



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 12:37 PM EDT

PDB ID : 5NDW
Title : Crystal structure of aminoglycoside TC007 bound to the yeast 80S ribosome
Authors : Prokhorova, I.; Djumagulov, M.; Urzhumtsev, A.; Yusupov, M.; Yusupova, G.
Deposited on : 2017-03-09
Resolution : 3.70 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

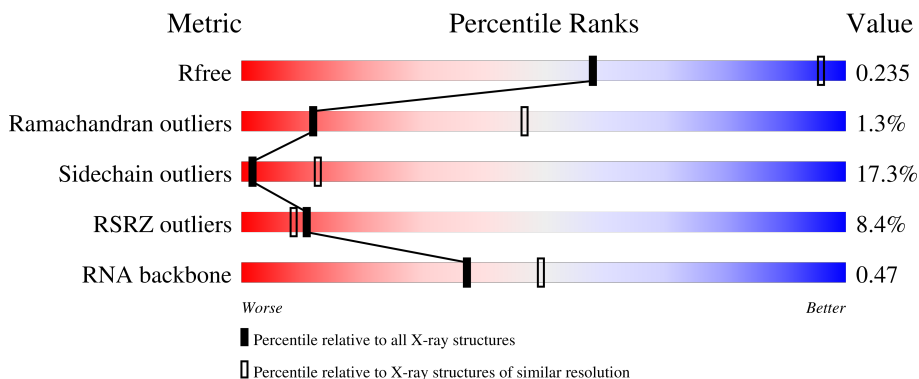
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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.






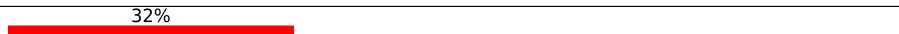
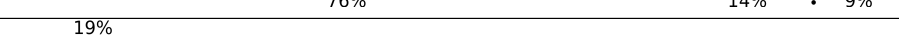
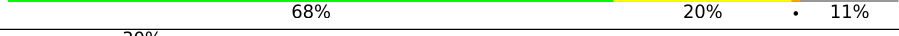



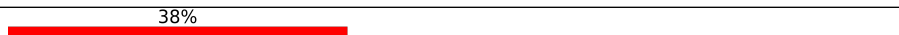
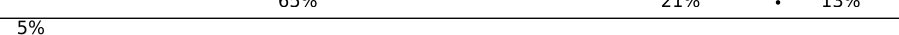




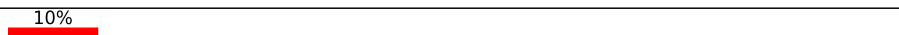






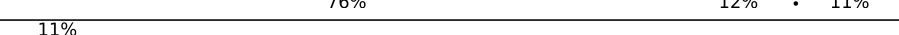


| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 1049 (3.88-3.52) |
| Ramachandran outliers | 138981 | 1069 (3.88-3.52) |
| Sidechain outliers | 138945 | 1065 (3.88-3.52) |
| RSRZ outliers | 127900 | 1578 (3.90-3.50) |
| RNA backbone | 3102 | 1027 (4.40-3.00) |

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 | 57% 28% 6% 9% |
| 1 | 5 | 3396 | 59% 27% 6% 9% |
| 2 | 2 | 1800 | 3% 64% 29% 6% . |
| 2 | 6 | 1800 | % 66% 25% 5% . |
| 3 | 3 | 121 | 67% 31% . |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 3 | 7 | 121 |  79% 20% |
| 4 | 4 | 158 |  64% 31% 5% |
| 4 | 8 | 158 |  64% 32% 2% |
| 5 | C0 | 105 |  76% 14% 32% 9% |
| 5 | c0 | 105 |  68% 20% 19% 11% |
| 6 | C1 | 156 |  87% 11% 30% |
| 6 | c1 | 156 |  74% 19% 13% 6% |
| 7 | C2 | 143 |  62% 20% 39% 17% |
| 7 | c2 | 143 |  65% 21% 38% 13% |
| 8 | C3 | 150 |  83% 17% 5% |
| 8 | c3 | 150 |  84% 15% 9% |
| 9 | C4 | 128 |  79% 19% 5% |
| 9 | c4 | 128 |  84% 16% 21% |
| 10 | C5 | 141 |  70% 17% 10% 12% |
| 10 | c5 | 141 |  74% 13% 13% 11% |
| 11 | C6 | 141 |  78% 21% 33% |
| 11 | c6 | 141 |  80% 18% 30% |
| 12 | C7 | 136 |  71% 14% 15% 12% |
| 12 | c7 | 136 |  76% 12% 5% 11% |
| 13 | C8 | 145 |  77% 20% 11% |
| 13 | c8 | 145 |  81% 17% 10% |
| 14 | C9 | 143 |  87% 12% 10% |
| 14 | c9 | 143 |  85% 14% 8% |
| 15 | D0 | 107 |  77% 20% 37% |
| 15 | d0 | 107 |  74% 21% 9% |

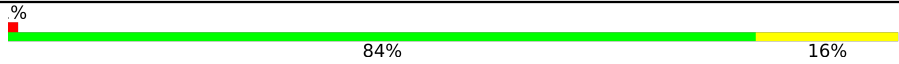

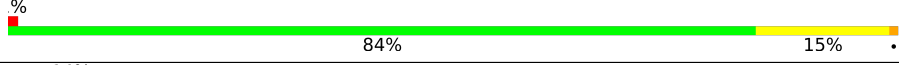

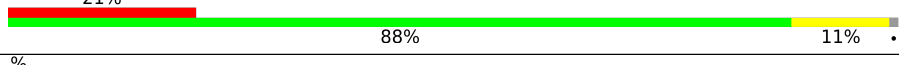
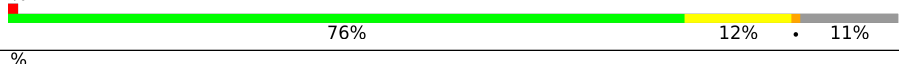
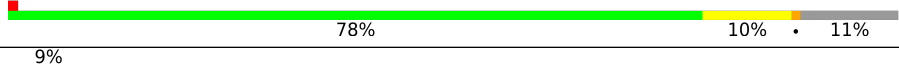
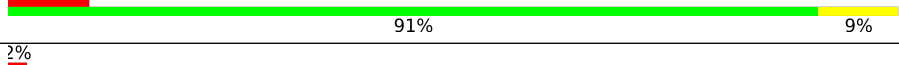
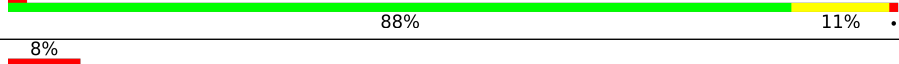


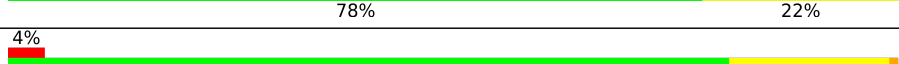
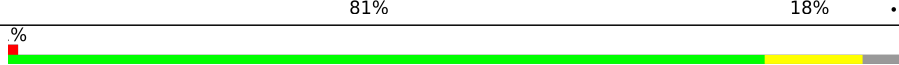
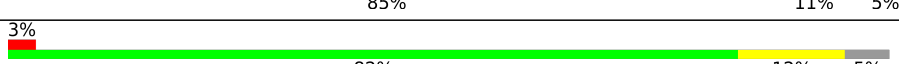

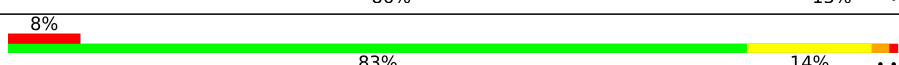
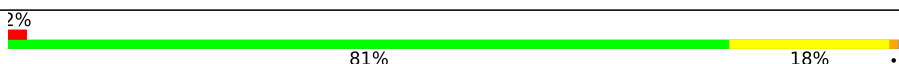
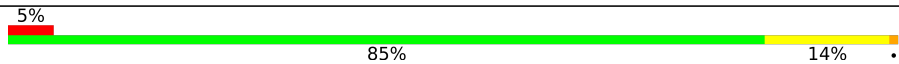
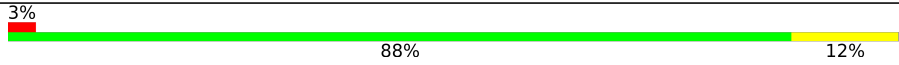
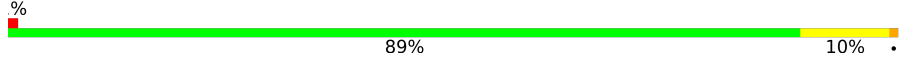

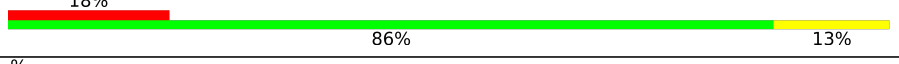
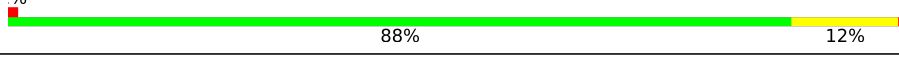
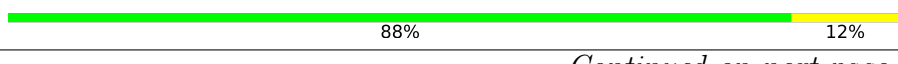

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--------------------------|
| 16 | D1 | 87 | 10% 86% 14% |
| 16 | d1 | 87 | 10% 87% 13% |
| 17 | D2 | 129 | 16% 84% 13% |
| 17 | d2 | 129 | 13% 88% 11% |
| 18 | D3 | 144 | 7% 83% 17% |
| 18 | d3 | 144 | 3% 88% 12% |
| 19 | D4 | 134 | 11% 81% 16% |
| 19 | d4 | 134 | 6% 84% 16% |
| 20 | D5 | 70 | 31% 71% 29% |
| 20 | d5 | 70 | 17% 76% 21% |
| 21 | D6 | 97 | 12% 73% 22% |
| 21 | d6 | 97 | 31% 82% 18% |
| 22 | D7 | 81 | 6% 85% 14% |
| 22 | d7 | 81 | 21% 85% 15% |
| 23 | D8 | 63 | 22% 76% 24% |
| 23 | d8 | 63 | 8% 73% 25% |
| 24 | D9 | 53 | 32% 85% 13% |
| 24 | d9 | 53 | 15% 83% 13% |
| 25 | E0 | 61 | 16% 84% 13% |
| 25 | e0 | 61 | 13% 85% 13% |
| 26 | E1 | 73 | 33% 63% 25% 8% |
| 26 | e1 | 73 | 29% 70% 19% 11% |
| 27 | L2 | 252 | 2% 88% 12% |
| 27 | l2 | 252 | 3% 85% 15% |
| 28 | L3 | 386 | 7% 85% 15% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 28 | l3 | 386 |  % 84% 16% |
| 29 | L4 | 361 |  % 86% 14% |
| 29 | l4 | 361 |  % 84% 15% . |
| 30 | L5 | 296 |  14% 82% 18% |
| 30 | l5 | 296 |  21% 88% 11% . |
| 31 | L6 | 176 |  % 76% 12% . 11% |
| 31 | l6 | 176 |  % 78% 10% . 11% |
| 32 | L7 | 223 |  9% 91% 9% |
| 32 | l7 | 223 |  2% 88% 11% . |
| 33 | L8 | 233 |  8% 86% 14% |
| 33 | l8 | 233 |  10% 86% 13% . |
| 34 | L9 | 191 |  9% 78% 22% |
| 34 | l9 | 191 |  4% 81% 18% . |
| 35 | M0 | 221 |  % 85% 11% 5% |
| 35 | m0 | 221 |  3% 82% 12% 5% |
| 36 | M1 | 169 |  6% 86% 13% . |
| 36 | m1 | 169 |  8% 83% 14% . . |
| 37 | M3 | 194 |  2% 81% 18% . . |
| 37 | m3 | 194 |  5% 85% 14% . |
| 38 | M4 | 137 |  3% 88% 12% . |
| 38 | m4 | 137 |  % 89% 10% . |
| 39 | M5 | 203 |  14% 88% 12% |
| 39 | m5 | 203 |  18% 86% 13% |
| 40 | M6 | 197 |  % 88% 12% . |
| 40 | m6 | 197 |  % 88% 12% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---------------------------|
| 41 | M7 | 184 | 2% 83% 16% .. |
| 41 | m7 | 184 | 2% 85% 14% . |
| 42 | M8 | 185 | 13% 88% 12% |
| 42 | m8 | 185 | 15% 90% 10% |
| 43 | M9 | 188 | 5% 88% 12% . |
| 43 | m9 | 188 | 6% 83% 15% . |
| 44 | N0 | 172 | 11% 81% 17% . |
| 44 | n0 | 172 | 4% 85% 15% . |
| 45 | N1 | 159 | 20% 77% 23% |
| 45 | n1 | 159 | 30% 85% 15% |
| 46 | N2 | 100 | 12% 82% 18% |
| 46 | n2 | 100 | 13% 81% 16% .. |
| 47 | N3 | 136 | 4% 90% 10% |
| 47 | n3 | 136 | 2% 93% 7% . |
| 48 | N4 | 155 | 16% 77% 7% 16% |
| 48 | n4 | 155 | 12% 77% 5% . 16% |
| 49 | N5 | 121 | 7% 84% 15% . |
| 49 | n5 | 121 | 29% 74% 26% . |
| 50 | N6 | 126 | 3% 84% 13% . |
| 50 | n6 | 126 | 8% 80% 17% . |
| 51 | N7 | 135 | 19% 84% 13% . |
| 51 | n7 | 135 | 11% 82% 16% . |
| 52 | N8 | 148 | 7% 89% 11% |
| 52 | n8 | 148 | 12% 87% 13% |
| 53 | N9 | 58 | 24% 81% 19% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------------|
| 53 | n9 | 58 | 36% 86% 10% |
| 54 | O0 | 100 | 8% 84% 13% |
| 54 | o0 | 100 | 7% 87% 13% |
| 55 | O1 | 109 | 7% 84% 14% |
| 55 | o1 | 109 | 7% 80% 18% |
| 56 | O2 | 127 | 89% 11% |
| 56 | o2 | 127 | 2% 86% 13% |
| 57 | O3 | 106 | % 90% 10% |
| 57 | o3 | 106 | 87% 13% |
| 58 | O4 | 112 | 22% 87% 13% |
| 58 | o4 | 112 | 10% 88% 10% |
| 59 | O5 | 119 | 3% 81% 19% |
| 59 | o5 | 119 | 10% 77% 21% |
| 60 | O6 | 99 | 5% 79% 21% |
| 60 | o6 | 99 | 8% 75% 25% |
| 61 | O7 | 87 | 80% 20% |
| 61 | o7 | 87 | 3% 85% 10% 5% |
| 62 | O8 | 77 | 17% 79% 21% |
| 62 | o8 | 77 | 21% 86% 14% |
| 63 | O9 | 50 | 4% 84% 14% |
| 63 | o9 | 50 | 20% 90% 10% |
| 64 | Q0 | 52 | 2% 87% 13% |
| 64 | q0 | 52 | 4% 87% 12% |
| 65 | Q1 | 25 | 84% 16% |
| 65 | q1 | 25 | 4% 84% 16% |


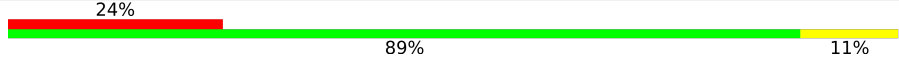
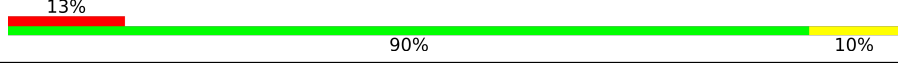
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|-------------------------|
| 66 | Q2 | 105 | 17% 81% 19% |
| 66 | q2 | 105 | 27% 87% 12% |
| 67 | Q3 | 91 | 88% 12% |
| 67 | q3 | 91 | 85% 15% |
| 68 | S0 | 206 | 10% 83% 17% |
| 68 | s0 | 206 | 11% 84% 15% |
| 69 | S1 | 216 | 15% 75% 22% |
| 69 | s1 | 216 | 32% 83% 15% |
| 70 | S2 | 217 | 13% 80% 19% |
| 70 | s2 | 217 | 10% 84% 15% |
| 71 | S3 | 223 | 21% 83% 17% |
| 71 | s3 | 223 | 11% 82% 16% |
| 72 | S4 | 260 | 21% 84% 15% |
| 72 | s4 | 260 | 6% 87% 13% |
| 73 | S5 | 206 | 20% 85% 15% |
| 73 | s5 | 206 | 17% 82% 18% |
| 74 | S6 | 236 | 19% 80% 16% |
| 74 | s6 | 236 | 14% 78% 14% 8% |
| 75 | S7 | 184 | 18% 79% 20% |
| 75 | s7 | 184 | 10% 83% 16% |
| 76 | S8 | 200 | 18% 83% 10% 6% |
| 76 | s8 | 200 | 14% 80% 12% 8% |
| 77 | S9 | 185 | 19% 84% 16% |
| 77 | s9 | 185 | 16% 86% 13% |
| 78 | SM | 272 | 8% 48% 10% 42% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 78 | sM | 272 |  |
| 79 | SR | 318 |  |
| 79 | sR | 318 |  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 80 | MG | 1 | 3413 | - | - | - | X |
| 80 | MG | 1 | 3418 | - | - | - | X |
| 80 | MG | 1 | 3431 | - | - | - | X |
| 80 | MG | 1 | 3441 | - | - | - | X |
| 80 | MG | 1 | 3448 | - | - | - | X |
| 80 | MG | 1 | 3461 | - | - | - | X |
| 80 | MG | 1 | 3480 | - | - | - | X |
| 80 | MG | 1 | 3492 | - | - | - | X |
| 80 | MG | 1 | 3498 | - | - | - | X |
| 80 | MG | 1 | 3504 | - | - | - | X |
| 80 | MG | 1 | 3505 | - | - | - | X |
| 80 | MG | 1 | 3515 | - | - | - | X |
| 80 | MG | 1 | 3517 | - | - | - | X |
| 80 | MG | 1 | 3523 | - | - | - | X |
| 80 | MG | 1 | 3544 | - | - | - | X |
| 80 | MG | 1 | 3548 | - | - | - | X |
| 80 | MG | 1 | 3550 | - | - | - | X |
| 80 | MG | 1 | 3551 | - | - | - | X |
| 80 | MG | 1 | 3552 | - | - | - | X |
| 80 | MG | 1 | 3559 | - | - | - | X |
| 80 | MG | 1 | 3564 | - | - | - | X |
| 80 | MG | 1 | 3567 | - | - | - | X |
| 80 | MG | 1 | 3569 | - | - | - | X |
| 80 | MG | 1 | 3571 | - | - | - | X |
| 80 | MG | 1 | 3576 | - | - | - | X |
| 80 | MG | 1 | 3580 | - | - | - | X |
| 80 | MG | 1 | 3590 | - | - | - | X |
| 80 | MG | 1 | 3598 | - | - | - | X |
| 80 | MG | 1 | 3608 | - | - | - | X |
| 80 | MG | 1 | 3609 | - | - | - | X |
| 80 | MG | 1 | 3623 | - | - | - | X |
| 80 | MG | 1 | 3658 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 80 | MG | 1 | 3659 | - | - | - | X |
| 80 | MG | 1 | 3664 | - | - | - | X |
| 80 | MG | 1 | 3667 | - | - | - | X |
| 80 | MG | 1 | 3674 | - | - | - | X |
| 80 | MG | 1 | 3687 | - | - | - | X |
| 80 | MG | 1 | 3690 | - | - | - | X |
| 80 | MG | 1 | 3699 | - | - | - | X |
| 80 | MG | 1 | 3706 | - | - | - | X |
| 80 | MG | 1 | 3708 | - | - | - | X |
| 80 | MG | 1 | 3709 | - | - | - | X |
| 80 | MG | 1 | 3712 | - | - | - | X |
| 80 | MG | 1 | 3713 | - | - | - | X |
| 80 | MG | 1 | 3737 | - | - | - | X |
| 80 | MG | 1 | 3739 | - | - | - | X |
| 80 | MG | 1 | 3740 | - | - | - | X |
| 80 | MG | 1 | 3741 | - | - | - | X |
| 80 | MG | 1 | 3744 | - | - | - | X |
| 80 | MG | 1 | 3761 | - | - | - | X |
| 80 | MG | 1 | 3763 | - | - | - | X |
| 80 | MG | 1 | 3775 | - | - | - | X |
| 80 | MG | 1 | 3829 | - | - | - | X |
| 80 | MG | 1 | 3841 | - | - | - | X |
| 80 | MG | 1 | 3842 | - | - | - | X |
| 80 | MG | 1 | 3853 | - | - | - | X |
| 80 | MG | 1 | 3854 | - | - | - | X |
| 80 | MG | 1 | 3856 | - | - | - | X |
| 80 | MG | 1 | 3858 | - | - | - | X |
| 80 | MG | 1 | 3860 | - | - | - | X |
| 80 | MG | 1 | 3862 | - | - | - | X |
| 80 | MG | 1 | 3864 | - | - | - | X |
| 80 | MG | 1 | 3867 | - | - | - | X |
| 80 | MG | 1 | 3868 | - | - | - | X |
| 80 | MG | 1 | 3876 | - | - | - | X |
| 80 | MG | 1 | 3877 | - | - | - | X |
| 80 | MG | 1 | 3880 | - | - | - | X |
| 80 | MG | 2 | 1908 | - | - | - | X |
| 80 | MG | 2 | 1944 | - | - | - | X |
| 80 | MG | 2 | 1947 | - | - | - | X |
| 80 | MG | 2 | 1968 | - | - | - | X |
| 80 | MG | 2 | 1973 | - | - | - | X |
| 80 | MG | 2 | 1977 | - | - | - | X |
| 80 | MG | 2 | 2022 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 80 | MG | 2 | 2026 | - | - | - | X |
| 80 | MG | 2 | 2027 | - | - | - | X |
| 80 | MG | 3 | 201 | - | - | - | X |
| 80 | MG | 4 | 202 | - | - | - | X |
| 80 | MG | 4 | 203 | - | - | - | X |
| 80 | MG | 4 | 206 | - | - | - | X |
| 80 | MG | 4 | 207 | - | - | - | X |
| 80 | MG | 4 | 214 | - | - | - | X |
| 80 | MG | 5 | 3426 | - | - | - | X |
| 80 | MG | 5 | 3430 | - | - | - | X |
| 80 | MG | 5 | 3431 | - | - | - | X |
| 80 | MG | 5 | 3437 | - | - | - | X |
| 80 | MG | 5 | 3445 | - | - | - | X |
| 80 | MG | 5 | 3457 | - | - | - | X |
| 80 | MG | 5 | 3459 | - | - | - | X |
| 80 | MG | 5 | 3463 | - | - | - | X |
| 80 | MG | 5 | 3464 | - | - | - | X |
| 80 | MG | 5 | 3466 | - | - | - | X |
| 80 | MG | 5 | 3471 | - | - | - | X |
| 80 | MG | 5 | 3480 | - | - | - | X |
| 80 | MG | 5 | 3481 | - | - | - | X |
| 80 | MG | 5 | 3488 | - | - | - | X |
| 80 | MG | 5 | 3491 | - | - | - | X |
| 80 | MG | 5 | 3493 | - | - | - | X |
| 80 | MG | 5 | 3506 | - | - | - | X |
| 80 | MG | 5 | 3513 | - | - | - | X |
| 80 | MG | 5 | 3516 | - | - | - | X |
| 80 | MG | 5 | 3543 | - | - | - | X |
| 80 | MG | 5 | 3556 | - | - | - | X |
| 80 | MG | 5 | 3565 | - | - | - | X |
| 80 | MG | 5 | 3588 | - | - | - | X |
| 80 | MG | 5 | 3595 | - | - | - | X |
| 80 | MG | 5 | 3598 | - | - | - | X |
| 80 | MG | 5 | 3601 | - | - | - | X |
| 80 | MG | 5 | 3603 | - | - | - | X |
| 80 | MG | 5 | 3614 | - | - | - | X |
| 80 | MG | 5 | 3619 | - | - | - | X |
| 80 | MG | 5 | 3627 | - | - | - | X |
| 80 | MG | 5 | 3635 | - | - | - | X |
| 80 | MG | 5 | 3640 | - | - | - | X |
| 80 | MG | 5 | 3650 | - | - | - | X |
| 80 | MG | 5 | 3664 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 80 | MG | 5 | 3667 | - | - | - | X |
| 80 | MG | 5 | 3694 | - | - | - | X |
| 80 | MG | 5 | 3696 | - | - | - | X |
| 80 | MG | 5 | 3697 | - | - | - | X |
| 80 | MG | 5 | 3698 | - | - | - | X |
| 80 | MG | 5 | 3701 | - | - | - | X |
| 80 | MG | 5 | 3702 | - | - | - | X |
| 80 | MG | 5 | 3705 | - | - | - | X |
| 80 | MG | 5 | 3707 | - | - | - | X |
| 80 | MG | 5 | 3713 | - | - | - | X |
| 80 | MG | 5 | 3725 | - | - | - | X |
| 80 | MG | 5 | 3728 | - | - | - | X |
| 80 | MG | 5 | 3731 | - | - | - | X |
| 80 | MG | 5 | 3735 | - | - | - | X |
| 80 | MG | 5 | 3736 | - | - | - | X |
| 80 | MG | 5 | 3738 | - | - | - | X |
| 80 | MG | 5 | 3740 | - | - | - | X |
| 80 | MG | 5 | 3750 | - | - | - | X |
| 80 | MG | 5 | 3764 | - | - | - | X |
| 80 | MG | 5 | 3768 | - | - | - | X |
| 80 | MG | 5 | 3800 | - | - | - | X |
| 80 | MG | 5 | 3822 | - | - | - | X |
| 80 | MG | 5 | 3829 | - | - | - | X |
| 80 | MG | 5 | 3832 | - | - | - | X |
| 80 | MG | 5 | 3834 | - | - | - | X |
| 80 | MG | 5 | 3843 | - | - | - | X |
| 80 | MG | 5 | 3846 | - | - | - | X |
| 80 | MG | 5 | 3847 | - | - | - | X |
| 80 | MG | 6 | 1901 | - | - | - | X |
| 80 | MG | 6 | 1904 | - | - | - | X |
| 80 | MG | 6 | 1908 | - | - | - | X |
| 80 | MG | 6 | 1913 | - | - | - | X |
| 80 | MG | 6 | 1915 | - | - | - | X |
| 80 | MG | 6 | 1921 | - | - | - | X |
| 80 | MG | 6 | 1939 | - | - | - | X |
| 80 | MG | 6 | 1940 | - | - | - | X |
| 80 | MG | 6 | 1965 | - | - | - | X |
| 80 | MG | 6 | 1967 | - | - | - | X |
| 80 | MG | 6 | 1979 | - | - | - | X |
| 80 | MG | 6 | 1981 | - | - | - | X |
| 80 | MG | 6 | 1995 | - | - | - | X |
| 80 | MG | 6 | 1996 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 80 | MG | 6 | 2009 | - | - | - | X |
| 80 | MG | 6 | 2033 | - | - | - | X |
| 80 | MG | 6 | 2038 | - | - | - | X |
| 80 | MG | 6 | 2041 | - | - | - | X |
| 80 | MG | 6 | 2046 | - | - | - | X |
| 80 | MG | 6 | 2047 | - | - | - | X |
| 80 | MG | 6 | 2050 | - | - | - | X |
| 80 | MG | 6 | 2054 | - | - | - | X |
| 80 | MG | 6 | 2060 | - | - | - | X |
| 80 | MG | 8 | 203 | - | - | - | X |
| 80 | MG | 8 | 206 | - | - | - | X |
| 80 | MG | C4 | 202 | - | - | - | X |
| 80 | MG | M6 | 201 | - | - | - | X |
| 80 | MG | N0 | 201 | - | - | - | X |
| 80 | MG | O1 | 201 | - | - | - | X |
| 80 | MG | O1 | 202 | - | - | - | X |
| 80 | MG | O3 | 202 | - | - | - | X |
| 80 | MG | O4 | 502 | - | - | - | X |
| 80 | MG | c1 | 201 | - | - | - | X |
| 80 | MG | c1 | 202 | - | - | - | X |
| 80 | MG | d2 | 201 | - | - | - | X |
| 80 | MG | d3 | 201 | - | - | - | X |
| 80 | MG | l3 | 401 | - | - | - | X |
| 80 | MG | l5 | 301 | - | - | - | X |
| 80 | MG | m6 | 201 | - | - | - | X |
| 80 | MG | n1 | 201 | - | - | - | X |
| 80 | MG | n6 | 201 | - | - | - | X |
| 80 | MG | n8 | 201 | - | - | - | X |
| 80 | MG | o3 | 201 | - | - | - | X |
| 80 | MG | q2 | 503 | - | - | - | X |
| 80 | MG | q2 | 504 | - | - | - | X |

2 Entry composition [i](#)

There are 83 unique types of molecules in this entry. The entry contains 400111 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 | 3090 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 66081 | 29518 | 11903 | 21570 | 3090 | | | |
| 1 | 5 | 3080 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 65880 | 29427 | 11878 | 21495 | 3080 | | | |

- Molecule 2 is a RNA chain called 18S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| | | | Total | C | N | O | P | | | |
| 2 | 2 | 1770 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 37692 | 16850 | 6663 | 12409 | 1770 | | | |
| 2 | 6 | 1736 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 36971 | 16529 | 6541 | 12165 | 1736 | | | |

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 4 is a RNA chain called 5.8S ribosomal RNA.

