,138,138,138 | 0 |
| 85 | MG | AR | 3843 | 1/1 | 0.94 | 0.35 | 30,30,30,30 | 0 |
| 85 | MG | 6 | 2096 | 1/1 | 0.94 | 0.57 | 68,68,68,68 | 0 |
| 85 | MG | 6 | 2097 | 1/1 | 0.94 | 0.42 | 46,46,46,46 | 0 |
| 84 | OHX | 1 | 3660 | 7/7 | 0.94 | 0.28 | 153,153,154,154 | 0 |
| 85 | MG | A | 2082 | 1/1 | 0.94 | 0.23 | 61,61,61,61 | 0 |
| 85 | MG | 1 | 4126 | 1/1 | 0.94 | 0.98 | 33,33,33,33 | 0 |
| 85 | MG | AR | 3854 | 1/1 | 0.94 | 0.40 | 48,48,48,48 | 0 |
| 85 | MG | AR | 3859 | 1/1 | 0.94 | 0.49 | 29,29,29,29 | 0 |
| 85 | MG | 6 | 2102 | 1/1 | 0.94 | 0.46 | 45,45,45,45 | 0 |
| 85 | MG | 1 | 3791 | 1/1 | 0.94 | 0.60 | 54,54,54,54 | 0 |
| 84 | OHX | 6 | 2016 | 7/7 | 0.94 | 0.25 | 120,120,121,121 | 0 |
| 85 | MG | 1 | 3794 | 1/1 | 0.94 | 0.53 | 34,34,34,34 | 0 |
| 85 | MG | AR | 3872 | 1/1 | 0.94 | 0.34 | 43,43,43,43 | 0 |
| 85 | MG | 6 | 2108 | 1/1 | 0.94 | 0.56 | 50,50,50,50 | 0 |
| 85 | MG | AR | 3875 | 1/1 | 0.94 | 0.16 | 45,45,45,45 | 0 |
| 85 | MG | AR | 3879 | 1/1 | 0.94 | 0.64 | 22,22,22,22 | 0 |
| 85 | MG | 1 | 3795 | 1/1 | 0.94 | 0.29 | 26,26,26,26 | 0 |
| 85 | MG | AR | 3883 | 1/1 | 0.94 | 0.54 | 32,32,32,32 | 0 |
| 85 | MG | A | 2096 | 1/1 | 0.94 | 0.41 | 62,62,62,62 | 0 |
| 85 | MG | A | 2097 | 1/1 | 0.94 | 0.57 | 53,53,53,53 | 0 |
| 85 | MG | AR | 3888 | 1/1 | 0.94 | 0.67 | 24,24,24,24 | 0 |
| 84 | OHX | 1 | 3629 | 7/7 | 0.94 | 0.22 | 148,148,148,149 | 0 |
| 84 | OHX | 6 | 2019 | 7/7 | 0.94 | 0.30 | 140,140,141,141 | 0 |
| 84 | OHX | CG | 301 | 7/7 | 0.94 | 0.16 | 142,143,143,144 | 0 |
| 85 | MG | 6 | 2113 | 1/1 | 0.94 | 0.23 | 77,77,77,77 | 0 |
| 85 | MG | AR | 3893 | 1/1 | 0.94 | 0.95 | 50,50,50,50 | 0 |
| 84 | OHX | 4 | 214 | 7/7 | 0.94 | 0.46 | 140,140,140,140 | 0 |
| 84 | OHX | CM | 201 | 7/7 | 0.94 | 0.34 | 150,150,151,151 | 0 |
| 85 | MG | 1 | 4139 | 1/1 | 0.94 | 0.28 | 31,31,31,31 | 0 |
| 84 | OHX | 1 | 3663 | 7/7 | 0.94 | 0.19 | 111,111,111,111 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85 | MG | AR | 3900 | 1/1 | 0.94 | 0.81 | 37,37,37,37 | 0 |
| 84 | OHX | 1 | 3631 | 7/7 | 0.94 | 0.32 | 116,116,117,117 | 0 |
| 85 | MG | A | 2111 | 1/1 | 0.94 | 0.26 | 90,90,90,90 | 0 |
| 84 | OHX | A | 1953 | 7/7 | 0.94 | 0.41 | 146,147,147,147 | 0 |
| 85 | MG | 1 | 3978 | 1/1 | 0.94 | 0.35 | 46,46,46,46 | 0 |
| 84 | OHX | A | 1959 | 7/7 | 0.94 | 0.20 | 137,138,139,139 | 0 |
| 85 | MG | 1 | 3808 | 1/1 | 0.94 | 0.47 | 43,43,43,43 | 0 |
| 85 | MG | AR | 3912 | 1/1 | 0.94 | 0.54 | 23,23,23,23 | 0 |
| 84 | OHX | A | 1963 | 7/7 | 0.94 | 0.18 | 150,151,152,152 | 0 |
| 84 | OHX | 1 | 3632 | 7/7 | 0.94 | 0.34 | 156,156,156,156 | 0 |
| 85 | MG | AR | 3917 | 1/1 | 0.94 | 0.50 | 42,42,42,42 | 0 |
| 85 | MG | AR | 4162 | 1/1 | 0.94 | 0.60 | 56,56,56,56 | 0 |
| 84 | OHX | AR | 3651 | 7/7 | 0.94 | 0.31 | 150,151,151,151 | 0 |
| 84 | OHX | 6 | 2025 | 7/7 | 0.94 | 0.39 | 120,120,121,121 | 0 |
| 85 | MG | 1 | 3986 | 1/1 | 0.94 | 0.26 | 42,42,42,42 | 0 |
| 85 | MG | AR | 3923 | 1/1 | 0.94 | 0.66 | 38,38,38,38 | 0 |
| 84 | OHX | A | 1974 | 7/7 | 0.94 | 0.14 | 167,167,168,168 | 0 |
| 84 | OHX | AR | 3654 | 7/7 | 0.94 | 0.50 | 137,137,138,138 | 0 |
| 84 | OHX | AR | 3655 | 7/7 | 0.94 | 0.24 | 129,129,130,130 | 0 |
| 84 | OHX | A | 1991 | 7/7 | 0.94 | 0.24 | 157,157,158,158 | 0 |
| 84 | OHX | 6 | 2028 | 7/7 | 0.94 | 0.40 | 123,124,124,124 | 0 |
| 84 | OHX | AR | 3659 | 7/7 | 0.94 | 0.54 | 136,136,137,137 | 0 |
| 84 | OHX | AR | 3660 | 7/7 | 0.94 | 0.43 | 123,123,124,124 | 0 |
| 85 | MG | 1 | 3829 | 1/1 | 0.94 | 0.53 | 16,16,16,16 | 0 |
| 85 | MG | 1 | 4166 | 1/1 | 0.94 | 0.16 | 47,47,47,47 | 0 |
| 85 | MG | 1 | 4167 | 1/1 | 0.94 | 0.23 | 23,23,23,23 | 0 |
| 85 | MG | 1 | 4169 | 1/1 | 0.94 | 0.27 | 30,30,30,30 | 0 |
| 84 | OHX | r | 301 | 7/7 | 0.94 | 0.20 | 115,115,115,115 | 0 |
| 85 | MG | 1 | 3831 | 1/1 | 0.94 | 0.47 | 26,26,26,26 | 0 |
| 85 | MG | AR | 3949 | 1/1 | 0.94 | 0.19 | 32,32,32,32 | 0 |
| 84 | OHX | 6 | 2031 | 7/7 | 0.94 | 0.31 | 125,126,126,126 | 0 |
| 85 | MG | 1 | 4181 | 1/1 | 0.94 | 0.35 | 23,23,23,23 | 0 |
| 84 | OHX | 1 | 3705 | 7/7 | 0.94 | 0.38 | 131,131,132,132 | 0 |
| 85 | MG | 6 | 2155 | 1/1 | 0.94 | 0.86 | 58,58,58,58 | 0 |
| 84 | OHX | A | 2013 | 7/7 | 0.94 | 0.34 | 132,133,133,133 | 0 |
| 84 | OHX | A | 2014 | 7/7 | 0.94 | 0.35 | 127,128,128,128 | 0 |
| 85 | MG | A | 2153 | 1/1 | 0.94 | 0.58 | 51,51,51,51 | 0 |
| 85 | MG | AR | 3959 | 1/1 | 0.94 | 0.28 | 32,32,32,32 | 0 |
| 85 | MG | 6 | 2159 | 1/1 | 0.94 | 0.08 | 82,82,82,82 | 0 |
| 84 | OHX | AR | 3666 | 7/7 | 0.94 | 0.27 | 130,131,131,131 | 0 |
| 84 | OHX | AR | 3667 | 7/7 | 0.94 | 0.38 | 146,147,147,147 | 0 |
| 85 | MG | AR | 3963 | 1/1 | 0.94 | 0.20 | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 84 | OHX | A | 2018 | 7/7 | 0.94 | 0.34 | 155,155,156,156 | 0 |
| 85 | MG | 1 | 4194 | 1/1 | 0.94 | 0.50 | 22,22,22,22 | 0 |
| 85 | MG | 1 | 4195 | 1/1 | 0.94 | 0.46 | 29,29,29,29 | 0 |
| 85 | MG | AR | 4203 | 1/1 | 0.94 | 0.24 | 29,29,29,29 | 0 |
| 84 | OHX | 1 | 3605 | 7/7 | 0.94 | 0.33 | 129,130,130,130 | 0 |
| 85 | MG | 1 | 4201 | 1/1 | 0.94 | 0.49 | 28,28,28,28 | 0 |
| 85 | MG | AR | 3969 | 1/1 | 0.94 | 0.13 | 60,60,60,60 | 0 |
| 84 | OHX | y | 201 | 7/7 | 0.94 | 0.32 | 128,129,129,129 | 0 |
| 84 | OHX | 1 | 3639 | 7/7 | 0.94 | 0.32 | 132,132,132,132 | 0 |
| 85 | MG | 1 | 4206 | 1/1 | 0.94 | 0.30 | 30,30,30,30 | 0 |
| 84 | OHX | A | 2022 | 7/7 | 0.94 | 0.36 | 167,167,167,167 | 0 |
| 85 | MG | AR | 4213 | 1/1 | 0.94 | 0.14 | 53,53,53,53 | 0 |
| 84 | OHX | 6 | 1919 | 7/7 | 0.94 | 0.21 | 121,121,122,122 | 0 |
| 85 | MG | AR | 3978 | 1/1 | 0.94 | 0.36 | 49,49,49,49 | 0 |
| 85 | MG | d3 | 201 | 1/1 | 0.94 | 0.25 | 49,49,49,49 | 0 |
| 85 | MG | 1 | 4010 | 1/1 | 0.94 | 0.46 | 30,30,30,30 | 0 |
| 85 | MG | 1 | 4212 | 1/1 | 0.94 | 0.42 | 39,39,39,39 | 0 |
| 85 | MG | AR | 3981 | 1/1 | 0.94 | 0.14 | 33,33,33,33 | 0 |
| 84 | OHX | 6 | 1929 | 7/7 | 0.94 | 0.11 | 157,158,159,159 | 0 |
| 84 | OHX | 1 | 3669 | 7/7 | 0.94 | 0.39 | 131,131,131,131 | 0 |
| 84 | OHX | A | 2028 | 7/7 | 0.94 | 0.34 | 157,157,158,158 | 0 |
| 84 | OHX | AR | 3681 | 7/7 | 0.94 | 0.23 | 140,140,140,141 | 0 |
| 85 | MG | 1 | 3860 | 1/1 | 0.94 | 0.47 | 36,36,36,36 | 0 |
| 85 | MG | 1 | 4220 | 1/1 | 0.94 | 0.57 | 35,35,35,35 | 0 |
| 85 | MG | AR | 3993 | 1/1 | 0.94 | 0.35 | 28,28,28,28 | 0 |
| 85 | MG | AR | 4012 | 1/1 | 0.95 | 0.35 | 30,30,30,30 | 0 |
| 85 | MG | 1 | 404 | 1/1 | 0.95 | 0.34 | 35,35,35,35 | 0 |
| 85 | MG | 1 | 4071 | 1/1 | 0.95 | 0.20 | 40,40,40,40 | 0 |
| 84 | OHX | AR | 3605 | 7/7 | 0.95 | 0.16 | 128,128,128,129 | 0 |
| 84 | OHX | 1 | 3604 | 7/7 | 0.95 | 0.34 | 116,116,117,117 | 0 |
| 85 | MG | 1 | 4075 | 1/1 | 0.95 | 0.43 | 41,41,41,41 | 0 |
| 85 | MG | 1 | 3924 | 1/1 | 0.95 | 0.37 | 60,60,60,60 | 0 |
| 85 | MG | AR | 4247 | 1/1 | 0.95 | 0.46 | 22,22,22,22 | 0 |
| 85 | MG | 1 | 3749 | 1/1 | 0.95 | 0.26 | 24,24,24,24 | 0 |
| 84 | OHX | 6 | 2020 | 7/7 | 0.95 | 0.18 | 135,136,136,137 | 0 |
| 84 | OHX | 1 | 3539 | 7/7 | 0.95 | 0.28 | 119,119,119,119 | 0 |
| 84 | OHX | AR | 3610 | 7/7 | 0.95 | 0.38 | 137,138,138,138 | 0 |
| 84 | OHX | 1 | 3606 | 7/7 | 0.95 | 0.40 | 138,138,138,138 | 0 |
| 85 | MG | w | 201 | 1/1 | 0.95 | 0.42 | 37,37,37,37 | 0 |
| 84 | OHX | 1 | 3469 | 7/7 | 0.95 | 0.21 | 117,117,118,118 | 0 |
| 84 | OHX | AR | 3618 | 7/7 | 0.95 | 0.21 | 113,113,114,114 | 0 |
| 84 | OHX | 1 | 3544 | 7/7 | 0.95 | 0.16 | 116,117,117,117 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85 | MG | AR | 4259 | 1/1 | 0.95 | 0.49 | 16,16,16,16 | 0 |
| 85 | MG | AS | 212 | 1/1 | 0.95 | 0.33 | 41,41,41,41 | 0 |
| 84 | OHX | AR | 3624 | 7/7 | 0.95 | 0.33 | 150,150,151,151 | 0 |
| 84 | OHX | 1 | 3612 | 7/7 | 0.95 | 0.31 | 122,122,122,122 | 0 |
| 84 | OHX | 6 | 2026 | 7/7 | 0.95 | 0.25 | 146,146,147,147 | 0 |
| 84 | OHX | 6 | 2027 | 7/7 | 0.95 | 0.47 | 146,147,147,148 | 0 |
| 84 | OHX | 1 | 3657 | 7/7 | 0.95 | 0.28 | 123,123,124,124 | 0 |
| 84 | OHX | AT | 214 | 7/7 | 0.95 | 0.33 | 131,131,131,132 | 0 |
| 84 | OHX | AR | 3637 | 7/7 | 0.95 | 0.40 | 129,129,129,129 | 0 |
| 85 | MG | AS | 221 | 1/1 | 0.95 | 0.16 | 60,60,60,60 | 0 |
| 84 | OHX | AT | 216 | 7/7 | 0.95 | 0.40 | 132,132,132,132 | 0 |
| 84 | OHX | AR | 3638 | 7/7 | 0.95 | 0.42 | 119,119,119,119 | 0 |
| 85 | MG | AR | 3793 | 1/1 | 0.95 | 0.31 | 29,29,29,29 | 0 |
| 85 | MG | 6 | 2062 | 1/1 | 0.95 | 0.42 | 51,51,51,51 | 0 |
| 84 | OHX | 1 | 3545 | 7/7 | 0.95 | 0.21 | 120,120,120,120 | 0 |
| 85 | MG | 1 | 3769 | 1/1 | 0.95 | 0.19 | 45,45,45,45 | 0 |
| 84 | OHX | 1 | 3550 | 7/7 | 0.95 | 0.18 | 115,115,115,116 | 0 |
| 84 | OHX | 1 | 3706 | 7/7 | 0.95 | 0.30 | 136,137,137,138 | 0 |
| 85 | MG | AR | 3802 | 1/1 | 0.95 | 0.12 | 40,40,40,40 | 0 |
| 85 | MG | 1 | 4106 | 1/1 | 0.95 | 0.34 | 67,67,67,67 | 0 |
| 84 | OHX | 1 | 3616 | 7/7 | 0.95 | 0.31 | 146,146,147,147 | 0 |
| 84 | OHX | 6 | 1954 | 7/7 | 0.95 | 0.09 | 178,178,178,178 | 0 |
| 85 | MG | 1 | 3774 | 1/1 | 0.95 | 0.54 | 43,43,43,43 | 0 |
| 85 | MG | 6 | 2073 | 1/1 | 0.95 | 0.52 | 48,48,48,48 | 0 |
| 84 | OHX | CL | 301 | 7/7 | 0.95 | 0.21 | 121,122,122,122 | 0 |
| 84 | OHX | 6 | 1956 | 7/7 | 0.95 | 0.12 | 174,174,175,175 | 0 |
| 84 | OHX | A | 1909 | 7/7 | 0.95 | 0.24 | 151,151,152,153 | 0 |
| 84 | OHX | A | 1915 | 7/7 | 0.95 | 0.21 | 142,143,143,144 | 0 |
| 84 | OHX | 1 | 3662 | 7/7 | 0.95 | 0.31 | 116,116,116,116 | 0 |
| 84 | OHX | A | 1935 | 7/7 | 0.95 | 0.23 | 140,140,141,141 | 0 |
| 84 | OHX | 1 | 3487 | 7/7 | 0.95 | 0.17 | 115,115,116,116 | 0 |
| 85 | MG | 1 | 3788 | 1/1 | 0.95 | 0.53 | 45,45,45,45 | 0 |
| 84 | OHX | 1 | 3554 | 7/7 | 0.95 | 0.24 | 129,129,130,130 | 0 |
| 85 | MG | CE | 405 | 1/1 | 0.95 | 0.89 | 26,26,26,26 | 0 |
| 85 | MG | AR | 4062 | 1/1 | 0.95 | 0.17 | 42,42,42,42 | 0 |
| 84 | OHX | A | 1958 | 7/7 | 0.95 | 0.22 | 173,173,173,173 | 0 |
| 85 | MG | AR | 3822 | 1/1 | 0.95 | 0.31 | 46,46,46,46 | 0 |
| 85 | MG | AR | 4065 | 1/1 | 0.95 | 0.25 | 31,31,31,31 | 0 |
| 85 | MG | AR | 4066 | 1/1 | 0.95 | 0.14 | 56,56,56,56 | 0 |
| 84 | OHX | 6 | 1966 | 7/7 | 0.95 | 0.15 | 133,133,134,134 | 0 |
| 84 | OHX | A | 1960 | 7/7 | 0.95 | 0.18 | 151,151,151,152 | 0 |