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

- Molecule 5 is a protein called 40S ribosomal protein S10-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | C0 | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 772 | 499 | 126 | 145 | 2 | | | |
| 5 | c0 | 93 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 746 | 481 | 122 | 141 | 2 | | | |

- Molecule 6 is a protein called 40S ribosomal protein S11-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | C1 | 154 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1207 | 771 | 229 | 204 | 3 | | | |
| 6 | c1 | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1168 | 747 | 221 | 197 | 3 | | | |

- Molecule 7 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | C2 | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 865 | 545 | 151 | 167 | 2 | | | |
| 7 | c2 | 124 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 890 | 560 | 156 | 172 | 2 | | | |

- Molecule 8 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | C3 | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1192 | 759 | 224 | 207 | 2 | | | |
| 8 | c3 | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1192 | 759 | 224 | 207 | 2 | | | |

- Molecule 9 is a protein called 40S ribosomal protein S14-B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9 | C4 | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 891 | 545 | 182 | 163 | 1 | | | |
| 9 | c4 | 128 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 949 | 582 | 188 | 176 | 3 | | | |

- Molecule 10 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | C5 | 124 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 977 | 622 | 182 | 166 | 7 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | c5 | 125 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 987 | 627 | 186 | 167 | 7 | | | |

- Molecule 11 is a protein called 40S ribosomal protein S16-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | C6 | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1105 | 708 | 203 | 194 | | | | |
| 11 | c6 | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1105 | 708 | 203 | 194 | | | | |

- Molecule 12 is a protein called 40S ribosomal protein S17-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | C7 | 120 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 926 | 577 | 177 | 170 | 2 | | | |
| 12 | c7 | 121 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 926 | 575 | 178 | 171 | 2 | | | |

- Molecule 13 is a protein called 40S ribosomal protein S18-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | C8 | 145 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1192 | 743 | 237 | 210 | 2 | | | |
| 13 | c8 | 145 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1192 | 743 | 237 | 210 | 2 | | | |

- Molecule 14 is a protein called 40S ribosomal protein S19-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14 | C9 | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1112 | 694 | 208 | 208 | 2 | | | |
| 14 | c9 | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1112 | 694 | 208 | 208 | 2 | | | |

- Molecule 15 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | d0 | 104 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 828 | 524 | 150 | 153 | 1 | | | |
| 15 | D0 | 105 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 841 | 532 | 153 | 155 | 1 | | | |

- Molecule 16 is a protein called 40S ribosomal protein S21-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | d1 | 87 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 684 | 420 | 125 | 137 | 2 | | | |
| 16 | D1 | 87 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 684 | 420 | 125 | 137 | 2 | | | |

- Molecule 17 is a protein called 40S ribosomal protein S22-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | d2 | 129 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1021 | 650 | 188 | 180 | 3 | | | |
| 17 | D2 | 129 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1021 | 650 | 188 | 180 | 3 | | | |

- Molecule 18 is a protein called 40S ribosomal protein S23-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18 | d3 | 144 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1121 | 708 | 220 | 191 | 2 | | | |
| 18 | D3 | 144 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1121 | 708 | 220 | 191 | 2 | | | |

- Molecule 19 is a protein called 40S ribosomal protein S24-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 19 | d4 | 134 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1073 | 676 | 208 | 189 | | | |
| 19 | D4 | 134 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1073 | 676 | 208 | 189 | | | |

- Molecule 20 is a protein called 40S ribosomal protein S25-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 20 | d5 | 69 | Total | C | N | O | 0 | 0 | 0 |
| | | | 558 | 357 | 103 | 98 | | | |
| 20 | D5 | 70 | Total | C | N | O | 0 | 0 | 0 |
| | | | 563 | 360 | 104 | 99 | | | |

- Molecule 21 is a protein called 40S ribosomal protein S26-B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21 | d6 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 769 | 475 | 160 | 129 | 5 | | | |
| 21 | D6 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 769 | 475 | 160 | 129 | 5 | | | |

- Molecule 22 is a protein called 40S ribosomal protein S27-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22 | d7 | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 610 | 382 | 110 | 113 | 5 | | | |
| 22 | D7 | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 610 | 382 | 110 | 113 | 5 | | | |

- Molecule 23 is a protein called 40S ribosomal protein S28-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 23 | d8 | 63 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 497 | 306 | 99 | 91 | 1 | | | |
| 23 | D8 | 63 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 497 | 306 | 99 | 91 | 1 | | | |

- Molecule 24 is a protein called 40S ribosomal protein S29-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 24 | d9 | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 442 | 274 | 92 | 72 | 4 | | | |
| 24 | D9 | 52 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 433 | 269 | 91 | 69 | 4 | | | |

- Molecule 25 is a protein called 40S ribosomal protein S30-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 25 | e0 | 61 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 482 | 304 | 99 | 78 | 1 | | | |
| 25 | E0 | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 475 | 299 | 98 | 77 | 1 | | | |

- Molecule 26 is a protein called Ubiquitin-40S ribosomal protein S31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 26 | e1 | 73 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 586 | 374 | 112 | 96 | 4 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|---------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 26 | E1 | 71 | Total 566 | C 362 | N 106 | O 94 | S 4 | 0 | 0 | 0 |

- Molecule 27 is a protein called 60S ribosomal protein L2-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 27 | l2 | 252 | Total 1912 | C 1190 | N 388 | O 333 | S 1 | 0 | 0 | 0 |
| 27 | L2 | 252 | Total 1914 | C 1191 | N 388 | O 334 | S 1 | 0 | 0 | 0 |

- Molecule 28 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 28 | l3 | 386 | Total 3075 | C 1950 | N 584 | O 533 | S 8 | 0 | 0 | 0 |
| 28 | L3 | 386 | Total 3075 | C 1950 | N 584 | O 533 | S 8 | 0 | 0 | 0 |

- Molecule 29 is a protein called 60S ribosomal protein L4-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 29 | l4 | 361 | Total 2748 | C 1729 | N 522 | O 494 | S 3 | 0 | 0 | 0 |
| 29 | L4 | 361 | Total 2748 | C 1729 | N 522 | O 494 | S 3 | 0 | 0 | 0 |

- Molecule 30 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 30 | l5 | 294 | Total 2359 | C 1489 | N 412 | O 456 | S 2 | 0 | 0 | 0 |
| 30 | L5 | 296 | Total 2375 | C 1501 | N 414 | O 458 | S 2 | 0 | 0 | 0 |

- Molecule 31 is a protein called 60S ribosomal protein L6-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 31 | l6 | 157 | Total 1248 | C 806 | N 224 | O 217 | S 1 | 0 | 0 | 0 |
| 31 | L6 | 157 | Total 1248 | C 806 | N 224 | O 217 | S 1 | 0 | 0 | 0 |

- Molecule 32 is a protein called 60S ribosomal protein L7-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 32 | l7 | 223 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1791 | 1155 | 325 | 310 | 1 | | | |
| 32 | L7 | 222 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1784 | 1151 | 324 | 308 | 1 | | | |

- Molecule 33 is a protein called 60S ribosomal protein L8-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 33 | l8 | 231 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1764 | 1130 | 316 | 315 | 3 | | | |
| 33 | L8 | 233 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1804 | 1151 | 323 | 327 | 3 | | | |

- Molecule 34 is a protein called 60S ribosomal protein L9-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 34 | l9 | 191 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1518 | 963 | 274 | 277 | 4 | | | |
| 34 | L9 | 191 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1518 | 963 | 274 | 277 | 4 | | | |

- Molecule 35 is a protein called 60S ribosomal protein L10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 35 | m0 | 209 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1696 | 1077 | 321 | 293 | 5 | | | |
| 35 | M0 | 211 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1705 | 1083 | 322 | 294 | 6 | | | |

- Molecule 36 is a protein called 60S ribosomal protein L11-B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 36 | m1 | 169 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1353 | 847 | 253 | 249 | 4 | | | |
| 36 | M1 | 169 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1353 | 847 | 253 | 249 | 4 | | | |

- Molecule 37 is a protein called 60S ribosomal protein L13-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 37 | m3 | 194 | 1548 | 965 | 316 | 267 | 0 | 0 | 0 |
| 37 | M3 | 193 | 1543 | 962 | 315 | 266 | 0 | 0 | 0 |

- Molecule 38 is a protein called 60S ribosomal protein L14-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 38 | m4 | 137 | 1059 | 678 | 200 | 179 | 2 | 0 | 0 | 0 |
| 38 | M4 | 136 | 1053 | 675 | 199 | 177 | 2 | 0 | 0 | 0 |

- Molecule 39 is a protein called 60S ribosomal protein L15-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 39 | m5 | 203 | 1720 | 1077 | 361 | 281 | 1 | 0 | 0 | 0 |
| 39 | M5 | 203 | 1720 | 1077 | 361 | 281 | 1 | 0 | 0 | 0 |

- Molecule 40 is a protein called 60S ribosomal protein L16-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 40 | m6 | 197 | 1555 | 1003 | 289 | 262 | 1 | 0 | 0 | 0 |
| 40 | M6 | 197 | 1555 | 1003 | 289 | 262 | 1 | 0 | 0 | 0 |

- Molecule 41 is a protein called 60S ribosomal protein L17-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 41 | m7 | 183 | 1420 | 882 | 281 | 257 | 0 | 0 | 0 |
| 41 | M7 | 183 | 1420 | 882 | 281 | 257 | 0 | 0 | 0 |

- Molecule 42 is a protein called 60S ribosomal protein L18-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 42 | m8 | 185 | 1441 | 908 | 290 | 241 | 2 | 0 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 42 | M8 | 185 | 1441 | 908 | 290 | 241 | 2 | 0 | 0 | 0 |

- Molecule 43 is a protein called 60S ribosomal protein L19-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 43 | m9 | 184 | 1490 | 917 | 321 | 252 | | 0 | 0 | 0 |
| 43 | M9 | 188 | 1521 | 935 | 326 | 260 | | 0 | 0 | 0 |

- Molecule 44 is a protein called 60S ribosomal protein L20-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 44 | n0 | 171 | 1437 | 925 | 266 | 243 | 3 | 0 | 0 | 0 |
| 44 | N0 | 172 | 1445 | 930 | 267 | 244 | 4 | 0 | 0 | 0 |

- Molecule 45 is a protein called 60S ribosomal protein L21-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 45 | n1 | 159 | 1276 | 805 | 246 | 221 | 4 | 0 | 0 | 0 |
| 45 | N1 | 159 | 1276 | 805 | 246 | 221 | 4 | 0 | 0 | 0 |

- Molecule 46 is a protein called 60S ribosomal protein L22-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 46 | n2 | 98 | 778 | 505 | 127 | 146 | 0 | 0 | 0 |
| 46 | N2 | 100 | 796 | 516 | 131 | 149 | 0 | 0 | 0 |

- Molecule 47 is a protein called 60S ribosomal protein L23-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 47 | n3 | 135 | 997 | 625 | 188 | 177 | 7 | 0 | 0 | 0 |
| 47 | N3 | 136 | 1003 | 628 | 189 | 179 | 7 | 0 | 0 | 0 |

- Molecule 48 is a protein called 60S ribosomal protein L24-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 48 | n4 | 130 | Total 1007 | C 634 | N 200 | O 172 | S 1 | 0 | 0 | 0 |
| 48 | N4 | 130 | Total 965 | C 606 | N 192 | O 166 | S 1 | 0 | 0 | 0 |

- Molecule 49 is a protein called 60S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 49 | n5 | 120 | Total 959 | C 617 | N 168 | O 172 | S 2 | 0 | 0 | 0 |
| 49 | N5 | 121 | Total 964 | C 620 | N 169 | O 173 | S 2 | 0 | 0 | 0 |

- Molecule 50 is a protein called 60S ribosomal protein L26-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 50 | n6 | 122 | Total 963 | C 606 | N 187 | O 170 | 0 | 0 | 0 |
| 50 | N6 | 126 | Total 993 | C 625 | N 192 | O 176 | 0 | 0 | 0 |

- Molecule 51 is a protein called 60S ribosomal protein L27-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 51 | n7 | 135 | Total 1092 | C 710 | N 202 | O 180 | 0 | 0 | 0 |
| 51 | N7 | 135 | Total 1092 | C 710 | N 202 | O 180 | 0 | 0 | 0 |

- Molecule 52 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 52 | n8 | 148 | Total 1173 | C 749 | N 231 | O 190 | S 3 | 0 | 0 | 0 |
| 52 | N8 | 148 | Total 1173 | C 749 | N 231 | O 190 | S 3 | 0 | 0 | 0 |

- Molecule 53 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 53 | n9 | 56 | Total | C | N | O | 0 | 0 | 0 |
| | | | 444 | 277 | 96 | 71 | | | |
| 53 | N9 | 58 | Total | C | N | O | 0 | 0 | 0 |
| | | | 462 | 289 | 100 | 73 | | | |

- Molecule 54 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 54 | o0 | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 767 | 492 | 128 | 146 | 1 | | | |
| 54 | O0 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 743 | 479 | 124 | 139 | 1 | | | |

- Molecule 55 is a protein called 60S ribosomal protein L31-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 55 | o1 | 109 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 883 | 559 | 167 | 156 | 1 | | | |
| 55 | O1 | 109 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 876 | 556 | 167 | 152 | 1 | | | |

- Molecule 56 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 56 | o2 | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1020 | 647 | 205 | 167 | 1 | | | |
| 56 | O2 | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1020 | 647 | 205 | 167 | 1 | | | |

- Molecule 57 is a protein called 60S ribosomal protein L33-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 57 | o3 | 106 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 850 | 540 | 165 | 144 | 1 | | | |
| 57 | O3 | 106 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 850 | 540 | 165 | 144 | 1 | | | |

- Molecule 58 is a protein called 60S ribosomal protein L34-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 58 | o4 | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 880 | 545 | 179 | 152 | 4 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 58 | O4 | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 880 | 545 | 179 | 152 | 4 | | | |

- Molecule 59 is a protein called 60S ribosomal protein L35-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 59 | o5 | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 965 | 612 | 185 | 167 | 1 | | | |
| 59 | O5 | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 969 | 615 | 186 | 167 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 60 | o6 | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 770 | 481 | 156 | 131 | 2 | | | |
| 60 | O6 | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 771 | 481 | 156 | 132 | 2 | | | |

- Molecule 61 is a protein called 60S ribosomal protein L37-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 61 | o7 | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 656 | 399 | 143 | 109 | 5 | | | |
| 61 | O7 | 87 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 681 | 414 | 148 | 114 | 5 | | | |

- Molecule 62 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 62 | o8 | 77 | Total | C | N | O | 0 | 0 | 0 |
| | | | 608 | 388 | 114 | 106 | | | |
| 62 | O8 | 77 | Total | C | N | O | 0 | 0 | 0 |
| | | | 612 | 391 | 115 | 106 | | | |

- Molecule 63 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 63 | o9 | 50 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 436 | 272 | 97 | 65 | 2 | | | |
| 63 | O9 | 50 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 436 | 272 | 97 | 65 | 2 | | | |

- Molecule 64 is a protein called Ubiquitin-60S ribosomal protein L40.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 64 | q0 | 52 | Total 417 | C 259 | N 86 | O 67 | S 5 | 0 | 0 | 0 |
| 64 | Q0 | 52 | Total 417 | C 259 | N 86 | O 67 | S 5 | 0 | 0 | 0 |

- Molecule 65 is a protein called 60S ribosomal protein L41-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 65 | q1 | 25 | Total 233 | C 142 | N 63 | O 27 | S 1 | 0 | 0 | 0 |
| 65 | Q1 | 25 | Total 233 | C 142 | N 63 | O 27 | S 1 | 0 | 0 | 0 |

- Molecule 66 is a protein called 60S ribosomal protein L42-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 66 | q2 | 104 | Total 836 | C 525 | N 169 | O 137 | S 5 | 0 | 0 | 0 |
| 66 | Q2 | 105 | Total 847 | C 534 | N 170 | O 138 | S 5 | 0 | 0 | 0 |

- Molecule 67 is a protein called 60S ribosomal protein L43-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 67 | q3 | 91 | Total 694 | C 429 | N 138 | O 121 | S 6 | 0 | 0 | 0 |
| 67 | Q3 | 91 | Total 694 | C 429 | N 138 | O 121 | S 6 | 0 | 0 | 0 |

- Molecule 68 is a protein called 40S ribosomal protein S0-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 68 | S0 | 206 | Total 1577 | C 1014 | N 278 | O 283 | S 2 | 0 | 0 | 0 |
| 68 | s0 | 206 | Total 1583 | C 1017 | N 281 | O 283 | S 2 | 0 | 0 | 0 |

- Molecule 69 is a protein called 40S ribosomal protein S1-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 69 | S1 | 214 | Total 1709 | C 1084 | N 310 | O 311 | S 4 | 0 | 0 | 0 |
| 69 | s1 | 216 | Total 1722 | C 1091 | N 312 | O 315 | S 4 | 0 | 0 | 0 |

- Molecule 70 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 70 | S2 | 217 | Total 1635 | C 1047 | N 289 | O 297 | S 2 | 0 | 0 | 0 |
| 70 | s2 | 217 | Total 1635 | C 1047 | N 289 | O 297 | S 2 | 0 | 0 | 0 |

- Molecule 71 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 71 | S3 | 223 | Total 1734 | C 1101 | N 313 | O 314 | S 6 | 0 | 0 | 0 |
| 71 | s3 | 223 | Total 1734 | C 1101 | N 313 | O 314 | S 6 | 0 | 0 | 0 |

- Molecule 72 is a protein called 40S ribosomal protein S4-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 72 | S4 | 260 | Total 2068 | C 1316 | N 389 | O 360 | S 3 | 0 | 0 | 0 |
| 72 | s4 | 260 | Total 2068 | C 1316 | N 389 | O 360 | S 3 | 0 | 0 | 0 |

- Molecule 73 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 73 | S5 | 206 | Total 1609 | C 1007 | N 300 | O 299 | S 3 | 0 | 0 | 0 |
| 73 | s5 | 206 | Total 1609 | C 1007 | N 300 | O 299 | S 3 | 0 | 0 | 0 |

- Molecule 74 is a protein called 40S ribosomal protein S6-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 74 | S6 | 226 | Total 1799 | C 1129 | N 346 | O 321 | S 3 | 0 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 74 | s6 | 218 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1755 | 1102 | 337 | 313 | 3 | | | |

- Molecule 75 is a protein called 40S ribosomal protein S7-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 75 | s7 | 184 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1481 | 951 | 265 | 265 | | | |
| 75 | S7 | 184 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1481 | 951 | 265 | 265 | | | |

- Molecule 76 is a protein called 40S ribosomal protein S8-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 76 | s8 | 185 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1466 | 910 | 293 | 261 | 2 | | | |
| 76 | S8 | 188 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1489 | 925 | 298 | 264 | 2 | | | |

- Molecule 77 is a protein called 40S ribosomal protein S9-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 77 | S9 | 185 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1494 | 943 | 289 | 261 | 1 | | | |
| 77 | s9 | 185 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1494 | 943 | 289 | 261 | 1 | | | |

- Molecule 78 is a protein called Suppressor protein STM1.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 78 | sM | 131 | Total | C | N | O | 0 | 0 | 0 |
| | | | 958 | 564 | 193 | 201 | | | |
| 78 | SM | 159 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1104 | 652 | 221 | 231 | | | |

- Molecule 79 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 79 | sR | 316 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2427 | 1535 | 415 | 469 | 8 | | | |
| 79 | SR | 318 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2437 | 1541 | 418 | 470 | 8 | | | |

- Molecule 80 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|---------------------|---------|---------|
| 80 | 1 | 485 | Total Mg 485 485 | 0 | 0 |
| 80 | 2 | 128 | Total Mg 128 128 | 0 | 0 |
| 80 | 3 | 13 | Total Mg 13 13 | 0 | 0 |
| 80 | 4 | 19 | Total Mg 19 19 | 1 | 0 |
| 80 | 5 | 449 | Total Mg 449 449 | 1 | 0 |
| 80 | 6 | 160 | Total Mg 160 160 | 0 | 0 |
| 80 | 7 | 8 | Total Mg 8 8 | 0 | 0 |
| 80 | 8 | 10 | Total Mg 10 10 | 0 | 0 |
| 80 | c1 | 2 | Total Mg 2 2 | 0 | 0 |
| 80 | c3 | 1 | Total Mg 1 1 | 0 | 0 |
| 80 | C4 | 3 | Total Mg 3 3 | 0 | 0 |
| 80 | C6 | 1 | Total Mg 1 1 | 0 | 0 |
| 80 | c7 | 1 | Total Mg 1 1 | 0 | 0 |
| 80 | C8 | 1 | Total Mg 1 1 | 0 | 0 |
| 80 | c8 | 2 | Total Mg 2 2 | 0 | 0 |
| 80 | C9 | 1 | Total Mg 1 1 | 0 | 0 |
| 80 | c9 | 1 | Total Mg 1 1 | 0 | 0 |
| 80 | d2 | 1 | Total Mg 1 1 | 0 | 0 |
| 80 | D2 | 1 | Total Mg 1 1 | 0 | 0 |
| 80 | d3 | 1 | Total Mg 1 1 | 0 | 0 |
| 80 | d9 | 2 | Total Mg 2 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 80 | l2 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 80 | L2 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 80 | l3 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 80 | L3 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 80 | l4 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 80 | l5 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 80 | L6 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 80 | l7 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 80 | L7 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 80 | L9 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 80 | m0 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 80 | M0 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 80 | m5 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 80 | M5 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 80 | m6 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 80 | M6 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 80 | m7 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 80 | M7 | 4 | Total 4 | Mg 4 | 0 | 0 |
| 80 | M8 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 80 | N0 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 80 | n1 | 1 | Total 1 | Mg 1 | 0 | 0 |

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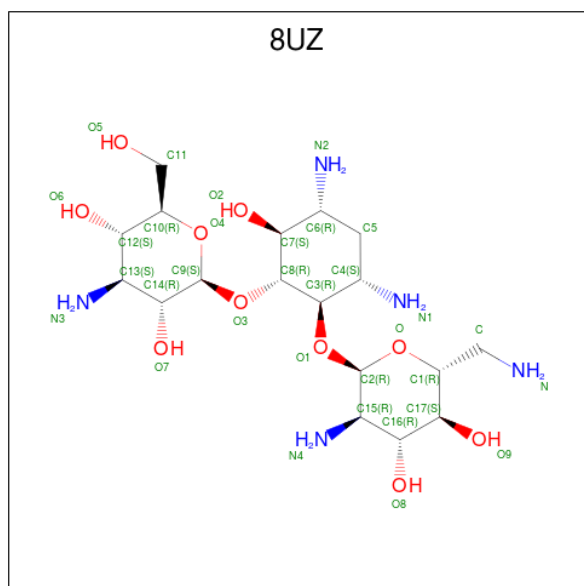
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 80 | n3 | 1 | Total Mg 1 1 | 0 | 0 |
| 80 | N3 | 1 | Total Mg 1 1 | 0 | 0 |
| 80 | n6 | 1 | Total Mg 1 1 | 0 | 0 |
| 80 | N6 | 1 | Total Mg 1 1 | 0 | 0 |
| 80 | n7 | 1 | Total Mg 1 1 | 0 | 0 |
| 80 | N7 | 1 | Total Mg 1 1 | 0 | 0 |
| 80 | n8 | 1 | Total Mg 1 1 | 0 | 0 |
| 80 | N8 | 1 | Total Mg 1 1 | 0 | 0 |
| 80 | O1 | 2 | Total Mg 2 2 | 0 | 0 |
| 80 | o2 | 2 | Total Mg 2 2 | 0 | 0 |
| 80 | O2 | 1 | Total Mg 1 1 | 0 | 0 |
| 80 | o3 | 2 | Total Mg 2 2 | 0 | 0 |
| 80 | O3 | 2 | Total Mg 2 2 | 0 | 0 |
| 80 | o4 | 1 | Total Mg 1 1 | 0 | 0 |
| 80 | O4 | 1 | Total Mg 1 1 | 0 | 0 |
| 80 | O5 | 1 | Total Mg 1 1 | 0 | 0 |
| 80 | O6 | 1 | Total Mg 1 1 | 0 | 0 |
| 80 | o7 | 2 | Total Mg 2 2 | 0 | 0 |
| 80 | O7 | 2 | Total Mg 2 2 | 0 | 0 |
| 80 | q2 | 3 | Total Mg 3 3 | 0 | 0 |
| 80 | Q2 | 1 | Total Mg 1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 80 | s0 | 1 | Total Mg 1 1 | 0 | 0 |
| 80 | S1 | 1 | Total Mg 1 1 | 0 | 0 |
| 80 | S4 | 1 | Total Mg 1 1 | 0 | 0 |
| 80 | s4 | 1 | Total Mg 1 1 | 0 | 0 |
| 80 | S6 | 1 | Total Mg 1 1 | 0 | 0 |
| 80 | s6 | 1 | Total Mg 1 1 | 0 | 0 |
| 80 | s8 | 1 | Total Mg 1 1 | 0 | 0 |
| 80 | SM | 2 | Total Mg 2 2 | 0 | 0 |

- Molecule 81 is TC007 (three-letter code: 8UZ) (formula: C₁₈H₃₇N₅O₁₀).



| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|---------------------------|---------|---------|
| 81 | 1 | 1 | Total C N O 33 18 5 10 | 0 | 0 |
| 81 | 1 | 1 | Total C N O 33 18 5 10 | 0 | 0 |
| 81 | 1 | 1 | Total C N O 33 18 5 10 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
| 81 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 33 | 18 | 5 | 10 | | |
| 81 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 33 | 18 | 5 | 10 | | |
| 81 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 33 | 18 | 5 | 10 | | |
| 81 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 33 | 18 | 5 | 10 | | |
| 81 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 33 | 18 | 5 | 10 | | |
| 81 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 33 | 18 | 5 | 10 | | |
| 81 | 2 | 1 | Total | C | N | O | 0 | 0 |
| | | | 33 | 18 | 5 | 10 | | |
| 81 | 2 | 1 | Total | C | N | O | 0 | 0 |
| | | | 33 | 18 | 5 | 10 | | |
| 81 | 2 | 1 | Total | C | N | O | 0 | 0 |
| | | | 33 | 18 | 5 | 10 | | |
| 81 | 3 | 1 | Total | C | N | O | 0 | 0 |
| | | | 33 | 18 | 5 | 10 | | |
| 81 | 4 | 1 | Total | C | N | O | 0 | 0 |
| | | | 33 | 18 | 5 | 10 | | |
| 81 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 33 | 18 | 5 | 10 | | |
| 81 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 33 | 18 | 5 | 10 | | |
| 81 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 33 | 18 | 5 | 10 | | |
| 81 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 33 | 18 | 5 | 10 | | |
| 81 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 33 | 18 | 5 | 10 | | |
| 81 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 33 | 18 | 5 | 10 | | |
| 81 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 33 | 18 | 5 | 10 | | |
| 81 | 6 | 1 | Total | C | N | O | 0 | 0 |
| | | | 33 | 18 | 5 | 10 | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
| | | | Total | C | N | O | | |
| 81 | 7 | 1 | 33 | 18 | 5 | 10 | 0 | 0 |

- Molecule 82 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 82 | d6 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 82 | D6 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 82 | D7 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 82 | d9 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 82 | D9 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 82 | e1 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 82 | E1 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 82 | o4 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 82 | O4 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 82 | o7 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 82 | O7 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 82 | q0 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 82 | Q0 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 82 | q2 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 82 | Q2 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 82 | q3 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 82 | Q3 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 83 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 83 | 1 | 597 | Total O 597 597 | 3 | 0 |
| 83 | 2 | 154 | Total O 154 154 | 0 | 0 |
| 83 | 3 | 23 | Total O 23 23 | 0 | 0 |
| 83 | 4 | 7 | Total O 7 7 | 0 | 0 |
| 83 | 5 | 556 | Total O 556 556 | 0 | 0 |
| 83 | 6 | 204 | Total O 204 204 | 0 | 0 |
| 83 | 7 | 19 | Total O 19 19 | 0 | 0 |
| 83 | 8 | 10 | Total O 10 10 | 0 | 0 |
| 83 | C3 | 2 | Total O 2 2 | 0 | 0 |
| 83 | C4 | 1 | Total O 1 1 | 0 | 0 |
| 83 | c4 | 1 | Total O 1 1 | 0 | 0 |
| 83 | C6 | 1 | Total O 1 1 | 0 | 0 |
| 83 | c6 | 1 | Total O 1 1 | 0 | 0 |
| 83 | C7 | 1 | Total O 1 1 | 0 | 0 |
| 83 | c8 | 1 | Total O 1 1 | 0 | 0 |
| 83 | C9 | 3 | Total O 3 3 | 0 | 0 |
| 83 | c9 | 4 | Total O 4 4 | 0 | 0 |
| 83 | D0 | 1 | Total O 1 1 | 0 | 0 |
| 83 | d3 | 1 | Total O 1 1 | 0 | 0 |
| 83 | D3 | 2 | Total O 2 2 | 0 | 0 |
| 83 | d6 | 3 | Total O 3 3 | 0 | 0 |
| 83 | D6 | 1 | Total O 1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 83 | d9 | 2 | Total O 2 2 | 0 | 0 |
| 83 | l2 | 4 | Total O 4 4 | 0 | 0 |
| 83 | L2 | 3 | Total O 3 3 | 0 | 0 |
| 83 | l3 | 4 | Total O 4 4 | 0 | 0 |
| 83 | L3 | 1 | Total O 1 1 | 0 | 0 |
| 83 | l4 | 3 | Total O 3 3 | 0 | 0 |
| 83 | L4 | 1 | Total O 1 1 | 0 | 0 |
| 83 | l5 | 3 | Total O 3 3 | 0 | 0 |
| 83 | L5 | 2 | Total O 2 2 | 0 | 0 |
| 83 | l9 | 2 | Total O 2 2 | 0 | 0 |
| 83 | M0 | 2 | Total O 2 2 | 0 | 0 |
| 83 | M3 | 3 | Total O 3 3 | 0 | 0 |
| 83 | m5 | 3 | Total O 3 3 | 0 | 0 |
| 83 | M5 | 1 | Total O 1 1 | 0 | 0 |
| 83 | M6 | 3 | Total O 3 3 | 0 | 0 |
| 83 | m7 | 3 | Total O 3 3 | 0 | 0 |
| 83 | M7 | 4 | Total O 4 4 | 0 | 0 |
| 83 | m8 | 1 | Total O 1 1 | 0 | 0 |
| 83 | m9 | 5 | Total O 5 5 | 0 | 0 |
| 83 | M9 | 2 | Total O 2 2 | 0 | 0 |
| 83 | n1 | 2 | Total O 2 2 | 0 | 0 |

Continued on next page...

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 83 | N1 | 3 | Total O 3 3 | 0 | 0 |
| 83 | n3 | 3 | Total O 3 3 | 0 | 0 |
| 83 | N3 | 3 | Total O 3 3 | 0 | 0 |
| 83 | N5 | 1 | Total O 1 1 | 0 | 0 |
| 83 | N6 | 3 | Total O 3 3 | 0 | 0 |
| 83 | n8 | 3 | Total O 3 3 | 0 | 0 |
| 83 | N8 | 1 | Total O 1 1 | 0 | 0 |
| 83 | o1 | 3 | Total O 3 3 | 0 | 0 |
| 83 | O1 | 5 | Total O 5 5 | 0 | 0 |
| 83 | o2 | 5 | Total O 5 5 | 0 | 0 |
| 83 | O2 | 3 | Total O 3 3 | 0 | 0 |
| 83 | o4 | 4 | Total O 4 4 | 0 | 0 |
| 83 | O4 | 1 | Total O 1 1 | 0 | 0 |
| 83 | O5 | 1 | Total O 1 1 | 0 | 0 |
| 83 | o6 | 3 | Total O 3 3 | 0 | 0 |
| 83 | o7 | 1 | Total O 1 1 | 0 | 0 |
| 83 | O7 | 4 | Total O 4 4 | 0 | 0 |
| 83 | O9 | 2 | Total O 2 2 | 0 | 0 |
| 83 | q0 | 1 | Total O 1 1 | 0 | 0 |
| 83 | q2 | 1 | Total O 1 1 | 0 | 0 |
| 83 | Q2 | 1 | Total O 1 1 | 0 | 0 |

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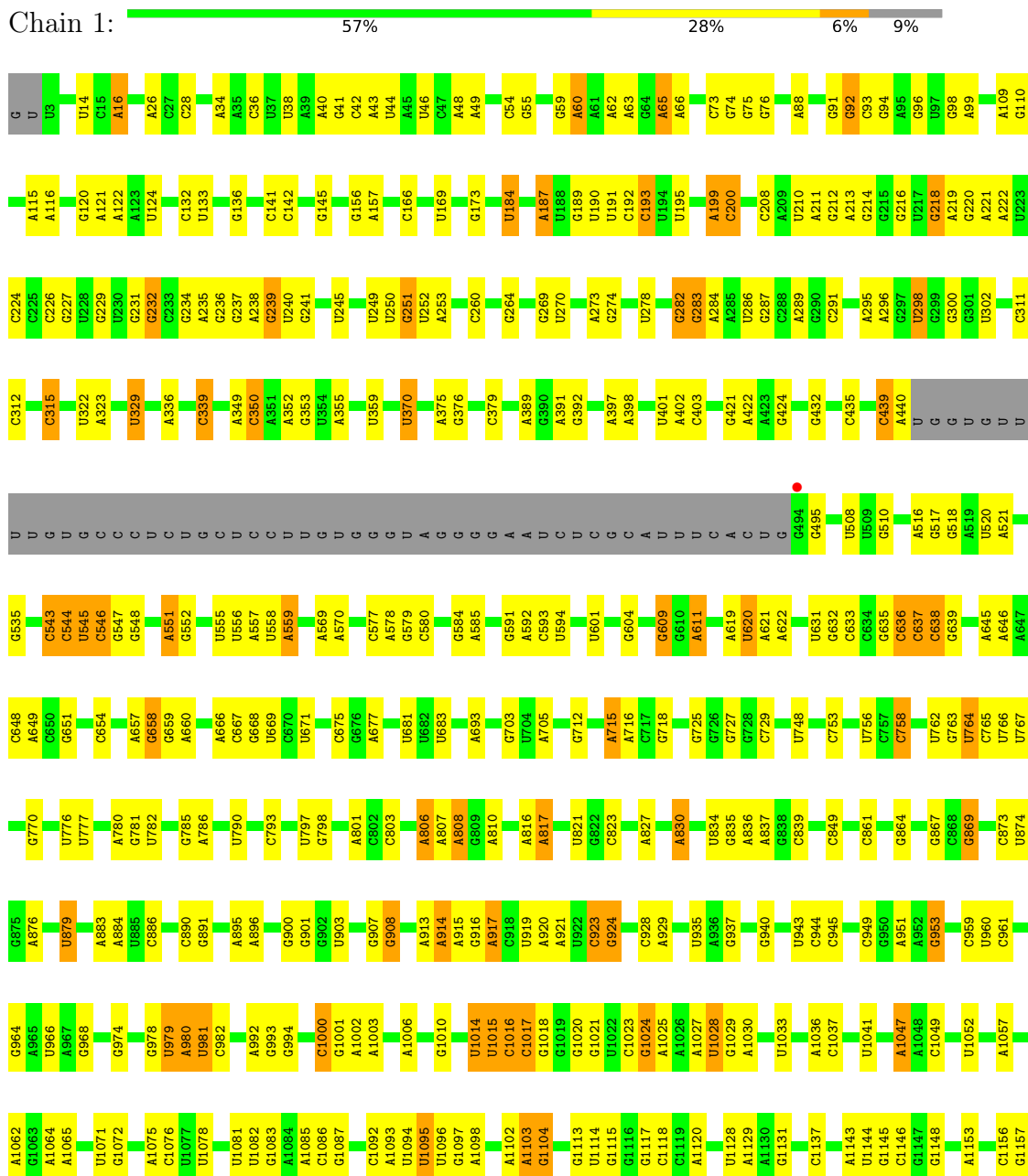
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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|------------|--------------|-----------------|----------------|----------------|----------------|
| 83 | S6 | 1 | Total O 1 1 | 0 | 0 |
| 83 | S9 | 1 | Total O 1 1 | 0 | 0 |
| 83 | sM | 3 | Total O 3 3 | 0 | 0 |
| 83 | SM | 1 | Total O 1 1 | 0 | 0 |

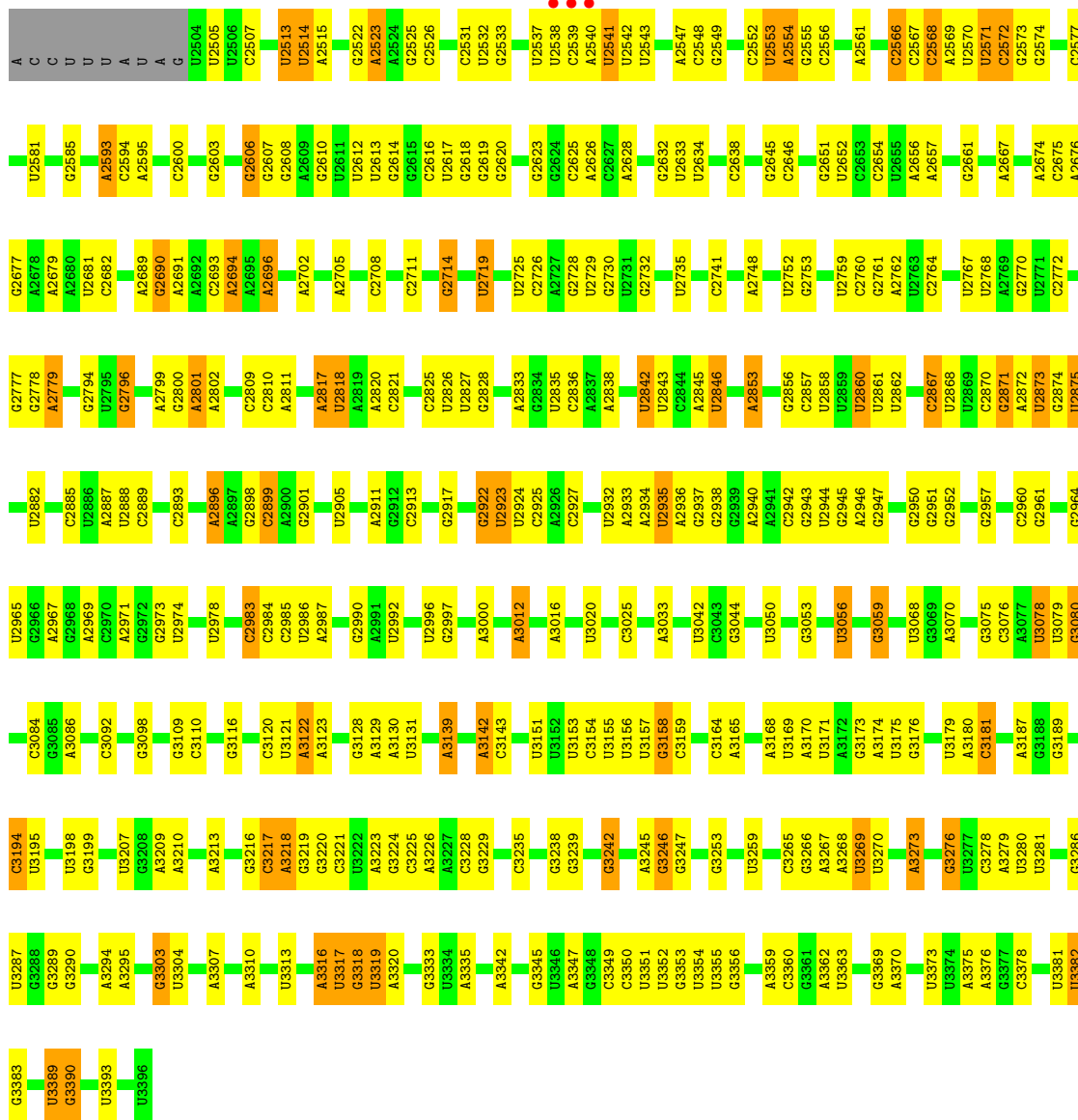
3 Residue-property plots

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

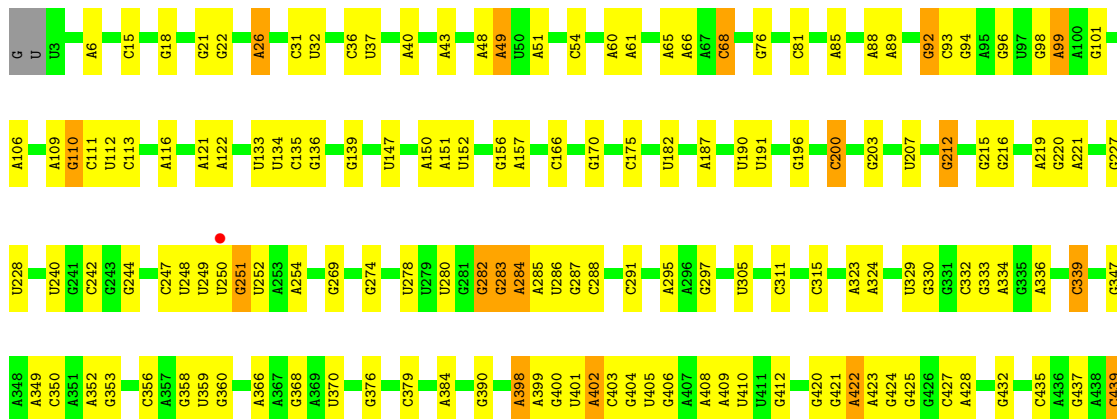
- Molecule 1: 25S ribosomal RNA



| | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| U2491 | U2334 | U2209 | G2110 | G1898 | G1796 | G1644 | U1564 | G1486 | C1316 | A1158 |
| C2422 | G2356 | G2210 | G2111 | G1899 | A1797 | U1645 | G1565 | G1486 | A1317 | A1169 |
| U2423 | U2336 | U2211 | U2211 | G1906 | A1800 | A1654 | A1566 | G1487 | G1487 | C1160 |
| A2424 | C2337 | C2212 | U2112 | C1907 | U1801 | A1655 | U1567 | G1488 | G1319 | G1161 |
| G2425 | C2337 | C2212 | A2113 | U1908 | U1801 | A1656 | U1568 | A1489 | A | A |
| G2435 | U2340 | A2222 | C2114 | A1909 | G1808 | C1657 | U1570 | A1490 | U1322 | G1166 |
| G2436 | A2348 | U2225 | A2120 | A1910 | A1809 | G1662 | A1571 | G1493 | U1324 | A1169 |
| G2437 | U2351 | U2226 | G2121 | A1911 | A1810 | C1663 | U1572 | U1494 | U1325 | G |
| C2444 | A2352 | A2227 | G2122 | U1912 | A1814 | C1664 | C1574 | U1495 | U1326 | G1174 |
| A | U2353 | A2228 | A2125 | A1913 | U1815 | C1664 | C1574 | U1496 | A1326 | G1175 |
| A | C2354 | C2237 | U2127 | A1914 | U1816 | C1665 | A1575 | C1497 | U1328 | G1176 |
| G | G2355 | U2127 | U | U1916 | G1817 | G1677 | G1577 | A1503 | A1330 | G1177 |
| G | A2358 | G2240 | U | U1818 | U1818 | A1683 | C1578 | G1507 | C1338 | A1179 |
| G | C2359 | U2241 | U | U1819 | U1819 | A1683 | C1579 | C1507 | C1339 | A1180 |
| G | C2360 | A2244 | U | U1820 | A1820 | U1687 | A1580 | C1508 | U1181 | U1181 |
| U | A2361 | C2245 | U | U1821 | U1821 | U1687 | C1582 | A1418 | A1182 | A1182 |
| U | C2362 | G2246 | U | A1835 | A1835 | A1699 | A1583 | A1419 | A | A |
| U | A2363 | C2247 | U | G1838 | U1702 | A1699 | G1586 | A1422 | C1342 | U1191 |
| G | C2366 | C2248 | U | A1839 | A1587 | U1702 | A1587 | G1422 | G1345 | C1192 |
| A | A2372 | U2140 | U | U1840 | U1588 | U1716 | A1588 | C1423 | A | A1193 |
| A | A2373 | U2141 | U | A1841 | A1589 | U1717 | A1589 | C1424 | U | G1194 |
| A | C2374 | A2142 | U | A1842 | A1593 | U1720 | A1593 | A1428 | G | C1196 |
| U | C2375 | A2144 | U | G1845 | A1594 | U1720 | A1594 | A1428 | A | A1197 |
| U | A2255 | A2147 | U | A1594 | U1595 | U1724 | U1595 | C1432 | U | C1201 |
| U | G2376 | A2256 | U | A1595 | U1600 | C1725 | U1600 | A1433 | U | A1202 |
| A | C2377 | C2257 | U | U1601 | A1602 | C1725 | A1602 | A1434 | A | A1203 |
| G | C2378 | G2258 | U | G1603 | A1603 | A1729 | U1603 | A1435 | U | A1204 |
| G | U2379 | C2263 | U | A1604 | U1606 | A1729 | U1606 | A1436 | C | A1205 |
| G | U2380 | C2263 | U | A1605 | A1607 | A1750 | U1607 | A1437 | A | A1206 |
| G | G2381 | G2272 | U | C1606 | C1607 | A1751 | C1607 | C1437 | A | G1206 |
| G | G2382 | G2273 | U | U1609 | C1608 | G1751 | C1608 | U1443 | U | G1209 |
| G | C2383 | C2274 | U | G1610 | G1609 | C1759 | G1610 | G1444 | C | U1210 |
| G | A2384 | C2275 | U | C1614 | G1610 | A1759 | G1614 | G1445 | U | U1211 |
| U | G2385 | C2276 | U | U1620 | U1620 | C1762 | U1620 | A1446 | U | A1221 |
| U | C2389 | A2279 | U | U1625 | U1625 | U1764 | U1625 | A1447 | C | A1222 |
| U | A2280 | A2280 | U | A1625 | A1625 | U1764 | A1625 | A1449 | U | A1225 |
| U | A2281 | A2281 | U | U1629 | U1629 | U1766 | U1629 | G1450 | U | A1229 |
| G | A2390 | U2282 | U | A1632 | A1633 | U1766 | A1632 | C1451 | G | G |
| G | G2391 | G2283 | U | G1633 | G1633 | C1767 | G1633 | C1452 | U | A |
| C | C2392 | C2284 | U | G1635 | G1635 | U1768 | G1635 | A1453 | U | C |
| G | G2393 | C2284 | U | C1639 | C1639 | U1768 | C1639 | A1454 | U | G |
| C | A2397 | C2287 | U | G1640 | G1640 | G1769 | G1640 | A1467 | U | A |
| C | A2397 | G2288 | U | U1641 | U1641 | G1770 | U1641 | A1467 | U | A |
| A | G2400 | G2288 | U | U1642 | U1642 | G1770 | U1642 | A1467 | U | A |
| A | A2401 | U2298 | U | U1643 | U1643 | U1770 | U1643 | A1467 | U | A |
| U | A2402 | G2307 | U | U1644 | U1644 | G1775 | U1644 | A1467 | U | A |
| G | G2403 | U2186 | U | U1645 | U1645 | G1775 | U1645 | A1467 | U | A |
| A | A2404 | C2192 | U | U1646 | U1646 | G1775 | U1646 | A1467 | U | A |
| A | U2411 | G2201 | U | U1647 | U1647 | G1775 | U1647 | A1467 | U | A |
| A | U2411 | A2312 | U | U1648 | U1648 | G1775 | U1648 | A1467 | U | A |
| A | C2415 | U2205 | U | U1649 | U1649 | G1775 | U1649 | A1467 | U | A |
| C | C2415 | G2315 | U | U1650 | U1650 | G1775 | U1650 | A1467 | U | A |
| C | G2418 | A2206 | U | U1651 | U1651 | G1775 | U1651 | A1467 | U | A |
| A | A2419 | A2207 | U | U1652 | U1652 | G1775 | U1652 | A1467 | U | A |
| U | C2420 | A2208 | U | U1653 | U1653 | G1775 | U1653 | A1467 | U | A |

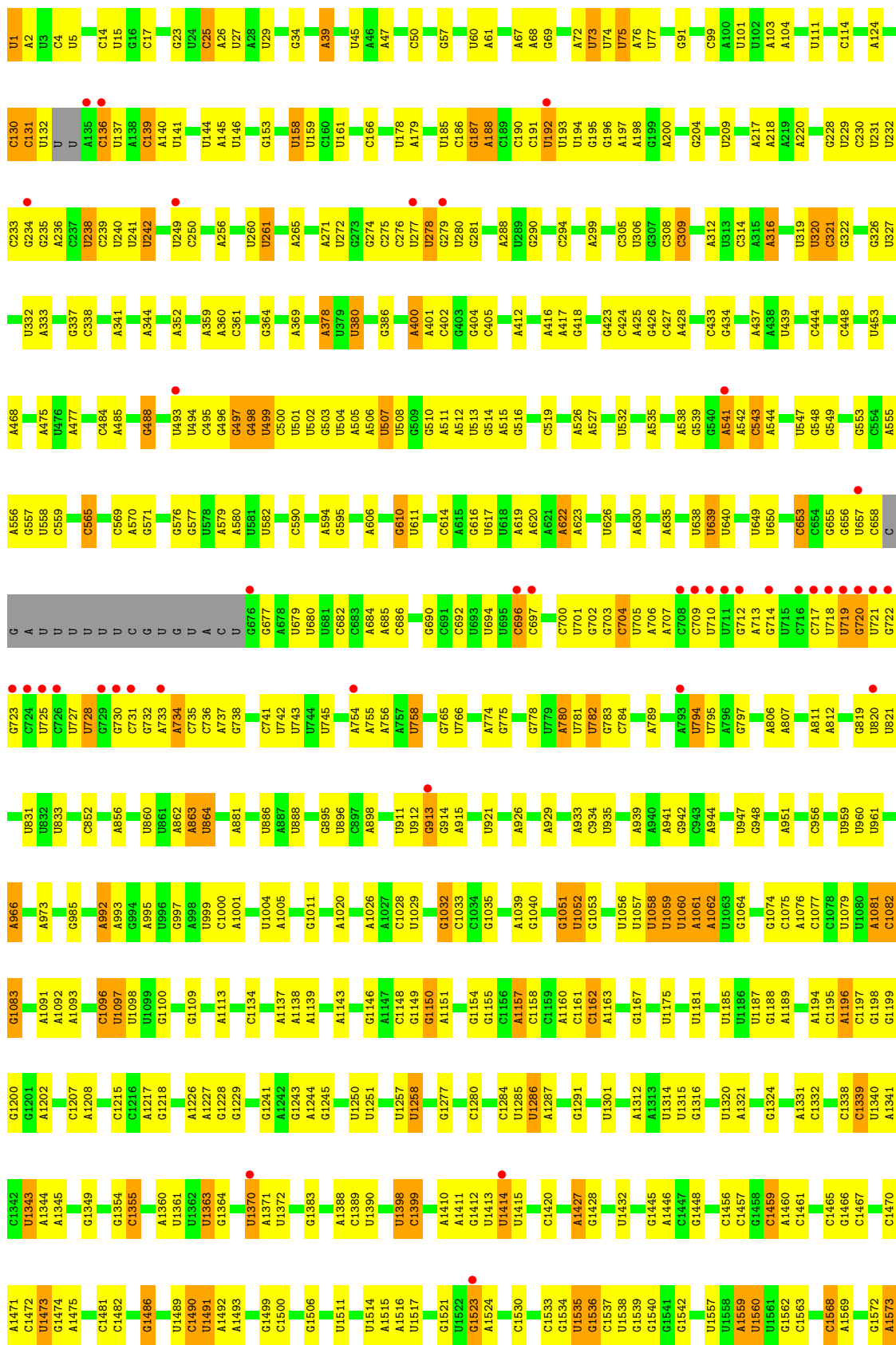


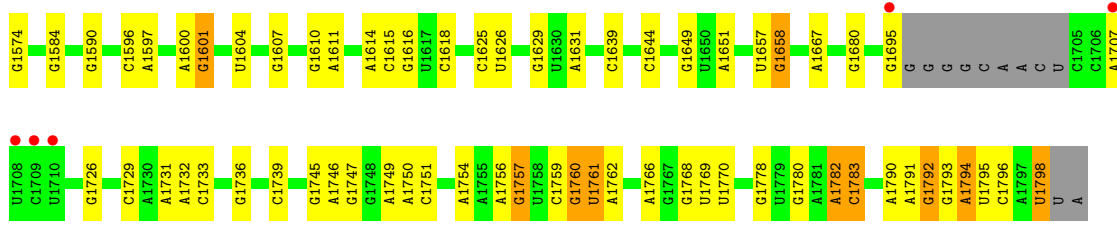
• Molecule 1: 25S ribosomal RNA



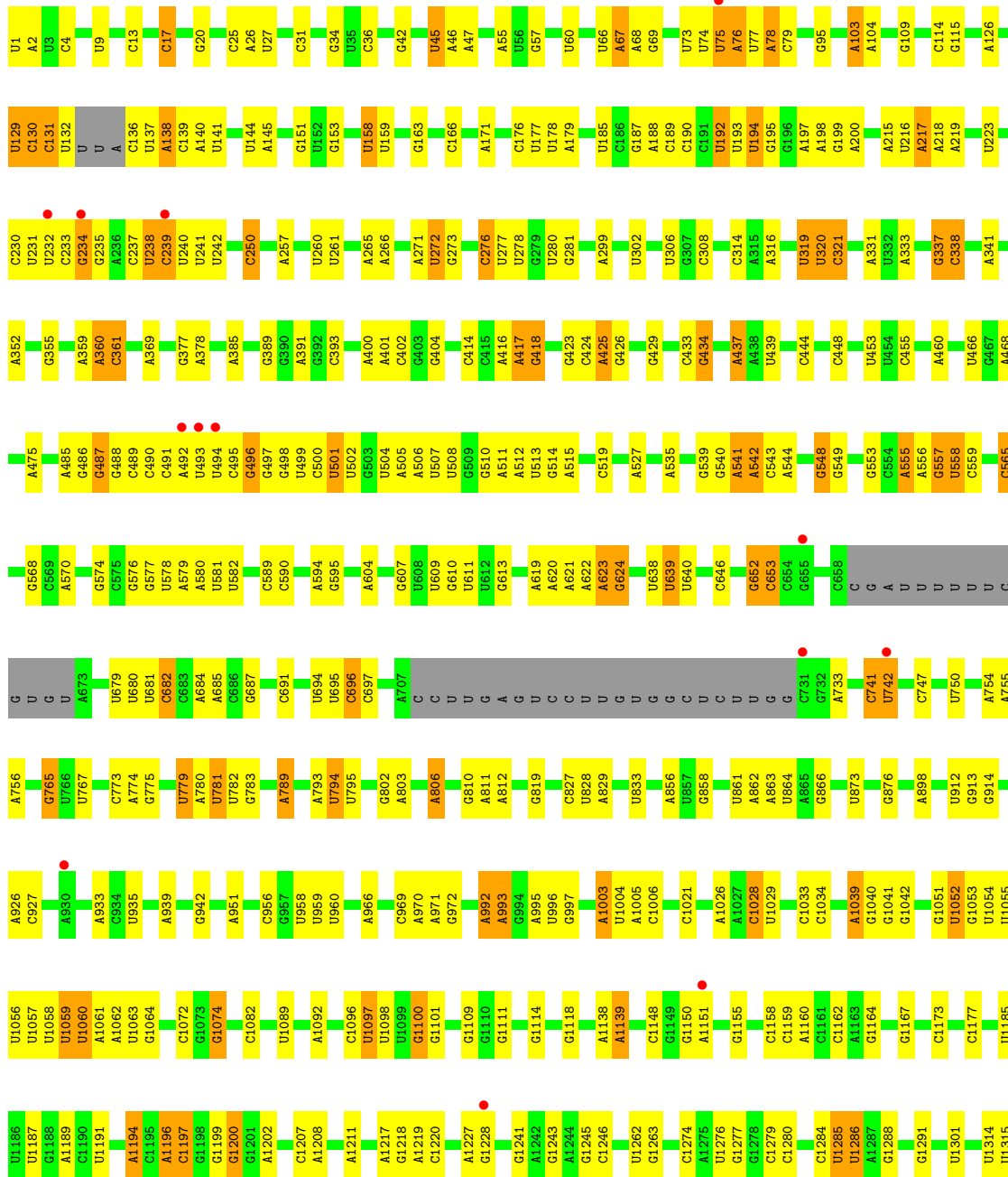
| | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|---|
| U3319 | U3320 | A3123 | G2990 | U2891 | A2813 | A2656 | G2549 | U2410 | A2326 | G2239 | G2110 | U |
| A3320 | G3221 | G3124 | G2993 | A2892 | G2814 | A2657 | U2850 | U2411 | G2330 | G2289 | G2111 | U |
| A3335 | G3224 | C3126 | G2994 | A2896 | G2815 | G2662 | U2852 | G2412 | C2331 | U2241 | U2112 | G |
| G3337 | C3228 | A3127 | U2995 | C2899 | A2817 | G2663 | C2555 | C2413 | A2332 | U2244 | A2113 | U |
| C3338 | G3229 | G3128 | U2996 | C2899 | U2818 | G2667 | G2555 | G2414 | G2333 | C2245 | G2121 | G |
| A3339 | G3230 | A3129 | G2997 | C2899 | U2819 | A2667 | C2566 | U2415 | U2334 | C2246 | G2122 | U |
| G3340 | U3231 | U3130 | C3004 | A2910 | C2821 | U2668 | C2567 | U2417 | G2335 | G2247 | G | |
| U3341 | G3235 | G3134 | A3008 | A2911 | U2822 | U2669 | C2568 | A2418 | A2345 | C2248 | A2131 | A |
| A3342 | G3236 | U3135 | G3008 | G2917 | G2823 | A2674 | U2569 | A2419 | G2346 | G2249 | C2132 | C |
| G3343 | G3239 | G3136 | G3022 | U2920 | U2824 | G2677 | U2570 | C2420 | U2347 | G2251 | G | |
| U3351 | A3243 | C3137 | C3039 | U2923 | U2827 | C2682 | C2572 | U2421 | A2348 | A2252 | C | |
| U3352 | A3244 | A3142 | G3059 | U2923 | G2830 | U2683 | G2573 | U2427 | G2355 | U2253 | C | |
| G3353 | A3245 | C3143 | C3043 | C2927 | G2831 | U2683 | G2574 | A2430 | G2355 | U2254 | C | |
| U3354 | G3246 | G3144 | C3047 | C2928 | U2832 | A2689 | G2575 | C2431 | A2255 | A2256 | U | |
| U3355 | G3247 | U3047 | C3049 | C2929 | A2837 | G2690 | G2584 | U2433 | C2359 | C2257 | U | |
| G3356 | G3248 | A3048 | A3049 | U2932 | G2840 | A2691 | G2585 | U2434 | C2362 | U2258 | U | |
| U3362 | G3252 | U3151 | A3052 | U2933 | G2841 | A2694 | G2589 | G2435 | A2363 | A2259 | A | |
| U3363 | G3253 | U3152 | G3052 | A2933 | U2842 | A2695 | U2593 | U2436 | G2364 | U2260 | G | |
| U3365 | G3259 | C3154 | G3053 | A2934 | A2845 | A2696 | A2593 | G2437 | C2365 | G2157 | G | |
| G3366 | G3260 | U3155 | U3056 | U2935 | U2846 | G2714 | C2594 | A2438 | C2366 | U2159 | C | |
| G3369 | G3261 | U3157 | G3059 | C2942 | A2847 | A2715 | G2598 | A2439 | G2371 | U2160 | U | |
| C3378 | G3266 | G3158 | G3059 | C2943 | G2848 | A2716 | U2599 | C2440 | A2372 | G2272 | C | |
| U3382 | A3267 | A3170 | G3062 | U2944 | C2849 | A2717 | U2599 | G2442 | A2373 | G2273 | C | |
| G3383 | A3268 | U3171 | C3063 | U2944 | U2852 | U2727 | G2600 | A | A2374 | U2170 | U | |
| G3386 | U3269 | A3172 | G3069 | C2948 | A2856 | A2728 | A2601 | A | G2375 | U2176 | G | |
| U3387 | U3270 | G3173 | G3075 | U2949 | G2857 | A2729 | A2609 | U | G2376 | U2177 | U | |
| U3388 | G3271 | A3174 | C3076 | U2950 | C2857 | U2729 | A2609 | G | U2379 | A2280 | A | |
| U3389 | C3272 | U3175 | G3077 | G2951 | U2858 | U2737 | U2610 | A | G2380 | U2282 | G | |
| U3394 | A3273 | G3176 | A3077 | G2952 | U2859 | U2752 | U2611 | G | G2381 | G2283 | A | |
| G3395 | A3274 | U3179 | U3078 | U2953 | U2861 | G2752 | U2612 | U | G2382 | C2284 | C | |
| G3396 | U3275 | A3180 | U3079 | U2954 | U2862 | G2753 | U2613 | G | G2383 | U2285 | G | |
| U3397 | U3277 | C3181 | G3080 | U2957 | U2862 | A2762 | U2614 | U | G2386 | C2287 | C | |
| U3398 | C3278 | A3187 | A3086 | C2957 | U2866 | A2762 | U2617 | A | A2388 | G2288 | C | |
| U3399 | U3280 | U3196 | A3087 | G2964 | C2867 | U2771 | G2618 | U | A2390 | U2298 | U | |
| U3400 | U3281 | G3197 | G3088 | U2965 | U2868 | C2772 | A2619 | G | G2393 | U2305 | G | |
| C3285 | C3286 | U3198 | C3089 | G2968 | C2870 | C2773 | G2620 | A | G2394 | G2306 | G | |
| A3294 | A3294 | U3199 | A3091 | G2968 | G2871 | G2778 | G2624 | U | G2395 | C2307 | C | |
| U3304 | U3304 | G3205 | C3092 | A2971 | U2873 | A2779 | A2626 | A | G2397 | U2209 | A | |
| A3307 | U3307 | G3206 | C3093 | A2976 | G2877 | G2796 | G2627 | G | A2398 | A2309 | C | |
| C3311 | C3311 | U3207 | C3099 | A2977 | G2878 | C2797 | A2628 | U | A2399 | U2310 | A | |
| A3316 | U3316 | G3208 | U3100 | G2977 | G2878 | C2798 | C2539 | G | G2400 | A2313 | A | |
| A3218 | G3218 | A3209 | G3101 | U2978 | C2881 | A2799 | A2540 | G | A2401 | U2314 | U | |
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| | | A3218 | A3122 | A2987 | A2889 | A2547 | C2546 | U | U2408 | A2229 | U | |
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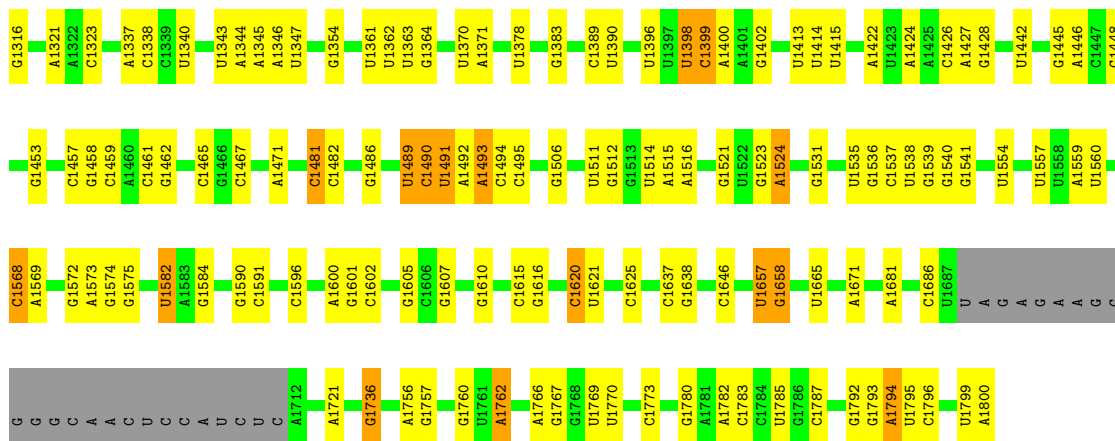
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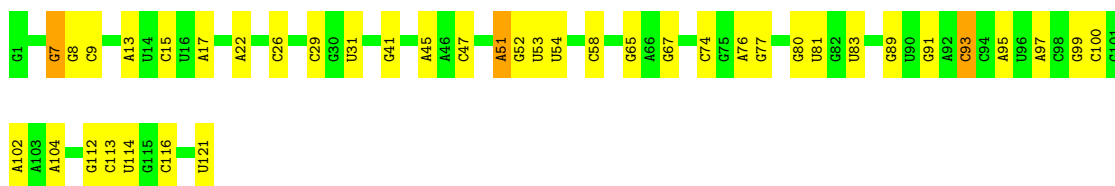


• Molecule 2: 18S ribosomal RNA

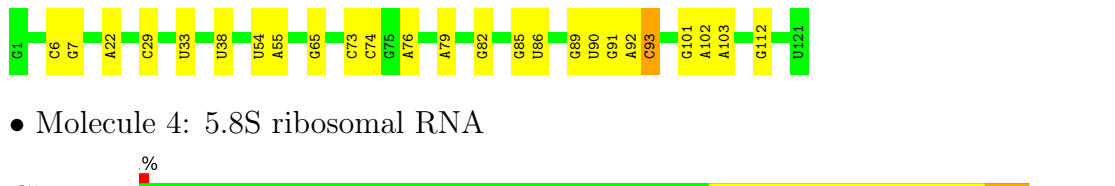
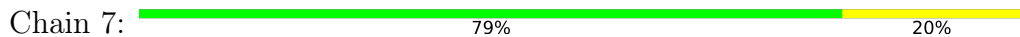