| 84 | OHX | 1 | 3481 | 7/7 | 0.95 | 0.19 | 116,117,117,117 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85 | MG | AR | 3826 | 1/1 | 0.95 | 0.32 | 23,23,23,23 | 0 |
| 85 | MG | CM | 203 | 1/1 | 0.95 | 0.21 | 55,55,55,55 | 0 |
| 85 | MG | 6 | 2089 | 1/1 | 0.95 | 0.44 | 44,44,44,44 | 0 |
| 85 | MG | CP | 504 | 1/1 | 0.95 | 0.23 | 46,46,46,46 | 0 |
| 84 | OHX | A | 1964 | 7/7 | 0.95 | 0.28 | 122,122,123,123 | 0 |
| 85 | MG | 1 | 3796 | 1/1 | 0.95 | 0.54 | 18,18,18,18 | 0 |
| 85 | MG | CQ | 203 | 1/1 | 0.95 | 0.15 | 34,34,34,34 | 0 |
| 84 | OHX | 1 | 3621 | 7/7 | 0.95 | 0.23 | 125,126,126,126 | 0 |
| 84 | OHX | A | 1969 | 7/7 | 0.95 | 0.34 | 144,144,145,145 | 0 |
| 84 | OHX | 6 | 1972 | 7/7 | 0.95 | 0.42 | 142,143,143,144 | 0 |
| 84 | OHX | AR | 3658 | 7/7 | 0.95 | 0.35 | 122,123,123,123 | 0 |
| 84 | OHX | A | 1973 | 7/7 | 0.95 | 0.28 | 167,168,169,169 | 0 |
| 84 | OHX | 6 | 1973 | 7/7 | 0.95 | 0.22 | 137,138,138,138 | 0 |
| 84 | OHX | A | 1977 | 7/7 | 0.95 | 0.25 | 153,154,154,155 | 0 |
| 84 | OHX | 1 | 3667 | 7/7 | 0.95 | 0.30 | 127,127,128,128 | 0 |
| 85 | MG | 1 | 4141 | 1/1 | 0.95 | 0.38 | 64,64,64,64 | 0 |
| 85 | MG | 1 | 4144 | 1/1 | 0.95 | 0.16 | 53,53,53,53 | 0 |
| 84 | OHX | 1 | 3559 | 7/7 | 0.95 | 0.17 | 143,143,143,144 | 0 |
| 85 | MG | 6 | 2107 | 1/1 | 0.95 | 0.55 | 43,43,43,43 | 0 |
| 85 | MG | AR | 4088 | 1/1 | 0.95 | 0.40 | 25,25,25,25 | 0 |
| 84 | OHX | A | 1986 | 7/7 | 0.95 | 0.29 | 168,169,170,170 | 0 |
| 85 | MG | 1 | 3809 | 1/1 | 0.95 | 0.27 | 39,39,39,39 | 0 |
| 85 | MG | DH | 203 | 1/1 | 0.95 | 0.28 | 31,31,31,31 | 0 |
| 85 | MG | 1 | 3977 | 1/1 | 0.95 | 0.14 | 48,48,48,48 | 0 |
| 85 | MG | AR | 3853 | 1/1 | 0.95 | 0.26 | 43,43,43,43 | 0 |
| 84 | OHX | 1 | 3715 | 7/7 | 0.95 | 0.09 | 166,166,167,167 | 0 |
| 85 | MG | AR | 3855 | 1/1 | 0.95 | 0.43 | 33,33,33,33 | 0 |
| 85 | MG | AR | 3856 | 1/1 | 0.95 | 0.71 | 27,27,27,27 | 0 |
| 85 | MG | AR | 3857 | 1/1 | 0.95 | 0.53 | 20,20,20,20 | 0 |
| 84 | OHX | 6 | 1984 | 7/7 | 0.95 | 0.26 | 150,150,151,151 | 0 |
| 84 | OHX | A | 1995 | 7/7 | 0.95 | 0.17 | 151,152,152,152 | 0 |
| 84 | OHX | 1 | 3517 | 7/7 | 0.95 | 0.26 | 119,119,120,120 | 0 |
| 84 | OHX | A | 2000 | 7/7 | 0.95 | 0.24 | 140,141,141,141 | 0 |
| 85 | MG | AR | 3865 | 1/1 | 0.95 | 0.41 | 24,24,24,24 | 0 |
| 85 | MG | AR | 3867 | 1/1 | 0.95 | 0.55 | 18,18,18,18 | 0 |
| 85 | MG | AR | 4105 | 1/1 | 0.95 | 0.14 | 42,42,42,42 | 0 |
| 84 | OHX | A | 2002 | 7/7 | 0.95 | 0.31 | 147,148,149,149 | 0 |
| 84 | OHX | 1 | 3671 | 7/7 | 0.95 | 0.24 | 149,150,150,150 | 0 |
| 84 | OHX | 1 | 3567 | 7/7 | 0.95 | 0.24 | 128,129,129,129 | 0 |
| 84 | OHX | AH | 201 | 7/7 | 0.95 | 0.44 | 129,129,129,130 | 0 |
| 85 | MG | AR | 4111 | 1/1 | 0.95 | 0.35 | 37,37,37,37 | 0 |
| 85 | MG | AR | 3877 | 1/1 | 0.95 | 0.34 | 22,22,22,22 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 85 | MG | 1 | 3824 | 1/1 | 0.95 | 0.39 | 25,25,25,25 | 0 |
| 85 | MG | AR | 3880 | 1/1 | 0.95 | 0.47 | 42,42,42,42 | 0 |
| 85 | MG | AR | 3881 | 1/1 | 0.95 | 0.29 | 30,30,30,30 | 0 |
| 85 | MG | A | 2059 | 1/1 | 0.95 | 0.61 | 53,53,53,53 | 0 |
| 84 | OHX | AR | 3673 | 7/7 | 0.95 | 0.19 | 125,125,125,125 | 0 |
| 84 | OHX | AK | 102 | 7/7 | 0.95 | 0.18 | 105,105,105,105 | 0 |
| 85 | MG | AR | 3886 | 1/1 | 0.95 | 0.70 | 30,30,30,30 | 0 |
| 85 | MG | A | 2063 | 1/1 | 0.95 | 0.50 | 51,51,51,51 | 0 |
| 85 | MG | A | 2064 | 1/1 | 0.95 | 0.34 | 65,65,65,65 | 0 |
| 85 | MG | AR | 4121 | 1/1 | 0.95 | 0.30 | 27,27,27,27 | 0 |
| 84 | OHX | 1 | 3575 | 7/7 | 0.95 | 0.27 | 116,117,117,117 | 0 |
| 85 | MG | 6 | 2126 | 1/1 | 0.95 | 0.29 | 53,53,53,53 | 0 |
| 84 | OHX | AR | 3427 | 7/7 | 0.95 | 0.29 | 110,110,111,111 | 0 |
| 85 | MG | 6 | 2128 | 1/1 | 0.95 | 0.23 | 47,47,47,47 | 0 |
| 84 | OHX | AR | 3460 | 7/7 | 0.95 | 0.20 | 112,112,112,112 | 0 |
| 84 | OHX | AR | 3680 | 7/7 | 0.95 | 0.42 | 141,141,142,142 | 0 |
| 85 | MG | A | 2073 | 1/1 | 0.95 | 0.57 | 50,50,50,50 | 0 |
| 84 | OHX | AR | 3472 | 7/7 | 0.95 | 0.16 | 111,111,111,112 | 0 |
| 85 | MG | AR | 4129 | 1/1 | 0.95 | 0.36 | 26,26,26,26 | 0 |
| 84 | OHX | AR | 3474 | 7/7 | 0.95 | 0.19 | 114,114,114,115 | 0 |
| 85 | MG | 1 | 4171 | 1/1 | 0.95 | 0.24 | 85,85,85,85 | 0 |
| 85 | MG | 6 | 2135 | 1/1 | 0.95 | 0.24 | 49,49,49,49 | 0 |
| 85 | MG | 1 | 4173 | 1/1 | 0.95 | 0.54 | 36,36,36,36 | 0 |
| 85 | MG | AR | 3901 | 1/1 | 0.95 | 0.45 | 29,29,29,29 | 0 |
| 85 | MG | AR | 4138 | 1/1 | 0.95 | 0.47 | 28,28,28,28 | 0 |
| 84 | OHX | AR | 3495 | 7/7 | 0.95 | 0.17 | 113,113,114,114 | 0 |
| 85 | MG | 1 | 4175 | 1/1 | 0.95 | 0.44 | 39,39,39,39 | 0 |
| 85 | MG | AR | 3904 | 1/1 | 0.95 | 0.52 | 21,21,21,21 | 0 |
| 85 | MG | 1 | 3839 | 1/1 | 0.95 | 0.19 | 27,27,27,27 | 0 |
| 85 | MG | 1 | 4179 | 1/1 | 0.95 | 0.23 | 38,38,38,38 | 0 |
| 84 | OHX | AR | 3688 | 7/7 | 0.95 | 0.29 | 136,136,137,137 | 0 |
| 85 | MG | 1 | 3841 | 1/1 | 0.95 | 0.59 | 29,29,29,29 | 0 |
| 84 | OHX | AR | 3499 | 7/7 | 0.95 | 0.15 | 125,126,126,126 | 0 |
| 85 | MG | 1 | 4186 | 1/1 | 0.95 | 0.52 | 25,25,25,25 | 0 |
| 85 | MG | AR | 3915 | 1/1 | 0.95 | 0.61 | 28,28,28,28 | 0 |
| 84 | OHX | A | 2024 | 7/7 | 0.95 | 0.24 | 151,152,153,153 | 0 |
| 85 | MG | AR | 3918 | 1/1 | 0.95 | 0.48 | 27,27,27,27 | 0 |
| 85 | MG | AR | 4151 | 1/1 | 0.95 | 0.10 | 148,148,148,148 | 0 |
| 85 | MG | 6 | 2147 | 1/1 | 0.95 | 0.12 | 57,57,57,57 | 0 |
| 85 | MG | 6 | 2148 | 1/1 | 0.95 | 0.43 | 48,48,48,48 | 0 |
| 85 | MG | 1 | 3846 | 1/1 | 0.95 | 0.28 | 39,39,39,39 | 0 |
| 84 | OHX | AR | 3503 | 7/7 | 0.95 | 0.17 | 120,120,121,121 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84 | OHX | 1 | 3674 | 7/7 | 0.95 | 0.28 | 136,136,137,137 | 0 |
| 85 | MG | 6 | 2153 | 1/1 | 0.95 | 0.27 | 97,97,97,97 | 0 |
| 84 | OHX | A | 2027 | 7/7 | 0.95 | 0.33 | 159,160,161,161 | 0 |
| 84 | OHX | AR | 3511 | 7/7 | 0.95 | 0.26 | 108,108,108,108 | 0 |
| 85 | MG | 6 | 2156 | 1/1 | 0.95 | 0.16 | 101,101,101,101 | 0 |
| 84 | OHX | 6 | 1997 | 7/7 | 0.95 | 0.36 | 132,132,133,133 | 0 |
| 84 | OHX | 1 | 3577 | 7/7 | 0.95 | 0.31 | 118,118,119,119 | 0 |
| 85 | MG | AR | 3937 | 1/1 | 0.95 | 0.67 | 27,27,27,27 | 0 |
| 85 | MG | AR | 3942 | 1/1 | 0.95 | 0.56 | 31,31,31,31 | 0 |
| 84 | OHX | A | 2031 | 7/7 | 0.95 | 0.35 | 159,160,161,161 | 0 |
| 84 | OHX | 1 | 3634 | 7/7 | 0.95 | 0.17 | 132,132,132,133 | 0 |
| 84 | OHX | AR | 3700 | 7/7 | 0.95 | 0.47 | 135,135,135,135 | 0 |
| 85 | MG | 1 | 4207 | 1/1 | 0.95 | 0.28 | 36,36,36,36 | 0 |
| 85 | MG | 1 | 4208 | 1/1 | 0.95 | 0.32 | 37,37,37,37 | 0 |
| 85 | MG | 1 | 3859 | 1/1 | 0.95 | 0.44 | 28,28,28,28 | 0 |
| 84 | OHX | 1 | 3581 | 7/7 | 0.95 | 0.22 | 112,113,113,113 | 0 |
| 85 | MG | A | 2120 | 1/1 | 0.95 | 0.22 | 85,85,85,85 | 0 |
| 84 | OHX | 1 | 3681 | 7/7 | 0.95 | 0.32 | 127,127,127,128 | 0 |
| 84 | OHX | AR | 3703 | 7/7 | 0.95 | 0.51 | 136,136,136,136 | 0 |
| 84 | OHX | AR | 3532 | 7/7 | 0.95 | 0.14 | 135,136,136,137 | 0 |
| 84 | OHX | AR | 3537 | 7/7 | 0.95 | 0.15 | 131,132,132,132 | 0 |
| 84 | OHX | AR | 3538 | 7/7 | 0.95 | 0.17 | 123,123,124,124 | 0 |
| 84 | OHX | AR | 3544 | 7/7 | 0.95 | 0.16 | 109,109,110,110 | 0 |
| 85 | MG | 1 | 3867 | 1/1 | 0.95 | 0.43 | 35,35,35,35 | 0 |
| 85 | MG | 1 | 4024 | 1/1 | 0.95 | 0.21 | 61,61,61,61 | 0 |
| 84 | OHX | 1 | 3583 | 7/7 | 0.95 | 0.16 | 131,132,132,132 | 0 |
| 85 | MG | 6 | 2179 | 1/1 | 0.95 | 0.36 | 43,43,43,43 | 0 |
| 84 | OHX | 1 | 3588 | 7/7 | 0.95 | 0.19 | 128,128,128,128 | 0 |
| 84 | OHX | 1 | 3525 | 7/7 | 0.95 | 0.21 | 114,114,114,115 | 0 |
| 84 | OHX | AR | 3565 | 7/7 | 0.95 | 0.20 | 113,113,113,113 | 0 |
| 85 | MG | 1 | 3872 | 1/1 | 0.95 | 0.59 | 32,32,32,32 | 0 |
| 84 | OHX | AR | 3568 | 7/7 | 0.95 | 0.25 | 117,117,117,117 | 0 |
| 84 | OHX | 4 | 210 | 7/7 | 0.95 | 0.27 | 108,108,108,108 | 0 |
| 84 | OHX | AR | 3714 | 7/7 | 0.95 | 0.33 | 132,132,133,133 | 0 |
| 85 | MG | 1 | 3879 | 1/1 | 0.95 | 0.38 | 45,45,45,45 | 0 |
| 85 | MG | AR | 3972 | 1/1 | 0.95 | 0.53 | 39,39,39,39 | 0 |
| 84 | OHX | AR | 3575 | 7/7 | 0.95 | 0.28 | 119,120,120,120 | 0 |
| 85 | MG | 4 | 218 | 1/1 | 0.95 | 0.60 | 49,49,49,49 | 0 |
| 85 | MG | AR | 4199 | 1/1 | 0.95 | 0.36 | 45,45,45,45 | 0 |
| 85 | MG | A | 2148 | 1/1 | 0.95 | 0.37 | 64,64,64,64 | 0 |
| 85 | MG | 4 | 219 | 1/1 | 0.95 | 0.68 | 42,42,42,42 | 0 |
| 84 | OHX | AR | 3577 | 7/7 | 0.95 | 0.09 | 156,157,158,158 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85 | MG | AR | 4202 | 1/1 | 0.95 | 0.56 | 29,29,29,29 | 0 |
| 84 | OHX | AR | 3579 | 7/7 | 0.95 | 0.35 | 130,130,130,130 | 0 |
| 84 | OHX | AR | 3583 | 7/7 | 0.95 | 0.22 | 113,114,114,114 | 0 |
| 84 | OHX | AR | 3587 | 7/7 | 0.95 | 0.24 | 126,126,126,126 | 0 |
| 85 | MG | 4 | 224 | 1/1 | 0.95 | 0.40 | 33,33,33,33 | 0 |
| 84 | OHX | 6 | 2009 | 7/7 | 0.95 | 0.18 | 126,127,127,128 | 0 |
| 85 | MG | 1 | 3894 | 1/1 | 0.95 | 0.48 | 22,22,22,22 | 0 |
| 84 | OHX | AR | 3592 | 7/7 | 0.95 | 0.34 | 114,114,114,114 | 0 |
| 84 | OHX | 1 | 3527 | 7/7 | 0.95 | 0.12 | 135,135,136,136 | 0 |
| 85 | MG | AR | 4212 | 1/1 | 0.95 | 0.27 | 31,31,31,31 | 0 |
| 85 | MG | AR | 3989 | 1/1 | 0.95 | 0.23 | 44,44,44,44 | 0 |
| 85 | MG | AR | 3990 | 1/1 | 0.95 | 0.08 | 39,39,39,39 | 0 |
| 85 | MG | 1 | 4048 | 1/1 | 0.95 | 0.83 | 33,33,33,33 | 0 |
| 84 | OHX | AR | 3724 | 7/7 | 0.95 | 0.27 | 130,130,131,131 | 0 |
| 84 | OHX | AR | 3595 | 7/7 | 0.95 | 0.31 | 131,131,131,132 | 0 |
| 85 | MG | 1 | 3733 | 1/1 | 0.95 | 0.49 | 26,26,26,26 | 0 |
| 85 | MG | 1 | 3902 | 1/1 | 0.95 | 0.50 | 35,35,35,35 | 0 |
| 84 | OHX | 6 | 2012 | 7/7 | 0.95 | 0.21 | 136,136,137,137 | 0 |
| 85 | MG | AR | 3746 | 1/1 | 0.95 | 0.26 | 58,58,58,58 | 0 |
| 84 | OHX | 1 | 3537 | 7/7 | 0.95 | 0.25 | 115,115,115,116 | 0 |
| 85 | MG | 1 | 3907 | 1/1 | 0.95 | 0.33 | 40,40,40,40 | 0 |
| 84 | OHX | 6 | 2014 | 7/7 | 0.95 | 0.34 | 129,129,129,130 | 0 |
| 84 | OHX | 6 | 2015 | 7/7 | 0.95 | 0.35 | 135,135,136,136 | 0 |
| 84 | OHX | AR | 3601 | 7/7 | 0.95 | 0.42 | 127,127,128,128 | 0 |
| 85 | MG | AR | 4228 | 1/1 | 0.95 | 0.38 | 27,27,27,27 | 0 |
| 85 | MG | 1 | 3914 | 1/1 | 0.95 | 0.50 | 19,19,19,19 | 0 |
| 86 | HN8 | 1 | 4223 | 22/22 | 0.95 | 0.24 | 32,32,32,32 | 0 |
| 86 | HN8 | AR | 4263 | 22/22 | 0.95 | 0.26 | 27,27,27,27 | 22 |
| 84 | OHX | 1 | 3599 | 7/7 | 0.95 | 0.43 | 115,116,116,116 | 0 |
| 85 | MG | 1 | 3741 | 1/1 | 0.95 | 0.25 | 37,37,37,37 | 0 |