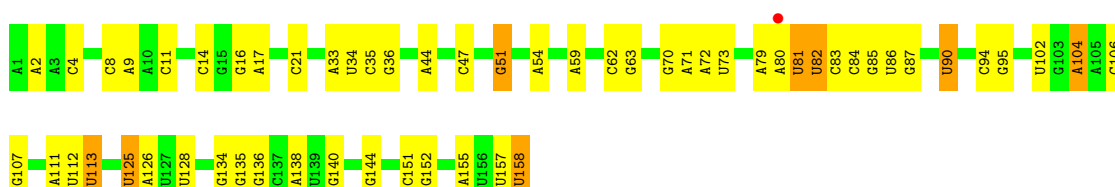
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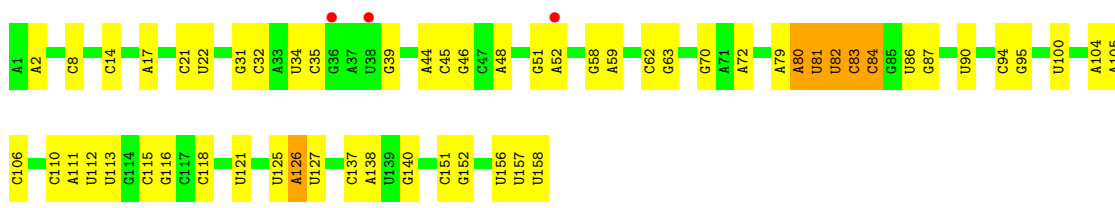
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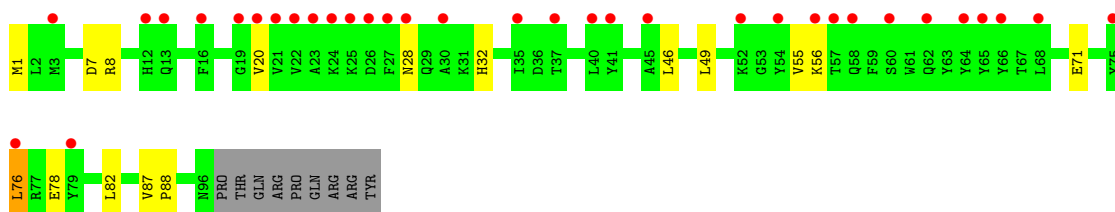
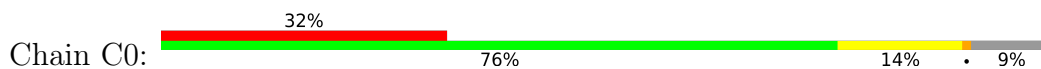
• Molecule 4: 5.8S ribosomal RNA



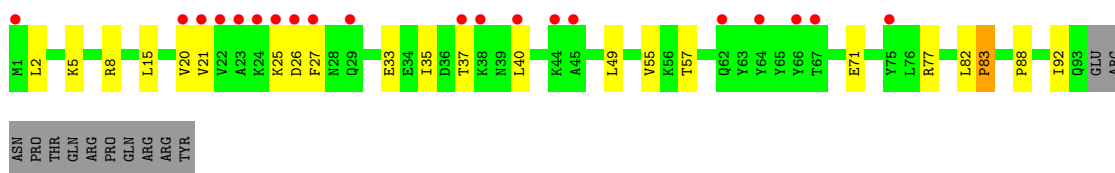
• Molecule 4: 5.8S ribosomal RNA



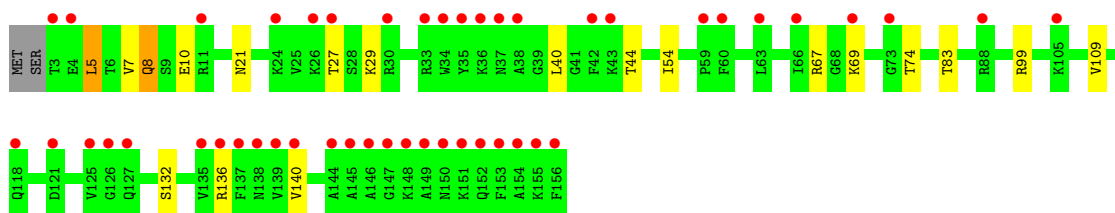
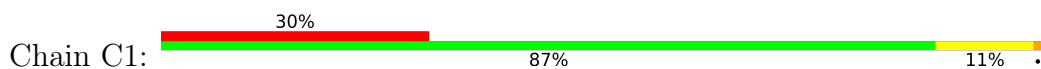
- Molecule 5: 40S ribosomal protein S10-A



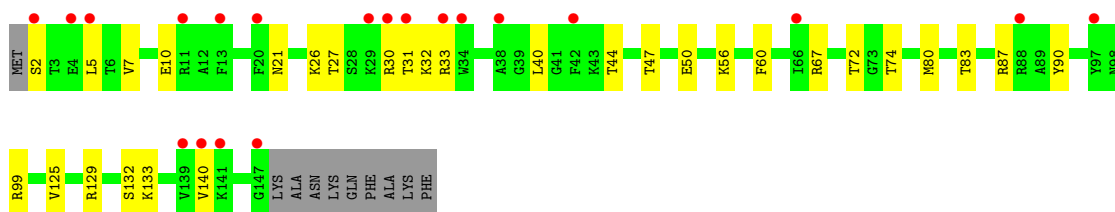
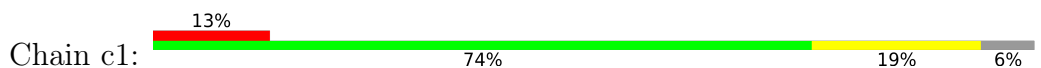
- Molecule 5: 40S ribosomal protein S10-A



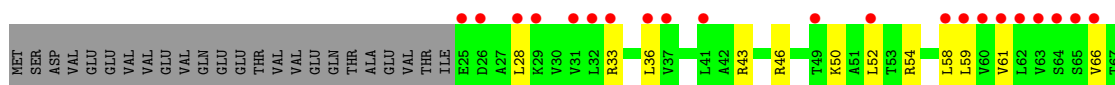
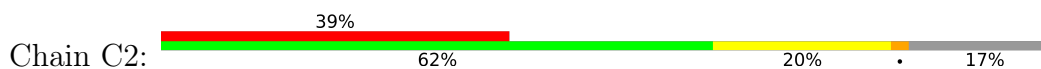
- Molecule 6: 40S ribosomal protein S11-A



- Molecule 6: 40S ribosomal protein S11-A

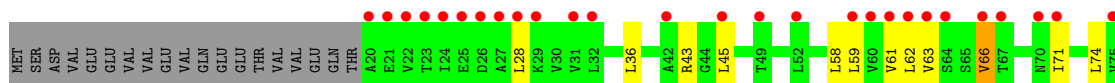
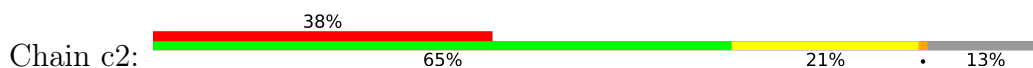


- Molecule 7: 40S ribosomal protein S12

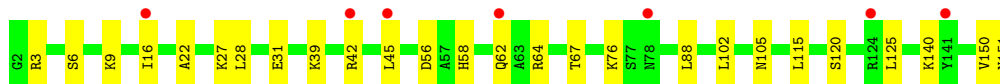
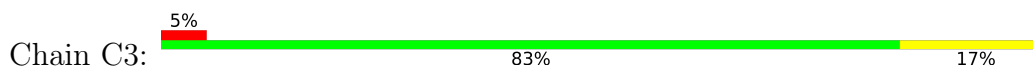




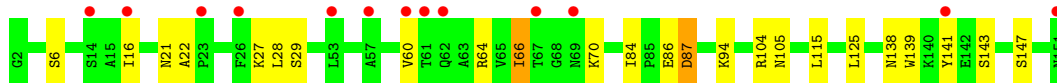
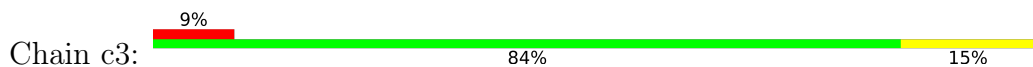
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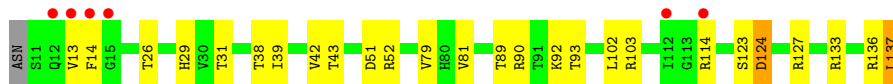
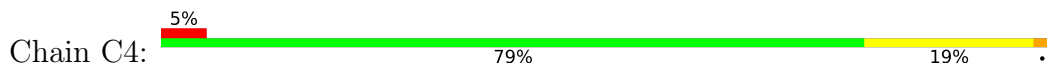
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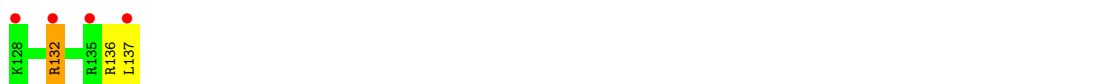
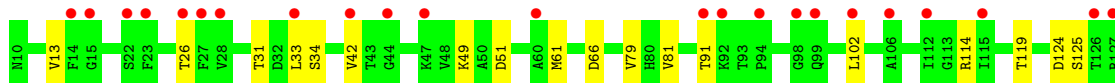
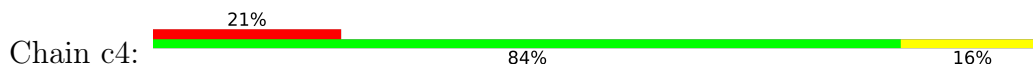
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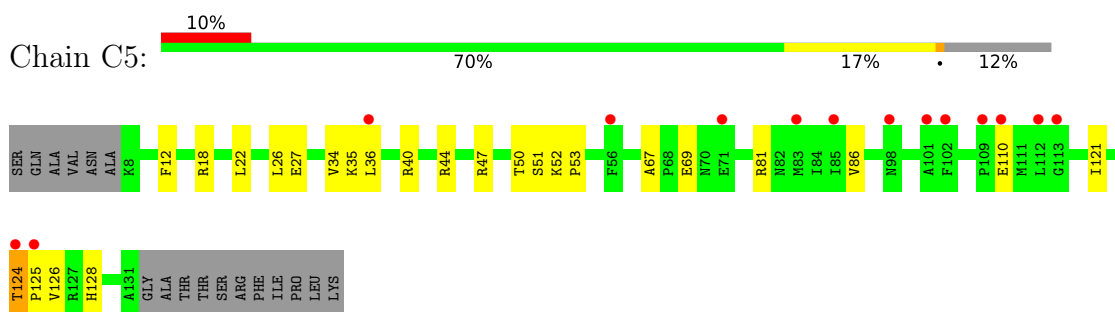
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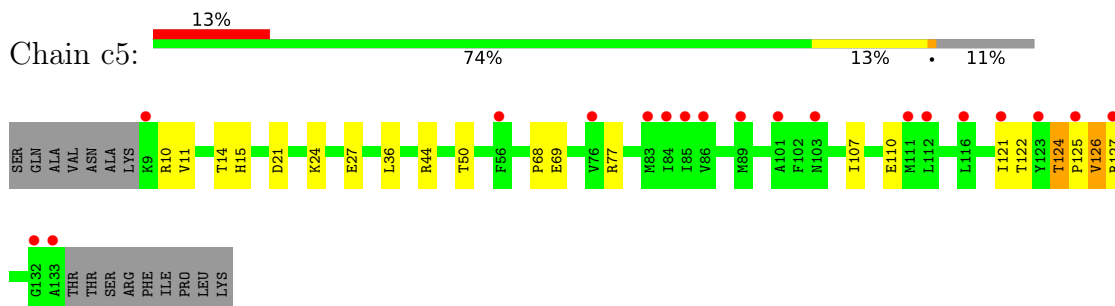
- Molecule 9: 40S ribosomal protein S14-B



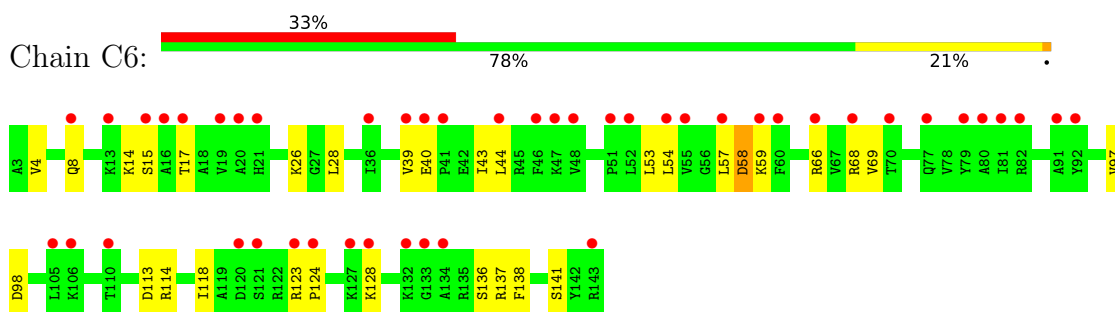
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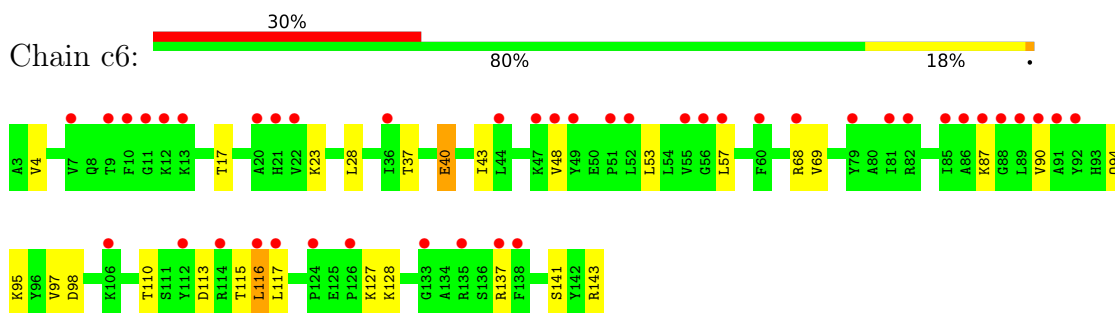
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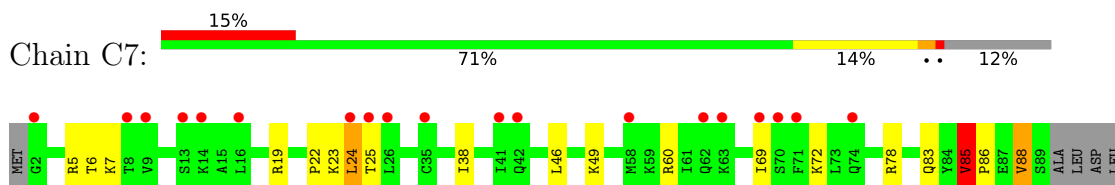
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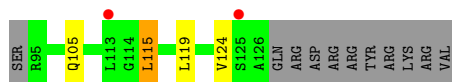


- Molecule 11: 40S ribosomal protein S16-A

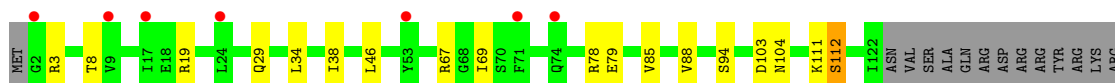
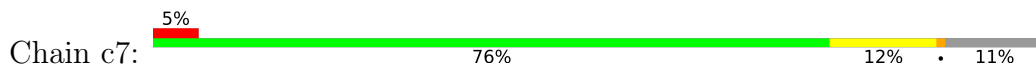


- Molecule 12: 40S ribosomal protein S17-A



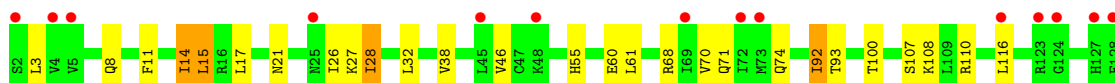
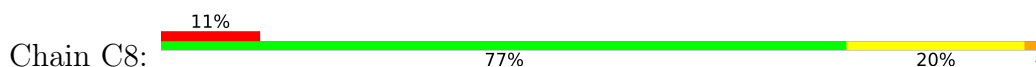


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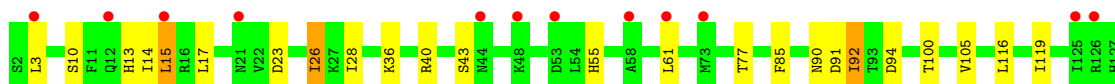
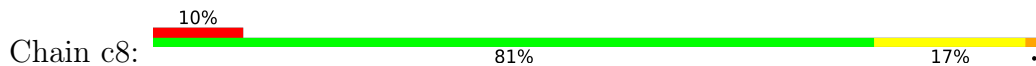


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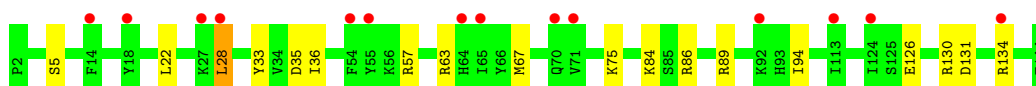
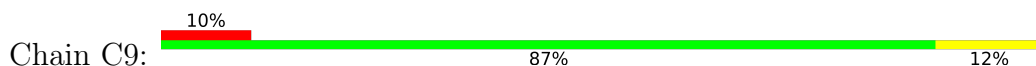
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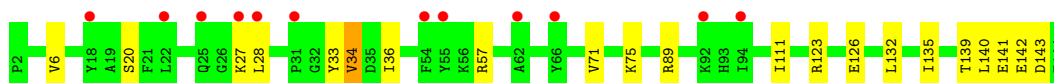
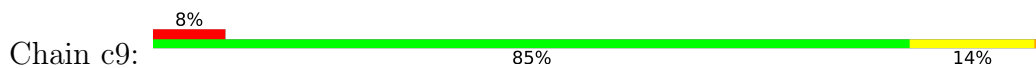
- Molecule 13: 40S ribosomal protein S18-A



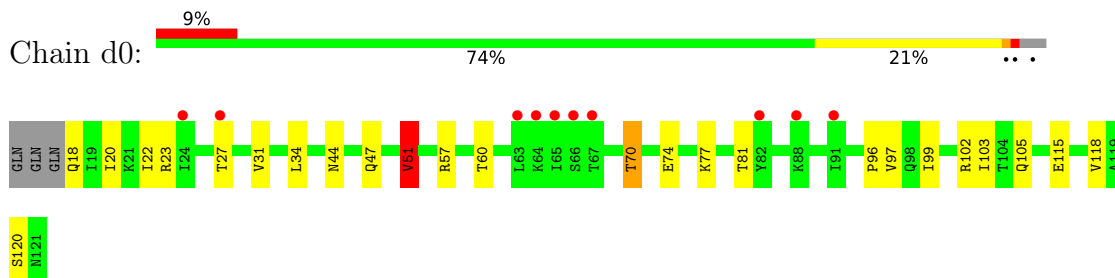
- Molecule 14: 40S ribosomal protein S19-A



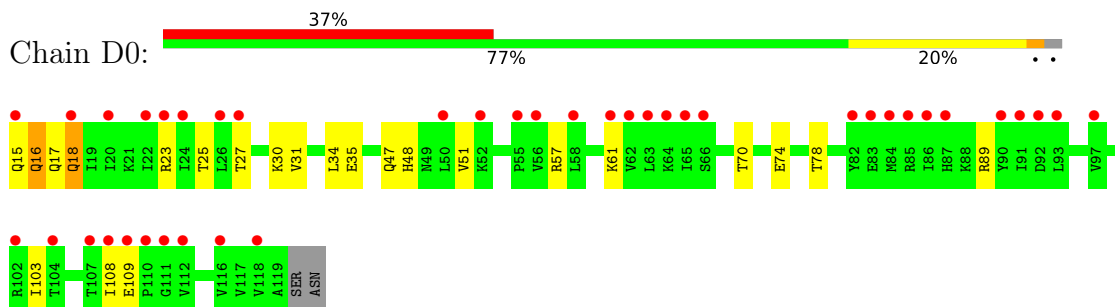
- Molecule 14: 40S ribosomal protein S19-A



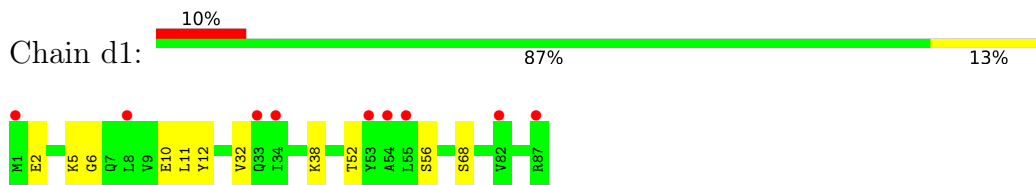
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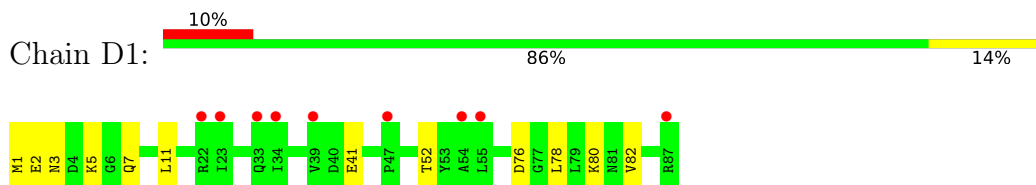
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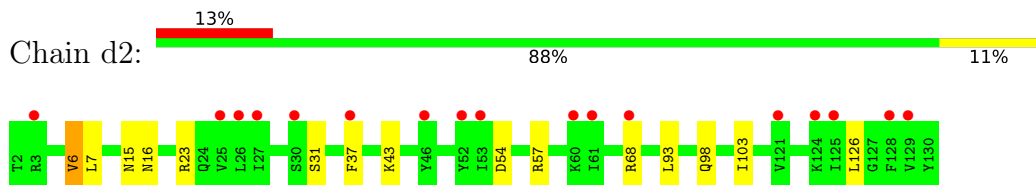
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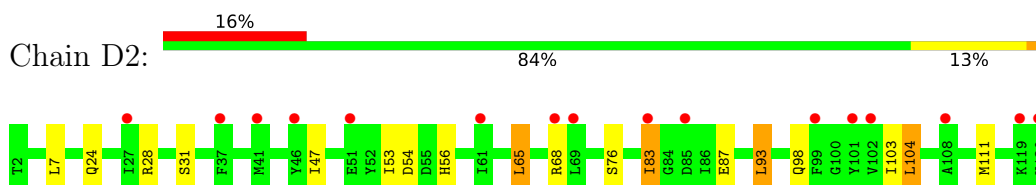
- Molecule 16: 40S ribosomal protein S21-A



- Molecule 17: 40S ribosomal protein S22-A

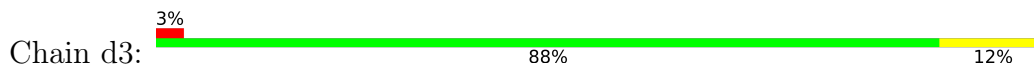


- Molecule 17: 40S ribosomal protein S22-A

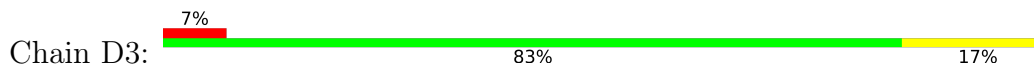




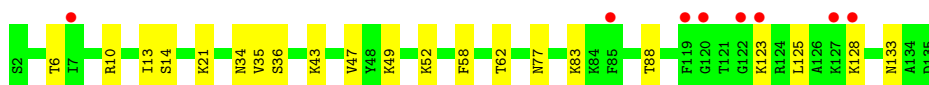
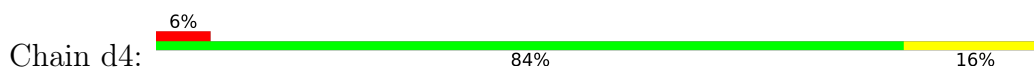
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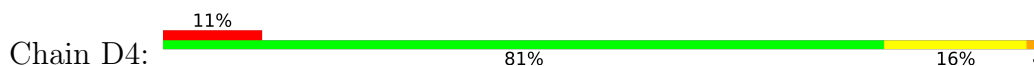
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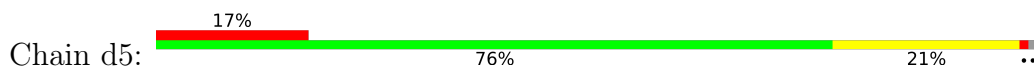
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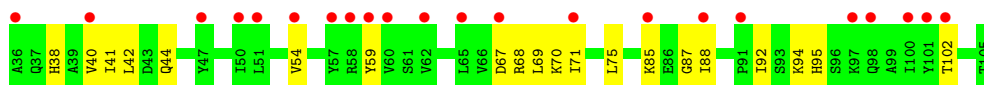
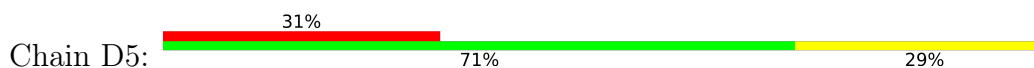
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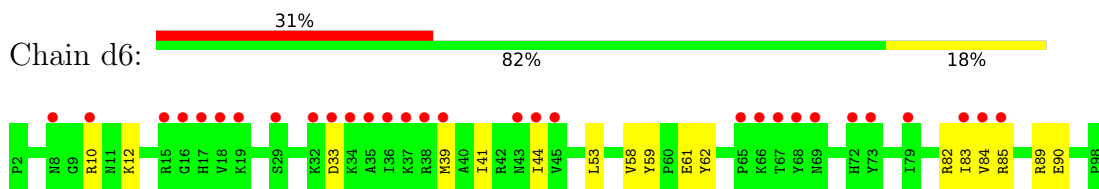
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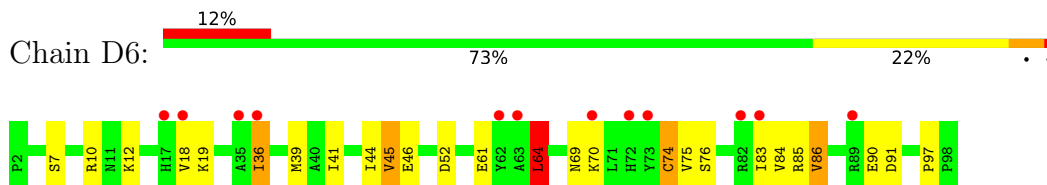
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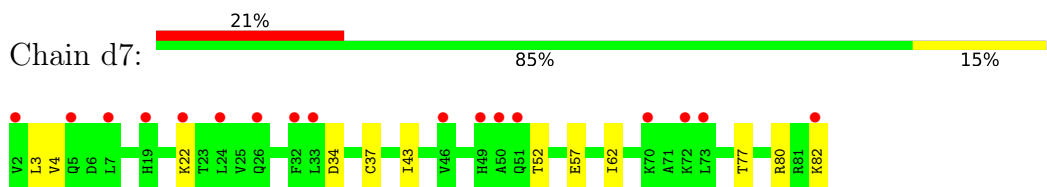
- Molecule 21: 40S ribosomal protein S26-B



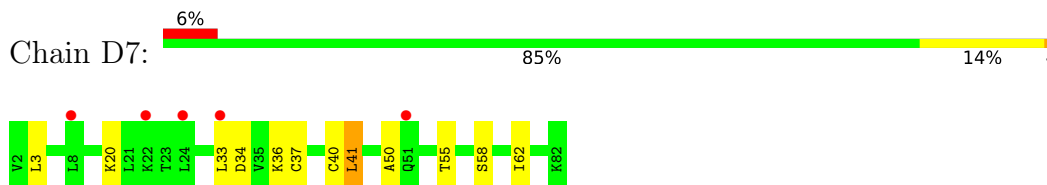
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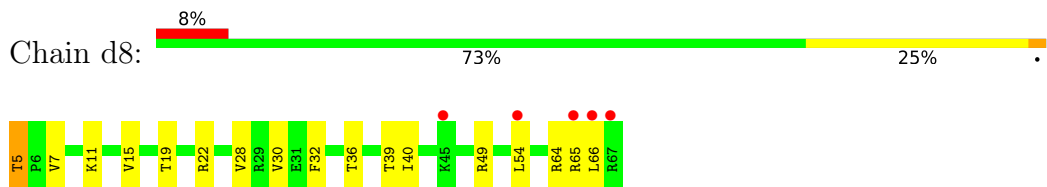
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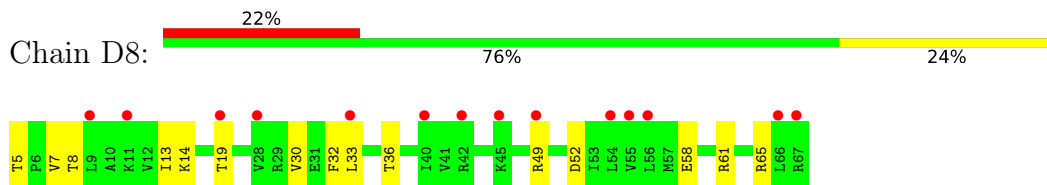
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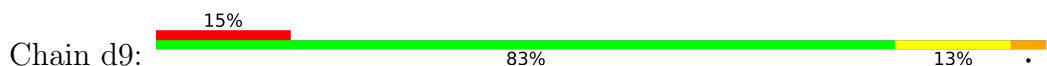
- Molecule 23: 40S ribosomal protein S28-A

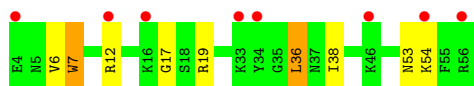


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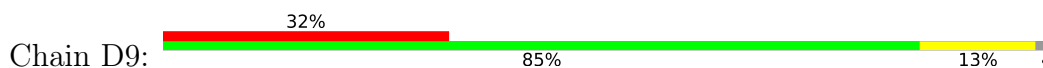


- Molecule 24: 40S ribosomal protein S29-A

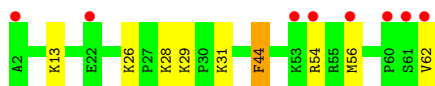
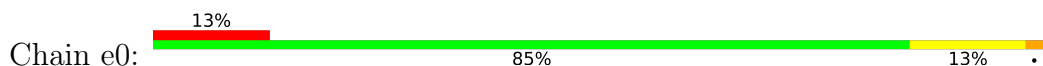




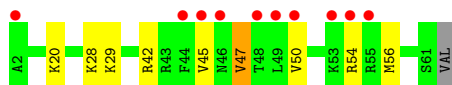
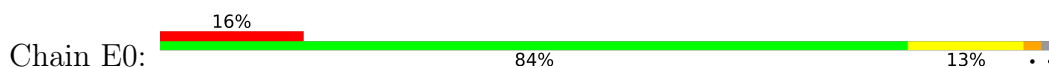
- Molecule 24: 40S ribosomal protein S29-A



- Molecule 25: 40S ribosomal protein S30-A



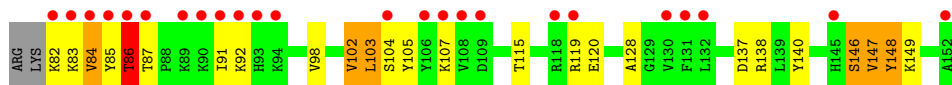
- Molecule 25: 40S ribosomal protein S30-A



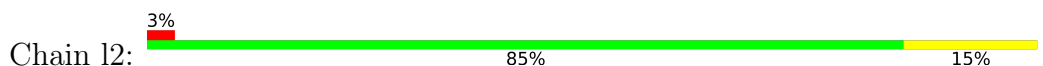
- Molecule 26: Ubiquitin-40S ribosomal protein S31

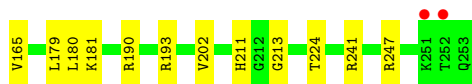


- Molecule 26: Ubiquitin-40S ribosomal protein S31

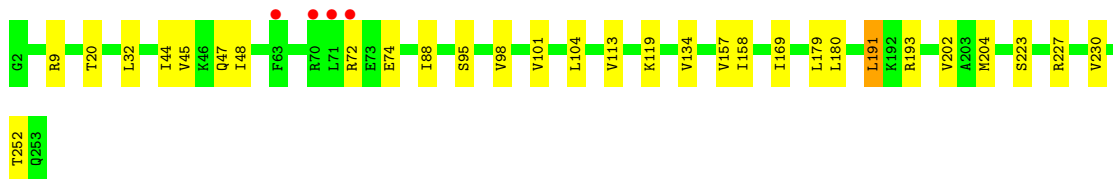
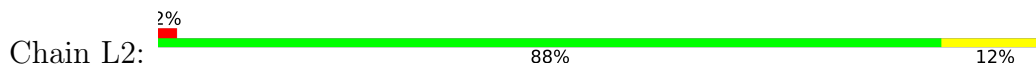