| 85 | MG | 1 | 3919 | 1/1 | 0.95 | 0.27 | 33,33,33,33 | 0 |
| 85 | MG | k | 404 | 1/1 | 0.95 | 0.67 | 32,32,32,32 | 0 |
| 84 | OHX | AR | 3603 | 7/7 | 0.95 | 0.24 | 107,107,107,107 | 0 |
| 85 | MG | AR | 4237 | 1/1 | 0.95 | 0.21 | 39,39,39,39 | 0 |
| 88 | ZN | g | 501 | 1/1 | 0.95 | 0.06 | 119,119,119,119 | 0 |
| 84 | OHX | 1 | 3649 | 7/7 | 0.95 | 0.35 | 113,113,113,113 | 0 |
| 84 | OHX | AR | 3682 | 7/7 | 0.96 | 0.52 | 144,144,144,145 | 0 |
| 84 | OHX | AR | 3684 | 7/7 | 0.96 | 0.52 | 124,125,125,125 | 0 |
| 84 | OHX | 1 | 3519 | 7/7 | 0.96 | 0.22 | 116,116,116,116 | 0 |
| 84 | OHX | O | 201 | 7/7 | 0.96 | 0.28 | 158,159,159,160 | 0 |
| 84 | OHX | 6 | 1978 | 7/7 | 0.96 | 0.29 | 117,117,117,118 | 0 |
| 85 | MG | AR | 4217 | 1/1 | 0.96 | 0.60 | 80,80,80,80 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 84 | OHX | T | 201 | 7/7 | 0.96 | 0.19 | 145,146,146,147 | 0 |
| 85 | MG | AR | 3951 | 1/1 | 0.96 | 0.53 | 29,29,29,29 | 0 |
| 85 | MG | AR | 3952 | 1/1 | 0.96 | 0.36 | 28,28,28,28 | 0 |
| 84 | OHX | e | 101 | 7/7 | 0.96 | 0.41 | 143,144,145,145 | 0 |
| 84 | OHX | AR | 3687 | 7/7 | 0.96 | 0.37 | 121,121,122,122 | 0 |
| 85 | MG | 1 | 4143 | 1/1 | 0.96 | 0.21 | 29,29,29,29 | 0 |
| 84 | OHX | c1 | 201 | 7/7 | 0.96 | 0.41 | 147,148,148,149 | 0 |
| 84 | OHX | 1 | 3703 | 7/7 | 0.96 | 0.46 | 131,131,132,132 | 0 |
| 84 | OHX | 6 | 1980 | 7/7 | 0.96 | 0.34 | 116,116,116,116 | 0 |
| 84 | OHX | AR | 3512 | 7/7 | 0.96 | 0.18 | 118,118,119,119 | 0 |
| 84 | OHX | AR | 3514 | 7/7 | 0.96 | 0.19 | 112,112,112,113 | 0 |
| 84 | OHX | 6 | 1982 | 7/7 | 0.96 | 0.17 | 147,147,148,148 | 0 |
| 84 | OHX | AR | 3693 | 7/7 | 0.96 | 0.41 | 131,131,131,131 | 0 |
| 84 | OHX | AR | 3521 | 7/7 | 0.96 | 0.28 | 117,118,118,118 | 0 |
| 84 | OHX | AR | 3522 | 7/7 | 0.96 | 0.13 | 114,114,115,115 | 0 |
| 85 | MG | 6 | 2151 | 1/1 | 0.96 | 0.15 | 60,60,60,60 | 0 |
| 84 | OHX | AR | 3697 | 7/7 | 0.96 | 0.25 | 114,115,115,115 | 0 |
| 84 | OHX | 1 | 3584 | 7/7 | 0.96 | 0.25 | 114,114,114,114 | 0 |
| 84 | OHX | AR | 3699 | 7/7 | 0.96 | 0.36 | 117,117,117,117 | 0 |
| 84 | OHX | AR | 3526 | 7/7 | 0.96 | 0.18 | 117,117,117,118 | 0 |
| 84 | OHX | 6 | 1985 | 7/7 | 0.96 | 0.33 | 130,130,131,131 | 0 |
| 84 | OHX | 1 | 3586 | 7/7 | 0.96 | 0.23 | 121,122,122,122 | 0 |
| 84 | OHX | AR | 3530 | 7/7 | 0.96 | 0.17 | 112,113,113,113 | 0 |
| 84 | OHX | 1 | 3520 | 7/7 | 0.96 | 0.18 | 123,123,124,124 | 0 |
| 84 | OHX | 6 | 1988 | 7/7 | 0.96 | 0.14 | 133,133,133,134 | 0 |
| 84 | OHX | AR | 3534 | 7/7 | 0.96 | 0.16 | 109,109,109,109 | 0 |
| 84 | OHX | AR | 3536 | 7/7 | 0.96 | 0.22 | 123,124,124,124 | 0 |
| 84 | OHX | 1 | 3589 | 7/7 | 0.96 | 0.23 | 113,113,113,113 | 0 |
| 85 | MG | AR | 4249 | 1/1 | 0.96 | 0.44 | 24,24,24,24 | 0 |
| 85 | MG | 1 | 4168 | 1/1 | 0.96 | 0.45 | 20,20,20,20 | 0 |
| 85 | MG | 1 | 3743 | 1/1 | 0.96 | 0.28 | 79,79,79,79 | 0 |
| 84 | OHX | 6 | 1990 | 7/7 | 0.96 | 0.29 | 129,130,130,130 | 0 |
| 84 | OHX | AR | 3541 | 7/7 | 0.96 | 0.19 | 125,125,125,125 | 0 |
| 85 | MG | 1 | 4172 | 1/1 | 0.96 | 0.41 | 67,67,67,67 | 0 |
| 84 | OHX | AR | 3543 | 7/7 | 0.96 | 0.24 | 123,123,123,123 | 0 |
| 84 | OHX | 1 | 3473 | 7/7 | 0.96 | 0.15 | 114,115,115,115 | 0 |
| 85 | MG | 6 | 2172 | 1/1 | 0.96 | 0.26 | 38,38,38,38 | 0 |
| 85 | MG | AR | 4258 | 1/1 | 0.96 | 0.54 | 34,34,34,34 | 0 |
| 84 | OHX | AR | 3545 | 7/7 | 0.96 | 0.24 | 108,108,108,108 | 0 |
| 85 | MG | 1 | 4176 | 1/1 | 0.96 | 0.62 | 34,34,34,34 | 0 |
| 85 | MG | 1 | 4177 | 1/1 | 0.96 | 0.44 | 27,27,27,27 | 0 |
| 85 | MG | 6 | 2177 | 1/1 | 0.96 | 0.19 | 68,68,68,68 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 84 | OHX | AR | 3546 | 7/7 | 0.96 | 0.21 | 123,124,124,124 | 0 |
| 85 | MG | AS | 216 | 1/1 | 0.96 | 0.50 | 23,23,23,23 | 0 |
| 84 | OHX | AR | 3715 | 7/7 | 0.96 | 0.29 | 118,118,119,119 | 0 |
| 84 | OHX | AR | 3548 | 7/7 | 0.96 | 0.16 | 121,121,122,122 | 0 |
| 84 | OHX | AR | 3551 | 7/7 | 0.96 | 0.14 | 129,129,130,130 | 0 |
| 85 | MG | AR | 4000 | 1/1 | 0.96 | 0.43 | 25,25,25,25 | 0 |
| 84 | OHX | 1 | 3592 | 7/7 | 0.96 | 0.33 | 117,117,117,117 | 0 |
| 84 | OHX | AR | 3553 | 7/7 | 0.96 | 0.29 | 113,113,113,113 | 0 |
| 85 | MG | 6 | 2187 | 1/1 | 0.96 | 0.18 | 82,82,82,82 | 0 |
| 85 | MG | 1 | 3968 | 1/1 | 0.96 | 0.47 | 29,29,29,29 | 0 |
| 85 | MG | 1 | 4188 | 1/1 | 0.96 | 0.36 | 28,28,28,28 | 0 |
| 85 | MG | 1 | 3757 | 1/1 | 0.96 | 0.19 | 38,38,38,38 | 0 |
| 85 | MG | AR | 4007 | 1/1 | 0.96 | 0.28 | 29,29,29,29 | 0 |
| 85 | MG | AS | 229 | 1/1 | 0.96 | 0.24 | 46,46,46,46 | 0 |
| 84 | OHX | AR | 3555 | 7/7 | 0.96 | 0.21 | 115,115,115,115 | 0 |
| 84 | OHX | AR | 3556 | 7/7 | 0.96 | 0.21 | 109,109,109,109 | 0 |
| 84 | OHX | AR | 3557 | 7/7 | 0.96 | 0.17 | 123,123,124,124 | 0 |
| 84 | OHX | AR | 3562 | 7/7 | 0.96 | 0.24 | 124,124,124,124 | 0 |
| 85 | MG | 1 | 4197 | 1/1 | 0.96 | 0.34 | 32,32,32,32 | 0 |
| 84 | OHX | 6 | 1994 | 7/7 | 0.96 | 0.25 | 170,170,170,170 | 0 |
| 85 | MG | 1 | 4199 | 1/1 | 0.96 | 0.59 | 24,24,24,24 | 0 |
| 84 | OHX | 6 | 1995 | 7/7 | 0.96 | 0.24 | 133,134,134,135 | 0 |
| 84 | OHX | 6 | 1996 | 7/7 | 0.96 | 0.20 | 154,154,155,155 | 0 |
| 84 | OHX | AR | 3567 | 7/7 | 0.96 | 0.15 | 121,121,121,121 | 0 |
| 84 | OHX | 1 | 3593 | 7/7 | 0.96 | 0.15 | 166,167,167,167 | 0 |
| 84 | OHX | AR | 3570 | 7/7 | 0.96 | 0.25 | 120,121,121,121 | 0 |
| 85 | MG | 1 | 3980 | 1/1 | 0.96 | 0.26 | 73,73,73,73 | 0 |
| 84 | OHX | 6 | 1998 | 7/7 | 0.96 | 0.33 | 146,146,147,147 | 0 |
| 84 | OHX | AR | 3731 | 7/7 | 0.96 | 0.19 | 117,117,117,117 | 0 |
| 84 | OHX | 1 | 3526 | 7/7 | 0.96 | 0.29 | 114,115,115,115 | 0 |
| 84 | OHX | 6 | 2000 | 7/7 | 0.96 | 0.17 | 130,130,131,131 | 0 |
| 84 | OHX | 1 | 3654 | 7/7 | 0.96 | 0.14 | 136,136,136,137 | 0 |
| 84 | OHX | AR | 3580 | 7/7 | 0.96 | 0.20 | 117,118,118,118 | 0 |
| 85 | MG | AK | 103 | 1/1 | 0.96 | 0.44 | 36,36,36,36 | 0 |
| 85 | MG | AP | 503 | 1/1 | 0.96 | 0.28 | 27,27,27,27 | 0 |
| 85 | MG | 1 | 4216 | 1/1 | 0.96 | 0.39 | 23,23,23,23 | 0 |
| 85 | MG | 1 | 3775 | 1/1 | 0.96 | 0.29 | 32,32,32,32 | 0 |
| 84 | OHX | AR | 3581 | 7/7 | 0.96 | 0.18 | 109,109,109,109 | 0 |
| 84 | OHX | 1 | 3595 | 7/7 | 0.96 | 0.11 | 140,140,140,140 | 0 |
| 85 | MG | CK | 202 | 1/1 | 0.96 | 0.20 | 44,44,44,44 | 0 |
| 84 | OHX | AR | 3586 | 7/7 | 0.96 | 0.24 | 119,119,120,120 | 0 |
| 85 | MG | 1 | 4221 | 1/1 | 0.96 | 0.52 | 35,35,35,35 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85 | MG | 1 | 4222 | 1/1 | 0.96 | 0.65 | 13,13,13,13 | 0 |
| 85 | MG | CO | 201 | 1/1 | 0.96 | 0.19 | 44,44,44,44 | 0 |
| 85 | MG | 1 | 3781 | 1/1 | 0.96 | 0.39 | 33,33,33,33 | 0 |
| 84 | OHX | 1 | 3445 | 7/7 | 0.96 | 0.26 | 111,112,112,112 | 0 |
| 85 | MG | CP | 505 | 1/1 | 0.96 | 0.27 | 71,71,71,71 | 0 |
| 84 | OHX | AR | 3588 | 7/7 | 0.96 | 0.27 | 112,112,112,113 | 0 |
| 85 | MG | 3 | 213 | 1/1 | 0.96 | 0.45 | 48,48,48,48 | 0 |
| 84 | OHX | 1 | 3597 | 7/7 | 0.96 | 0.39 | 117,117,118,118 | 0 |
| 85 | MG | 3 | 215 | 1/1 | 0.96 | 0.57 | 31,31,31,31 | 0 |
| 84 | OHX | 1 | 3531 | 7/7 | 0.96 | 0.19 | 114,114,114,114 | 0 |
| 84 | OHX | AR | 3743 | 7/7 | 0.96 | 0.33 | 109,109,109,109 | 0 |
| 85 | MG | 3 | 219 | 1/1 | 0.96 | 0.21 | 56,56,56,56 | 0 |
| 84 | OHX | 1 | 3601 | 7/7 | 0.96 | 0.30 | 112,112,112,112 | 0 |
| 84 | OHX | 1 | 3483 | 7/7 | 0.96 | 0.12 | 113,113,113,113 | 0 |
| 85 | MG | AR | 3766 | 1/1 | 0.96 | 0.14 | 96,96,96,96 | 0 |
| 84 | OHX | 1 | 3446 | 7/7 | 0.96 | 0.19 | 116,116,116,116 | 0 |
| 85 | MG | 1 | 3792 | 1/1 | 0.96 | 0.52 | 37,37,37,37 | 0 |
| 84 | OHX | 1 | 3451 | 7/7 | 0.96 | 0.22 | 111,111,111,111 | 0 |
| 84 | OHX | AT | 210 | 7/7 | 0.96 | 0.20 | 119,119,120,120 | 0 |
| 84 | OHX | AT | 211 | 7/7 | 0.96 | 0.11 | 137,138,138,138 | 0 |
| 85 | MG | AR | 3772 | 1/1 | 0.96 | 0.52 | 37,37,37,37 | 0 |
| 84 | OHX | AR | 3598 | 7/7 | 0.96 | 0.18 | 117,118,118,118 | 0 |
| 84 | OHX | 6 | 2011 | 7/7 | 0.96 | 0.43 | 146,146,147,147 | 0 |
| 85 | MG | DH | 202 | 1/1 | 0.96 | 0.26 | 40,40,40,40 | 0 |
| 84 | OHX | 1 | 3541 | 7/7 | 0.96 | 0.26 | 119,119,120,120 | 0 |
| 84 | OHX | 1 | 3543 | 7/7 | 0.96 | 0.22 | 119,119,120,120 | 0 |
| 84 | OHX | 1 | 3611 | 7/7 | 0.96 | 0.21 | 119,119,119,120 | 0 |
| 85 | MG | 4 | 226 | 1/1 | 0.96 | 0.59 | 42,42,42,42 | 0 |
| 84 | OHX | 1 | 3455 | 7/7 | 0.96 | 0.16 | 127,127,127,128 | 0 |
| 84 | OHX | 1 | 3489 | 7/7 | 0.96 | 0.21 | 113,113,114,114 | 0 |
| 84 | OHX | 6 | 2017 | 7/7 | 0.96 | 0.29 | 135,135,136,136 | 0 |
| 84 | OHX | 1 | 3547 | 7/7 | 0.96 | 0.11 | 120,121,121,121 | 0 |
| 85 | MG | AR | 3787 | 1/1 | 0.96 | 0.69 | 31,31,31,31 | 0 |
| 84 | OHX | 3 | 207 | 7/7 | 0.96 | 0.20 | 137,138,138,138 | 0 |
| 84 | OHX | 1 | 3670 | 7/7 | 0.96 | 0.24 | 111,111,111,111 | 0 |
| 85 | MG | AR | 3790 | 1/1 | 0.96 | 0.34 | 22,22,22,22 | 0 |
| 84 | OHX | CK | 201 | 7/7 | 0.96 | 0.21 | 118,118,119,119 | 0 |
| 84 | OHX | 4 | 206 | 7/7 | 0.96 | 0.16 | 116,116,116,116 | 0 |
| 85 | MG | 1 | 3812 | 1/1 | 0.96 | 0.64 | 64,64,64,64 | 0 |
| 84 | OHX | 1 | 3497 | 7/7 | 0.96 | 0.11 | 125,125,126,126 | 0 |
| 85 | MG | AR | 3795 | 1/1 | 0.96 | 0.66 | 49,49,49,49 | 0 |
| 84 | OHX | CX | 202 | 7/7 | 0.96 | 0.27 | 117,118,118,118 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84 | OHX | AR | 3612 | 7/7 | 0.96 | 0.34 | 111,111,111,111 | 0 |
| 85 | MG | AR | 4079 | 1/1 | 0.96 | 0.31 | 34,34,34,34 | 0 |
| 85 | MG | 4 | 239 | 1/1 | 0.96 | 0.69 | 43,43,43,43 | 0 |
| 84 | OHX | AR | 3613 | 7/7 | 0.96 | 0.29 | 112,112,112,112 | 0 |
| 84 | OHX | AR | 3614 | 7/7 | 0.96 | 0.20 | 114,114,114,114 | 0 |
| 84 | OHX | A | 1933 | 7/7 | 0.96 | 0.13 | 122,122,122,123 | 0 |
| 84 | OHX | 4 | 211 | 7/7 | 0.96 | 0.14 | 138,139,139,140 | 0 |
| 84 | OHX | A | 1936 | 7/7 | 0.96 | 0.17 | 126,127,127,128 | 0 |
| 84 | OHX | A | 1944 | 7/7 | 0.96 | 0.12 | 138,139,139,140 | 0 |
| 84 | OHX | AR | 3617 | 7/7 | 0.96 | 0.28 | 123,123,123,123 | 0 |
| 84 | OHX | A | 1947 | 7/7 | 0.96 | 0.27 | 129,129,130,130 | 0 |
| 85 | MG | 1 | 4032 | 1/1 | 0.96 | 0.31 | 42,42,42,42 | 0 |
| 85 | MG | A | 2066 | 1/1 | 0.96 | 0.59 | 79,79,79,79 | 0 |
| 85 | MG | AR | 4091 | 1/1 | 0.96 | 0.31 | 35,35,35,35 | 0 |
| 84 | OHX | 1 | 3617 | 7/7 | 0.96 | 0.23 | 122,122,122,122 | 0 |
| 84 | OHX | A | 1955 | 7/7 | 0.96 | 0.13 | 145,146,147,147 | 0 |
| 84 | OHX | AR | 3619 | 7/7 | 0.96 | 0.35 | 122,123,123,124 | 0 |
| 85 | MG | AR | 4095 | 1/1 | 0.96 | 0.22 | 25,25,25,25 | 0 |
| 84 | OHX | AR | 3621 | 7/7 | 0.96 | 0.35 | 135,135,136,136 | 0 |
| 84 | OHX | 1 | 3458 | 7/7 | 0.96 | 0.20 | 116,116,116,117 | 0 |
| 85 | MG | A | 2074 | 1/1 | 0.96 | 0.41 | 55,55,55,55 | 0 |
| 84 | OHX | AR | 3623 | 7/7 | 0.96 | 0.29 | 138,139,139,139 | 0 |
| 84 | OHX | 1 | 3553 | 7/7 | 0.96 | 0.29 | 121,122,122,122 | 0 |
| 85 | MG | 1 | 3838 | 1/1 | 0.96 | 0.57 | 33,33,33,33 | 0 |
| 84 | OHX | AR | 3626 | 7/7 | 0.96 | 0.30 | 122,123,123,123 | 0 |
| 84 | OHX | AR | 3627 | 7/7 | 0.96 | 0.32 | 127,128,128,128 | 0 |
| 84 | OHX | AR | 3628 | 7/7 | 0.96 | 0.32 | 147,148,148,148 | 0 |
| 85 | MG | 1 | 3842 | 1/1 | 0.96 | 0.55 | 25,25,25,25 | 0 |
| 84 | OHX | AR | 3629 | 7/7 | 0.96 | 0.14 | 141,141,141,142 | 0 |
| 84 | OHX | 1 | 3500 | 7/7 | 0.96 | 0.16 | 119,120,120,120 | 0 |
| 85 | MG | AR | 3828 | 1/1 | 0.96 | 0.61 | 60,60,60,60 | 0 |
| 84 | OHX | AR | 3632 | 7/7 | 0.96 | 0.35 | 117,117,118,118 | 0 |
| 85 | MG | 1 | 4052 | 1/1 | 0.96 | 0.29 | 21,21,21,21 | 0 |
| 84 | OHX | A | 1975 | 7/7 | 0.96 | 0.10 | 156,158,158,158 | 0 |
| 85 | MG | AR | 4112 | 1/1 | 0.96 | 0.15 | 54,54,54,54 | 0 |
| 84 | OHX | A | 1976 | 7/7 | 0.96 | 0.18 | 123,124,124,124 | 0 |
| 84 | OHX | AR | 3633 | 7/7 | 0.96 | 0.28 | 124,125,125,125 | 0 |
| 84 | OHX | A | 1978 | 7/7 | 0.96 | 0.26 | 143,144,144,145 | 0 |
| 85 | MG | IR | 201 | 1/1 | 0.96 | 0.36 | 26,26,26,26 | 0 |
| 84 | OHX | A | 1980 | 7/7 | 0.96 | 0.26 | 137,137,138,138 | 0 |
| 85 | MG | 6 | 2055 | 1/1 | 0.96 | 0.73 | 49,49,49,49 | 0 |
| 84 | OHX | k | 401 | 7/7 | 0.96 | 0.27 | 118,118,118,118 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 84 | OHX | A | 1983 | 7/7 | 0.96 | 0.24 | 142,142,143,143 | 0 |
| 85 | MG | 1 | 3854 | 1/1 | 0.96 | 0.62 | 34,34,34,34 | 0 |
| 85 | MG | 6 | 2061 | 1/1 | 0.96 | 0.32 | 100,100,100,100 | 0 |
| 85 | MG | AR | 3844 | 1/1 | 0.96 | 0.40 | 27,27,27,27 | 0 |
| 84 | OHX | 6 | 2029 | 7/7 | 0.96 | 0.41 | 152,153,153,154 | 0 |
| 85 | MG | AR | 3846 | 1/1 | 0.96 | 0.56 | 33,33,33,33 | 0 |
| 85 | MG | 1 | 3856 | 1/1 | 0.96 | 0.68 | 24,24,24,24 | 0 |
| 84 | OHX | 1 | 3431 | 7/7 | 0.96 | 0.30 | 114,114,114,114 | 0 |
| 84 | OHX | A | 1989 | 7/7 | 0.96 | 0.37 | 154,155,155,155 | 0 |
| 84 | OHX | 1 | 3677 | 7/7 | 0.96 | 0.33 | 116,116,117,117 | 0 |
| 85 | MG | AR | 4133 | 1/1 | 0.96 | 0.27 | 25,25,25,25 | 0 |
| 85 | MG | 1 | 4069 | 1/1 | 0.96 | 0.43 | 46,46,46,46 | 0 |
| 84 | OHX | 1 | 3622 | 7/7 | 0.96 | 0.27 | 153,154,154,154 | 0 |
| 84 | OHX | A | 1994 | 7/7 | 0.96 | 0.28 | 142,143,144,144 | 0 |
| 84 | OHX | 1 | 3680 | 7/7 | 0.96 | 0.32 | 122,122,122,122 | 0 |
| 84 | OHX | 6 | 2034 | 7/7 | 0.96 | 0.19 | 155,155,155,155 | 0 |
| 84 | OHX | A | 1997 | 7/7 | 0.96 | 0.28 | 139,140,140,140 | 0 |
| 85 | MG | 6 | 2075 | 1/1 | 0.96 | 0.14 | 76,76,76,76 | 0 |
| 84 | OHX | A | 1999 | 7/7 | 0.96 | 0.24 | 146,146,147,147 | 0 |
| 84 | OHX | 1 | 3623 | 7/7 | 0.96 | 0.23 | 114,114,115,115 | 0 |
| 85 | MG | A | 2119 | 1/1 | 0.96 | 0.35 | 57,57,57,57 | 0 |
| 84 | OHX | A | 2001 | 7/7 | 0.96 | 0.20 | 136,137,137,138 | 0 |
| 84 | OHX | 1 | 3683 | 7/7 | 0.96 | 0.33 | 118,118,118,118 | 0 |
| 85 | MG | AR | 3871 | 1/1 | 0.96 | 0.40 | 28,28,28,28 | 0 |
| 84 | OHX | A | 2003 | 7/7 | 0.96 | 0.32 | 129,130,130,130 | 0 |
| 84 | OHX | A | 2005 | 7/7 | 0.96 | 0.32 | 131,132,132,132 | 0 |
| 85 | MG | AR | 3874 | 1/1 | 0.96 | 0.60 | 27,27,27,27 | 0 |
| 84 | OHX | 1 | 3684 | 7/7 | 0.96 | 0.41 | 141,141,141,141 | 0 |
| 84 | OHX | 6 | 1921 | 7/7 | 0.96 | 0.17 | 141,141,142,143 | 0 |
| 85 | MG | 6 | 2084 | 1/1 | 0.96 | 0.22 | 48,48,48,48 | 0 |
| 84 | OHX | A | 2009 | 7/7 | 0.96 | 0.38 | 126,126,127,127 | 0 |
| 85 | MG | 1 | 3876 | 1/1 | 0.96 | 0.40 | 37,37,37,37 | 0 |
| 84 | OHX | AR | 3648 | 7/7 | 0.96 | 0.55 | 130,131,131,131 | 0 |
| 84 | OHX | 1 | 3685 | 7/7 | 0.96 | 0.41 | 121,121,121,121 | 0 |
| 84 | OHX | 1 | 3624 | 7/7 | 0.96 | 0.20 | 136,136,136,137 | 0 |
| 84 | OHX | 1 | 3507 | 7/7 | 0.96 | 0.23 | 113,113,114,114 | 0 |
| 84 | OHX | 6 | 1941 | 7/7 | 0.96 | 0.13 | 120,120,121,121 | 0 |
| 84 | OHX | A | 2016 | 7/7 | 0.96 | 0.28 | 142,143,143,144 | 0 |
| 85 | MG | A | 2137 | 1/1 | 0.96 | 0.48 | 58,58,58,58 | 0 |
| 85 | MG | A | 2138 | 1/1 | 0.96 | 0.46 | 66,66,66,66 | 0 |
| 85 | MG | 6 | 2093 | 1/1 | 0.96 | 0.33 | 47,47,47,47 | 0 |
| 85 | MG | 1 | 4094 | 1/1 | 0.96 | 0.15 | 78,78,78,78 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85 | MG | 1 | 4095 | 1/1 | 0.96 | 0.20 | 61,61,61,61 | 0 |
| 85 | MG | 1 | 4096 | 1/1 | 0.96 | 0.41 | 27,27,27,27 | 0 |
| 85 | MG | A | 2144 | 1/1 | 0.96 | 0.39 | 69,69,69,69 | 0 |
| 85 | MG | AR | 3895 | 1/1 | 0.96 | 0.28 | 43,43,43,43 | 0 |
| 84 | OHX | 6 | 1946 | 7/7 | 0.96 | 0.17 | 127,128,128,129 | 0 |
| 84 | OHX | 6 | 2044 | 7/7 | 0.96 | 0.35 | 140,141,141,141 | 0 |
| 84 | OHX | 6 | 1947 | 7/7 | 0.96 | 0.14 | 121,122,122,122 | 0 |
| 85 | MG | 6 | 2101 | 1/1 | 0.96 | 0.51 | 53,53,53,53 | 0 |
| 84 | OHX | 6 | 1949 | 7/7 | 0.96 | 0.11 | 135,136,136,136 | 0 |
| 84 | OHX | 1 | 3509 | 7/7 | 0.96 | 0.14 | 119,120,120,120 | 0 |
| 85 | MG | 6 | 2104 | 1/1 | 0.96 | 0.20 | 70,70,70,70 | 0 |
| 85 | MG | 1 | 4103 | 1/1 | 0.96 | 0.27 | 60,60,60,60 | 0 |
| 84 | OHX | 6 | 1952 | 7/7 | 0.96 | 0.14 | 148,148,148,148 | 0 |
| 85 | MG | 1 | 4105 | 1/1 | 0.96 | 0.49 | 26,26,26,26 | 0 |
| 84 | OHX | AR | 3662 | 7/7 | 0.96 | 0.22 | 111,111,112,112 | 0 |
| 84 | OHX | 1 | 3628 | 7/7 | 0.96 | 0.26 | 144,145,145,145 | 0 |
| 84 | OHX | 1 | 3565 | 7/7 | 0.96 | 0.25 | 131,131,131,131 | 0 |
| 84 | OHX | 1 | 3510 | 7/7 | 0.96 | 0.16 | 111,111,111,111 | 0 |
| 84 | OHX | 1 | 3435 | 7/7 | 0.96 | 0.27 | 114,114,114,114 | 0 |
| 85 | MG | AR | 3916 | 1/1 | 0.96 | 0.58 | 19,19,19,19 | 0 |
| 84 | OHX | 1 | 3693 | 7/7 | 0.96 | 0.27 | 118,118,118,118 | 0 |
| 85 | MG | 6 | 2114 | 1/1 | 0.96 | 0.47 | 46,46,46,46 | 0 |
| 85 | MG | AR | 3919 | 1/1 | 0.96 | 0.43 | 34,34,34,34 | 0 |
| 84 | OHX | 1 | 3471 | 7/7 | 0.96 | 0.21 | 112,112,113,113 | 0 |
| 84 | OHX | AR | 3669 | 7/7 | 0.96 | 0.17 | 175,176,176,176 | 0 |
| 84 | OHX | 1 | 3579 | 7/7 | 0.96 | 0.17 | 119,120,120,120 | 0 |
| 84 | OHX | AR | 3671 | 7/7 | 0.96 | 0.28 | 113,113,113,113 | 0 |
| 84 | OHX | 1 | 3637 | 7/7 | 0.96 | 0.15 | 140,140,140,141 | 0 |
| 85 | MG | 1 | 3916 | 1/1 | 0.96 | 0.29 | 26,26,26,26 | 0 |
| 85 | MG | AR | 3926 | 1/1 | 0.96 | 0.37 | 33,33,33,33 | 0 |
| 85 | MG | 1 | 4120 | 1/1 | 0.96 | 0.40 | 27,27,27,27 | 0 |
| 85 | MG | d3 | 202 | 1/1 | 0.96 | 0.33 | 47,47,47,47 | 0 |
| 84 | OHX | AR | 3441 | 7/7 | 0.96 | 0.18 | 116,117,117,117 | 0 |
| 84 | OHX | 1 | 3518 | 7/7 | 0.96 | 0.15 | 109,110,110,110 | 0 |
| 85 | MG | AR | 3931 | 1/1 | 0.96 | 0.29 | 17,17,17,17 | 0 |
| 85 | MG | AR | 3933 | 1/1 | 0.96 | 0.47 | 24,24,24,24 | 0 |
| 84 | OHX | AR | 3676 | 7/7 | 0.96 | 0.29 | 122,122,123,123 | 0 |
| 84 | OHX | AR | 3466 | 7/7 | 0.96 | 0.18 | 120,120,121,121 | 0 |
| 85 | MG | AR | 3936 | 1/1 | 0.96 | 0.52 | 20,20,20,20 | 0 |
| 84 | OHX | 1 | 3640 | 7/7 | 0.96 | 0.35 | 124,124,124,125 | 0 |
| 85 | MG | AR | 3939 | 1/1 | 0.96 | 0.31 | 31,31,31,31 | 0 |
| 85 | MG | AR | 3941 | 1/1 | 0.96 | 0.46 | 36,36,36,36 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 84 | OHX | AR | 3679 | 7/7 | 0.96 | 0.25 | 153,153,153,154 | 0 |
| 84 | OHX | 1 | 3582 | 7/7 | 0.96 | 0.29 | 121,121,121,121 | 0 |
| 84 | OHX | 6 | 1976 | 7/7 | 0.96 | 0.13 | 146,147,147,148 | 0 |
| 88 | ZN | e1 | 501 | 1/1 | 0.96 | 0.06 | 153,153,153,153 | 0 |
| 84 | OHX | AR | 3625 | 7/7 | 0.97 | 0.36 | 134,134,134,134 | 0 |
| 84 | OHX | A | 1968 | 7/7 | 0.97 | 0.34 | 125,125,126,126 | 0 |
| 84 | OHX | 1 | 3506 | 7/7 | 0.97 | 0.29 | 109,109,110,110 | 0 |
| 84 | OHX | 1 | 3466 | 7/7 | 0.97 | 0.16 | 114,115,115,115 | 0 |
| 84 | OHX | 6 | 1953 | 7/7 | 0.97 | 0.12 | 132,133,133,134 | 0 |
| 85 | MG | AR | 3930 | 1/1 | 0.97 | 0.62 | 29,29,29,29 | 0 |
| 84 | OHX | 1 | 3638 | 7/7 | 0.97 | 0.33 | 122,123,123,123 | 0 |
| 85 | MG | AR | 3932 | 1/1 | 0.97 | 0.28 | 63,63,63,63 | 0 |
| 84 | OHX | AR | 3630 | 7/7 | 0.97 | 0.13 | 124,125,125,125 | 0 |
| 84 | OHX | AG | 201 | 7/7 | 0.97 | 0.21 | 114,115,115,115 | 0 |
| 84 | OHX | 6 | 1955 | 7/7 | 0.97 | 0.13 | 179,179,179,179 | 0 |
| 84 | OHX | 1 | 3585 | 7/7 | 0.97 | 0.23 | 115,115,116,116 | 0 |
| 84 | OHX | 6 | 1957 | 7/7 | 0.97 | 0.14 | 129,130,130,131 | 0 |
| 85 | MG | AR | 3938 | 1/1 | 0.97 | 0.39 | 34,34,34,34 | 0 |
| 84 | OHX | A | 1979 | 7/7 | 0.97 | 0.22 | 142,143,144,144 | 0 |
| 84 | OHX | AP | 502 | 7/7 | 0.97 | 0.17 | 112,113,113,113 | 0 |
| 84 | OHX | 6 | 1959 | 7/7 | 0.97 | 0.17 | 137,138,138,139 | 0 |
| 85 | MG | 1 | 4112 | 1/1 | 0.97 | 0.43 | 32,32,32,32 | 0 |
| 84 | OHX | A | 1982 | 7/7 | 0.97 | 0.30 | 121,122,122,122 | 0 |
| 85 | MG | 1 | 4114 | 1/1 | 0.97 | 0.23 | 52,52,52,52 | 0 |
| 84 | OHX | AR | 3432 | 7/7 | 0.97 | 0.27 | 117,117,117,118 | 0 |
| 84 | OHX | 1 | 3542 | 7/7 | 0.97 | 0.17 | 119,119,120,120 | 0 |
| 84 | OHX | AR | 3442 | 7/7 | 0.97 | 0.22 | 112,112,112,112 | 0 |
| 85 | MG | AR | 4229 | 1/1 | 0.97 | 0.70 | 34,34,34,34 | 0 |
| 84 | OHX | A | 1987 | 7/7 | 0.97 | 0.15 | 128,128,129,129 | 0 |
| 84 | OHX | A | 1988 | 7/7 | 0.97 | 0.23 | 139,140,141,141 | 0 |
| 84 | OHX | AR | 3445 | 7/7 | 0.97 | 0.18 | 107,107,107,107 | 0 |
| 85 | MG | 6 | 2136 | 1/1 | 0.97 | 0.23 | 52,52,52,52 | 0 |
| 85 | MG | AR | 3953 | 1/1 | 0.97 | 0.19 | 34,34,34,34 | 0 |
| 85 | MG | AR | 4235 | 1/1 | 0.97 | 0.37 | 26,26,26,26 | 0 |
| 85 | MG | 1 | 4122 | 1/1 | 0.97 | 0.25 | 78,78,78,78 | 0 |
| 85 | MG | 1 | 3878 | 1/1 | 0.97 | 0.58 | 24,24,24,24 | 0 |
| 84 | OHX | A | 1990 | 7/7 | 0.97 | 0.27 | 135,135,136,136 | 0 |
| 84 | OHX | AR | 3447 | 7/7 | 0.97 | 0.25 | 112,112,112,112 | 0 |
| 84 | OHX | A | 1992 | 7/7 | 0.97 | 0.21 | 140,141,142,142 | 0 |
| 85 | MG | 1 | 3883 | 1/1 | 0.97 | 0.41 | 22,22,22,22 | 0 |
| 84 | OHX | AR | 3642 | 7/7 | 0.97 | 0.24 | 122,122,122,122 | 0 |
| 84 | OHX | AR | 3643 | 7/7 | 0.97 | 0.30 | 120,121,121,121 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 85 | MG | 1 | 3887 | 1/1 | 0.97 | 0.83 | 42,42,42,42 | 0 |