- Molecule 27: 60S ribosomal protein L2-A

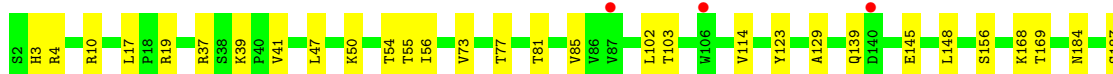
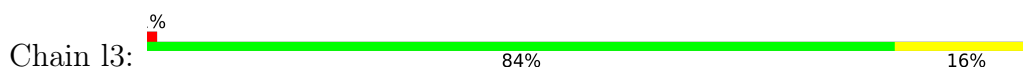




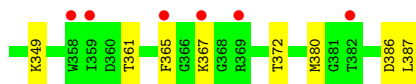
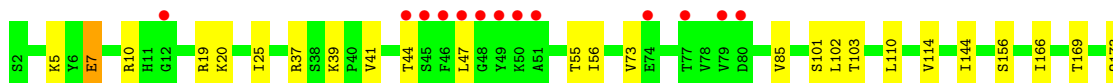
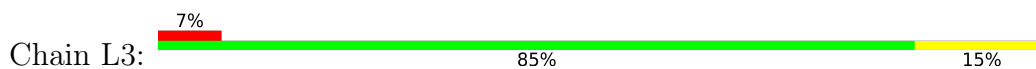
- Molecule 27: 60S ribosomal protein L2-A



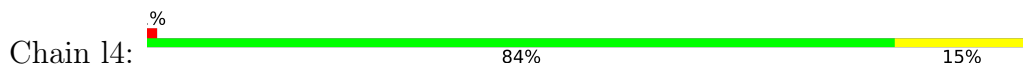
- Molecule 28: 60S ribosomal protein L3

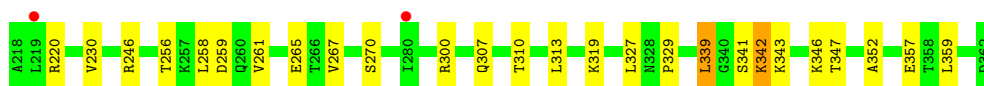


- Molecule 28: 60S ribosomal protein L3

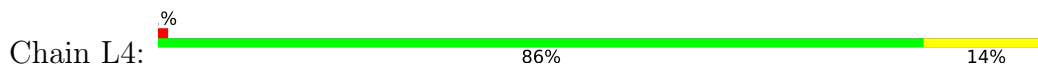


- Molecule 29: 60S ribosomal protein L4-A

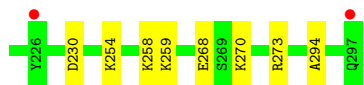
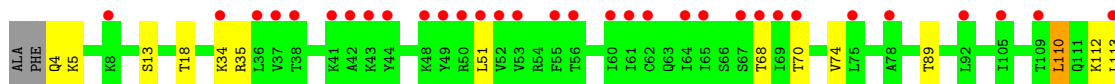
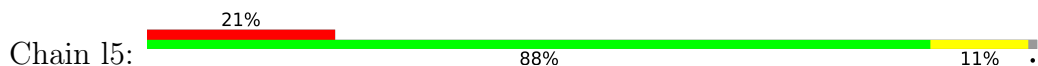




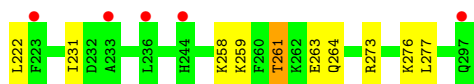
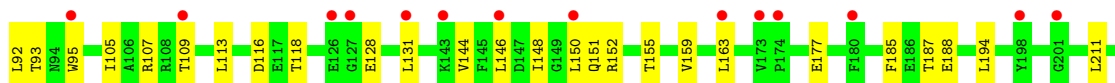
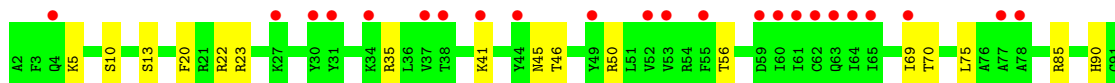
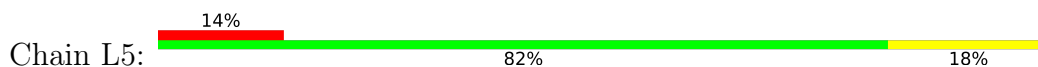
• Molecule 29: 60S ribosomal protein L4-A



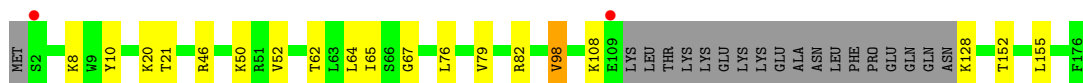
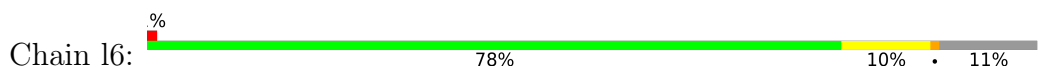
• Molecule 30: 60S ribosomal protein L5



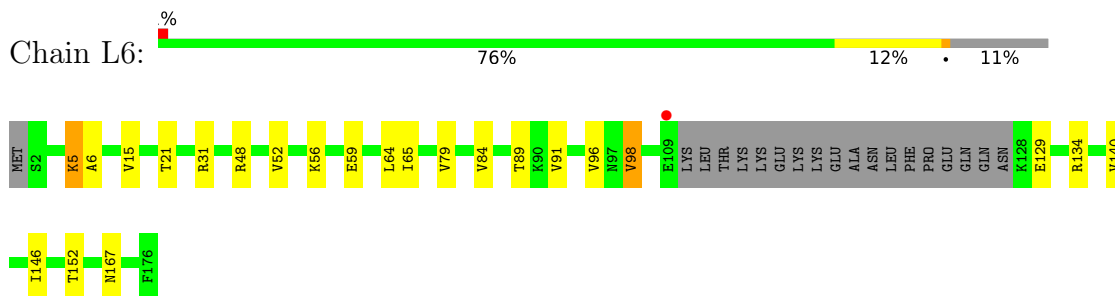
• Molecule 30: 60S ribosomal protein L5



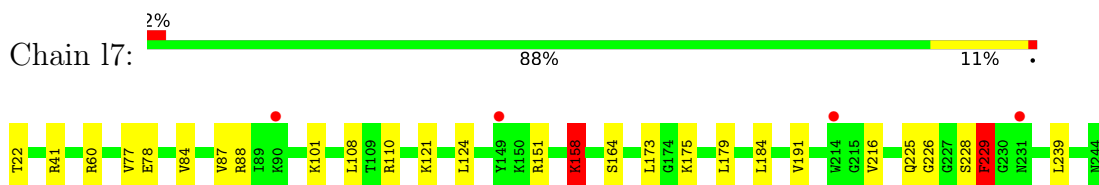
• Molecule 31: 60S ribosomal protein L6-A



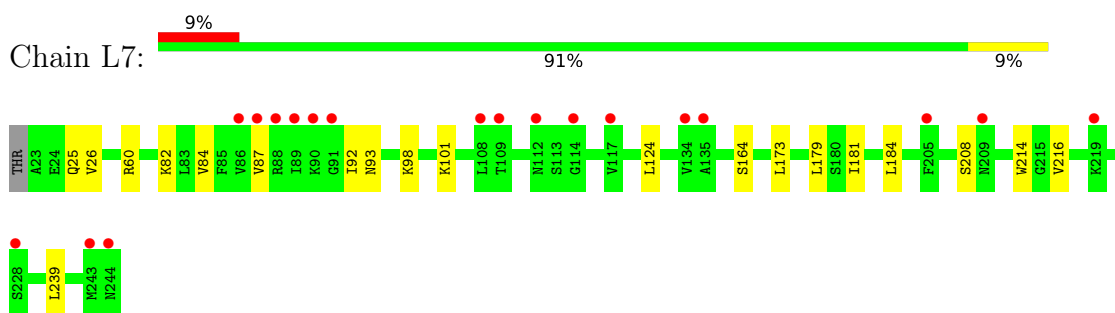
- Molecule 31: 60S ribosomal protein L6-A



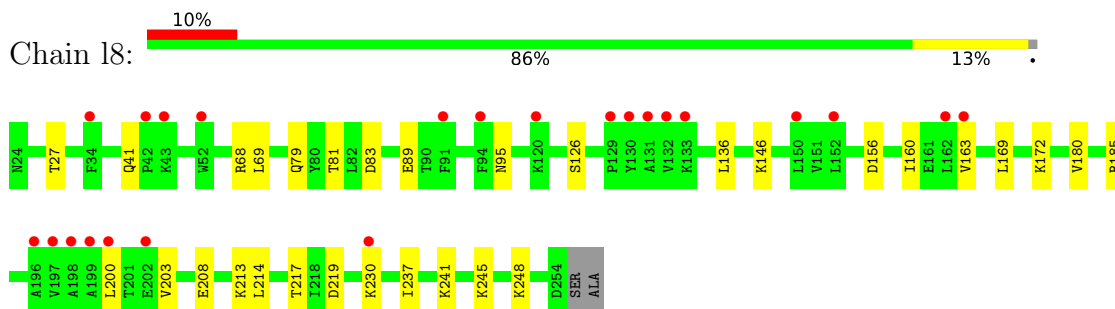
- Molecule 32: 60S ribosomal protein L7-A



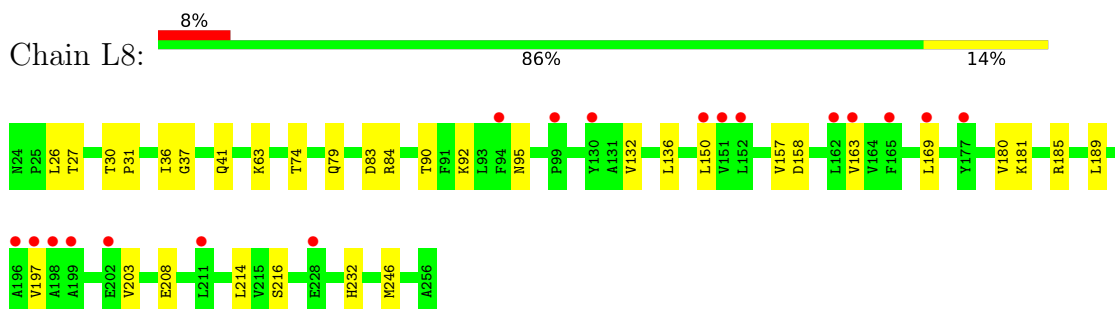
- Molecule 32: 60S ribosomal protein L7-A



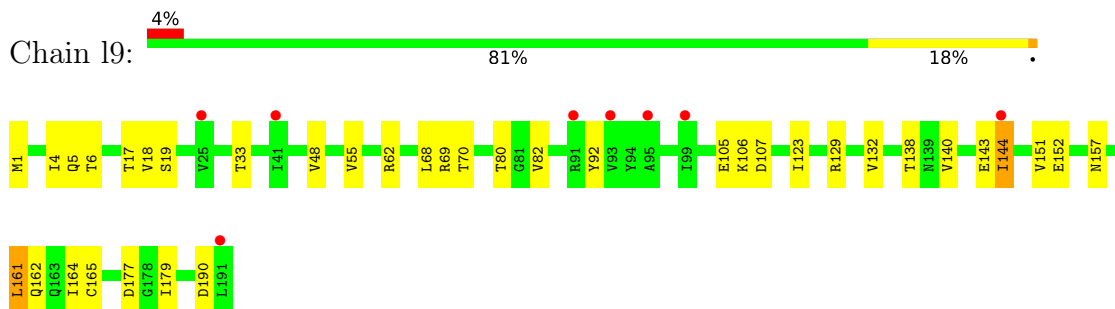
- Molecule 33: 60S ribosomal protein L8-A



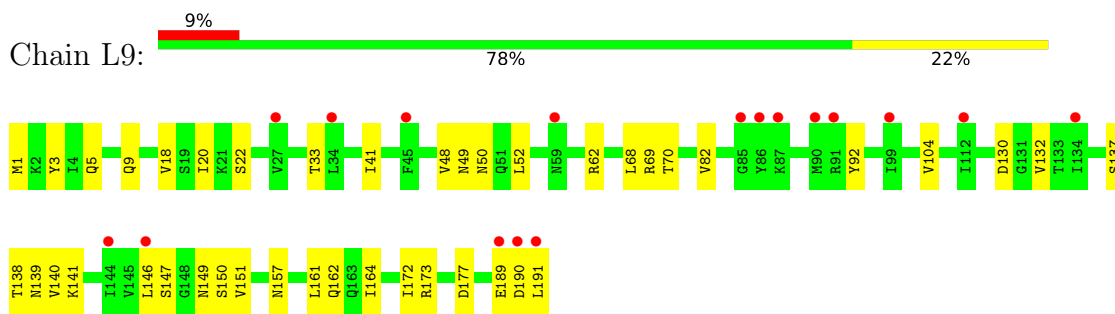
- Molecule 33: 60S ribosomal protein L8-A



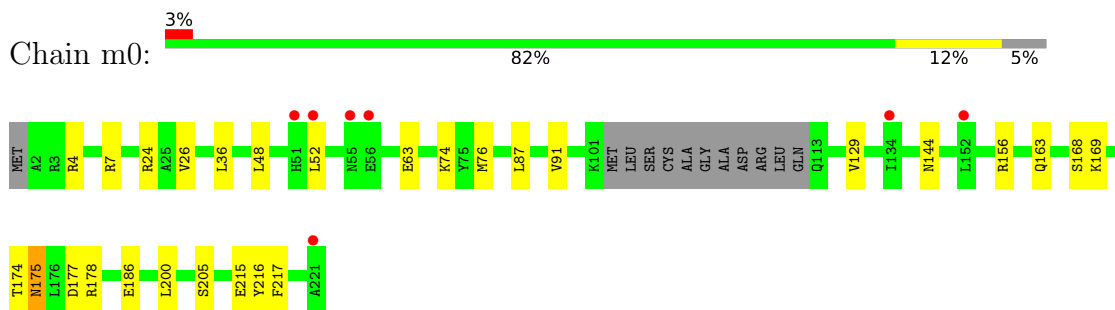
• Molecule 34: 60S ribosomal protein L9-A



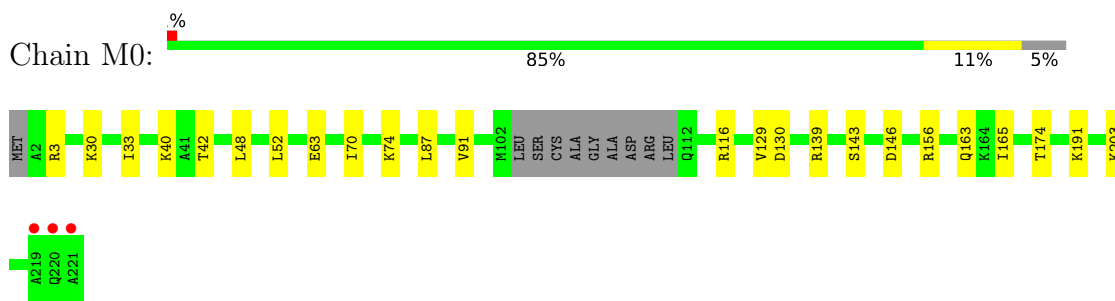
• Molecule 34: 60S ribosomal protein L9-A



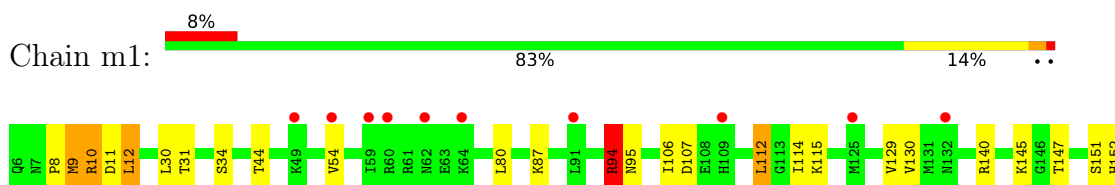
• Molecule 35: 60S ribosomal protein L10

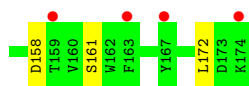


• Molecule 35: 60S ribosomal protein L10

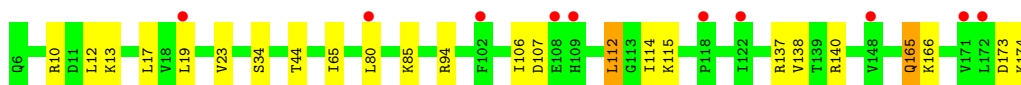
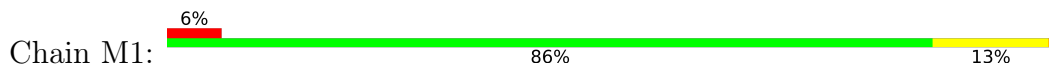


• Molecule 36: 60S ribosomal protein L11-B

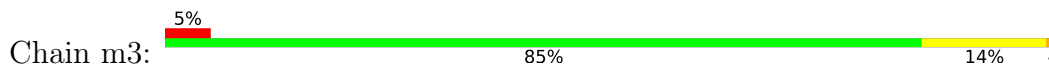




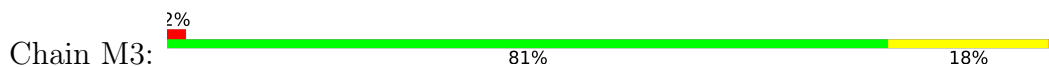
- Molecule 36: 60S ribosomal protein L11-B



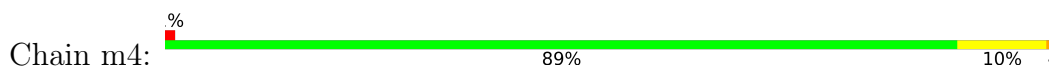
- Molecule 37: 60S ribosomal protein L13-A



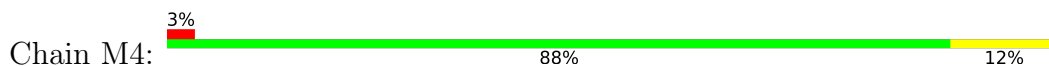
- Molecule 37: 60S ribosomal protein L13-A



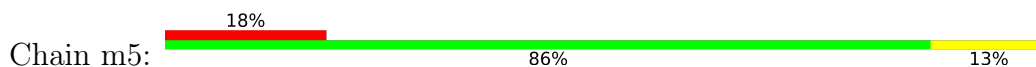
- Molecule 38: 60S ribosomal protein L14-A

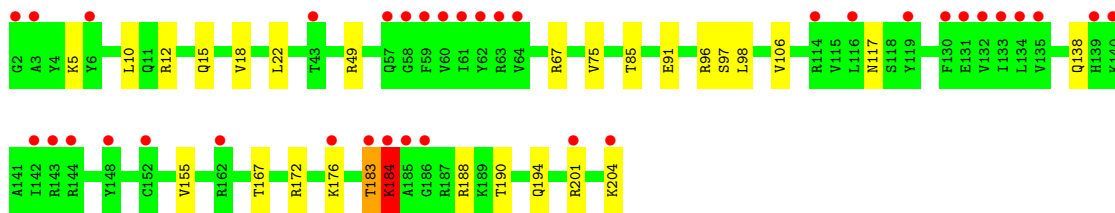


- Molecule 38: 60S ribosomal protein L14-A

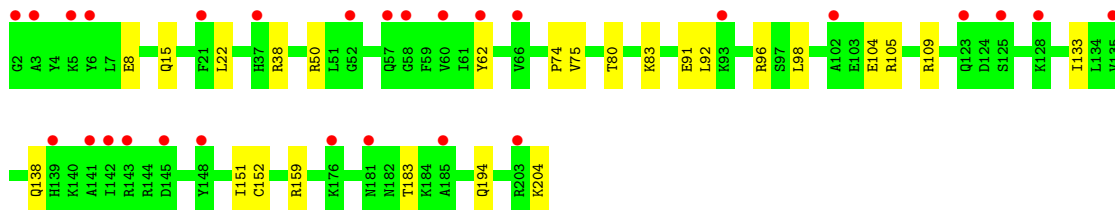
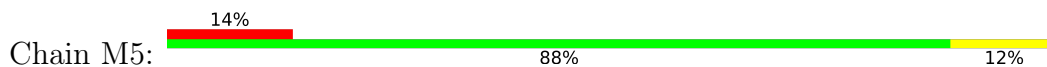


- Molecule 39: 60S ribosomal protein L15-A

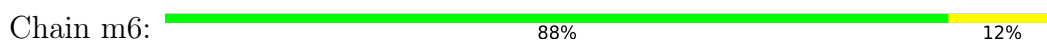




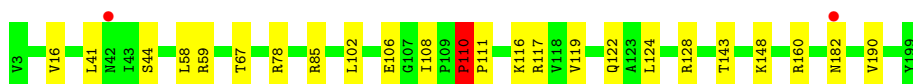
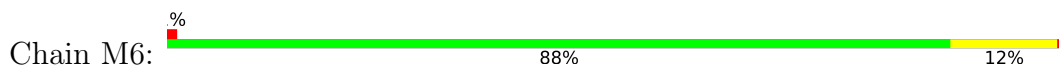
• Molecule 39: 60S ribosomal protein L15-A



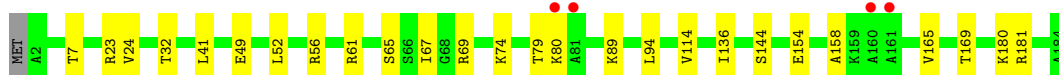
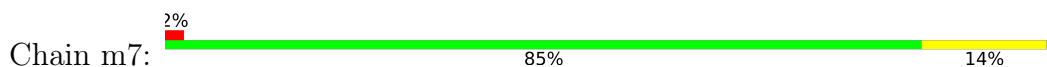
• Molecule 40: 60S ribosomal protein L16-A



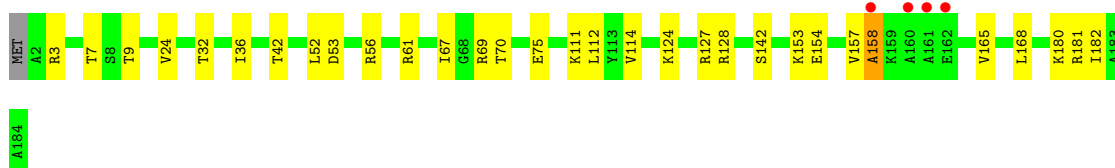
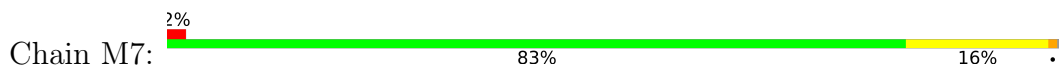
• Molecule 40: 60S ribosomal protein L16-A



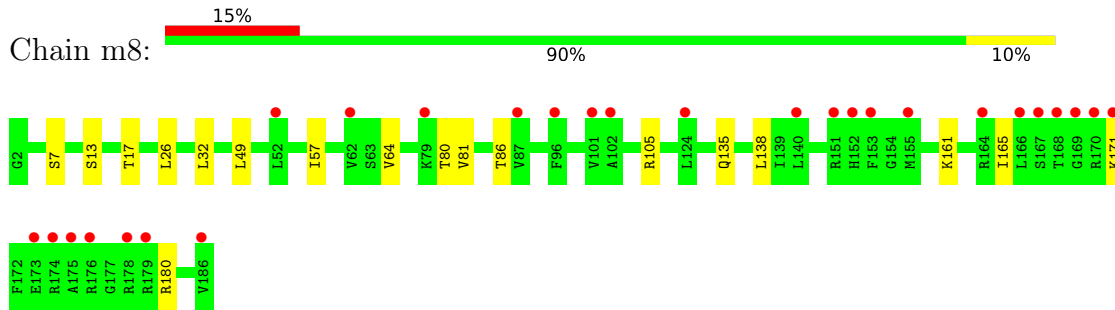
• Molecule 41: 60S ribosomal protein L17-A



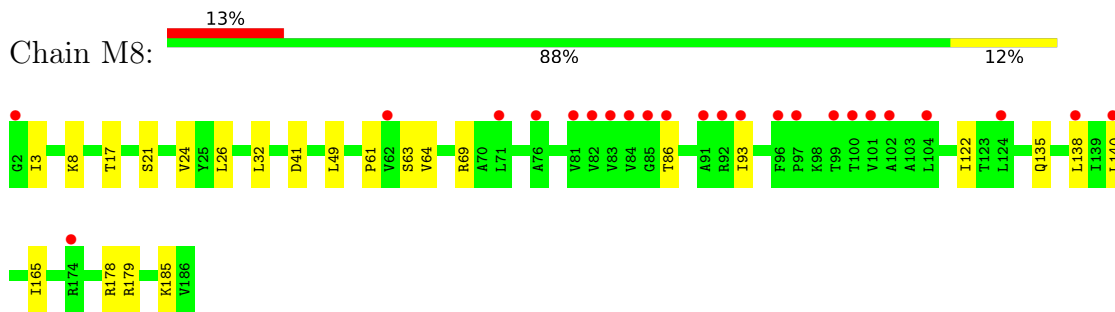
• Molecule 41: 60S ribosomal protein L17-A



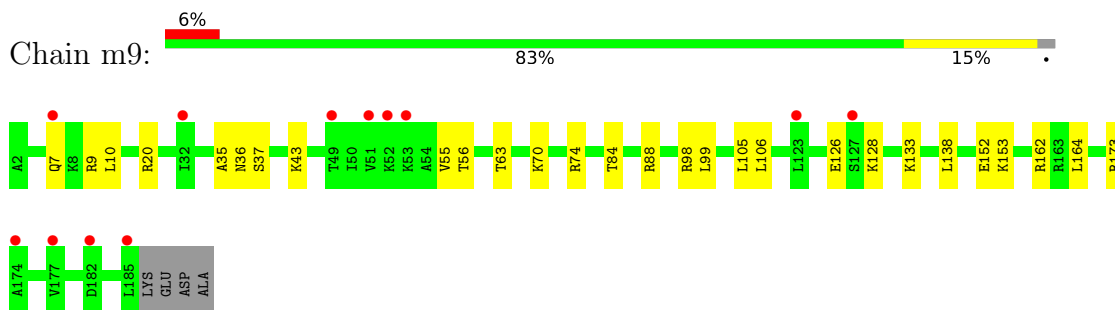
- Molecule 42: 60S ribosomal protein L18-A



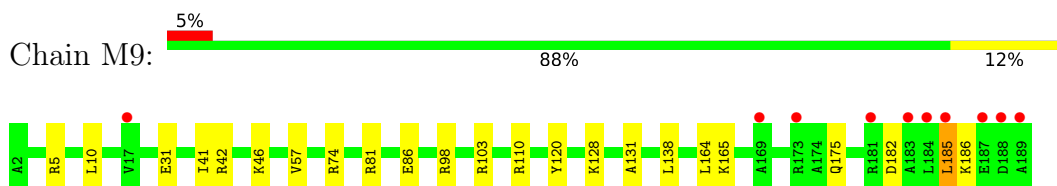
- Molecule 42: 60S ribosomal protein L18-A



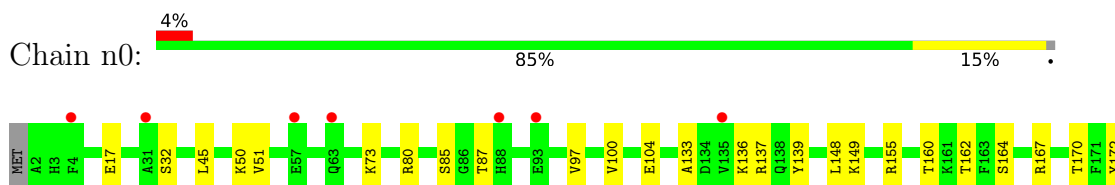
- Molecule 43: 60S ribosomal protein L19-A



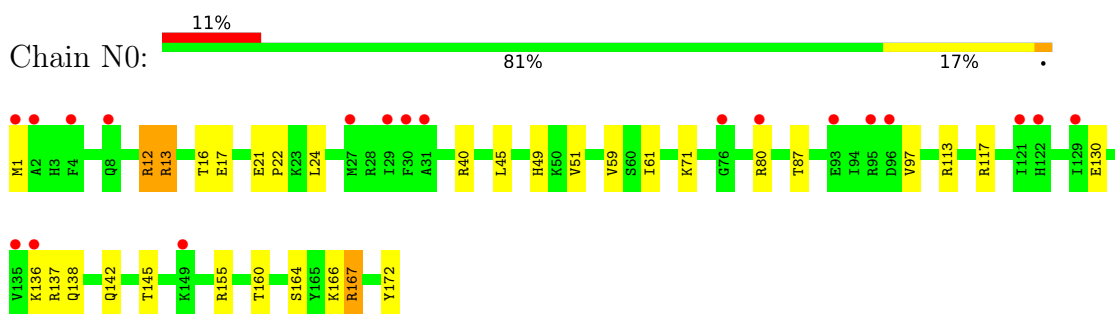
- Molecule 43: 60S ribosomal protein L19-A



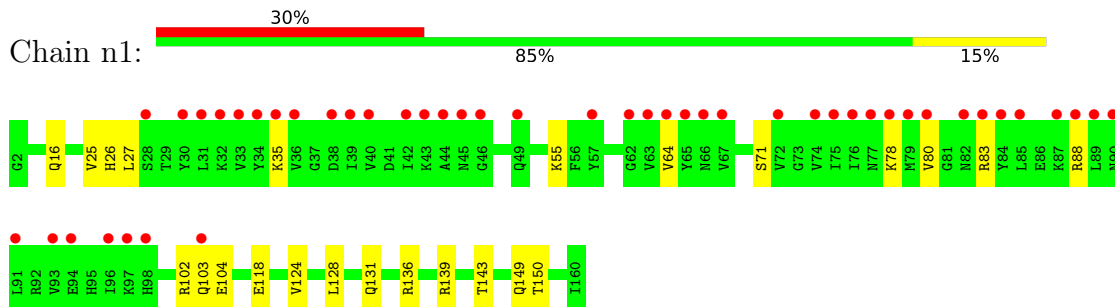
- Molecule 44: 60S ribosomal protein L20-A



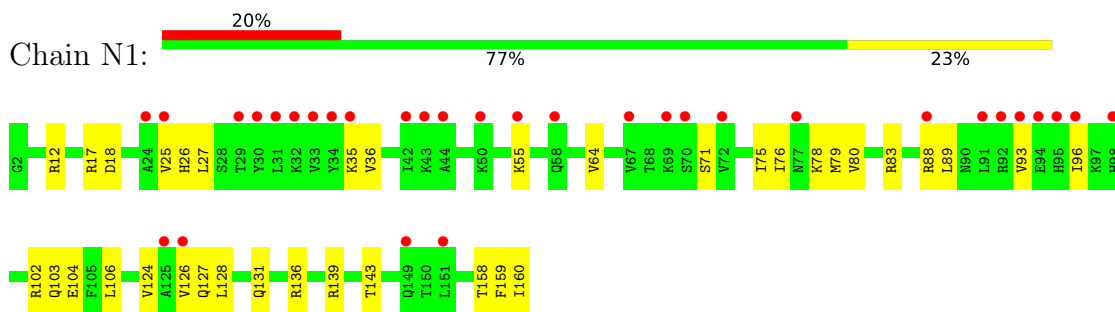
- Molecule 44: 60S ribosomal protein L20-A



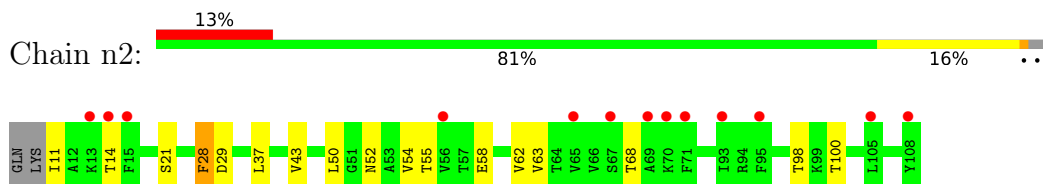
- Molecule 45: 60S ribosomal protein L21-A