| 84 | OHX | AR | 3455 | 7/7 | 0.97 | 0.22 | 111,112,112,112 | 0 |
| 84 | OHX | AR | 3456 | 7/7 | 0.97 | 0.19 | 117,117,117,117 | 0 |
| 84 | OHX | AR | 3458 | 7/7 | 0.97 | 0.19 | 114,114,114,115 | 0 |
| 85 | MG | 1 | 3895 | 1/1 | 0.97 | 0.42 | 28,28,28,28 | 0 |
| 84 | OHX | A | 1998 | 7/7 | 0.97 | 0.25 | 158,159,160,160 | 0 |
| 84 | OHX | AR | 3459 | 7/7 | 0.97 | 0.26 | 114,114,115,115 | 0 |
| 84 | OHX | 1 | 3699 | 7/7 | 0.97 | 0.40 | 130,131,131,131 | 0 |
| 85 | MG | AR | 3970 | 1/1 | 0.97 | 0.23 | 50,50,50,50 | 0 |
| 84 | OHX | AR | 3463 | 7/7 | 0.97 | 0.17 | 110,110,111,111 | 0 |
| 85 | MG | 1 | 3900 | 1/1 | 0.97 | 0.34 | 42,42,42,42 | 0 |
| 84 | OHX | 1 | 3442 | 7/7 | 0.97 | 0.24 | 120,121,121,121 | 0 |
| 85 | MG | AR | 3974 | 1/1 | 0.97 | 0.42 | 81,81,81,81 | 0 |
| 84 | OHX | AR | 3467 | 7/7 | 0.97 | 0.13 | 108,109,109,109 | 0 |
| 84 | OHX | A | 2004 | 7/7 | 0.97 | 0.22 | 139,139,140,140 | 0 |
| 84 | OHX | AR | 3653 | 7/7 | 0.97 | 0.30 | 120,120,121,121 | 0 |
| 84 | OHX | AR | 3469 | 7/7 | 0.97 | 0.14 | 121,122,122,122 | 0 |
| 84 | OHX | 6 | 1964 | 7/7 | 0.97 | 0.12 | 123,123,124,124 | 0 |
| 85 | MG | 1 | 3909 | 1/1 | 0.97 | 0.57 | 25,25,25,25 | 0 |
| 84 | OHX | A | 2008 | 7/7 | 0.97 | 0.16 | 132,132,133,133 | 0 |
| 84 | OHX | AR | 3656 | 7/7 | 0.97 | 0.31 | 134,134,134,134 | 0 |
| 84 | OHX | AR | 3473 | 7/7 | 0.97 | 0.11 | 111,111,112,112 | 0 |
| 85 | MG | AR | 3985 | 1/1 | 0.97 | 0.49 | 35,35,35,35 | 0 |
| 84 | OHX | 6 | 1965 | 7/7 | 0.97 | 0.24 | 116,117,117,117 | 0 |
| 85 | MG | AR | 3987 | 1/1 | 0.97 | 0.30 | 31,31,31,31 | 0 |
| 84 | OHX | AR | 3478 | 7/7 | 0.97 | 0.17 | 110,110,110,111 | 0 |
| 85 | MG | 1 | 4157 | 1/1 | 0.97 | 0.48 | 60,60,60,60 | 0 |
| 84 | OHX | AR | 3479 | 7/7 | 0.97 | 0.15 | 110,110,110,110 | 0 |
| 85 | MG | 1 | 3918 | 1/1 | 0.97 | 0.20 | 31,31,31,31 | 0 |
| 84 | OHX | AR | 3661 | 7/7 | 0.97 | 0.46 | 112,112,112,113 | 0 |
| 84 | OHX | AR | 3480 | 7/7 | 0.97 | 0.12 | 113,114,114,114 | 0 |
| 84 | OHX | AR | 3483 | 7/7 | 0.97 | 0.17 | 111,111,111,111 | 0 |
| 84 | OHX | AR | 3484 | 7/7 | 0.97 | 0.19 | 114,114,114,114 | 0 |
| 85 | MG | AS | 231 | 1/1 | 0.97 | 0.19 | 56,56,56,56 | 0 |
| 84 | OHX | AR | 3491 | 7/7 | 0.97 | 0.13 | 108,108,109,109 | 0 |
| 84 | OHX | AR | 3492 | 7/7 | 0.97 | 0.15 | 116,116,117,117 | 0 |
| 84 | OHX | AR | 3493 | 7/7 | 0.97 | 0.25 | 114,114,114,114 | 0 |
| 84 | OHX | AR | 3494 | 7/7 | 0.97 | 0.15 | 124,125,125,125 | 0 |
| 84 | OHX | 1 | 3425 | 7/7 | 0.97 | 0.25 | 108,109,109,109 | 0 |
| 84 | OHX | AR | 3496 | 7/7 | 0.97 | 0.24 | 112,113,113,113 | 0 |
| 84 | OHX | 6 | 1967 | 7/7 | 0.97 | 0.17 | 126,127,127,127 | 0 |
| 84 | OHX | AR | 3501 | 7/7 | 0.97 | 0.31 | 113,113,114,114 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 84 | OHX | 6 | 1968 | 7/7 | 0.97 | 0.26 | 122,122,123,123 | 0 |
| 84 | OHX | AR | 3504 | 7/7 | 0.97 | 0.18 | 110,110,110,110 | 0 |
| 84 | OHX | 1 | 3438 | 7/7 | 0.97 | 0.25 | 117,117,117,117 | 0 |
| 84 | OHX | 1 | 3546 | 7/7 | 0.97 | 0.17 | 127,127,127,127 | 0 |
| 84 | OHX | 1 | 3645 | 7/7 | 0.97 | 0.34 | 125,126,126,126 | 0 |
| 84 | OHX | AR | 3513 | 7/7 | 0.97 | 0.09 | 150,151,151,151 | 0 |
| 84 | OHX | 1 | 3646 | 7/7 | 0.97 | 0.25 | 117,118,118,118 | 0 |
| 84 | OHX | AR | 3516 | 7/7 | 0.97 | 0.15 | 112,112,112,112 | 0 |
| 85 | MG | 1 | 4182 | 1/1 | 0.97 | 0.30 | 25,25,25,25 | 0 |
| 84 | OHX | 6 | 1974 | 7/7 | 0.97 | 0.15 | 121,121,122,122 | 0 |
| 84 | OHX | AR | 3683 | 7/7 | 0.97 | 0.36 | 126,127,127,127 | 0 |
| 85 | MG | 1 | 4185 | 1/1 | 0.97 | 0.50 | 27,27,27,27 | 0 |
| 84 | OHX | AR | 3519 | 7/7 | 0.97 | 0.15 | 108,109,109,109 | 0 |
| 84 | OHX | AR | 3520 | 7/7 | 0.97 | 0.31 | 112,112,113,113 | 0 |
| 84 | OHX | 1 | 3647 | 7/7 | 0.97 | 0.23 | 118,118,118,118 | 0 |
| 84 | OHX | 1 | 3492 | 7/7 | 0.97 | 0.19 | 117,118,118,118 | 0 |
| 84 | OHX | 1 | 3548 | 7/7 | 0.97 | 0.11 | 134,134,134,134 | 0 |
| 85 | MG | 1 | 4191 | 1/1 | 0.97 | 0.44 | 29,29,29,29 | 0 |
| 85 | MG | 1 | 4192 | 1/1 | 0.97 | 0.66 | 21,21,21,21 | 0 |
| 84 | OHX | 1 | 3549 | 7/7 | 0.97 | 0.15 | 120,120,120,120 | 0 |
| 84 | OHX | 1 | 3494 | 7/7 | 0.97 | 0.13 | 119,119,120,120 | 0 |
| 84 | OHX | J | 301 | 7/7 | 0.97 | 0.25 | 157,157,158,158 | 0 |
| 85 | MG | CP | 503 | 1/1 | 0.97 | 0.41 | 38,38,38,38 | 0 |
| 84 | OHX | 1 | 3551 | 7/7 | 0.97 | 0.27 | 118,118,119,119 | 0 |
| 84 | OHX | M | 201 | 7/7 | 0.97 | 0.38 | 137,137,138,138 | 0 |
| 84 | OHX | 1 | 3598 | 7/7 | 0.97 | 0.27 | 127,127,127,127 | 0 |
| 85 | MG | 1 | 4200 | 1/1 | 0.97 | 0.49 | 22,22,22,22 | 0 |
| 84 | OHX | 6 | 1983 | 7/7 | 0.97 | 0.18 | 128,129,129,129 | 0 |
| 84 | OHX | 1 | 3495 | 7/7 | 0.97 | 0.14 | 114,115,115,115 | 0 |
| 84 | OHX | AR | 3533 | 7/7 | 0.97 | 0.18 | 111,111,111,111 | 0 |
| 85 | MG | 1 | 4204 | 1/1 | 0.97 | 0.51 | 34,34,34,34 | 0 |
| 85 | MG | 1 | 4205 | 1/1 | 0.97 | 0.24 | 31,31,31,31 | 0 |
| 84 | OHX | h | 401 | 7/7 | 0.97 | 0.15 | 175,176,177,177 | 0 |
| 84 | OHX | AR | 3696 | 7/7 | 0.97 | 0.18 | 112,113,113,113 | 0 |
| 84 | OHX | 1 | 3600 | 7/7 | 0.97 | 0.15 | 150,150,150,150 | 0 |
| 85 | MG | CX | 203 | 1/1 | 0.97 | 0.39 | 19,19,19,19 | 0 |
| 84 | OHX | AR | 3535 | 7/7 | 0.97 | 0.13 | 114,115,115,115 | 0 |
| 84 | OHX | 1 | 3476 | 7/7 | 0.97 | 0.14 | 111,111,111,112 | 0 |
| 84 | OHX | 1 | 3602 | 7/7 | 0.97 | 0.23 | 128,128,128,129 | 0 |
| 84 | OHX | c8 | 201 | 7/7 | 0.97 | 0.20 | 146,147,147,148 | 0 |
| 84 | OHX | 1 | 3658 | 7/7 | 0.97 | 0.34 | 142,143,143,143 | 0 |
| 84 | OHX | AR | 3539 | 7/7 | 0.97 | 0.14 | 127,128,128,128 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84 | OHX | AR | 3540 | 7/7 | 0.97 | 0.16 | 108,108,108,108 | 0 |
| 85 | MG | AR | 3762 | 1/1 | 0.97 | 0.17 | 24,24,24,24 | 0 |
| 84 | OHX | 1 | 3603 | 7/7 | 0.97 | 0.17 | 123,123,124,124 | 0 |
| 84 | OHX | AR | 3542 | 7/7 | 0.97 | 0.11 | 152,152,152,153 | 0 |
| 85 | MG | AR | 4048 | 1/1 | 0.97 | 0.23 | 34,34,34,34 | 0 |
| 84 | OHX | 1 | 3480 | 7/7 | 0.97 | 0.14 | 119,119,119,120 | 0 |
| 84 | OHX | 1 | 3449 | 7/7 | 0.97 | 0.23 | 117,117,118,118 | 0 |
| 84 | OHX | 1 | 3558 | 7/7 | 0.97 | 0.17 | 134,134,135,135 | 0 |
| 85 | MG | AR | 4053 | 1/1 | 0.97 | 0.40 | 30,30,30,30 | 0 |
| 84 | OHX | 1 | 3607 | 7/7 | 0.97 | 0.17 | 122,122,122,122 | 0 |
| 84 | OHX | AR | 3547 | 7/7 | 0.97 | 0.28 | 116,116,116,117 | 0 |
| 84 | OHX | 1 | 3608 | 7/7 | 0.97 | 0.25 | 118,119,119,119 | 0 |
| 85 | MG | 1 | 3736 | 1/1 | 0.97 | 0.60 | 31,31,31,31 | 0 |
| 84 | OHX | AR | 3549 | 7/7 | 0.97 | 0.20 | 116,117,117,117 | 0 |
| 85 | MG | AR | 3775 | 1/1 | 0.97 | 0.23 | 22,22,22,22 | 0 |
| 84 | OHX | 1 | 3463 | 7/7 | 0.97 | 0.13 | 121,121,122,122 | 0 |
| 84 | OHX | 3 | 202 | 7/7 | 0.97 | 0.12 | 115,116,116,116 | 0 |
| 84 | OHX | 3 | 203 | 7/7 | 0.97 | 0.11 | 118,118,118,119 | 0 |
| 84 | OHX | AR | 3554 | 7/7 | 0.97 | 0.15 | 112,112,112,112 | 0 |
| 85 | MG | 3 | 218 | 1/1 | 0.97 | 0.22 | 54,54,54,54 | 0 |
| 84 | OHX | 3 | 204 | 7/7 | 0.97 | 0.15 | 124,125,125,125 | 0 |
| 84 | OHX | 1 | 3561 | 7/7 | 0.97 | 0.26 | 124,124,125,125 | 0 |
| 84 | OHX | 1 | 3562 | 7/7 | 0.97 | 0.14 | 121,121,121,121 | 0 |
| 84 | OHX | AR | 3558 | 7/7 | 0.97 | 0.16 | 137,137,137,137 | 0 |
| 85 | MG | AR | 3786 | 1/1 | 0.97 | 0.48 | 25,25,25,25 | 0 |
| 84 | OHX | AR | 3559 | 7/7 | 0.97 | 0.31 | 121,121,121,121 | 0 |
| 85 | MG | A | 2058 | 1/1 | 0.97 | 0.66 | 46,46,46,46 | 0 |
| 84 | OHX | AR | 3560 | 7/7 | 0.97 | 0.19 | 135,135,136,136 | 0 |
| 84 | OHX | AR | 3561 | 7/7 | 0.97 | 0.24 | 110,110,110,111 | 0 |
| 84 | OHX | 1 | 3528 | 7/7 | 0.97 | 0.12 | 119,120,120,120 | 0 |
| 84 | OHX | 6 | 2003 | 7/7 | 0.97 | 0.13 | 126,126,127,127 | 0 |
| 84 | OHX | 3 | 208 | 7/7 | 0.97 | 0.30 | 116,116,116,116 | 0 |
| 84 | OHX | 1 | 3613 | 7/7 | 0.97 | 0.47 | 120,120,121,121 | 0 |
| 84 | OHX | AR | 3566 | 7/7 | 0.97 | 0.24 | 115,115,115,116 | 0 |
| 84 | OHX | 4 | 203 | 7/7 | 0.97 | 0.16 | 106,107,107,107 | 0 |
| 84 | OHX | 4 | 204 | 7/7 | 0.97 | 0.15 | 108,108,108,108 | 0 |
| 85 | MG | AR | 3797 | 1/1 | 0.97 | 0.27 | 31,31,31,31 | 0 |
| 84 | OHX | AR | 3569 | 7/7 | 0.97 | 0.29 | 137,137,137,138 | 0 |
| 84 | OHX | 4 | 205 | 7/7 | 0.97 | 0.17 | 106,106,106,106 | 0 |
| 85 | MG | 1 | 3760 | 1/1 | 0.97 | 0.35 | 27,27,27,27 | 0 |
| 84 | OHX | 1 | 3564 | 7/7 | 0.97 | 0.24 | 126,126,127,127 | 0 |
| 84 | OHX | AR | 3574 | 7/7 | 0.97 | 0.17 | 112,113,113,113 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 84 | OHX | 4 | 208 | 7/7 | 0.97 | 0.36 | 106,106,106,106 | 0 |
| 84 | OHX | AR | 3576 | 7/7 | 0.97 | 0.32 | 128,128,129,129 | 0 |
| 85 | MG | AR | 3806 | 1/1 | 0.97 | 0.29 | 57,57,57,57 | 0 |
| 85 | MG | A | 2077 | 1/1 | 0.97 | 0.59 | 48,48,48,48 | 0 |
| 84 | OHX | 4 | 209 | 7/7 | 0.97 | 0.23 | 113,113,113,113 | 0 |
| 85 | MG | A | 2079 | 1/1 | 0.97 | 0.64 | 58,58,58,58 | 0 |
| 84 | OHX | 1 | 3529 | 7/7 | 0.97 | 0.17 | 115,115,115,116 | 0 |
| 84 | OHX | 1 | 3566 | 7/7 | 0.97 | 0.18 | 113,113,114,114 | 0 |
| 85 | MG | AR | 3810 | 1/1 | 0.97 | 0.51 | 27,27,27,27 | 0 |
| 84 | OHX | 4 | 212 | 7/7 | 0.97 | 0.28 | 128,128,128,128 | 0 |
| 84 | OHX | 1 | 3502 | 7/7 | 0.97 | 0.18 | 114,114,114,114 | 0 |
| 84 | OHX | AR | 3584 | 7/7 | 0.97 | 0.13 | 131,131,131,132 | 0 |
| 84 | OHX | AR | 3585 | 7/7 | 0.97 | 0.20 | 117,117,117,117 | 0 |
| 84 | OHX | 1 | 3568 | 7/7 | 0.97 | 0.28 | 115,116,116,116 | 0 |
| 84 | OHX | AS | 206 | 7/7 | 0.97 | 0.13 | 124,124,125,125 | 0 |
| 84 | OHX | AS | 208 | 7/7 | 0.97 | 0.10 | 138,139,139,139 | 0 |
| 84 | OHX | 1 | 3569 | 7/7 | 0.97 | 0.28 | 111,111,111,111 | 0 |
| 85 | MG | 1 | 3776 | 1/1 | 0.97 | 0.50 | 43,43,43,43 | 0 |
| 84 | OHX | 1 | 3571 | 7/7 | 0.97 | 0.18 | 111,111,112,112 | 0 |
| 84 | OHX | 1 | 3572 | 7/7 | 0.97 | 0.27 | 118,119,119,119 | 0 |
| 84 | OHX | AT | 203 | 7/7 | 0.97 | 0.14 | 117,117,117,117 | 0 |
| 85 | MG | 1 | 3780 | 1/1 | 0.97 | 0.33 | 17,17,17,17 | 0 |
| 84 | OHX | AT | 205 | 7/7 | 0.97 | 0.15 | 108,108,108,108 | 0 |
| 85 | MG | 1 | 4019 | 1/1 | 0.97 | 0.24 | 42,42,42,42 | 0 |
| 84 | OHX | AT | 206 | 7/7 | 0.97 | 0.11 | 123,124,124,124 | 0 |
| 85 | MG | 1 | 3784 | 1/1 | 0.97 | 0.45 | 26,26,26,26 | 0 |
| 84 | OHX | AT | 207 | 7/7 | 0.97 | 0.15 | 117,117,117,117 | 0 |
| 84 | OHX | AT | 208 | 7/7 | 0.97 | 0.32 | 114,114,114,114 | 0 |
| 85 | MG | AR | 4115 | 1/1 | 0.97 | 0.33 | 46,46,46,46 | 0 |
| 84 | OHX | AT | 209 | 7/7 | 0.97 | 0.11 | 121,121,122,122 | 0 |
| 84 | OHX | AR | 3591 | 7/7 | 0.97 | 0.25 | 112,112,112,112 | 0 |
| 85 | MG | v | 302 | 1/1 | 0.97 | 0.34 | 36,36,36,36 | 0 |
| 84 | OHX | 1 | 3678 | 7/7 | 0.97 | 0.15 | 117,117,118,118 | 0 |
| 85 | MG | AR | 3837 | 1/1 | 0.97 | 0.59 | 19,19,19,19 | 0 |
| 85 | MG | A | 2108 | 1/1 | 0.97 | 0.62 | 57,57,57,57 | 0 |
| 84 | OHX | 1 | 3573 | 7/7 | 0.97 | 0.18 | 131,131,132,132 | 0 |
| 84 | OHX | AR | 3594 | 7/7 | 0.97 | 0.20 | 114,114,115,115 | 0 |
| 84 | OHX | v | 301 | 7/7 | 0.97 | 0.20 | 113,113,114,114 | 0 |
| 84 | OHX | 1 | 3574 | 7/7 | 0.97 | 0.28 | 116,116,117,117 | 0 |
| 84 | OHX | 1 | 3534 | 7/7 | 0.97 | 0.19 | 113,113,113,113 | 0 |
| 84 | OHX | 1 | 3682 | 7/7 | 0.97 | 0.14 | 110,110,111,111 | 0 |
| 84 | OHX | 1 | 3625 | 7/7 | 0.97 | 0.22 | 135,135,135,135 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 84 | OHX | 6 | 1905 | 7/7 | 0.97 | 0.34 | 132,133,133,134 | 0 |
| 84 | OHX | 6 | 1907 | 7/7 | 0.97 | 0.32 | 135,136,136,137 | 0 |
| 84 | OHX | 6 | 1909 | 7/7 | 0.97 | 0.26 | 137,138,138,139 | 0 |
| 85 | MG | AR | 4132 | 1/1 | 0.97 | 0.15 | 49,49,49,49 | 0 |
| 85 | MG | AR | 3848 | 1/1 | 0.97 | 0.28 | 31,31,31,31 | 0 |
| 85 | MG | AR | 3849 | 1/1 | 0.97 | 0.45 | 35,35,35,35 | 0 |
| 85 | MG | AR | 3850 | 1/1 | 0.97 | 0.28 | 24,24,24,24 | 0 |
| 84 | OHX | 6 | 1911 | 7/7 | 0.97 | 0.24 | 134,135,135,135 | 0 |
| 85 | MG | 6 | 2053 | 1/1 | 0.97 | 0.57 | 41,41,41,41 | 0 |
| 84 | OHX | 1 | 3576 | 7/7 | 0.97 | 0.14 | 131,131,132,132 | 0 |
| 84 | OHX | 1 | 3536 | 7/7 | 0.97 | 0.22 | 109,109,109,109 | 0 |
| 84 | OHX | 6 | 1925 | 7/7 | 0.97 | 0.20 | 122,122,122,123 | 0 |
| 85 | MG | 6 | 2057 | 1/1 | 0.97 | 0.56 | 51,51,51,51 | 0 |
| 85 | MG | 6 | 2058 | 1/1 | 0.97 | 0.43 | 45,45,45,45 | 0 |
| 85 | MG | 1 | 4043 | 1/1 | 0.97 | 0.32 | 27,27,27,27 | 0 |
| 84 | OHX | 6 | 1927 | 7/7 | 0.97 | 0.22 | 124,124,125,125 | 0 |
| 85 | MG | 1 | 3806 | 1/1 | 0.97 | 0.46 | 51,51,51,51 | 0 |
| 84 | OHX | 1 | 3578 | 7/7 | 0.97 | 0.19 | 107,107,107,107 | 0 |
| 85 | MG | 6 | 2063 | 1/1 | 0.97 | 0.20 | 82,82,82,82 | 0 |
| 84 | OHX | A | 1910 | 7/7 | 0.97 | 0.23 | 138,139,139,140 | 0 |
| 84 | OHX | A | 1911 | 7/7 | 0.97 | 0.22 | 139,140,141,141 | 0 |
| 85 | MG | AR | 3869 | 1/1 | 0.97 | 0.40 | 31,31,31,31 | 0 |
| 84 | OHX | A | 1913 | 7/7 | 0.97 | 0.20 | 126,126,127,127 | 0 |
| 85 | MG | 1 | 4051 | 1/1 | 0.97 | 0.22 | 44,44,44,44 | 0 |
| 84 | OHX | 1 | 3503 | 7/7 | 0.97 | 0.10 | 127,128,128,129 | 0 |
| 84 | OHX | A | 1917 | 7/7 | 0.97 | 0.17 | 130,131,131,131 | 0 |
| 84 | OHX | 6 | 1933 | 7/7 | 0.97 | 0.13 | 116,116,117,117 | 0 |
| 85 | MG | 6 | 2071 | 1/1 | 0.97 | 0.49 | 45,45,45,45 | 0 |
| 85 | MG | 1 | 3815 | 1/1 | 0.97 | 0.14 | 40,40,40,40 | 0 |
| 84 | OHX | A | 1921 | 7/7 | 0.97 | 0.22 | 142,143,144,144 | 0 |
| 84 | OHX | A | 1926 | 7/7 | 0.97 | 0.08 | 127,127,127,128 | 0 |
| 84 | OHX | A | 1927 | 7/7 | 0.97 | 0.14 | 138,138,139,139 | 0 |
| 85 | MG | 1 | 4059 | 1/1 | 0.97 | 0.42 | 51,51,51,51 | 0 |
| 85 | MG | AR | 3885 | 1/1 | 0.97 | 0.37 | 33,33,33,33 | 0 |
| 84 | OHX | A | 1928 | 7/7 | 0.97 | 0.13 | 125,126,126,126 | 0 |
| 84 | OHX | A | 1930 | 7/7 | 0.97 | 0.10 | 122,122,123,123 | 0 |
| 85 | MG | A | 2154 | 1/1 | 0.97 | 0.93 | 45,45,45,45 | 0 |
| 85 | MG | 1 | 3822 | 1/1 | 0.97 | 0.49 | 18,18,18,18 | 0 |
| 84 | OHX | A | 1931 | 7/7 | 0.97 | 0.10 | 139,140,140,140 | 0 |
| 84 | OHX | A | 1932 | 7/7 | 0.97 | 0.18 | 141,142,142,143 | 0 |
| 84 | OHX | 6 | 1934 | 7/7 | 0.97 | 0.13 | 139,139,140,140 | 0 |
| 84 | OHX | A | 1934 | 7/7 | 0.97 | 0.12 | 132,132,133,133 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 84 | OHX | 6 | 1935 | 7/7 | 0.97 | 0.14 | 121,121,121,122 | 0 |
| 84 | OHX | 6 | 1936 | 7/7 | 0.97 | 0.15 | 116,116,117,117 | 0 |
| 84 | OHX | A | 1937 | 7/7 | 0.97 | 0.16 | 153,154,155,155 | 0 |
| 85 | MG | 1 | 4072 | 1/1 | 0.97 | 0.18 | 46,46,46,46 | 0 |
| 85 | MG | AR | 3898 | 1/1 | 0.97 | 0.63 | 28,28,28,28 | 0 |
| 84 | OHX | A | 1939 | 7/7 | 0.97 | 0.11 | 140,141,141,142 | 0 |
| 84 | OHX | A | 1940 | 7/7 | 0.97 | 0.28 | 137,138,138,139 | 0 |
| 85 | MG | AR | 4179 | 1/1 | 0.97 | 0.27 | 43,43,43,43 | 0 |
| 84 | OHX | A | 1941 | 7/7 | 0.97 | 0.12 | 136,137,137,137 | 0 |
| 85 | MG | 1 | 3835 | 1/1 | 0.97 | 0.47 | 30,30,30,30 | 0 |
| 85 | MG | s8 | 302 | 1/1 | 0.97 | 0.33 | 51,51,51,51 | 0 |
| 85 | MG | 1 | 3836 | 1/1 | 0.97 | 0.39 | 36,36,36,36 | 0 |
| 84 | OHX | A | 1943 | 7/7 | 0.97 | 0.21 | 133,133,134,134 | 0 |
| 84 | OHX | 6 | 1938 | 7/7 | 0.97 | 0.13 | 130,131,131,131 | 0 |
| 85 | MG | AR | 3906 | 1/1 | 0.97 | 0.36 | 33,33,33,33 | 0 |
| 84 | OHX | A | 1945 | 7/7 | 0.97 | 0.18 | 143,144,144,145 | 0 |
| 85 | MG | AR | 3908 | 1/1 | 0.97 | 0.53 | 25,25,25,25 | 0 |
| 84 | OHX | AR | 3616 | 7/7 | 0.97 | 0.34 | 109,110,110,110 | 0 |
| 84 | OHX | 6 | 1939 | 7/7 | 0.97 | 0.10 | 131,132,132,133 | 0 |
| 84 | OHX | A | 1948 | 7/7 | 0.97 | 0.13 | 139,140,140,140 | 0 |
| 85 | MG | d6 | 102 | 1/1 | 0.97 | 0.50 | 38,38,38,38 | 0 |
| 84 | OHX | A | 1951 | 7/7 | 0.97 | 0.24 | 145,145,146,146 | 0 |
| 84 | OHX | 1 | 3580 | 7/7 | 0.97 | 0.35 | 115,116,116,116 | 0 |
| 84 | OHX | A | 1954 | 7/7 | 0.97 | 0.17 | 135,136,136,136 | 0 |
| 84 | OHX | 1 | 3538 | 7/7 | 0.97 | 0.09 | 125,125,125,126 | 0 |
| 84 | OHX | A | 1956 | 7/7 | 0.97 | 0.14 | 133,133,134,134 | 0 |
| 84 | OHX | AR | 3620 | 7/7 | 0.97 | 0.33 | 143,144,144,144 | 0 |
| 84 | OHX | 6 | 1943 | 7/7 | 0.97 | 0.09 | 124,124,125,125 | 0 |
| 84 | OHX | 1 | 3633 | 7/7 | 0.97 | 0.30 | 134,134,135,135 | 0 |
| 84 | OHX | 1 | 3504 | 7/7 | 0.97 | 0.19 | 127,127,127,128 | 0 |
| 84 | OHX | 1 | 3635 | 7/7 | 0.97 | 0.28 | 122,122,123,123 | 0 |
| 88 | ZN | d9 | 102 | 1/1 | 0.97 | 0.13 | 83,83,83,83 | 0 |
| 84 | OHX | A | 1965 | 7/7 | 0.97 | 0.16 | 134,135,135,136 | 0 |
| 84 | OHX | 1 | 3496 | 7/7 | 0.98 | 0.16 | 115,115,115,115 | 0 |
| 84 | OHX | 1 | 3454 | 7/7 | 0.98 | 0.18 | 111,111,111,111 | 0 |
| 84 | OHX | AR | 3481 | 7/7 | 0.98 | 0.20 | 106,106,107,107 | 0 |
| 84 | OHX | AR | 3482 | 7/7 | 0.98 | 0.19 | 111,112,112,112 | 0 |
| 84 | OHX | 1 | 3404 | 7/7 | 0.98 | 0.35 | 120,120,121,121 | 0 |
| 84 | OHX | 1 | 3555 | 7/7 | 0.98 | 0.17 | 111,111,112,112 | 0 |
| 84 | OHX | AR | 3485 | 7/7 | 0.98 | 0.15 | 114,114,115,115 | 0 |
| 84 | OHX | AR | 3486 | 7/7 | 0.98 | 0.19 | 111,111,111,111 | 0 |
| 84 | OHX | A | 1938 | 7/7 | 0.98 | 0.15 | 126,127,127,127 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 85 | MG | 1 | 3798 | 1/1 | 0.98 | 0.23 | 32,32,32,32 | 0 |
| 84 | OHX | AR | 3487 | 7/7 | 0.98 | 0.13 | 107,107,107,107 | 0 |
| 84 | OHX | AR | 3488 | 7/7 | 0.98 | 0.09 | 118,118,119,119 | 0 |
| 84 | OHX | AR | 3489 | 7/7 | 0.98 | 0.15 | 114,114,114,114 | 0 |
| 84 | OHX | A | 1942 | 7/7 | 0.98 | 0.19 | 133,133,134,134 | 0 |
| 84 | OHX | AR | 3490 | 7/7 | 0.98 | 0.12 | 112,112,112,113 | 0 |
| 85 | MG | AR | 3763 | 1/1 | 0.98 | 0.59 | 17,17,17,17 | 0 |
| 85 | MG | AR | 4260 | 1/1 | 0.98 | 0.52 | 6,6,6,6 | 0 |
| 84 | OHX | 6 | 1991 | 7/7 | 0.98 | 0.29 | 133,134,134,135 | 0 |
| 84 | OHX | AR | 3645 | 7/7 | 0.98 | 0.35 | 118,118,118,118 | 0 |
| 84 | OHX | 1 | 3499 | 7/7 | 0.98 | 0.23 | 111,111,111,111 | 0 |
| 84 | OHX | 1 | 3557 | 7/7 | 0.98 | 0.16 | 117,118,118,118 | 0 |
| 84 | OHX | 1 | 3456 | 7/7 | 0.98 | 0.16 | 111,111,111,111 | 0 |
| 84 | OHX | A | 1949 | 7/7 | 0.98 | 0.08 | 148,149,149,149 | 0 |
| 85 | MG | 1 | 3810 | 1/1 | 0.98 | 0.12 | 32,32,32,32 | 0 |
| 84 | OHX | A | 1950 | 7/7 | 0.98 | 0.13 | 127,128,128,128 | 0 |
| 84 | OHX | 1 | 3457 | 7/7 | 0.98 | 0.18 | 126,127,127,128 | 0 |
| 84 | OHX | A | 1952 | 7/7 | 0.98 | 0.20 | 128,129,129,129 | 0 |
| 85 | MG | AS | 222 | 1/1 | 0.98 | 0.21 | 44,44,44,44 | 0 |
| 85 | MG | AR | 3774 | 1/1 | 0.98 | 0.15 | 30,30,30,30 | 0 |
| 84 | OHX | 1 | 3560 | 7/7 | 0.98 | 0.12 | 111,112,112,112 | 0 |
| 84 | OHX | AR | 3497 | 7/7 | 0.98 | 0.09 | 124,125,125,126 | 0 |
| 84 | OHX | AR | 3498 | 7/7 | 0.98 | 0.15 | 123,123,123,124 | 0 |
| 85 | MG | 1 | 3817 | 1/1 | 0.98 | 0.26 | 23,23,23,23 | 0 |
| 84 | OHX | 1 | 3432 | 7/7 | 0.98 | 0.27 | 117,117,117,117 | 0 |
| 84 | OHX | A | 1957 | 7/7 | 0.98 | 0.23 | 133,134,134,134 | 0 |
| 85 | MG | AR | 3781 | 1/1 | 0.98 | 0.25 | 23,23,23,23 | 0 |
| 84 | OHX | AR | 3500 | 7/7 | 0.98 | 0.12 | 115,115,115,115 | 0 |
| 84 | OHX | 1 | 3459 | 7/7 | 0.98 | 0.19 | 108,108,108,108 | 0 |
| 85 | MG | AT | 219 | 1/1 | 0.98 | 0.35 | 36,36,36,36 | 0 |
| 85 | MG | 1 | 4034 | 1/1 | 0.98 | 0.25 | 42,42,42,42 | 0 |
| 84 | OHX | AR | 3502 | 7/7 | 0.98 | 0.17 | 113,114,114,114 | 0 |
| 84 | OHX | A | 1961 | 7/7 | 0.98 | 0.11 | 149,150,151,151 | 0 |
| 84 | OHX | A | 1962 | 7/7 | 0.98 | 0.21 | 132,133,133,134 | 0 |
| 84 | OHX | 1 | 3460 | 7/7 | 0.98 | 0.16 | 118,118,118,119 | 0 |
| 85 | MG | 1 | 3827 | 1/1 | 0.98 | 0.73 | 32,32,32,32 | 0 |
| 84 | OHX | 1 | 3505 | 7/7 | 0.98 | 0.18 | 116,116,117,117 | 0 |
| 84 | OHX | AR | 3505 | 7/7 | 0.98 | 0.20 | 114,114,115,115 | 0 |
| 84 | OHX | 1 | 3461 | 7/7 | 0.98 | 0.18 | 110,110,111,111 | 0 |
| 84 | OHX | A | 1967 | 7/7 | 0.98 | 0.12 | 119,119,120,120 | 0 |
| 85 | MG | AT | 230 | 1/1 | 0.98 | 0.42 | 39,39,39,39 | 0 |
| 84 | OHX | AR | 3507 | 7/7 | 0.98 | 0.08 | 123,123,123,123 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 84 | OHX | AR | 3508 | 7/7 | 0.98 | 0.21 | 109,109,109,109 | 0 |
| 84 | OHX | AR | 3510 | 7/7 | 0.98 | 0.13 | 117,118,118,118 | 0 |
| 85 | MG | 1 | 4047 | 1/1 | 0.98 | 0.12 | 57,57,57,57 | 0 |
| 84 | OHX | 1 | 3434 | 7/7 | 0.98 | 0.25 | 126,127,127,127 | 0 |
| 84 | OHX | A | 1972 | 7/7 | 0.98 | 0.22 | 148,148,148,148 | 0 |
| 84 | OHX | 1 | 3508 | 7/7 | 0.98 | 0.10 | 113,114,114,114 | 0 |
| 84 | OHX | 6 | 1910 | 7/7 | 0.98 | 0.26 | 119,120,120,120 | 0 |
| 84 | OHX | 1 | 3630 | 7/7 | 0.98 | 0.33 | 113,113,114,114 | 0 |
| 84 | OHX | AR | 3515 | 7/7 | 0.98 | 0.22 | 113,113,114,114 | 0 |
| 84 | OHX | 6 | 1913 | 7/7 | 0.98 | 0.26 | 133,134,135,135 | 0 |
| 84 | OHX | 6 | 1916 | 7/7 | 0.98 | 0.21 | 119,120,120,120 | 0 |
| 84 | OHX | AR | 3518 | 7/7 | 0.98 | 0.10 | 118,119,119,119 | 0 |
| 85 | MG | AR | 4054 | 1/1 | 0.98 | 0.14 | 55,55,55,55 | 0 |