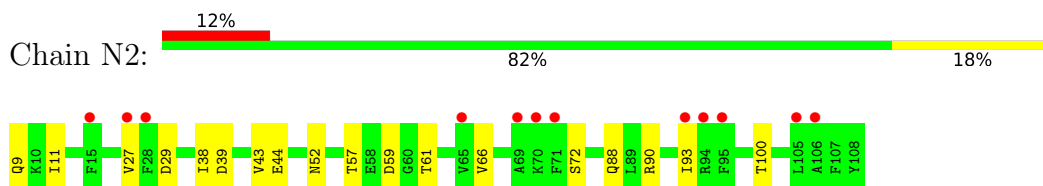
- Molecule 45: 60S ribosomal protein L21-A



- Molecule 46: 60S ribosomal protein L22-A



- Molecule 46: 60S ribosomal protein L22-A



- Molecule 47: 60S ribosomal protein L23-A

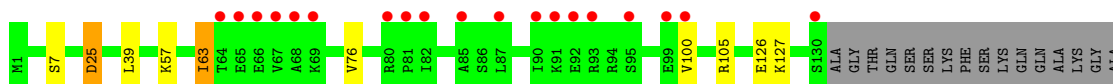
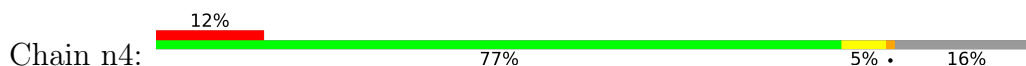




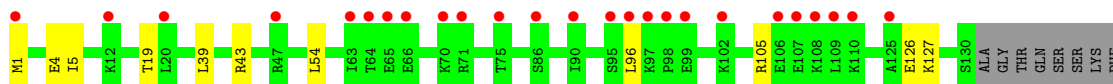
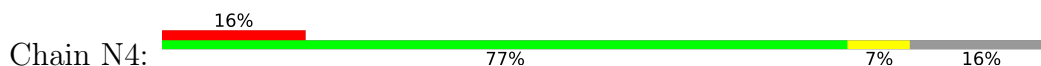
- Molecule 47: 60S ribosomal protein L23-A



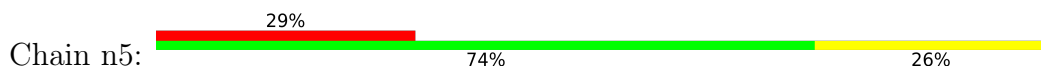
- Molecule 48: 60S ribosomal protein L24-A



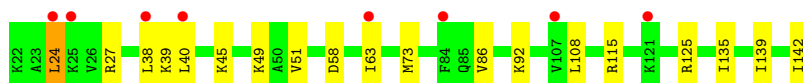
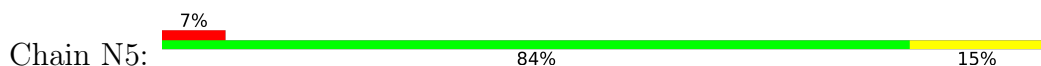
- Molecule 48: 60S ribosomal protein L24-A



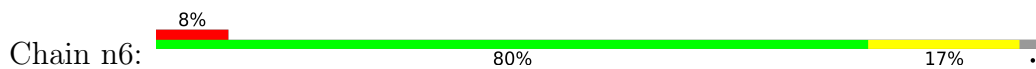
- Molecule 49: 60S ribosomal protein L25



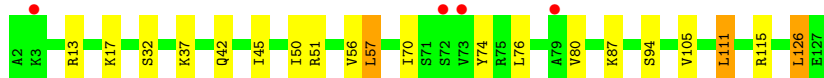
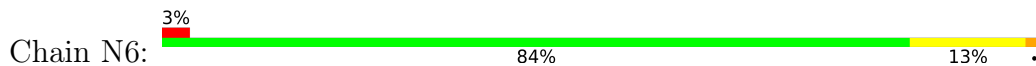
- Molecule 49: 60S ribosomal protein L25



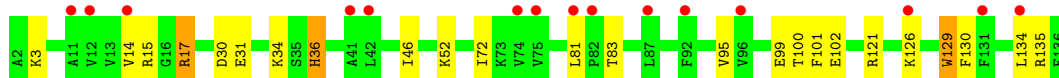
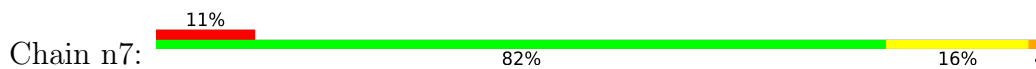
- Molecule 50: 60S ribosomal protein L26-A



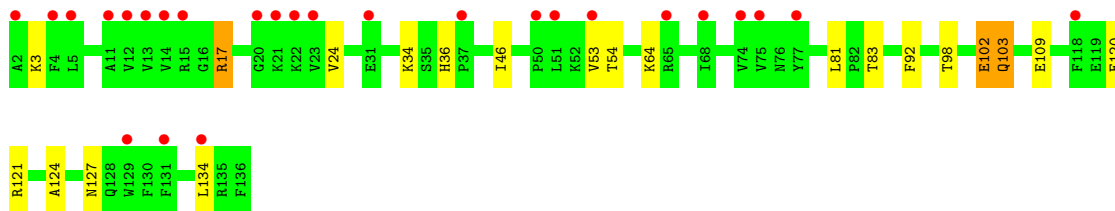
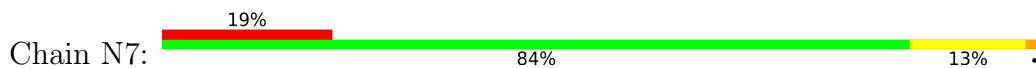
- Molecule 50: 60S ribosomal protein L26-A



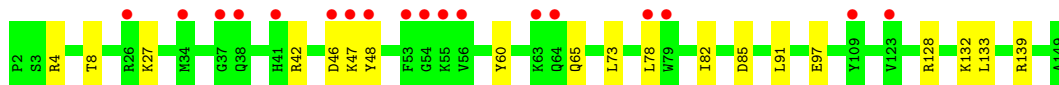
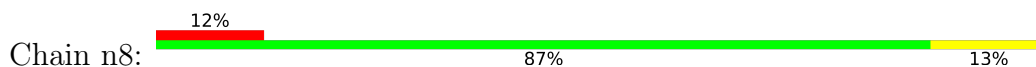
- Molecule 51: 60S ribosomal protein L27-A



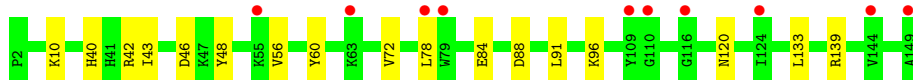
- Molecule 51: 60S ribosomal protein L27-A



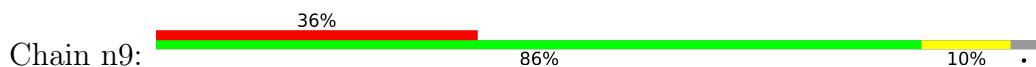
- Molecule 52: 60S ribosomal protein L28

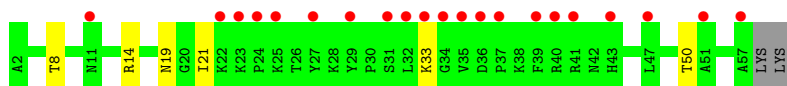


- Molecule 52: 60S ribosomal protein L28

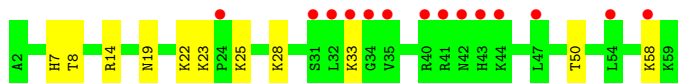
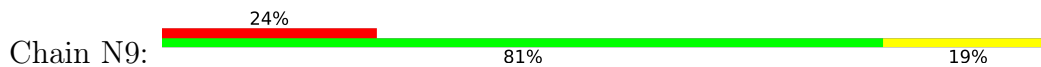


- Molecule 53: 60S ribosomal protein L29

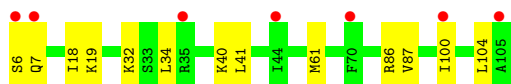
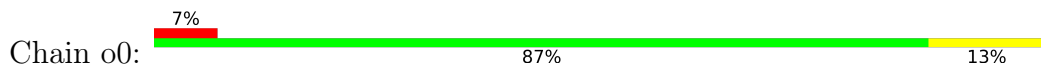




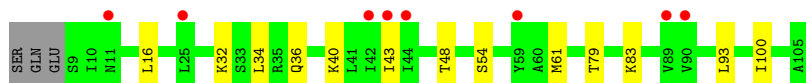
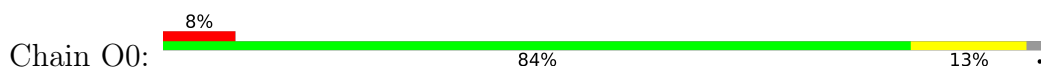
• Molecule 53: 60S ribosomal protein L29



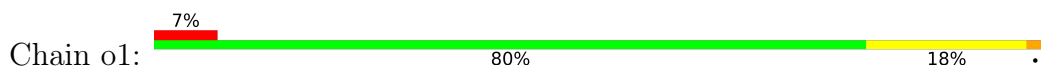
• Molecule 54: 60S ribosomal protein L30



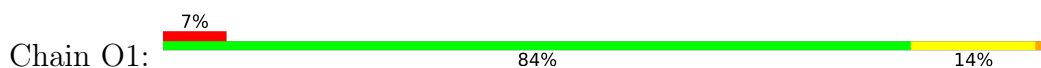
• Molecule 54: 60S ribosomal protein L30



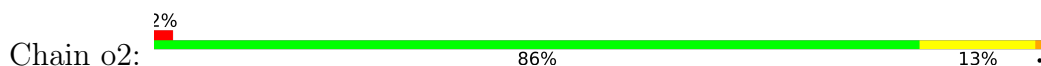
• Molecule 55: 60S ribosomal protein L31-A




• Molecule 55: 60S ribosomal protein L31-A



• Molecule 56: 60S ribosomal protein L32




• Molecule 56: 60S ribosomal protein L32

Chain O2:  89% 11%

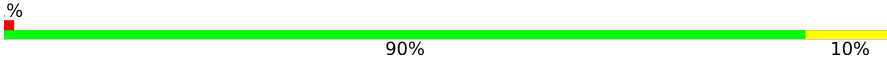


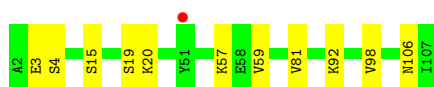
- Molecule 57: 60S ribosomal protein L33-A

Chain o3:  87% 13%




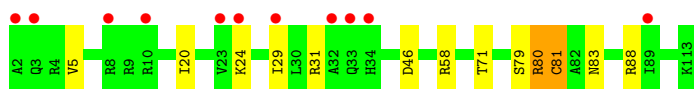
- Molecule 57: 60S ribosomal protein L33-A

Chain O3:  90% 10%




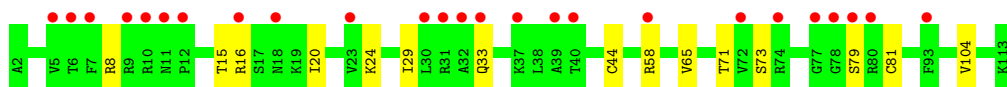
- Molecule 58: 60S ribosomal protein L34-A

Chain o4:  10% 88% 10%




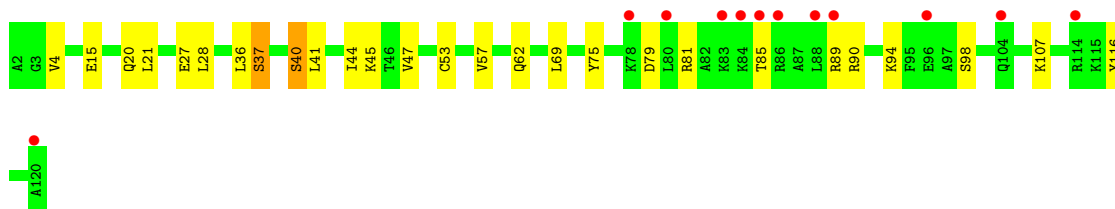
- Molecule 58: 60S ribosomal protein L34-A

Chain O4:  22% 87% 13%




- Molecule 59: 60S ribosomal protein L35-A

Chain o5:  10% 77% 21%



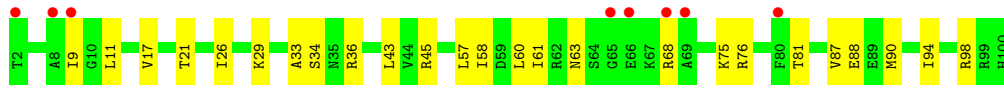
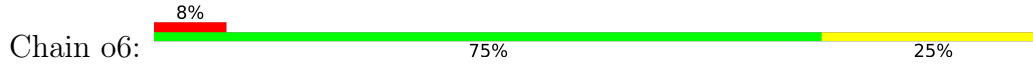
- Molecule 59: 60S ribosomal protein L35-A

Chain O5:  3% 81% 19%

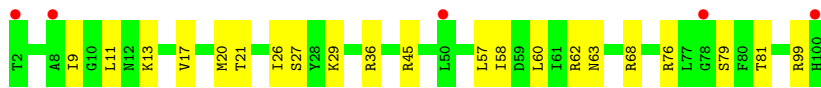
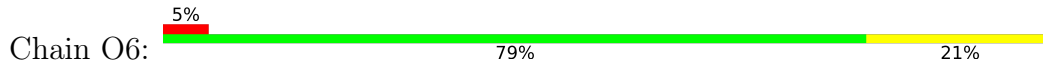




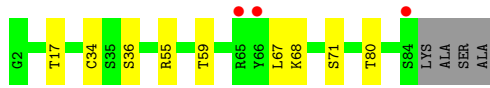
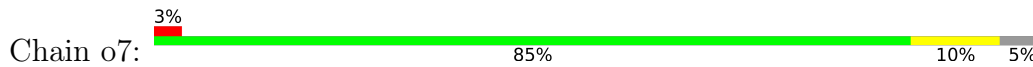
• Molecule 60: 60S ribosomal protein L36-A



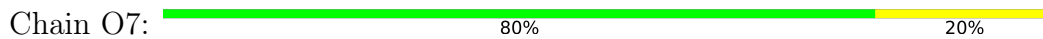
• Molecule 60: 60S ribosomal protein L36-A



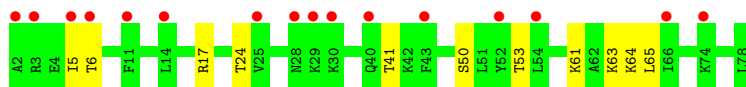
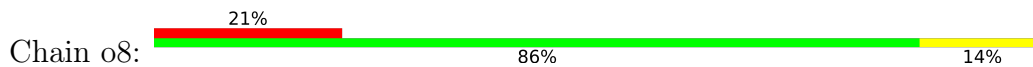
• Molecule 61: 60S ribosomal protein L37-A



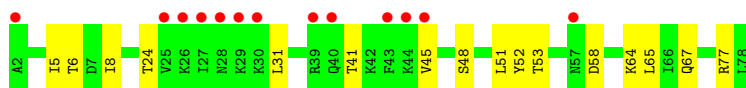
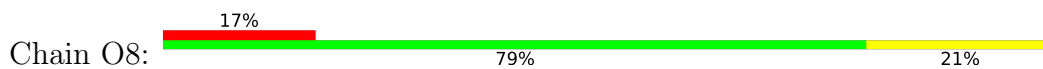
• Molecule 61: 60S ribosomal protein L37-A



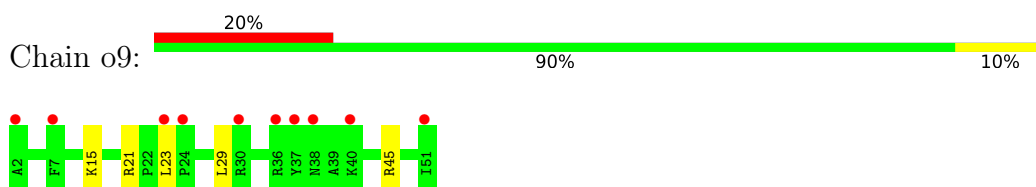
• Molecule 62: 60S ribosomal protein L38



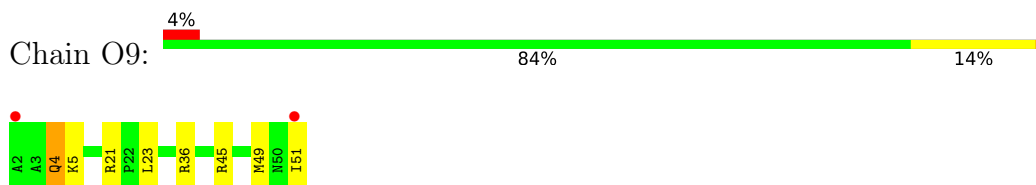
• Molecule 62: 60S ribosomal protein L38



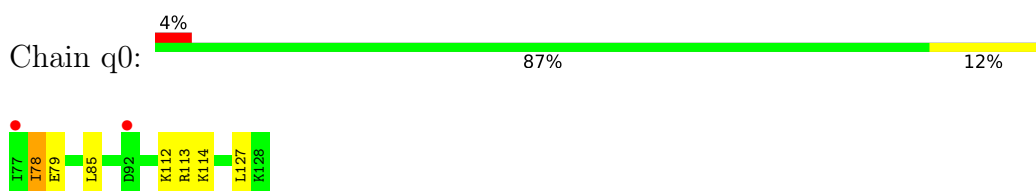
• Molecule 63: 60S ribosomal protein L39



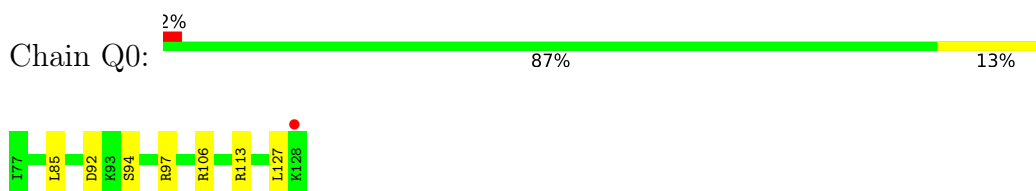
- Molecule 63: 60S ribosomal protein L39



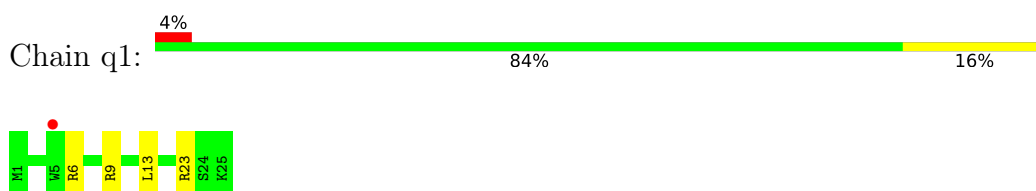
- Molecule 64: Ubiquitin-60S ribosomal protein L40



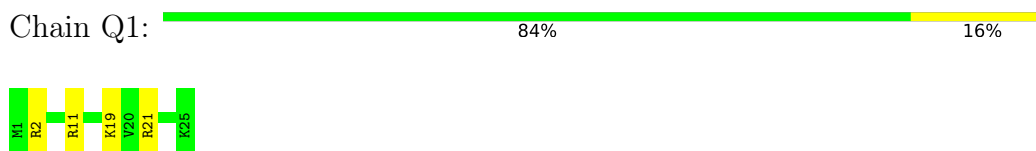
- Molecule 64: Ubiquitin-60S ribosomal protein L40



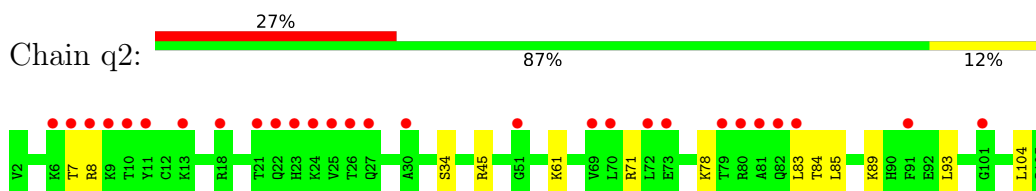
- Molecule 65: 60S ribosomal protein L41-A



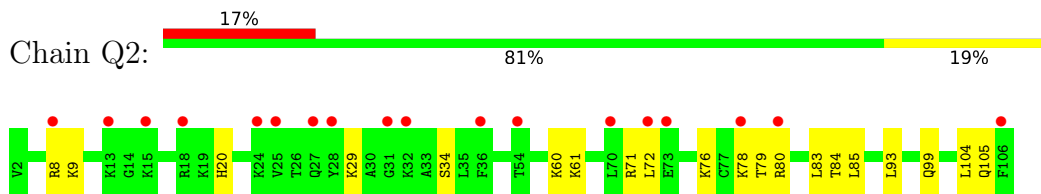
- Molecule 65: 60S ribosomal protein L41-A



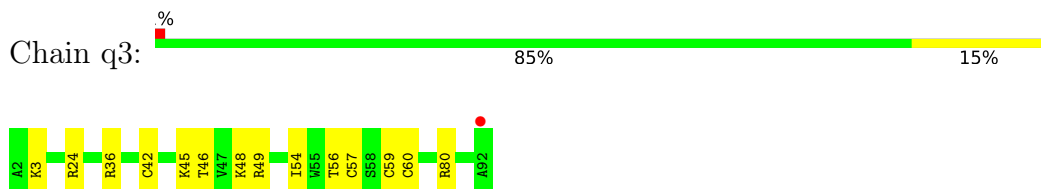
- Molecule 66: 60S ribosomal protein L42-A



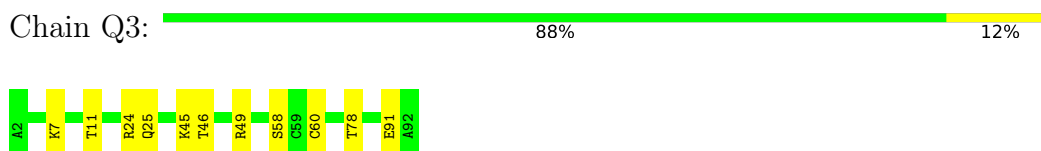
- Molecule 66: 60S ribosomal protein L42-A



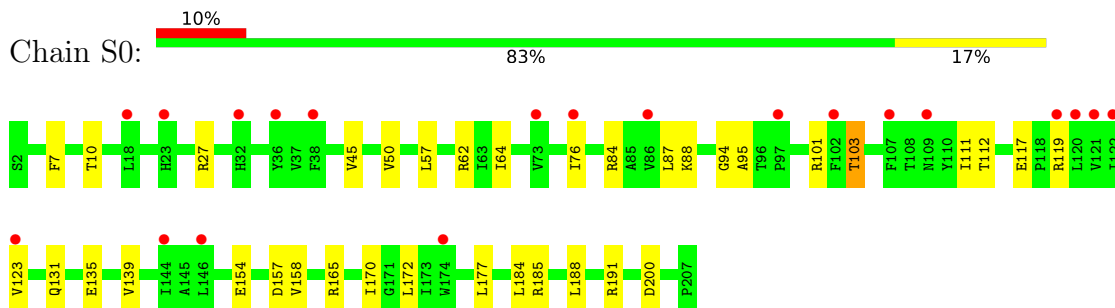
- Molecule 67: 60S ribosomal protein L43-A



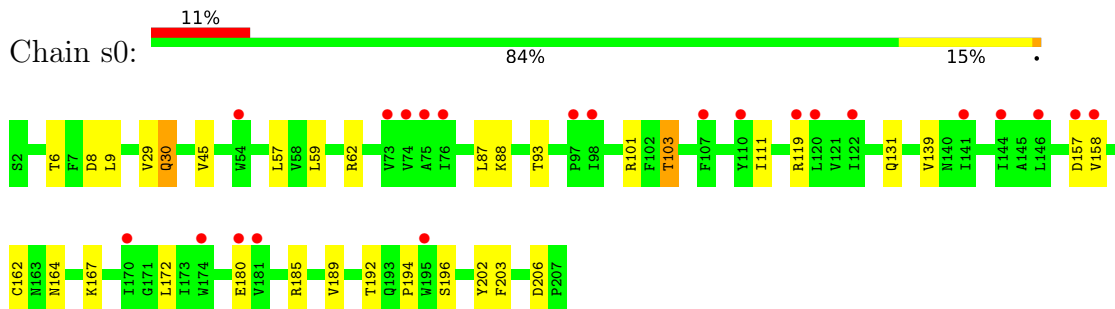
- Molecule 67: 60S ribosomal protein L43-A



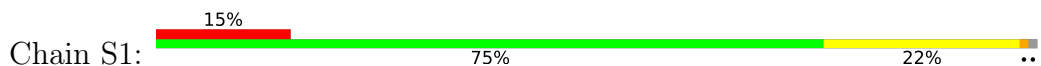
- Molecule 68: 40S ribosomal protein S0-A

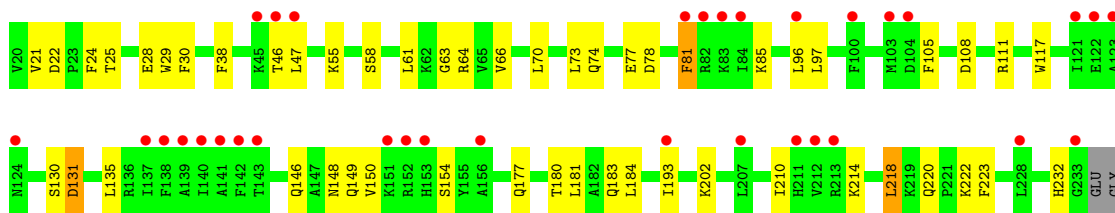


- Molecule 68: 40S ribosomal protein S0-A

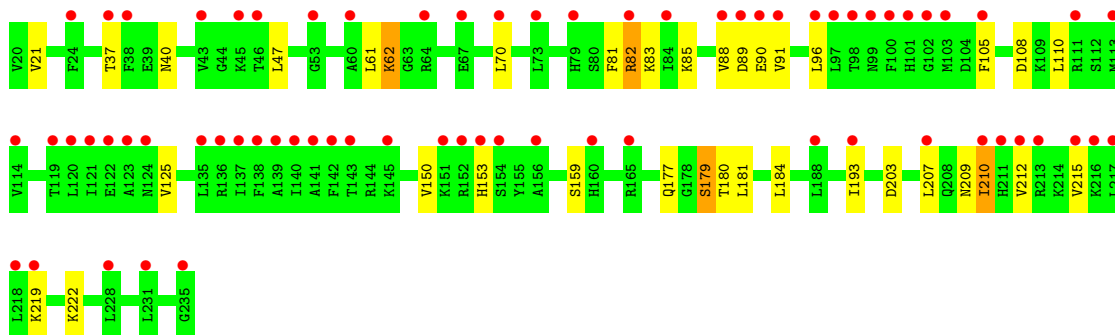
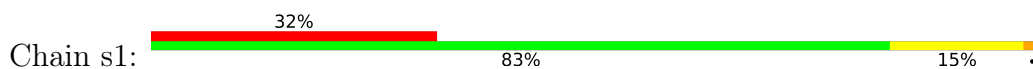


- Molecule 69: 40S ribosomal protein S1-A

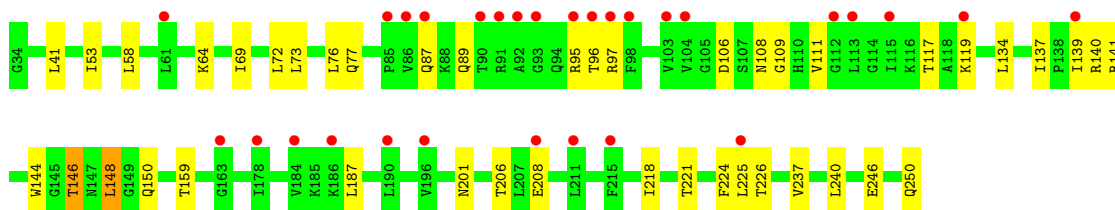
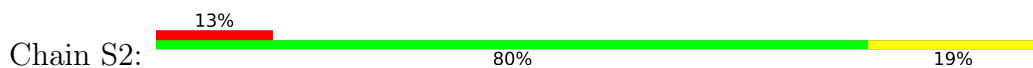




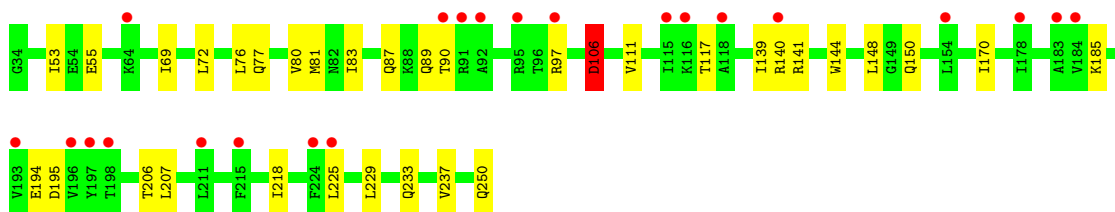
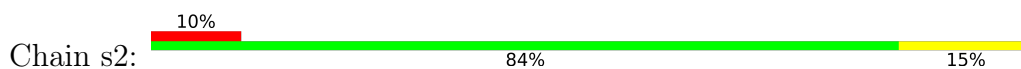
• Molecule 69: 40S ribosomal protein S1-A



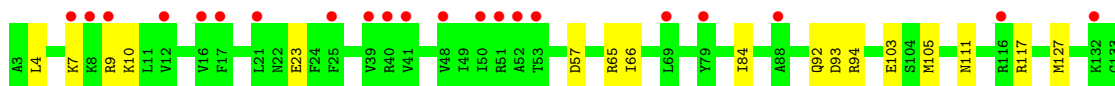
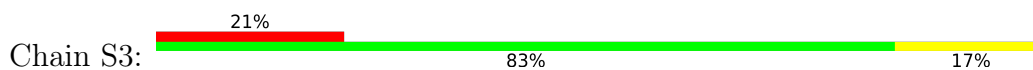
• Molecule 70: 40S ribosomal protein S2

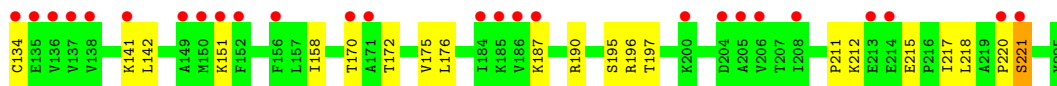


• Molecule 70: 40S ribosomal protein S2

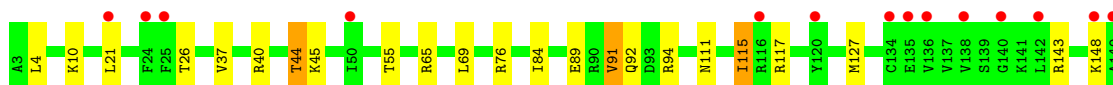
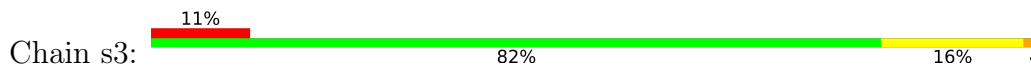


• Molecule 71: 40S ribosomal protein S3

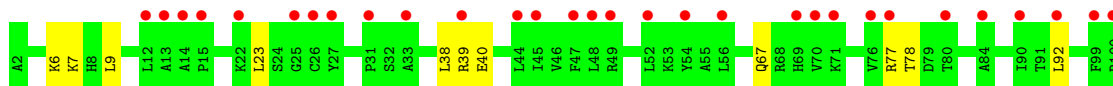
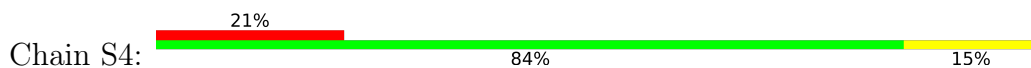




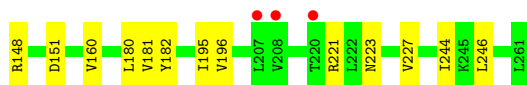
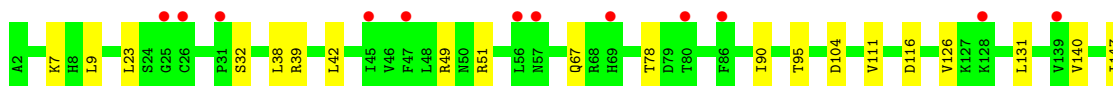
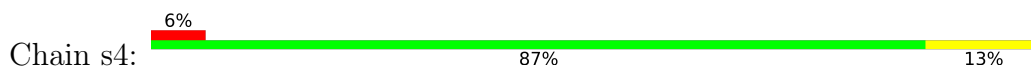
- Molecule 71: 40S ribosomal protein S3



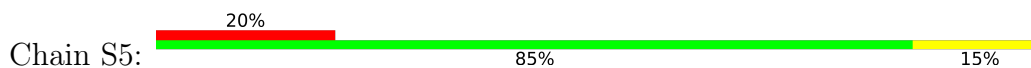
- Molecule 72: 40S ribosomal protein S4-A



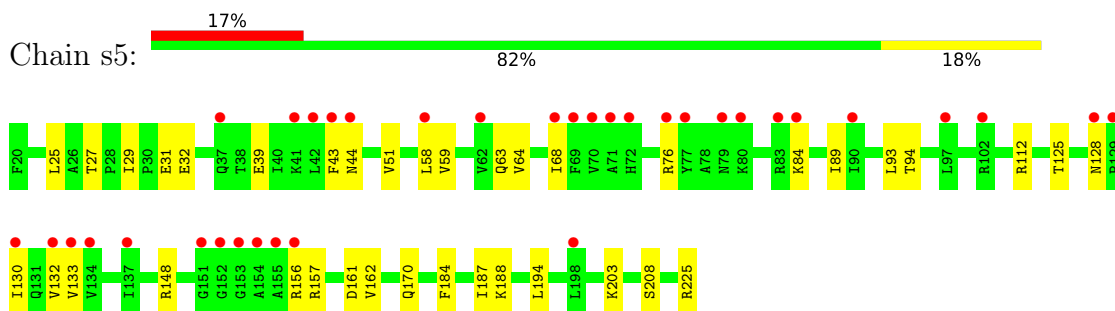
- Molecule 72: 40S ribosomal protein S4-A



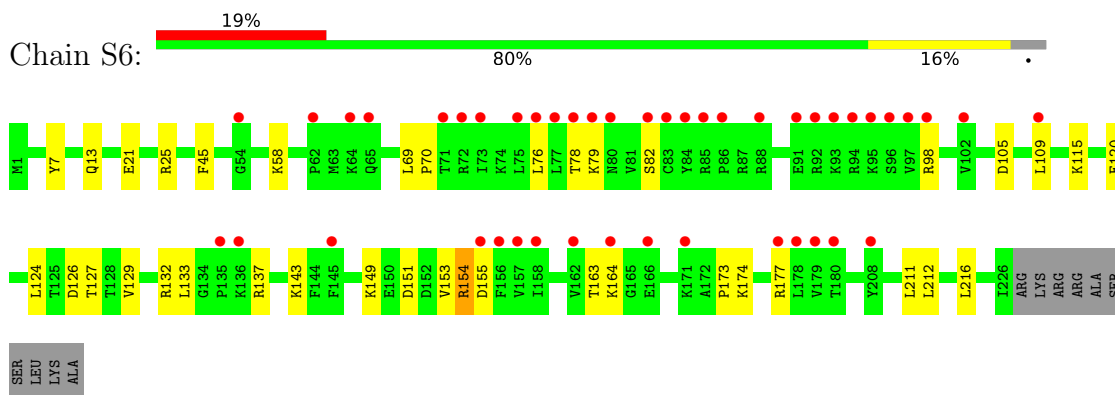
- Molecule 73: 40S ribosomal protein S5



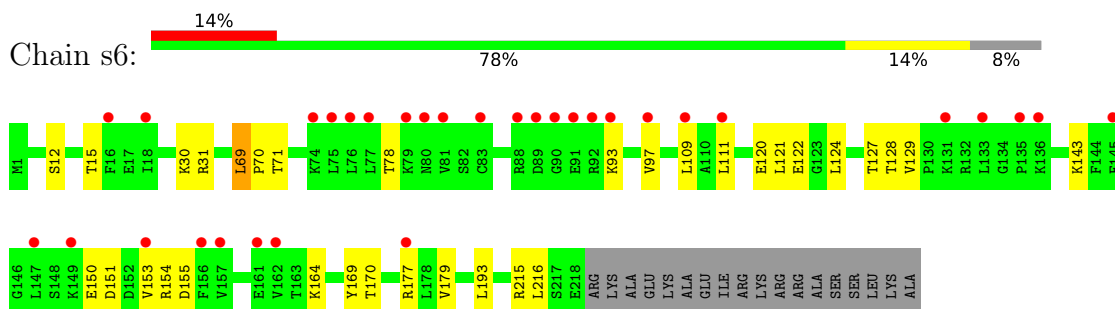
- Molecule 73: 40S ribosomal protein S5



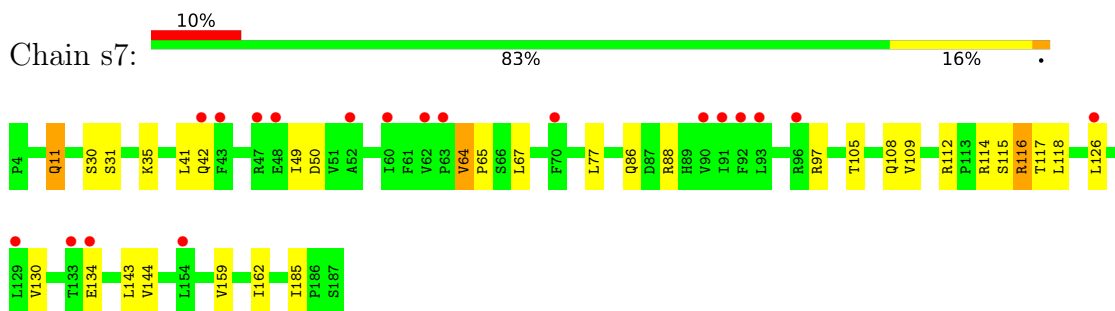
- Molecule 74: 40S ribosomal protein S6-A



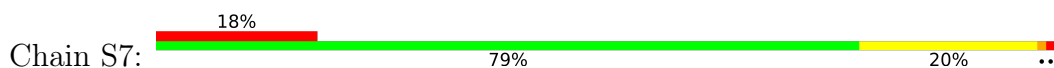
- Molecule 74: 40S ribosomal protein S6-A

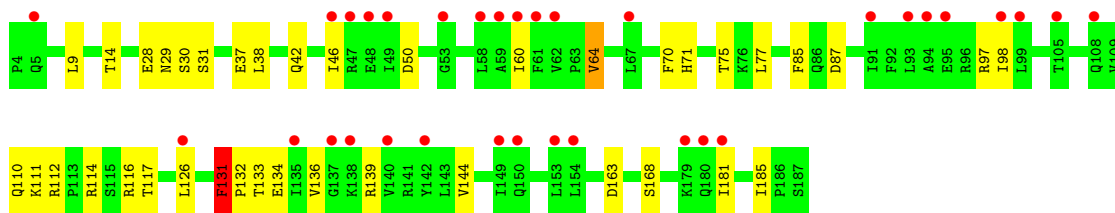


- Molecule 75: 40S ribosomal protein S7-A

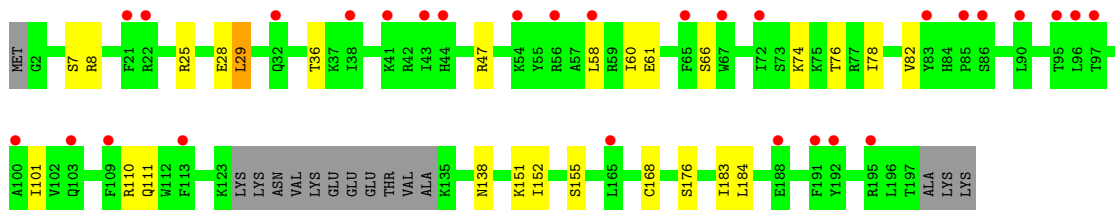
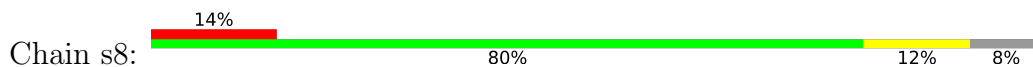


- Molecule 75: 40S ribosomal protein S7-A

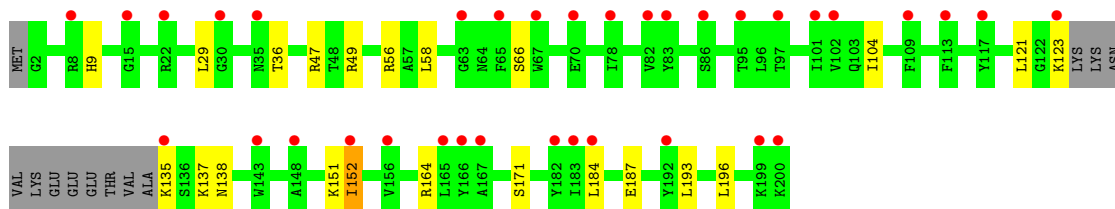
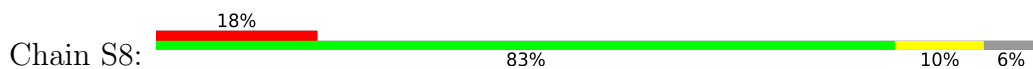




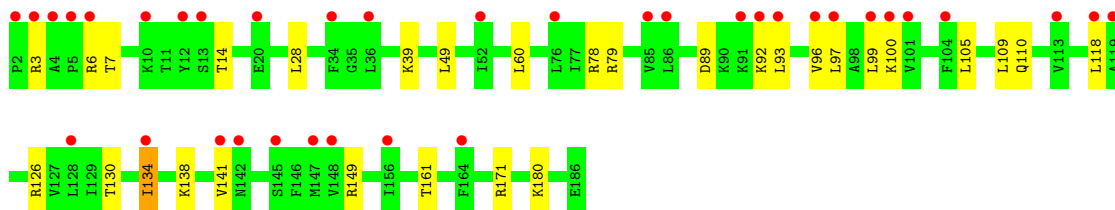
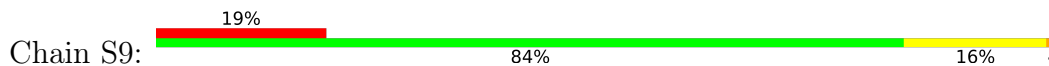
• Molecule 76: 40S ribosomal protein S8-A



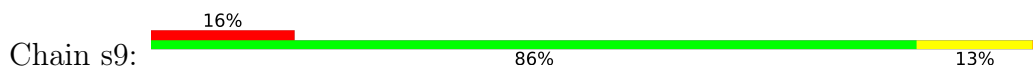
• Molecule 76: 40S ribosomal protein S8-A



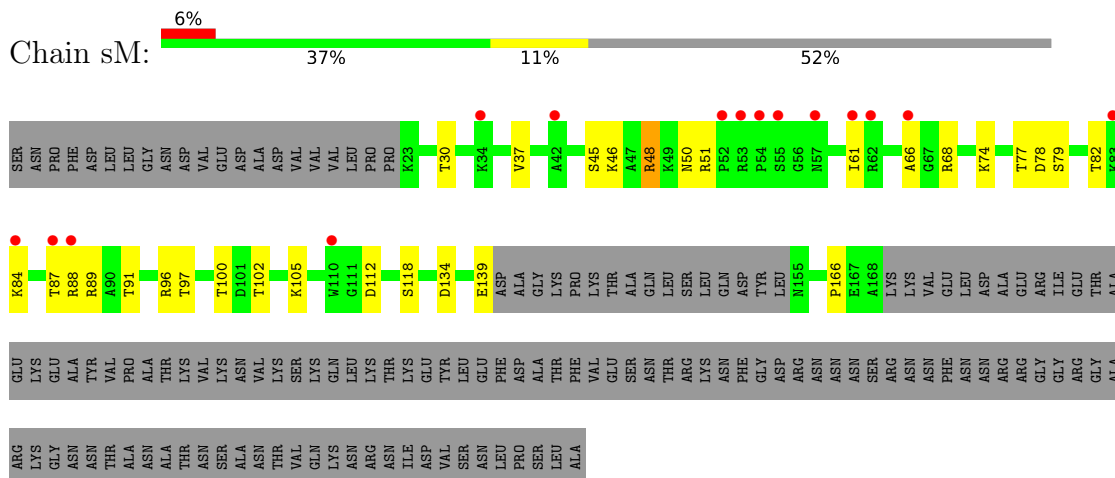
• Molecule 77: 40S ribosomal protein S9-A



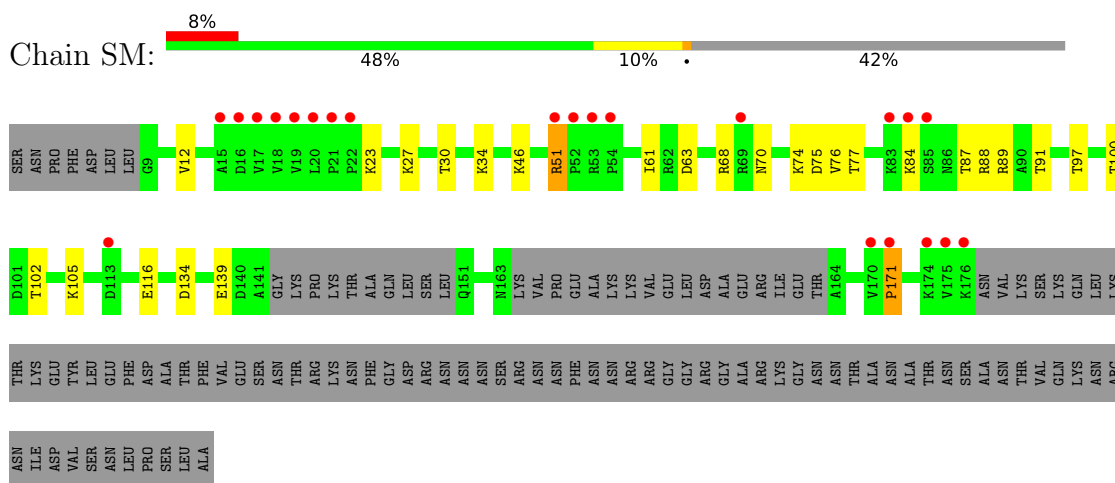
• Molecule 77: 40S ribosomal protein S9-A



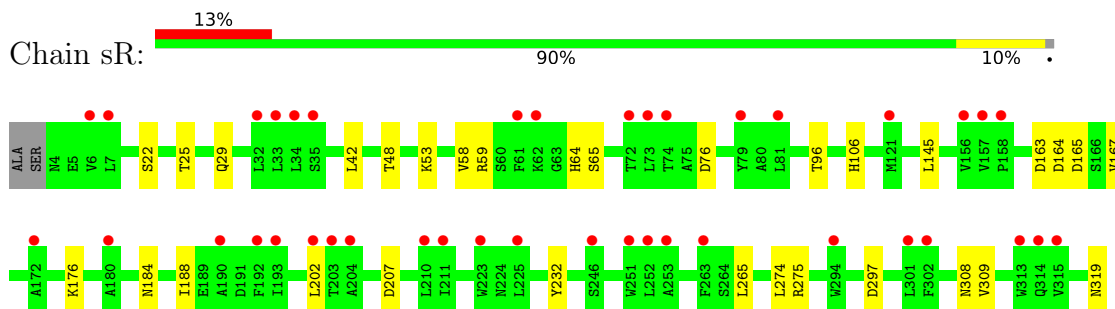
- Molecule 78: Suppressor protein STM1



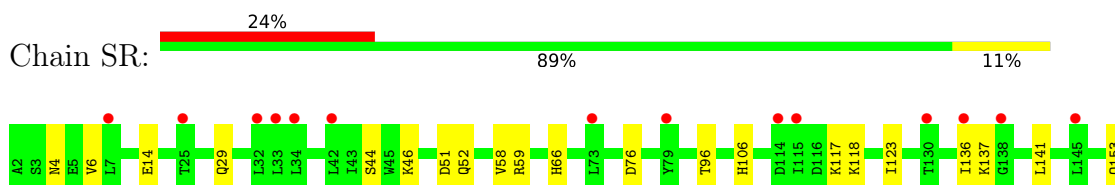
- Molecule 78: Suppressor protein STM1

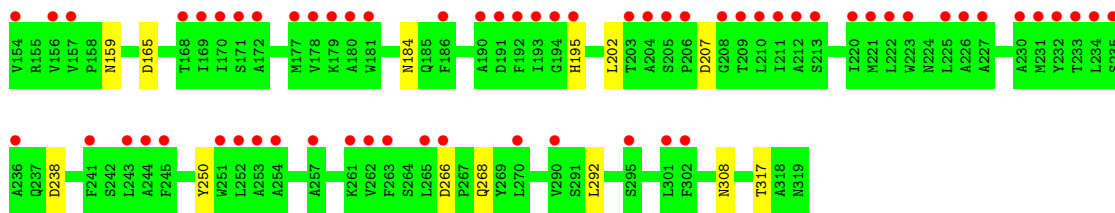


- Molecule 79: Guanine nucleotide-binding protein subunit beta-like protein



- Molecule 79: Guanine nucleotide-binding protein subunit beta-like protein





4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 442.14Å 298.76Å 299.77Å 90.00° 99.49° 90.00° | Depositor |
| Resolution (Å) | 147.83 – 3.70 147.83 – 3.70 | Depositor EDS |
| % Data completeness (in resolution range) | 99.9 (147.83-3.70) 92.7 (147.83-3.70) | Depositor EDS |
| R_{merge} | 0.30 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 0.75 (at 3.67Å) | Xtrriage |
| Refinement program | PHENIX | Depositor |
| R, R_{free} | 0.192 , 0.235 0.192 , 0.235 | Depositor DCC |
| R_{free} test set | 16291 reflections (2.00%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 118.6 | Xtrriage |
| Anisotropy | 0.323 | Xtrriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.28 , 98.8 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$ | Xtrriage |
| Estimated twinning fraction | No twinning to report. | Xtrriage |
| F_o, F_c correlation | 0.93 | EDS |
| Total number of atoms | 400111 | wwPDB-VP |
| Average B, all atoms (Å ²) | 150.0 | wwPDB-VP |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% 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: MG, 8UZ, 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 | 0.92 | 42/73963 (0.1%) | 1.53 | 1261/115306 (1.1%) |
| 1 | 5 | 0.84 | 20/73738 (0.0%) | 1.45 | 984/114951 (0.9%) |
| 2 | 2 | 0.68 | 6/42154 (0.0%) | 1.30 | 354/65680 (0.5%) |
| 2 | 6 | 0.68 | 4/41349 (0.0%) | 1.29 | 326/64423 (0.5%) |
| 3 | 3 | 0.81 | 0/2883 | 1.42 | 33/4491 (0.7%) |
| 3 | 7 | 0.66 | 0/2883 | 1.16 | 10/4491 (0.2%) |
| 4 | 4 | 0.84 | 0/3746 | 1.47 | 52/5832 (0.9%) |
| 4 | 8 | 0.81 | 0/3746 | 1.44 | 41/5832 (0.7%) |
| 5 | C0 | 0.39 | 0/789 | 0.66 | 1/1067 (0.1%) |
| 5 | c0 | 0.35 | 0/762 | 0.68 | 2/1029 (0.2%) |
| 6 | C1 | 0.51 | 0/1233 | 0.69 | 1/1665 (0.1%) |
| 6 | c1 | 0.49 | 0/1194 | 0.69 | 0/1610 |
| 7 | C2 | 0.36 | 0/873 | 0.71 | 1/1185 (0.1%) |
| 7 | c2 | 0.35 | 0/898 | 0.67 | 0/1220 |
| 8 | C3 | 0.46 | 0/1215 | 0.66 | 0/1638 |
| 8 | c3 | 0.44 | 0/1215 | 0.60 | 0/1638 |
| 9 | C4 | 0.41 | 0/901 | 0.71 | 2/1217 (0.2%) |
| 9 | c4 | 0.37 | 0/960 | 0.61 | 0/1290 |
| 10 | C5 | 0.48 | 1/998 (0.1%) | 0.63 | 0/1341 |
| 10 | c5 | 0.42 | 0/1008 | 0.68 | 0/1353 |
| 11 | C6 | 0.49 | 1/1125 (0.1%) | 0.66 | 1/1510 (0.1%) |
| 11 | c6 | 0.56 | 1/1125 (0.1%) | 0.64 | 0/1510 |
| 12 | C7 | 0.40 | 0/935 | 0.73 | 2/1254 (0.2%) |
| 12 | c7 | 0.40 | 0/935 | 0.62 | 0/1255 |
| 13 | C8 | 0.45 | 0/1211 | 0.71 | 1/1628 (0.1%) |
| 13 | c8 | 0.43 | 0/1211 | 0.69 | 1/1628 (0.1%) |
| 14 | C9 | 0.41 | 0/1130 | 0.63 | 1/1517 (0.1%) |
| 14 | c9 | 0.42 | 0/1130 | 0.60 | 0/1517 |
| 15 | D0 | 0.42 | 0/851 | 0.64 | 1/1150 (0.1%) |
| 15 | d0 | 0.40 | 0/838 | 0.62 | 0/1133 |
| 16 | D1 | 0.50 | 0/693 | 0.66 | 0/935 |
| 16 | d1 | 0.46 | 0/693 | 0.63 | 0/935 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | D2 | 0.44 | 0/1038 | 0.70 | 4/1395 (0.3%) |
| 17 | d2 | 0.44 | 0/1038 | 0.65 | 1/1395 (0.1%) |
| 18 | D3 | 0.52 | 0/1139 | 0.73 | 0/1518 |
| 18 | d3 | 0.48 | 0/1139 | 0.70 | 0/1518 |
| 19 | D4 | 0.41 | 0/1087 | 0.63 | 1/1449 (0.1%) |
| 19 | d4 | 0.42 | 0/1087 | 0.68 | 0/1449 |
| 20 | D5 | 0.41 | 0/571 | 0.71 | 0/768 |
| 20 | d5 | 0.35 | 0/566 | 0.63 | 1/761 (0.1%) |
| 21 | D6 | 0.50 | 0/782 | 0.82 | 2/1047 (0.2%) |
| 21 | d6 | 0.42 | 0/782 | 0.63 | 0/1047 |
| 22 | D7 | 0.36 | 0/620 | 0.65 | 1/838 (0.1%) |
| 22 | d7 | 0.40 | 0/620 | 0.66 | 0/838 |
| 23 | D8 | 0.40 | 0/499 | 0.63 | 0/670 |
| 23 | d8 | 0.68 | 1/499 (0.2%) | 0.66 | 1/670 (0.1%) |
| 24 | D9 | 0.57 | 0/443 | 0.70 | 0/588 |
| 24 | d9 | 0.54 | 0/452 | 0.72 | 1/600 (0.2%) |
| 25 | E0 | 0.43 | 0/483 | 0.66 | 0/643 |
| 25 | e0 | 0.45 | 0/490 | 0.67 | 0/653 |
| 26 | E1 | 0.46 | 0/577 | 0.88 | 3/770 (0.4%) |
| 26 | e1 | 0.42 | 0/597 | 0.81 | 1/795 (0.1%) |
| 27 | L2 | 0.53 | 0/1948 | 0.73 | 1/2617 (0.0%) |
| 27 | l2 | 0.55 | 0/1946 | 0.71 | 0/2614 |
| 28 | L3 | 0.60 | 2/3146 (0.1%) | 0.71 | 0/4228 |
| 28 | l3 | 0.58 | 0/3146 | 0.71 | 1/4228 (0.0%) |
| 29 | L4 | 0.57 | 0/2800 | 0.75 | 0/3790 |
| 29 | l4 | 0.53 | 0/2800 | 0.71 | 1/3790 (0.0%) |
| 30 | L5 | 0.50 | 0/2425 | 0.65 | 0/3271 |
| 30 | l5 | 0.38 | 0/2408 | 0.55 | 1/3248 (0.0%) |
| 31 | L6 | 0.59 | 0/1269 | 0.72 | 0/1705 |
| 31 | l6 | 0.59 | 0/1269 | 0.70 | 0/1705 |
| 32 | L7 | 0.57 | 1/1821 (0.1%) | 0.67 | 0/2451 |
| 32 | l7 | 0.55 | 0/1828 | 0.67 | 1/2461 (0.0%) |
| 33 | L8 | 0.47 | 1/1836 (0.1%) | 0.62 | 0/2481 |
| 33 | l8 | 0.41 | 0/1796 | 0.61 | 1/2430 (0.0%) |
| 34 | L9 | 0.54 | 0/1539 | 0.70 | 1/2073 (0.0%) |
| 34 | l9 | 0.54 | 0/1539 | 0.70 | 1/2073 (0.0%) |
| 35 | M0 | 0.59 | 0/1741 | 0.74 | 0/2335 |
| 35 | m0 | 0.53 | 0/1732 | 0.69 | 0/2323 |
| 36 | M1 | 0.46 | 0/1374 | 0.69 | 1/1842 (0.1%) |
| 36 | m1 | 0.37 | 0/1374 | 0.61 | 1/1842 (0.1%) |
| 37 | M3 | 0.54 | 1/1568 (0.1%) | 0.70 | 0/2106 |
| 37 | m3 | 0.49 | 0/1573 | 0.68 | 1/2113 (0.0%) |
| 38 | M4 | 0.50 | 0/1068 | 0.64 | 0/1438 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 38 | m4 | 0.53 | 0/1074 | 0.68 | 1/1446 (0.1%) |
| 39 | M5 | 0.58 | 2/1757 (0.1%) | 0.70 | 0/2354 |
| 39 | m5 | 0.51 | 0/1757 | 0.71 | 0/2354 |
| 40 | M6 | 0.66 | 0/1585 | 0.69 | 0/2128 |
| 40 | m6 | 0.70 | 0/1585 | 0.74 | 1/2128 (0.0%) |
| 41 | M7 | 0.59 | 0/1443 | 0.76 | 0/1944 |
| 41 | m7 | 0.59 | 0/1443 | 0.75 | 0/1944 |
| 42 | M8 | 0.50 | 0/1465 | 0.71 | 0/1965 |
| 42 | m8 | 0.45 | 0/1465 | 0.65 | 0/1965 |
| 43 | M9 | 0.48 | 0/1538 | 0.65 | 1/2050 (0.0%) |
| 43 | m9 | 0.45 | 0/1507 | 0.60 | 0/2009 |
| 44 | N0 | 0.57 | 0/1481 | 0.69 | 1/1990 (0.1%) |
| 44 | n0 | 0.56 | 0/1473 | 0.66 | 0/1980 |
| 45 | N1 | 0.51 | 0/1300 | 0.65 | 0/1743 |
| 45 | n1 | 0.49 | 0/1300 | 0.60 | 0/1743 |
| 46 | N2 | 0.46 | 0/812 | 0.64 | 0/1099 |
| 46 | n2 | 0.41 | 0/794 | 0.57 | 1/1076 (0.1%) |
| 47 | N3 | 0.62 | 0/1018 | 0.73 | 1/1369 (0.1%) |
| 47 | n3 | 0.60 | 0/1012 | 0.75 | 0/1361 |
| 48 | N4 | 0.50 | 0/978 | 0.60 | 0/1302 |
| 48 | n4 | 0.49 | 0/1021 | 0.60 | 0/1356 |
| 49 | N5 | 0.48 | 0/979 | 0.69 | 0/1321 |
| 49 | n5 | 0.48 | 0/974 | 0.72 | 0/1314 |
| 50 | N6 | 0.55 | 0/1004 | 0.76 | 3/1341 (0.2%) |
| 50 | n6 | 0.57 | 1/974 (0.1%) | 0.73 | 0/1302 |
| 51 | N7 | 0.47 | 1/1118 (0.1%) | 0.60 | 0/1497 |
| 51 | n7 | 0.77 | 1/1118 (0.1%) | 0.62 | 0/1497 |
| 52 | N8 | 0.54 | 0/1204 | 0.74 | 0/1612 |
| 52 | n8 | 0.49 | 0/1204 | 0.71 | 0/1612 |
| 53 | N9 | 0.52 | 0/473 | 0.65 | 0/629 |
| 53 | n9 | 0.43 | 0/455 | 0.68 | 0/607 |
| 54 | O0 | 0.46 | 0/751 | 0.63 | 0/1008 |
| 54 | o0 | 0.41 | 0/775 | 0.62 | 1/1040 (0.1%) |
| 55 | O1 | 0.58 | 0/890 | 0.70 | 0/1196 |
| 55 | o1 | 0.56 | 0/897 | 0.69 | 0/1205 |
| 56 | O2 | 0.57 | 0/1041 | 0.74 | 0/1394 |
| 56 | o2 | 0.56 | 0/1041 | 0.74 | 1/1394 (0.1%) |
| 57 | O3 | 0.62 | 0/868 | 0.78 | 0/1168 |
| 57 | o3 | 0.66 | 0/868 | 0.76 | 1/1168 (0.1%) |
| 58 | O4 | 0.48 | 0/890 | 0.64 | 0/1189 |
| 58 | o4 | 0.45 | 0/890 | 0.62 | 0/1189 |
| 59 | O5 | 0.52 | 0/978 | 0.66 | 0/1301 |
| 59 | o5 | 0.56 | 2/974 (0.2%) | 0.65 | 0/1297 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 60 | O6 | 0.48 | 0/778 | 0.66 | 0/1034 |
| 60 | o6 | 0.46 | 0/777 | 0.65 | 0/1033 |
| 61 | O7 | 0.65 | 2/696 (0.3%) | 0.79 | 0/923 |
| 61 | o7 | 0.60 | 0/671 | 0.76 | 0/890 |
| 62 | O8 | 0.44 | 0/618 | 0.59 | 0/826 |
| 62 | o8 | 0.42 | 0/614 | 0.59 | 0/822 |
| 63 | O9 | 0.56 | 0/443 | 0.75 | 0/588 |
| 63 | o9 | 0.51 | 0/443 | 0.64 | 0/588 |
| 64 | Q0 | 0.60 | 0/423 | 0.78 | 0/562 |
| 64 | q0 | 0.59 | 0/423 | 0.77 | 0/562 |
| 65 | Q1 | 0.59 | 0/234 | 0.77 | 0/300 |
| 65 | q1 | 0.55 | 0/234 | 0.69 | 0/300 |
| 66 | Q2 | 0.54 | 0/860 | 0.75 | 0/1136 |
| 66 | q2 | 0.45 | 0/848 | 0.61 | 0/1120 |
| 67 | Q3 | 0.59 | 0/701 | 0.68 | 0/934 |
| 67 | q3 | 0.48 | 0/701 | 0.70 | 0/934 |
| 68 | S0 | 0.42 | 0/1617 | 0.61 | 0/2215 |
| 68 | s0 | 0.42 | 1/1623 (0.1%) | 0.62 | 0/2222 |
| 69 | S1 | 0.39 | 0/1735 | 0.68 | 2/2335 (0.1%) |
| 69 | s1 | 0.36 | 0/1748 | 0.62 | 0/2352 |
| 70 | S2 | 0.44 | 0/1665 | 0.66 | 0/2263 |
| 70 | s2 | 0.43 | 0/1665 | 0.63 | 0/2263 |
| 71 | S3 | 0.45 | 0/1759 | 0.60 | 0/2368 |
| 71 | s3 | 0.42 | 0/1759 | 0.62 | 0/2368 |
| 72 | S4 | 0.41 | 0/2109 | 0.66 | 1/2839 (0.0%) |
| 72 | s4 | 0.43 | 0/2109 | 0.67 | 0/2839 |
| 73 | S5 | 0.38 | 0/1629 | 0.58 | 0/2202 |
| 73 | s5 | 0.42 | 0/1629 | 0.60 | 0/2202 |
| 74 | S6 | 0.40 | 0/1823 | 0.57 | 0/2439 |
| 74 | s6 | 0.43 | 0/1779 | 0.61 | 0/2379 |
| 75 | S7 | 0.42 | 0/1506 | 0.68 | 1/2028 (0.0%) |
| 75 | s7 | 0.39 | 0/1506 | 0.68 | 1/2028 (0.0%) |
| 76 | S8 | 0.44 | 0/1514 | 0.65 | 1/2021 (0.0%) |
| 76 | s8 | 0.46 | 0/1491 | 0.65 | 1/1992 (0.1%) |
| 77 | S9 | 0.41 | 0/1519 | 0.61 | 0/2035 |
| 77 | s9 | 0.42 | 0/1519 | 0.61 | 1/2035 (0.0%) |
| 78 | SM | 0.44 | 0/1113 | 0.70 | 2/1502 (0.1%) |
| 78 | sM | 0.43 | 0/964 | 0.67 | 2/1291 (0.2%) |
| 79 | SR | 0.33 | 0/2490 | 0.57 | 0/3389 |
| 79 | sR | 0.37 | 0/2480 | 0.59 | 1/3376 (0.0%) |
| All | All | 0.70 | 91/425229 (0.0%) | 1.19 | 3127/623929 (0.5%) |