| 85 | MG | 1 | 3844 | 1/1 | 0.98 | 0.41 | 28,28,28,28 | 0 |
| 84 | OHX | AR | 3672 | 7/7 | 0.98 | 0.29 | 109,110,110,110 | 0 |
| 84 | OHX | 6 | 1918 | 7/7 | 0.98 | 0.17 | 116,117,117,117 | 0 |
| 84 | OHX | 1 | 3407 | 7/7 | 0.98 | 0.31 | 106,106,107,107 | 0 |
| 84 | OHX | 6 | 1920 | 7/7 | 0.98 | 0.14 | 133,133,134,134 | 0 |
| 84 | OHX | A | 1984 | 7/7 | 0.98 | 0.10 | 130,130,131,131 | 0 |
| 85 | MG | 1 | 4063 | 1/1 | 0.98 | 0.09 | 38,38,38,38 | 0 |
| 84 | OHX | 1 | 3465 | 7/7 | 0.98 | 0.18 | 117,117,117,117 | 0 |
| 84 | OHX | AR | 3523 | 7/7 | 0.98 | 0.15 | 107,108,108,108 | 0 |
| 85 | MG | z | 202 | 1/1 | 0.98 | 0.28 | 59,59,59,59 | 0 |
| 85 | MG | AR | 3818 | 1/1 | 0.98 | 0.78 | 37,37,37,37 | 0 |
| 85 | MG | AR | 3819 | 1/1 | 0.98 | 0.36 | 37,37,37,37 | 0 |
| 84 | OHX | 6 | 1922 | 7/7 | 0.98 | 0.18 | 121,122,122,122 | 0 |
| 85 | MG | 1 | 4067 | 1/1 | 0.98 | 0.09 | 40,40,40,40 | 0 |
| 84 | OHX | AR | 3525 | 7/7 | 0.98 | 0.06 | 119,119,120,120 | 0 |
| 84 | OHX | 6 | 1923 | 7/7 | 0.98 | 0.17 | 121,121,122,122 | 0 |
| 84 | OHX | 6 | 1924 | 7/7 | 0.98 | 0.15 | 134,135,135,135 | 0 |
| 84 | OHX | 1 | 3570 | 7/7 | 0.98 | 0.09 | 144,144,145,145 | 0 |
| 84 | OHX | AR | 3529 | 7/7 | 0.98 | 0.12 | 108,109,109,109 | 0 |
| 84 | OHX | 6 | 1926 | 7/7 | 0.98 | 0.12 | 120,121,121,121 | 0 |
| 84 | OHX | 1 | 3697 | 7/7 | 0.98 | 0.25 | 119,119,120,120 | 0 |
| 84 | OHX | 6 | 1928 | 7/7 | 0.98 | 0.08 | 126,126,127,127 | 0 |
| 85 | MG | AR | 3830 | 1/1 | 0.98 | 0.46 | 42,42,42,42 | 0 |
| 84 | OHX | 1 | 3511 | 7/7 | 0.98 | 0.14 | 109,109,109,109 | 0 |
| 85 | MG | 1 | 4078 | 1/1 | 0.98 | 0.29 | 24,24,24,24 | 0 |
| 84 | OHX | 6 | 1930 | 7/7 | 0.98 | 0.21 | 121,121,122,122 | 0 |
| 85 | MG | AR | 4081 | 1/1 | 0.98 | 0.24 | 55,55,55,55 | 0 |
| 84 | OHX | 6 | 1931 | 7/7 | 0.98 | 0.10 | 115,116,116,116 | 0 |
| 84 | OHX | 1 | 3512 | 7/7 | 0.98 | 0.17 | 110,110,110,110 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84 | OHX | 1 | 3513 | 7/7 | 0.98 | 0.11 | 113,113,114,114 | 0 |
| 84 | OHX | 1 | 3410 | 7/7 | 0.98 | 0.32 | 112,112,112,112 | 0 |
| 84 | OHX | 1 | 3515 | 7/7 | 0.98 | 0.10 | 110,110,110,110 | 0 |
| 84 | OHX | 1 | 3516 | 7/7 | 0.98 | 0.12 | 116,117,117,117 | 0 |
| 84 | OHX | 6 | 1937 | 7/7 | 0.98 | 0.11 | 119,120,120,120 | 0 |
| 84 | OHX | 1 | 3467 | 7/7 | 0.98 | 0.17 | 123,123,124,124 | 0 |
| 84 | OHX | 1 | 3468 | 7/7 | 0.98 | 0.20 | 116,117,117,117 | 0 |
| 84 | OHX | 1 | 3439 | 7/7 | 0.98 | 0.19 | 109,109,109,109 | 0 |
| 84 | OHX | 1 | 3470 | 7/7 | 0.98 | 0.18 | 115,115,115,115 | 0 |
| 85 | MG | 1 | 3875 | 1/1 | 0.98 | 0.46 | 23,23,23,23 | 0 |
| 84 | OHX | 6 | 1942 | 7/7 | 0.98 | 0.16 | 135,135,136,136 | 0 |
| 84 | OHX | A | 2010 | 7/7 | 0.98 | 0.14 | 157,158,158,159 | 0 |
| 84 | OHX | 1 | 3521 | 7/7 | 0.98 | 0.14 | 116,117,117,117 | 0 |
| 84 | OHX | 6 | 1944 | 7/7 | 0.98 | 0.10 | 143,143,144,144 | 0 |
| 84 | OHX | 6 | 1945 | 7/7 | 0.98 | 0.17 | 126,127,127,128 | 0 |
| 84 | OHX | AR | 3550 | 7/7 | 0.98 | 0.14 | 107,107,107,107 | 0 |
| 84 | OHX | 1 | 3522 | 7/7 | 0.98 | 0.13 | 120,121,121,121 | 0 |
| 84 | OHX | 1 | 3523 | 7/7 | 0.98 | 0.19 | 119,119,120,120 | 0 |
| 85 | MG | 1 | 3885 | 1/1 | 0.98 | 0.49 | 20,20,20,20 | 0 |
| 84 | OHX | 6 | 1948 | 7/7 | 0.98 | 0.13 | 127,128,128,128 | 0 |
| 84 | OHX | 1 | 3524 | 7/7 | 0.98 | 0.21 | 116,117,117,117 | 0 |
| 85 | MG | 1 | 3888 | 1/1 | 0.98 | 0.40 | 29,29,29,29 | 0 |
| 85 | MG | AR | 4106 | 1/1 | 0.98 | 0.07 | 46,46,46,46 | 0 |
| 85 | MG | AR | 3858 | 1/1 | 0.98 | 0.32 | 36,36,36,36 | 0 |
| 85 | MG | 1 | 3889 | 1/1 | 0.98 | 0.54 | 23,23,23,23 | 0 |
| 85 | MG | AR | 3860 | 1/1 | 0.98 | 0.51 | 23,23,23,23 | 0 |
| 84 | OHX | 1 | 3440 | 7/7 | 0.98 | 0.22 | 110,110,111,111 | 0 |
| 85 | MG | 1 | 3891 | 1/1 | 0.98 | 0.60 | 17,17,17,17 | 0 |
| 85 | MG | AR | 3863 | 1/1 | 0.98 | 0.57 | 21,21,21,21 | 0 |
| 84 | OHX | 6 | 1951 | 7/7 | 0.98 | 0.14 | 134,134,135,135 | 0 |
| 85 | MG | 1 | 3893 | 1/1 | 0.98 | 0.26 | 26,26,26,26 | 0 |
| 84 | OHX | 1 | 3472 | 7/7 | 0.98 | 0.17 | 110,111,111,111 | 0 |
| 84 | OHX | 1 | 3587 | 7/7 | 0.98 | 0.23 | 133,133,133,134 | 0 |
| 84 | OHX | 1 | 3441 | 7/7 | 0.98 | 0.20 | 116,116,116,117 | 0 |
| 85 | MG | AR | 3870 | 1/1 | 0.98 | 0.70 | 33,33,33,33 | 0 |
| 84 | OHX | 1 | 3474 | 7/7 | 0.98 | 0.16 | 122,122,123,123 | 0 |
| 85 | MG | 6 | 2098 | 1/1 | 0.98 | 0.52 | 68,68,68,68 | 0 |
| 84 | OHX | 1 | 3590 | 7/7 | 0.98 | 0.12 | 137,138,138,138 | 0 |
| 84 | OHX | 1 | 3475 | 7/7 | 0.98 | 0.14 | 117,117,118,118 | 0 |
| 84 | OHX | 6 | 1958 | 7/7 | 0.98 | 0.15 | 126,127,127,127 | 0 |
| 85 | MG | AR | 3876 | 1/1 | 0.98 | 0.55 | 27,27,27,27 | 0 |
| 84 | OHX | 1 | 3530 | 7/7 | 0.98 | 0.13 | 138,138,139,139 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 84 | OHX | 1 | 3415 | 7/7 | 0.98 | 0.32 | 123,124,124,124 | 0 |
| 85 | MG | 1 | 3904 | 1/1 | 0.98 | 0.53 | 25,25,25,25 | 0 |
| 84 | OHX | 1 | 3532 | 7/7 | 0.98 | 0.07 | 159,159,159,159 | 0 |
| 85 | MG | 1 | 4121 | 1/1 | 0.98 | 0.10 | 64,64,64,64 | 0 |
| 84 | OHX | 1 | 3533 | 7/7 | 0.98 | 0.13 | 149,149,150,150 | 0 |
| 85 | MG | AR | 4131 | 1/1 | 0.98 | 0.09 | 39,39,39,39 | 0 |
| 85 | MG | AR | 3884 | 1/1 | 0.98 | 0.45 | 22,22,22,22 | 0 |
| 84 | OHX | AC | 101 | 7/7 | 0.98 | 0.30 | 114,115,115,115 | 0 |
| 84 | OHX | 6 | 1963 | 7/7 | 0.98 | 0.16 | 125,125,126,126 | 0 |
| 84 | OHX | 1 | 3477 | 7/7 | 0.98 | 0.12 | 109,109,109,109 | 0 |
| 85 | MG | 1 | 3910 | 1/1 | 0.98 | 0.58 | 19,19,19,19 | 0 |
| 84 | OHX | 1 | 3535 | 7/7 | 0.98 | 0.17 | 111,111,111,112 | 0 |
| 84 | OHX | AR | 3572 | 7/7 | 0.98 | 0.28 | 118,119,119,119 | 0 |
| 84 | OHX | AR | 3573 | 7/7 | 0.98 | 0.21 | 123,123,123,123 | 0 |
| 84 | OHX | 3 | 201 | 7/7 | 0.98 | 0.19 | 121,121,121,122 | 0 |
| 84 | OHX | 1 | 3479 | 7/7 | 0.98 | 0.17 | 108,109,109,109 | 0 |
| 85 | MG | 1 | 4132 | 1/1 | 0.98 | 0.13 | 86,86,86,86 | 0 |
| 85 | MG | 1 | 4133 | 1/1 | 0.98 | 0.09 | 51,51,51,51 | 0 |
| 85 | MG | 6 | 2119 | 1/1 | 0.98 | 0.47 | 74,74,74,74 | 0 |
| 84 | OHX | AR | 3401 | 7/7 | 0.98 | 0.39 | 121,121,121,122 | 0 |
| 84 | OHX | AR | 3406 | 7/7 | 0.98 | 0.34 | 112,112,113,113 | 0 |
| 84 | OHX | AR | 3407 | 7/7 | 0.98 | 0.34 | 113,113,113,113 | 0 |
| 84 | OHX | AR | 3411 | 7/7 | 0.98 | 0.30 | 106,106,106,106 | 0 |
| 84 | OHX | AR | 3412 | 7/7 | 0.98 | 0.28 | 109,109,109,109 | 0 |
| 84 | OHX | AR | 3582 | 7/7 | 0.98 | 0.27 | 114,114,114,114 | 0 |
| 84 | OHX | AR | 3414 | 7/7 | 0.98 | 0.30 | 113,113,114,114 | 0 |
| 85 | MG | 1 | 4142 | 1/1 | 0.98 | 0.26 | 38,38,38,38 | 0 |
| 84 | OHX | AR | 3415 | 7/7 | 0.98 | 0.35 | 109,109,110,110 | 0 |
| 84 | OHX | AR | 3417 | 7/7 | 0.98 | 0.26 | 111,112,112,112 | 0 |
| 84 | OHX | AR | 3425 | 7/7 | 0.98 | 0.23 | 105,106,106,106 | 0 |
| 85 | MG | 6 | 2131 | 1/1 | 0.98 | 0.24 | 44,44,44,44 | 0 |
| 84 | OHX | 1 | 3443 | 7/7 | 0.98 | 0.19 | 119,120,120,120 | 0 |
| 84 | OHX | AR | 3430 | 7/7 | 0.98 | 0.14 | 107,107,107,107 | 0 |
| 84 | OHX | AR | 3589 | 7/7 | 0.98 | 0.13 | 109,110,110,110 | 0 |
| 85 | MG | 1 | 4149 | 1/1 | 0.98 | 0.18 | 54,54,54,54 | 0 |
| 84 | OHX | 1 | 3444 | 7/7 | 0.98 | 0.23 | 116,116,117,117 | 0 |
| 84 | OHX | AR | 3744 | 7/7 | 0.98 | 0.17 | 109,110,110,110 | 0 |
| 84 | OHX | AR | 3433 | 7/7 | 0.98 | 0.21 | 110,110,110,111 | 0 |
| 84 | OHX | AS | 201 | 7/7 | 0.98 | 0.24 | 119,119,119,120 | 0 |
| 84 | OHX | AS | 202 | 7/7 | 0.98 | 0.22 | 124,124,125,125 | 0 |
| 85 | MG | 1 | 3935 | 1/1 | 0.98 | 0.23 | 47,47,47,47 | 0 |
| 84 | OHX | AS | 203 | 7/7 | 0.98 | 0.16 | 116,116,116,116 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 84 | OHX | sR | 401 | 7/7 | 0.98 | 0.22 | 161,161,162,162 | 0 |
| 84 | OHX | AS | 204 | 7/7 | 0.98 | 0.15 | 113,113,113,113 | 0 |
| 84 | OHX | AS | 205 | 7/7 | 0.98 | 0.12 | 113,113,114,114 | 0 |
| 84 | OHX | AR | 3435 | 7/7 | 0.98 | 0.22 | 112,113,113,113 | 0 |
| 84 | OHX | AS | 207 | 7/7 | 0.98 | 0.16 | 122,122,122,123 | 0 |
| 84 | OHX | AR | 3436 | 7/7 | 0.98 | 0.24 | 109,109,109,109 | 0 |
| 84 | OHX | AR | 3437 | 7/7 | 0.98 | 0.23 | 108,108,108,108 | 0 |
| 84 | OHX | AR | 3439 | 7/7 | 0.98 | 0.25 | 119,120,120,120 | 0 |
| 84 | OHX | 6 | 1970 | 7/7 | 0.98 | 0.26 | 126,126,127,127 | 0 |
| 84 | OHX | AT | 202 | 7/7 | 0.98 | 0.30 | 106,106,106,106 | 0 |
| 84 | OHX | 1 | 3482 | 7/7 | 0.98 | 0.18 | 117,117,117,117 | 0 |
| 84 | OHX | AT | 204 | 7/7 | 0.98 | 0.11 | 105,105,105,106 | 0 |
| 84 | OHX | AR | 3443 | 7/7 | 0.98 | 0.14 | 116,116,117,117 | 0 |
| 84 | OHX | AR | 3444 | 7/7 | 0.98 | 0.15 | 112,112,112,112 | 0 |
| 84 | OHX | 1 | 3417 | 7/7 | 0.98 | 0.31 | 116,117,117,117 | 0 |
| 84 | OHX | 1 | 3484 | 7/7 | 0.98 | 0.10 | 125,126,126,126 | 0 |
| 84 | OHX | AR | 3448 | 7/7 | 0.98 | 0.17 | 115,115,115,115 | 0 |
| 84 | OHX | AR | 3450 | 7/7 | 0.98 | 0.16 | 127,127,127,128 | 0 |
| 84 | OHX | AR | 3451 | 7/7 | 0.98 | 0.20 | 114,114,114,114 | 0 |
| 84 | OHX | AR | 3452 | 7/7 | 0.98 | 0.18 | 121,121,122,122 | 0 |
| 85 | MG | AR | 4190 | 1/1 | 0.98 | 0.19 | 30,30,30,30 | 0 |
| 84 | OHX | AR | 3453 | 7/7 | 0.98 | 0.10 | 106,106,107,107 | 0 |
| 84 | OHX | AR | 3454 | 7/7 | 0.98 | 0.17 | 112,112,113,113 | 0 |
| 85 | MG | 1 | 4180 | 1/1 | 0.98 | 0.35 | 45,45,45,45 | 0 |
| 84 | OHX | 1 | 3420 | 7/7 | 0.98 | 0.29 | 118,118,118,118 | 0 |
| 84 | OHX | 1 | 3486 | 7/7 | 0.98 | 0.14 | 116,117,117,117 | 0 |
| 84 | OHX | AR | 3457 | 7/7 | 0.98 | 0.18 | 108,108,108,109 | 0 |
| 84 | OHX | CE | 401 | 7/7 | 0.98 | 0.17 | 114,114,115,115 | 0 |
| 85 | MG | 6 | 2170 | 1/1 | 0.98 | 0.17 | 64,64,64,64 | 0 |
| 84 | OHX | 4 | 201 | 7/7 | 0.98 | 0.35 | 108,108,108,108 | 0 |
| 84 | OHX | 1 | 3447 | 7/7 | 0.98 | 0.20 | 113,113,113,113 | 0 |
| 84 | OHX | 1 | 3448 | 7/7 | 0.98 | 0.21 | 117,117,117,117 | 0 |
| 84 | OHX | AR | 3461 | 7/7 | 0.98 | 0.14 | 110,111,111,111 | 0 |
| 84 | OHX | 1 | 3403 | 7/7 | 0.98 | 0.30 | 113,113,113,114 | 0 |
| 84 | OHX | AR | 3464 | 7/7 | 0.98 | 0.17 | 106,106,106,106 | 0 |
| 84 | OHX | AR | 3465 | 7/7 | 0.98 | 0.17 | 118,118,118,118 | 0 |
| 85 | MG | AR | 4208 | 1/1 | 0.98 | 0.21 | 57,57,57,57 | 0 |
| 84 | OHX | 1 | 3491 | 7/7 | 0.98 | 0.18 | 120,120,121,121 | 0 |
| 84 | OHX | CP | 501 | 7/7 | 0.98 | 0.20 | 126,126,126,127 | 0 |
| 85 | MG | 6 | 2182 | 1/1 | 0.98 | 0.14 | 83,83,83,83 | 0 |
| 84 | OHX | CX | 201 | 7/7 | 0.98 | 0.17 | 116,116,116,116 | 0 |
| 85 | MG | 6 | 2184 | 1/1 | 0.98 | 0.22 | 83,83,83,83 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 84 | OHX | 6 | 1981 | 7/7 | 0.98 | 0.29 | 139,140,140,140 | 0 |
| 85 | MG | 1 | 4196 | 1/1 | 0.98 | 0.42 | 30,30,30,30 | 0 |
| 84 | OHX | DD | 101 | 7/7 | 0.98 | 0.29 | 113,114,114,114 | 0 |
| 84 | OHX | DH | 201 | 7/7 | 0.98 | 0.13 | 113,113,113,113 | 0 |
| 84 | OHX | DQ | 201 | 7/7 | 0.98 | 0.15 | 111,111,111,111 | 0 |
| 84 | OHX | A | 1901 | 7/7 | 0.98 | 0.29 | 127,127,127,128 | 0 |
| 84 | OHX | A | 1903 | 7/7 | 0.98 | 0.35 | 149,149,150,150 | 0 |
| 84 | OHX | A | 1908 | 7/7 | 0.98 | 0.24 | 141,142,143,143 | 0 |
| 84 | OHX | AR | 3468 | 7/7 | 0.98 | 0.16 | 124,124,125,125 | 0 |
| 84 | OHX | 4 | 207 | 7/7 | 0.98 | 0.12 | 118,119,119,119 | 0 |
| 84 | OHX | AR | 3470 | 7/7 | 0.98 | 0.17 | 115,116,116,116 | 0 |
| 84 | OHX | A | 1912 | 7/7 | 0.98 | 0.19 | 137,137,138,138 | 0 |
| 84 | OHX | AR | 3471 | 7/7 | 0.98 | 0.13 | 109,109,109,109 | 0 |
| 84 | OHX | A | 1914 | 7/7 | 0.98 | 0.23 | 126,127,127,127 | 0 |
| 84 | OHX | 1 | 3430 | 7/7 | 0.98 | 0.19 | 110,110,110,110 | 0 |
| 84 | OHX | A | 1916 | 7/7 | 0.98 | 0.18 | 136,137,137,138 | 0 |
| 84 | OHX | 1 | 3493 | 7/7 | 0.98 | 0.17 | 115,116,116,116 | 0 |
| 84 | OHX | 1 | 3452 | 7/7 | 0.98 | 0.16 | 109,109,109,109 | 0 |
| 84 | OHX | A | 1919 | 7/7 | 0.98 | 0.17 | 121,122,122,122 | 0 |
| 85 | MG | 1 | 3991 | 1/1 | 0.98 | 0.17 | 66,66,66,66 | 0 |
| 85 | MG | 1 | 4215 | 1/1 | 0.98 | 0.62 | 27,27,27,27 | 0 |
| 84 | OHX | AR | 3475 | 7/7 | 0.98 | 0.14 | 116,116,116,116 | 0 |
| 84 | OHX | A | 1922 | 7/7 | 0.98 | 0.11 | 123,124,124,124 | 0 |
| 85 | MG | 1 | 3783 | 1/1 | 0.98 | 0.46 | 18,18,18,18 | 0 |
| 84 | OHX | A | 1923 | 7/7 | 0.98 | 0.13 | 124,125,125,125 | 0 |
| 84 | OHX | AR | 3476 | 7/7 | 0.98 | 0.17 | 109,109,109,109 | 0 |
| 84 | OHX | AR | 3477 | 7/7 | 0.98 | 0.20 | 112,112,113,113 | 0 |
| 84 | OHX | 1 | 3453 | 7/7 | 0.98 | 0.14 | 120,120,120,120 | 0 |
| 84 | OHX | A | 1929 | 7/7 | 0.98 | 0.14 | 123,123,124,124 | 0 |
| 84 | OHX | 1 | 3408 | 7/7 | 0.99 | 0.32 | 112,112,112,113 | 0 |
| 85 | MG | AR | 4172 | 1/1 | 0.99 | 0.12 | 65,65,65,65 | 0 |
| 84 | OHX | 1 | 3450 | 7/7 | 0.99 | 0.17 | 121,122,122,123 | 0 |
| 84 | OHX | AR | 3402 | 7/7 | 0.99 | 0.39 | 113,113,113,113 | 0 |
| 85 | MG | AR | 3866 | 1/1 | 0.99 | 0.23 | 34,34,34,34 | 0 |
| 84 | OHX | AR | 3403 | 7/7 | 0.99 | 0.28 | 110,110,110,110 | 0 |
| 84 | OHX | AR | 3404 | 7/7 | 0.99 | 0.33 | 112,112,112,112 | 0 |
| 84 | OHX | AR | 3405 | 7/7 | 0.99 | 0.34 | 119,119,120,120 | 0 |
| 84 | OHX | 2 | 201 | 7/7 | 0.99 | 0.31 | 119,119,120,120 | 0 |
| 84 | OHX | 6 | 1901 | 7/7 | 0.99 | 0.34 | 119,120,120,120 | 0 |
| 84 | OHX | AR | 3609 | 7/7 | 0.99 | 0.16 | 107,107,107,107 | 0 |
| 84 | OHX | AR | 3408 | 7/7 | 0.99 | 0.33 | 107,107,107,107 | 0 |
| 84 | OHX | AR | 3409 | 7/7 | 0.99 | 0.34 | 120,120,120,121 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 84 | OHX | AR | 3410 | 7/7 | 0.99 | 0.31 | 109,109,109,110 | 0 |
| 84 | OHX | 6 | 1902 | 7/7 | 0.99 | 0.34 | 136,136,137,137 | 0 |
| 84 | OHX | 6 | 1903 | 7/7 | 0.99 | 0.29 | 117,118,118,118 | 0 |
| 85 | MG | AR | 3878 | 1/1 | 0.99 | 0.36 | 31,31,31,31 | 0 |
| 84 | OHX | AR | 3413 | 7/7 | 0.99 | 0.26 | 107,107,107,107 | 0 |
| 84 | OHX | 6 | 1904 | 7/7 | 0.99 | 0.27 | 124,124,124,125 | 0 |
| 84 | OHX | 1 | 3426 | 7/7 | 0.99 | 0.28 | 120,120,120,120 | 0 |
| 85 | MG | AR | 4191 | 1/1 | 0.99 | 0.17 | 58,58,58,58 | 0 |
| 85 | MG | AR | 3983 | 1/1 | 0.99 | 0.12 | 33,33,33,33 | 0 |
| 84 | OHX | AR | 3416 | 7/7 | 0.99 | 0.29 | 114,114,115,115 | 0 |
| 84 | OHX | AT | 201 | 7/7 | 0.99 | 0.33 | 109,109,110,110 | 0 |
| 85 | MG | AR | 4195 | 1/1 | 0.99 | 0.18 | 63,63,63,63 | 0 |
| 85 | MG | 1 | 4031 | 1/1 | 0.99 | 0.55 | 21,21,21,21 | 0 |
| 84 | OHX | 6 | 1906 | 7/7 | 0.99 | 0.29 | 122,123,123,124 | 0 |
| 85 | MG | 1 | 3858 | 1/1 | 0.99 | 0.37 | 25,25,25,25 | 0 |
| 85 | MG | AR | 3887 | 1/1 | 0.99 | 0.46 | 21,21,21,21 | 0 |
| 84 | OHX | AR | 3418 | 7/7 | 0.99 | 0.30 | 116,116,117,117 | 0 |
| 84 | OHX | AR | 3419 | 7/7 | 0.99 | 0.27 | 122,122,123,123 | 0 |
| 84 | OHX | AR | 3420 | 7/7 | 0.99 | 0.29 | 113,114,114,114 | 0 |
| 84 | OHX | AR | 3421 | 7/7 | 0.99 | 0.25 | 113,113,113,113 | 0 |
| 84 | OHX | AR | 3422 | 7/7 | 0.99 | 0.28 | 112,112,112,112 | 0 |
| 84 | OHX | AR | 3423 | 7/7 | 0.99 | 0.28 | 110,111,111,111 | 0 |
| 84 | OHX | AR | 3424 | 7/7 | 0.99 | 0.27 | 112,112,113,113 | 0 |
| 84 | OHX | 1 | 3478 | 7/7 | 0.99 | 0.14 | 125,125,125,126 | 0 |
| 84 | OHX | AR | 3426 | 7/7 | 0.99 | 0.27 | 111,112,112,112 | 0 |
| 85 | MG | AR | 3799 | 1/1 | 0.99 | 0.36 | 22,22,22,22 | 0 |
| 84 | OHX | 6 | 1908 | 7/7 | 0.99 | 0.25 | 120,120,121,121 | 0 |
| 85 | MG | 1 | 4134 | 1/1 | 0.99 | 0.20 | 63,63,63,63 | 0 |
| 84 | OHX | AR | 3428 | 7/7 | 0.99 | 0.21 | 115,115,115,116 | 0 |
| 84 | OHX | AR | 3429 | 7/7 | 0.99 | 0.19 | 112,112,112,112 | 0 |
| 85 | MG | 6 | 2175 | 1/1 | 0.99 | 0.10 | 118,118,118,118 | 0 |
| 84 | OHX | 1 | 3427 | 7/7 | 0.99 | 0.26 | 112,113,113,113 | 0 |
| 84 | OHX | AR | 3431 | 7/7 | 0.99 | 0.24 | 109,109,110,110 | 0 |
| 84 | OHX | 1 | 3428 | 7/7 | 0.99 | 0.28 | 126,126,127,127 | 0 |
| 84 | OHX | 1 | 3429 | 7/7 | 0.99 | 0.22 | 110,110,110,110 | 0 |
| 84 | OHX | AR | 3434 | 7/7 | 0.99 | 0.22 | 111,111,111,111 | 0 |
| 85 | MG | 6 | 2181 | 1/1 | 0.99 | 0.11 | 95,95,95,95 | 0 |
| 85 | MG | AR | 3909 | 1/1 | 0.99 | 0.57 | 25,25,25,25 | 0 |
| 85 | MG | AR | 3910 | 1/1 | 0.99 | 0.32 | 23,23,23,23 | 0 |
| 84 | OHX | 6 | 1912 | 7/7 | 0.99 | 0.18 | 122,122,123,123 | 0 |
| 84 | OHX | 1 | 3409 | 7/7 | 0.99 | 0.30 | 116,116,117,117 | 0 |
| 84 | OHX | 6 | 1914 | 7/7 | 0.99 | 0.20 | 133,133,134,134 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 84 | OHX | AR | 3438 | 7/7 | 0.99 | 0.22 | 108,108,108,108 | 0 |
| 84 | OHX | 6 | 1915 | 7/7 | 0.99 | 0.17 | 119,119,120,120 | 0 |
| 85 | MG | A | 2141 | 1/1 | 0.99 | 0.31 | 101,101,101,101 | 0 |
| 84 | OHX | AR | 3440 | 7/7 | 0.99 | 0.18 | 125,125,125,126 | 0 |
| 85 | MG | 1 | 3882 | 1/1 | 0.99 | 0.45 | 32,32,32,32 | 0 |
| 84 | OHX | 4 | 202 | 7/7 | 0.99 | 0.33 | 112,112,112,113 | 0 |
| 85 | MG | A | 2145 | 1/1 | 0.99 | 0.21 | 92,92,92,92 | 0 |
| 84 | OHX | 6 | 1917 | 7/7 | 0.99 | 0.16 | 131,131,132,132 | 0 |
| 84 | OHX | CV | 201 | 7/7 | 0.99 | 0.31 | 117,117,117,117 | 0 |
| 84 | OHX | AR | 3509 | 7/7 | 0.99 | 0.10 | 106,106,106,106 | 0 |
| 84 | OHX | 1 | 3402 | 7/7 | 0.99 | 0.35 | 114,115,115,115 | 0 |
| 84 | OHX | AR | 3578 | 7/7 | 0.99 | 0.14 | 109,109,110,110 | 0 |
| 84 | OHX | 1 | 3411 | 7/7 | 0.99 | 0.29 | 111,112,112,112 | 0 |
| 84 | OHX | 1 | 3433 | 7/7 | 0.99 | 0.26 | 118,119,119,119 | 0 |
| 84 | OHX | AR | 3446 | 7/7 | 0.99 | 0.17 | 112,113,113,113 | 0 |
| 85 | MG | 1 | 3725 | 1/1 | 0.99 | 0.38 | 34,34,34,34 | 0 |
| 84 | OHX | A | 1902 | 7/7 | 0.99 | 0.26 | 122,122,123,123 | 0 |
| 85 | MG | AR | 4241 | 1/1 | 0.99 | 0.39 | 17,17,17,17 | 0 |
| 84 | OHX | 1 | 3412 | 7/7 | 0.99 | 0.30 | 114,114,115,115 | 0 |
| 84 | OHX | A | 1904 | 7/7 | 0.99 | 0.23 | 133,134,134,134 | 0 |
| 84 | OHX | A | 1905 | 7/7 | 0.99 | 0.29 | 128,129,129,129 | 0 |
| 84 | OHX | A | 1906 | 7/7 | 0.99 | 0.23 | 142,143,143,143 | 0 |
| 85 | MG | 1 | 4164 | 1/1 | 0.99 | 0.22 | 58,58,58,58 | 0 |
| 84 | OHX | A | 1907 | 7/7 | 0.99 | 0.19 | 133,134,134,134 | 0 |
| 84 | OHX | 1 | 3413 | 7/7 | 0.99 | 0.32 | 112,113,113,113 | 0 |
| 84 | OHX | AR | 3449 | 7/7 | 0.99 | 0.14 | 116,117,117,117 | 0 |
| 85 | MG | 1 | 4076 | 1/1 | 0.99 | 0.24 | 64,64,64,64 | 0 |
| 84 | OHX | 1 | 3436 | 7/7 | 0.99 | 0.28 | 115,115,115,115 | 0 |
| 84 | OHX | 1 | 3437 | 7/7 | 0.99 | 0.24 | 116,117,117,117 | 0 |
| 85 | MG | AR | 3940 | 1/1 | 0.99 | 0.49 | 21,21,21,21 | 0 |
| 85 | MG | 1 | 3903 | 1/1 | 0.99 | 0.67 | 21,21,21,21 | 0 |
| 84 | OHX | 1 | 3490 | 7/7 | 0.99 | 0.17 | 113,113,113,113 | 0 |
| 84 | OHX | 1 | 3414 | 7/7 | 0.99 | 0.27 | 109,109,109,109 | 0 |
| 84 | OHX | 1 | 3464 | 7/7 | 0.99 | 0.20 | 109,109,109,109 | 0 |
| 84 | OHX | 1 | 3405 | 7/7 | 0.99 | 0.37 | 124,125,125,125 | 0 |
| 84 | OHX | 1 | 3416 | 7/7 | 0.99 | 0.24 | 109,109,109,109 | 0 |
| 84 | OHX | 1 | 3406 | 7/7 | 0.99 | 0.33 | 108,108,108,108 | 0 |
| 84 | OHX | 1 | 3418 | 7/7 | 0.99 | 0.27 | 114,115,115,115 | 0 |
| 85 | MG | 1 | 3911 | 1/1 | 0.99 | 0.65 | 21,21,21,21 | 0 |
| 85 | MG | AR | 4052 | 1/1 | 0.99 | 0.12 | 86,86,86,86 | 0 |
| 85 | MG | 1 | 3825 | 1/1 | 0.99 | 0.41 | 31,31,31,31 | 0 |
| 84 | OHX | 1 | 3419 | 7/7 | 0.99 | 0.26 | 107,107,107,107 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 84 | OHX | A | 1920 | 7/7 | 0.99 | 0.14 | 128,128,129,129 | 0 |
| 85 | MG | 1 | 3745 | 1/1 | 0.99 | 0.67 | 31,31,31,31 | 0 |
| 84 | OHX | 1 | 3401 | 7/7 | 0.99 | 0.38 | 114,114,115,115 | 0 |
| 84 | OHX | 1 | 3421 | 7/7 | 0.99 | 0.29 | 115,115,116,116 | 0 |
| 85 | MG | 1 | 3748 | 1/1 | 0.99 | 0.34 | 44,44,44,44 | 0 |
| 84 | OHX | AR | 3462 | 7/7 | 0.99 | 0.16 | 116,116,116,116 | 0 |
| 84 | OHX | A | 1924 | 7/7 | 0.99 | 0.09 | 132,132,133,133 | 0 |
| 88 | ZN | AP | 501 | 1/1 | 0.99 | 0.04 | 61,61,61,61 | 0 |
| 88 | ZN | DL | 101 | 1/1 | 0.99 | 0.20 | 41,41,41,41 | 0 |
| 88 | ZN | DO | 201 | 1/1 | 0.99 | 0.15 | 32,32,32,32 | 0 |
| 88 | ZN | DQ | 202 | 1/1 | 0.99 | 0.03 | 63,63,63,63 | 0 |
| 88 | ZN | DR | 501 | 1/1 | 0.99 | 0.15 | 59,59,59,59 | 0 |
| 88 | ZN | b | 102 | 1/1 | 0.99 | 0.16 | 71,71,71,71 | 0 |
| 85 | MG | 1 | 4097 | 1/1 | 0.99 | 0.22 | 70,70,70,70 | 0 |
| 88 | ZN | e | 102 | 1/1 | 0.99 | 0.08 | 79,79,79,79 | 0 |
| 84 | OHX | A | 1925 | 7/7 | 0.99 | 0.12 | 136,137,137,137 | 0 |
| 84 | OHX | 1 | 3422 | 7/7 | 0.99 | 0.26 | 116,116,117,117 | 0 |
| 84 | OHX | 1 | 3423 | 7/7 | 0.99 | 0.26 | 120,120,121,121 | 0 |
| 84 | OHX | 1 | 3424 | 7/7 | 0.99 | 0.23 | 115,115,115,115 | 0 |
| 88 | ZN | AQ | 501 | 1/1 | 1.00 | 0.13 | 56,56,56,56 | 0 |
| 88 | ZN | d6 | 103 | 1/1 | 1.00 | 0.13 | 53,53,53,53 | 0 |
| 88 | ZN | AK | 101 | 1/1 | 1.00 | 0.15 | 34,34,34,34 | 0 |
| 88 | ZN | AN | 500 | 1/1 | 1.00 | 0.13 | 38,38,38,38 | 0 |
| 85 | MG | AR | 4168 | 1/1 | 1.00 | 0.19 | 65,65,65,65 | 0 |

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.