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 | c0 | 0 | 1 |
| 7 | C2 | 0 | 2 |
| 7 | c2 | 0 | 1 |
| 9 | C4 | 0 | 2 |
| 9 | c4 | 0 | 1 |
| 10 | C5 | 0 | 1 |
| 10 | c5 | 0 | 3 |
| 11 | C6 | 0 | 2 |
| 11 | c6 | 0 | 1 |
| 12 | C7 | 0 | 3 |
| 12 | c7 | 0 | 3 |
| 13 | C8 | 0 | 1 |
| 13 | c8 | 0 | 1 |
| 15 | d0 | 0 | 3 |
| 17 | D2 | 0 | 1 |
| 17 | d2 | 0 | 1 |
| 18 | D3 | 0 | 1 |
| 19 | D4 | 0 | 2 |
| 20 | D5 | 0 | 3 |
| 20 | d5 | 0 | 2 |
| 21 | D6 | 0 | 3 |
| 22 | D7 | 0 | 1 |
| 24 | d9 | 0 | 1 |
| 25 | e0 | 0 | 1 |
| 26 | E1 | 0 | 4 |
| 26 | e1 | 0 | 6 |
| 27 | l2 | 0 | 3 |
| 28 | L3 | 0 | 3 |
| 28 | l3 | 0 | 1 |
| 29 | L4 | 0 | 1 |
| 29 | l4 | 0 | 3 |
| 30 | L5 | 0 | 1 |
| 30 | l5 | 0 | 2 |
| 31 | l6 | 0 | 1 |
| 32 | l7 | 0 | 2 |
| 33 | L8 | 0 | 1 |
| 34 | L9 | 0 | 1 |
| 36 | m1 | 0 | 3 |
| 37 | M3 | 0 | 1 |
| 37 | m3 | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 38 | m4 | 0 | 1 |
| 39 | m5 | 0 | 2 |
| 40 | M6 | 0 | 1 |
| 41 | M7 | 0 | 2 |
| 43 | M9 | 0 | 1 |
| 44 | N0 | 0 | 3 |
| 44 | n0 | 0 | 2 |
| 48 | n4 | 0 | 1 |
| 50 | n6 | 0 | 1 |
| 51 | N7 | 0 | 2 |
| 51 | n7 | 0 | 1 |
| 53 | N9 | 0 | 1 |
| 53 | n9 | 0 | 1 |
| 55 | O1 | 0 | 1 |
| 55 | o1 | 0 | 2 |
| 56 | o2 | 0 | 1 |
| 58 | o4 | 0 | 2 |
| 59 | O5 | 0 | 1 |
| 60 | O6 | 0 | 1 |
| 66 | Q2 | 0 | 1 |
| 67 | q3 | 0 | 1 |
| 68 | S0 | 0 | 2 |
| 69 | S1 | 0 | 2 |
| 70 | S2 | 0 | 2 |
| 70 | s2 | 0 | 2 |
| 71 | S3 | 0 | 1 |
| 71 | s3 | 0 | 4 |
| 72 | S4 | 0 | 1 |
| 73 | S5 | 0 | 4 |
| 73 | s5 | 0 | 1 |
| 74 | s6 | 0 | 1 |
| 75 | S7 | 0 | 4 |
| 75 | s7 | 0 | 4 |
| 77 | s9 | 0 | 3 |
| 78 | SM | 0 | 1 |
| 79 | SR | 0 | 1 |
| All | All | 0 | 137 |

All (91) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 51 | n7 | 36 | HIS | C-N | 20.49 | 1.73 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 23 | d8 | 5 | THR | C-N | 12.69 | 1.58 | 1.34 |
| 11 | c6 | 4 | VAL | C-N | 10.62 | 1.54 | 1.34 |
| 1 | 5 | 1103 | A | N9-C4 | 9.38 | 1.43 | 1.37 |
| 1 | 1 | 2093 | A | N9-C4 | 8.68 | 1.43 | 1.37 |
| 10 | C5 | 67 | ALA | C-N | 7.60 | 1.48 | 1.34 |
| 1 | 5 | 2401 | A | N3-C4 | 7.42 | 1.39 | 1.34 |
| 1 | 1 | 2983 | C | N1-C6 | -7.26 | 1.32 | 1.37 |
| 11 | C6 | 124 | PRO | C-N | 7.20 | 1.50 | 1.34 |
| 33 | L8 | 158 | ASP | C-N | -7.10 | 1.20 | 1.34 |
| 50 | n6 | 99 | LEU | C-N | -7.07 | 1.17 | 1.34 |
| 1 | 1 | 3012 | A | N9-C4 | -7.04 | 1.33 | 1.37 |
| 37 | M3 | 125 | VAL | C-N | -6.98 | 1.18 | 1.34 |
| 1 | 5 | 2872 | A | N9-C4 | 6.93 | 1.42 | 1.37 |
| 1 | 1 | 1302 | A | N9-C4 | -6.93 | 1.33 | 1.37 |
| 1 | 1 | 1654 | A | N9-C4 | -6.92 | 1.33 | 1.37 |
| 1 | 1 | 1858 | A | N9-C4 | 6.80 | 1.42 | 1.37 |
| 1 | 1 | 2911 | A | N9-C4 | -6.70 | 1.33 | 1.37 |
| 2 | 2 | 1749 | A | N9-C4 | -6.64 | 1.33 | 1.37 |
| 1 | 1 | 2820 | A | N9-C4 | -6.53 | 1.33 | 1.37 |
| 1 | 1 | 1589 | A | N9-C4 | -6.51 | 1.33 | 1.37 |
| 1 | 5 | 1839 | A | N9-C4 | -6.45 | 1.33 | 1.37 |
| 2 | 2 | 1746 | A | N9-C4 | -6.44 | 1.33 | 1.37 |
| 2 | 2 | 541 | A | N9-C4 | 6.41 | 1.41 | 1.37 |
| 61 | O7 | 62 | GLY | C-O | -6.38 | 1.13 | 1.23 |
| 1 | 1 | 3209 | A | C5-C4 | 6.31 | 1.43 | 1.38 |
| 1 | 5 | 1196 | C | C4-C5 | 6.28 | 1.48 | 1.43 |
| 59 | o5 | 37 | SER | C-N | 6.19 | 1.48 | 1.34 |
| 39 | M5 | 152 | CYS | CB-SG | -6.12 | 1.71 | 1.82 |
| 1 | 1 | 2853 | A | N9-C4 | -6.00 | 1.34 | 1.37 |
| 1 | 1 | 1907 | C | N1-C6 | -5.96 | 1.33 | 1.37 |
| 1 | 1 | 895 | A | C5-C6 | -5.96 | 1.35 | 1.41 |
| 1 | 5 | 1221 | A | N9-C4 | 5.94 | 1.41 | 1.37 |
| 28 | L3 | 7 | GLU | CB-CG | 5.94 | 1.63 | 1.52 |
| 2 | 6 | 541 | A | N9-C4 | 5.93 | 1.41 | 1.37 |
| 1 | 1 | 1911 | A | N7-C5 | -5.91 | 1.35 | 1.39 |
| 1 | 5 | 1412 | G | N7-C5 | -5.90 | 1.35 | 1.39 |
| 1 | 5 | 1412 | G | C5-C6 | -5.87 | 1.36 | 1.42 |
| 1 | 1 | 3142 | A | N9-C4 | -5.81 | 1.34 | 1.37 |
| 1 | 1 | 1524 | A | N9-C4 | -5.80 | 1.34 | 1.37 |
| 1 | 1 | 2811 | A | C5-C4 | -5.74 | 1.34 | 1.38 |
| 1 | 1 | 895 | A | N7-C5 | -5.73 | 1.35 | 1.39 |
| 1 | 1 | 2693 | C | N1-C6 | -5.73 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 1 | 1452 | A | N9-C4 | -5.71 | 1.34 | 1.37 |
| 1 | 1 | 1330 | A | N9-C4 | -5.61 | 1.34 | 1.37 |
| 1 | 5 | 2363 | A | N9-C4 | -5.59 | 1.34 | 1.37 |
| 1 | 1 | 284 | A | N7-C5 | -5.58 | 1.35 | 1.39 |
| 1 | 1 | 2139 | A | N9-C4 | -5.58 | 1.34 | 1.37 |
| 1 | 5 | 1152 | G | N9-C4 | -5.56 | 1.33 | 1.38 |
| 1 | 5 | 2911 | A | N9-C4 | -5.56 | 1.34 | 1.37 |
| 28 | L3 | 7 | GLU | CG-CD | 5.55 | 1.60 | 1.51 |
| 2 | 6 | 992 | A | N9-C4 | -5.52 | 1.34 | 1.37 |
| 1 | 1 | 2932 | U | C2-N3 | -5.49 | 1.33 | 1.37 |
| 1 | 1 | 2702 | A | N7-C5 | -5.49 | 1.35 | 1.39 |
| 2 | 6 | 234 | G | N9-C4 | 5.48 | 1.42 | 1.38 |
| 59 | o5 | 75 | TYR | C-N | 5.47 | 1.46 | 1.34 |
| 1 | 1 | 2377 | G | C6-N1 | -5.41 | 1.35 | 1.39 |
| 1 | 5 | 1343 | A | N9-C4 | -5.41 | 1.34 | 1.37 |
| 32 | L7 | 214 | TRP | CB-CG | -5.41 | 1.40 | 1.50 |
| 1 | 1 | 660 | A | N9-C4 | -5.39 | 1.34 | 1.37 |
| 1 | 1 | 1319 | G | C6-N1 | -5.35 | 1.35 | 1.39 |
| 61 | O7 | 62 | GLY | CA-C | 5.35 | 1.60 | 1.51 |
| 1 | 1 | 397 | A | C6-N1 | -5.34 | 1.31 | 1.35 |
| 1 | 5 | 2401 | A | C5-C4 | 5.34 | 1.42 | 1.38 |
| 1 | 1 | 810 | A | N7-C5 | -5.34 | 1.36 | 1.39 |
| 51 | N7 | 36 | HIS | C-N | 5.26 | 1.44 | 1.34 |
| 2 | 2 | 966 | A | N9-C4 | -5.25 | 1.34 | 1.37 |
| 1 | 5 | 2601 | A | N9-C4 | -5.21 | 1.34 | 1.37 |
| 1 | 1 | 1911 | A | C5-C6 | -5.20 | 1.36 | 1.41 |
| 39 | M5 | 8 | GLU | CG-CD | 5.18 | 1.59 | 1.51 |
| 1 | 5 | 94 | G | N9-C4 | -5.18 | 1.33 | 1.38 |
| 1 | 1 | 2625 | C | N3-C4 | -5.17 | 1.30 | 1.33 |
| 1 | 1 | 60 | A | N9-C4 | -5.17 | 1.34 | 1.37 |
| 2 | 2 | 1732 | A | N9-C4 | -5.15 | 1.34 | 1.37 |
| 1 | 1 | 1322 | U | C4-O4 | 5.15 | 1.27 | 1.23 |
| 1 | 1 | 817 | A | N9-C4 | 5.14 | 1.41 | 1.37 |
| 1 | 5 | 336 | A | N9-C4 | -5.14 | 1.34 | 1.37 |
| 1 | 1 | 1432 | C | N1-C6 | -5.14 | 1.34 | 1.37 |
| 68 | s0 | 192 | THR | C-N | 5.14 | 1.45 | 1.34 |
| 1 | 1 | 2391 | G | C6-N1 | -5.13 | 1.35 | 1.39 |
| 1 | 1 | 1399 | A | N9-C4 | -5.10 | 1.34 | 1.37 |
| 1 | 5 | 920 | A | C5-C6 | -5.08 | 1.36 | 1.41 |
| 1 | 5 | 1152 | G | C6-N1 | 5.08 | 1.43 | 1.39 |
| 1 | 1 | 806 | A | N9-C4 | -5.08 | 1.34 | 1.37 |
| 1 | 1 | 2679 | A | C5-C6 | -5.07 | 1.36 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 5 | 2635 | A | N9-C4 | 5.05 | 1.40 | 1.37 |
| 1 | 5 | 2968 | G | C5-C6 | -5.04 | 1.37 | 1.42 |
| 1 | 1 | 1839 | A | N9-C4 | -5.04 | 1.34 | 1.37 |
| 1 | 1 | 1882 | G | C6-N1 | -5.04 | 1.36 | 1.39 |
| 2 | 6 | 803 | A | N9-C4 | 5.02 | 1.40 | 1.37 |
| 2 | 2 | 400 | A | N9-C4 | -5.00 | 1.34 | 1.37 |

All (3127) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 2 | 2 | 1059 | U | O5'-P-OP2 | -30.24 | 74.41 | 110.70 |
| 2 | 2 | 1059 | U | OP1-P-OP2 | 17.12 | 145.28 | 119.60 |
| 2 | 2 | 1059 | U | O5'-P-OP1 | -16.80 | 90.55 | 110.70 |
| 2 | 2 | 1058 | U | OP2-P-O3' | -13.98 | 74.45 | 105.20 |
| 1 | 5 | 1152 | G | N3-C4-C5 | 13.14 | 135.17 | 128.60 |
| 1 | 5 | 1592 | G | C5-C6-O6 | -12.74 | 120.96 | 128.60 |
| 4 | 8 | 115 | C | C6-N1-C2 | 12.53 | 125.31 | 120.30 |
| 1 | 1 | 2212 | C | C5-C6-N1 | 12.46 | 127.23 | 121.00 |
| 1 | 1 | 2212 | C | N1-C2-O2 | 12.41 | 126.34 | 118.90 |
| 1 | 5 | 2400 | G | C4-C5-N7 | 11.71 | 115.49 | 110.80 |
| 1 | 5 | 2917 | G | O5'-P-OP2 | -11.59 | 95.27 | 105.70 |
| 1 | 5 | 2403 | G | N1-C6-O6 | 11.43 | 126.76 | 119.90 |
| 1 | 5 | 2548 | C | N1-C2-O2 | 11.32 | 125.69 | 118.90 |
| 1 | 5 | 1356 | U | N3-C2-O2 | -11.30 | 114.29 | 122.20 |
| 1 | 1 | 638 | C | O5'-P-OP2 | -11.26 | 95.56 | 105.70 |
| 1 | 5 | 2968 | G | C5-C6-O6 | -11.16 | 121.90 | 128.60 |
| 1 | 1 | 1413 | G | N1-C6-O6 | 11.15 | 126.59 | 119.90 |
| 1 | 1 | 1432 | C | C6-N1-C2 | -11.03 | 115.89 | 120.30 |
| 1 | 1 | 2871 | G | O5'-P-OP2 | -11.00 | 95.80 | 105.70 |
| 1 | 1 | 645 | A | N1-C6-N6 | -10.99 | 112.01 | 118.60 |
| 1 | 5 | 2400 | G | N9-C4-C5 | -10.93 | 101.03 | 105.40 |
| 1 | 1 | 1916 | U | O5'-P-OP2 | -10.90 | 95.89 | 105.70 |
| 1 | 5 | 2968 | G | N1-C6-O6 | 10.89 | 126.43 | 119.90 |
| 1 | 1 | 2861 | U | O5'-P-OP1 | -10.86 | 95.93 | 105.70 |
| 2 | 2 | 1058 | U | OP1-P-O3' | -10.77 | 81.51 | 105.20 |
| 1 | 5 | 1152 | G | C8-N9-C1' | 10.73 | 140.95 | 127.00 |
| 1 | 1 | 1443 | G | C5-C6-O6 | -10.70 | 122.18 | 128.60 |
| 1 | 5 | 2983 | C | O5'-P-OP1 | -10.66 | 96.11 | 105.70 |
| 1 | 5 | 1152 | G | C4-N9-C1' | -10.59 | 112.73 | 126.50 |
| 1 | 1 | 891 | G | C5-C6-O6 | -10.56 | 122.27 | 128.60 |
| 1 | 1 | 1160 | C | C6-N1-C2 | 10.54 | 124.51 | 120.30 |
| 1 | 1 | 1495 | U | C5-C6-N1 | -10.52 | 117.44 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1 | 5 | 1152 | G | N3-C4-N9 | -10.47 | 119.72 | 126.00 |
| 1 | 5 | 2821 | C | C6-N1-C2 | -10.46 | 116.12 | 120.30 |
| 2 | 6 | 1467 | C | C6-N1-C2 | -10.42 | 116.13 | 120.30 |
| 1 | 1 | 2310 | U | O5'-P-OP1 | -10.35 | 96.38 | 105.70 |
| 2 | 2 | 1280 | C | C6-N1-C2 | -10.35 | 116.16 | 120.30 |
| 1 | 5 | 1592 | G | N1-C6-O6 | 10.35 | 126.11 | 119.90 |
| 1 | 5 | 2400 | G | C5-C6-O6 | -10.21 | 122.47 | 128.60 |
| 2 | 6 | 129 | U | OP1-P-O3' | -10.21 | 82.75 | 105.20 |
| 1 | 1 | 1451 | C | C6-N1-C2 | 10.11 | 124.34 | 120.30 |
| 1 | 1 | 2996 | U | N1-C2-O2 | 10.03 | 129.82 | 122.80 |
| 1 | 5 | 2548 | C | C6-N1-C2 | -10.00 | 116.30 | 120.30 |
| 1 | 5 | 2403 | G | C6-C5-N7 | -9.98 | 124.41 | 130.40 |
| 2 | 2 | 309 | C | C6-N1-C2 | -9.95 | 116.32 | 120.30 |
| 4 | 4 | 158 | U | O4'-C1'-N1 | 9.94 | 116.15 | 108.20 |
| 1 | 1 | 981 | U | O5'-P-OP1 | -9.90 | 96.78 | 105.70 |
| 1 | 5 | 2548 | C | N3-C2-O2 | -9.88 | 114.98 | 121.90 |
| 1 | 1 | 1403 | C | C6-N1-C2 | 9.88 | 124.25 | 120.30 |
| 1 | 1 | 2913 | C | C6-N1-C2 | 9.85 | 124.24 | 120.30 |
| 2 | 2 | 1096 | C | N1-C2-O2 | 9.80 | 124.78 | 118.90 |
| 2 | 6 | 129 | U | OP2-P-O3' | -9.73 | 83.78 | 105.20 |
| 1 | 1 | 2192 | C | C6-N1-C2 | -9.72 | 116.41 | 120.30 |
| 1 | 5 | 1356 | U | N1-C2-O2 | 9.72 | 129.60 | 122.80 |
| 1 | 1 | 2827 | U | C5-C6-N1 | -9.68 | 117.86 | 122.70 |
| 1 | 5 | 700 | C | C6-N1-C2 | -9.66 | 116.44 | 120.30 |
| 1 | 5 | 1793 | C | C6-N1-C2 | 9.63 | 124.15 | 120.30 |
| 1 | 5 | 439 | C | C6-N1-C2 | -9.60 | 116.46 | 120.30 |
| 1 | 1 | 2821 | C | C6-N1-C2 | -9.59 | 116.47 | 120.30 |
| 2 | 2 | 405 | C | C6-N1-C2 | 9.56 | 124.13 | 120.30 |
| 1 | 1 | 891 | G | N1-C6-O6 | 9.53 | 125.62 | 119.90 |
| 1 | 1 | 2273 | G | O5'-P-OP2 | -9.52 | 97.13 | 105.70 |
| 1 | 5 | 439 | C | N1-C2-O2 | 9.52 | 124.61 | 118.90 |
| 1 | 1 | 966 | U | N3-C4-O4 | 9.49 | 126.04 | 119.40 |
| 1 | 1 | 631 | U | O5'-P-OP2 | -9.46 | 97.19 | 105.70 |
| 1 | 1 | 1926 | C | O5'-P-OP2 | -9.46 | 97.19 | 105.70 |
| 1 | 5 | 200 | C | C6-N1-C2 | -9.46 | 116.52 | 120.30 |
| 1 | 5 | 2572 | C | N1-C2-O2 | 9.42 | 124.55 | 118.90 |
| 1 | 5 | 2355 | G | N1-C6-O6 | 9.41 | 125.55 | 119.90 |
| 1 | 5 | 2400 | G | N1-C6-O6 | 9.40 | 125.54 | 119.90 |
| 1 | 5 | 3269 | U | C5-C6-N1 | 9.38 | 127.39 | 122.70 |
| 1 | 1 | 2679 | A | N1-C6-N6 | 9.35 | 124.21 | 118.60 |
| 1 | 1 | 2922 | G | C6-C5-N7 | -9.34 | 124.80 | 130.40 |
| 2 | 2 | 1751 | C | C6-N1-C2 | 9.31 | 124.03 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 1 | 1454 | A | C8-N9-C4 | 9.31 | 109.52 | 105.80 |
| 1 | 1 | 1338 | C | C6-N1-C2 | -9.27 | 116.59 | 120.30 |
| 1 | 5 | 439 | C | C2-N1-C1' | 9.27 | 128.99 | 118.80 |
| 1 | 5 | 1308 | A | C8-N9-C4 | -9.22 | 102.11 | 105.80 |
| 1 | 5 | 3278 | C | N1-C2-O2 | 9.21 | 124.42 | 118.90 |
| 1 | 1 | 55 | G | C8-N9-C4 | 9.19 | 110.08 | 106.40 |
| 1 | 1 | 945 | C | C6-N1-C2 | -9.19 | 116.63 | 120.30 |
| 2 | 2 | 453 | U | C2-N1-C1' | 9.16 | 128.69 | 117.70 |
| 1 | 1 | 645 | A | N9-C4-C5 | 9.15 | 109.46 | 105.80 |
| 1 | 1 | 2355 | G | N1-C6-O6 | 9.14 | 125.38 | 119.90 |
| 1 | 5 | 982 | C | C6-N1-C2 | -9.13 | 116.65 | 120.30 |
| 1 | 5 | 2403 | G | C4-C5-C6 | 9.13 | 124.28 | 118.80 |
| 1 | 1 | 639 | G | N1-C6-O6 | 9.11 | 125.36 | 119.90 |
| 1 | 5 | 424 | G | N1-C6-O6 | 9.10 | 125.36 | 119.90 |
| 4 | 4 | 125 | U | N1-C2-O2 | 9.10 | 129.17 | 122.80 |
| 1 | 1 | 914 | A | N1-C6-N6 | -9.09 | 113.15 | 118.60 |
| 4 | 4 | 140 | G | N1-C6-O6 | 9.08 | 125.35 | 119.90 |
| 3 | 3 | 15 | C | C6-N1-C2 | 9.07 | 123.93 | 120.30 |
| 1 | 1 | 1763 | U | C2-N1-C1' | 9.07 | 128.58 | 117.70 |
| 1 | 5 | 824 | C | C6-N1-C2 | -9.07 | 116.67 | 120.30 |
| 1 | 5 | 3217 | C | C6-N1-C2 | 9.06 | 123.93 | 120.30 |
| 4 | 4 | 54 | A | N1-C6-N6 | 9.05 | 124.03 | 118.60 |
| 1 | 1 | 1665 | C | C6-N1-C2 | 9.04 | 123.91 | 120.30 |
| 1 | 5 | 2156 | C | C6-N1-C2 | 9.03 | 123.91 | 120.30 |
| 1 | 5 | 408 | A | C8-N9-C4 | -9.02 | 102.19 | 105.80 |
| 1 | 5 | 2383 | C | C6-N1-C2 | -9.01 | 116.69 | 120.30 |
| 1 | 1 | 1422 | G | N1-C6-O6 | 9.00 | 125.30 | 119.90 |
| 1 | 5 | 833 | G | C8-N9-C4 | 9.00 | 110.00 | 106.40 |
| 2 | 6 | 320 | U | C5-C6-N1 | 8.98 | 127.19 | 122.70 |
| 1 | 1 | 884 | A | N1-C6-N6 | 8.98 | 123.99 | 118.60 |
| 13 | C8 | 15 | LEU | CA-CB-CG | 8.97 | 135.93 | 115.30 |
| 1 | 1 | 546 | C | O5'-P-OP1 | -8.93 | 97.67 | 105.70 |
| 1 | 5 | 2181 | C | C6-N1-C2 | 8.86 | 123.84 | 120.30 |
| 1 | 5 | 1312 | C | C6-N1-C2 | -8.83 | 116.77 | 120.30 |
| 1 | 1 | 1866 | C | N1-C2-O2 | 8.80 | 124.18 | 118.90 |
| 1 | 1 | 2693 | C | C6-N1-C2 | 8.79 | 123.82 | 120.30 |
| 1 | 1 | 1589 | A | C8-N9-C4 | 8.79 | 109.32 | 105.80 |
| 1 | 5 | 875 | G | O5'-P-OP2 | -8.77 | 97.81 | 105.70 |
| 1 | 1 | 3025 | C | C6-N1-C2 | 8.76 | 123.80 | 120.30 |
| 1 | 1 | 667 | C | C6-N1-C2 | 8.74 | 123.80 | 120.30 |
| 1 | 5 | 1413 | G | N1-C6-O6 | 8.74 | 125.14 | 119.90 |
| 1 | 5 | 860 | G | C4-C5-N7 | 8.71 | 114.28 | 110.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | 6 | 558 | U | C2-N1-C1' | 8.70 | 128.15 | 117.70 |
| 1 | 1 | 1306 | G | C6-C5-N7 | -8.69 | 125.18 | 130.40 |
| 1 | 1 | 3266 | G | C8-N9-C4 | -8.69 | 102.92 | 106.40 |
| 2 | 2 | 1420 | C | C6-N1-C2 | 8.69 | 123.78 | 120.30 |
| 1 | 1 | 2093 | A | C2-N3-C4 | 8.69 | 114.94 | 110.60 |
| 1 | 1 | 289 | A | O5'-P-OP1 | -8.67 | 97.90 | 105.70 |
| 1 | 1 | 1279 | C | C6-N1-C2 | -8.67 | 116.83 | 120.30 |
| 4 | 8 | 14 | C | O5'-P-OP2 | -8.64 | 97.93 | 105.70 |
| 1 | 5 | 2885 | C | O5'-P-OP2 | -8.63 | 97.94 | 105.70 |
| 1 | 1 | 2937 | G | C5-C6-O6 | -8.62 | 123.43 | 128.60 |
| 43 | M9 | 185 | LEU | CA-CB-CG | 8.61 | 135.10 | 115.30 |
| 2 | 6 | 794 | U | C2-N1-C1' | 8.61 | 128.03 | 117.70 |
| 1 | 1 | 924 | G | N1-C6-O6 | -8.59 | 114.75 | 119.90 |
| 1 | 1 | 1941 | C | C6-N1-C2 | -8.59 | 116.87 | 120.30 |
| 1 | 5 | 3093 | C | C6-N1-C2 | 8.58 | 123.73 | 120.30 |
| 1 | 1 | 2608 | G | C8-N9-C4 | 8.58 | 109.83 | 106.40 |
| 2 | 6 | 589 | C | C6-N1-C2 | -8.57 | 116.87 | 120.30 |
| 1 | 5 | 21 | G | N1-C6-O6 | -8.57 | 114.76 | 119.90 |
| 1 | 1 | 2171 | G | N1-C6-O6 | -8.57 | 114.76 | 119.90 |
| 1 | 5 | 835 | G | N3-C4-N9 | -8.56 | 120.86 | 126.00 |
| 4 | 4 | 134 | G | O5'-P-OP1 | -8.56 | 98.00 | 105.70 |
| 1 | 5 | 2821 | C | N3-C2-O2 | -8.56 | 115.91 | 121.90 |
| 1 | 5 | 2548 | C | C2-N1-C1' | 8.55 | 128.21 | 118.80 |
| 2 | 6 | 1490 | C | C6-N1-C2 | -8.54 | 116.89 | 120.30 |
| 1 | 1 | 312 | C | C6-N1-C2 | -8.53 | 116.89 | 120.30 |
| 1 | 1 | 753 | C | C6-N1-C2 | 8.51 | 123.70 | 120.30 |
| 1 | 1 | 979 | U | C6-N1-C2 | -8.50 | 115.90 | 121.00 |
| 4 | 8 | 45 | C | C6-N1-C2 | 8.50 | 123.70 | 120.30 |
| 1 | 1 | 1493 | G | N1-C6-O6 | -8.49 | 114.80 | 119.90 |
| 1 | 5 | 1412 | G | N1-C6-O6 | 8.49 | 124.99 | 119.90 |
| 1 | 1 | 2944 | U | C6-N1-C2 | -8.48 | 115.91 | 121.00 |
| 2 | 6 | 337 | G | C4-C5-N7 | 8.48 | 114.19 | 110.80 |
| 1 | 5 | 1911 | A | N1-C6-N6 | -8.47 | 113.52 | 118.60 |
| 6 | C1 | 5 | LEU | CA-CB-CG | 8.46 | 134.76 | 115.30 |
| 2 | 2 | 1077 | C | C6-N1-C2 | -8.46 | 116.92 | 120.30 |
| 1 | 5 | 2400 | G | C8-N9-C4 | 8.45 | 109.78 | 106.40 |
| 1 | 5 | 1839 | A | C8-N9-C4 | 8.44 | 109.18 | 105.80 |
| 1 | 5 | 3205 | G | N1-C6-O6 | 8.44 | 124.96 | 119.90 |
| 1 | 1 | 1507 | G | N1-C6-O6 | 8.44 | 124.96 | 119.90 |
| 1 | 1 | 924 | G | C5-C6-O6 | 8.43 | 133.66 | 128.60 |
| 3 | 3 | 47 | C | C6-N1-C2 | -8.42 | 116.93 | 120.30 |
| 1 | 5 | 2606 | G | N3-C4-N9 | 8.42 | 131.05 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 1 | 2400 | G | C5-C6-O6 | -8.41 | 123.55 | 128.60 |
| 1 | 1 | 1889 | G | N1-C6-O6 | 8.41 | 124.94 | 119.90 |
| 1 | 1 | 2862 | U | C6-N1-C2 | 8.41 | 126.05 | 121.00 |
| 1 | 1 | 42 | C | N3-C4-C5 | 8.40 | 125.26 | 121.90 |
| 2 | 6 | 697 | C | C6-N1-C2 | -8.39 | 116.94 | 120.30 |
| 4 | 8 | 81 | U | N3-C2-O2 | -8.39 | 116.33 | 122.20 |
| 1 | 1 | 979 | U | N3-C2-O2 | -8.38 | 116.33 | 122.20 |
| 29 | 14 | 339 | LEU | CA-CB-CG | 8.38 | 134.57 | 115.30 |
| 1 | 1 | 46 | U | O5'-P-OP1 | -8.37 | 98.17 | 105.70 |
| 1 | 1 | 1604 | G | N3-C4-C5 | -8.37 | 124.42 | 128.60 |
| 1 | 1 | 1306 | G | N3-C4-N9 | 8.37 | 131.02 | 126.00 |
| 1 | 1 | 92 | G | C4-C5-N7 | 8.36 | 114.14 | 110.80 |
| 1 | 5 | 1550 | C | C6-N1-C2 | -8.36 | 116.95 | 120.30 |
| 1 | 1 | 545 | U | C2-N1-C1' | 8.35 | 127.72 | 117.70 |
| 1 | 1 | 2212 | C | C2-N1-C1' | 8.35 | 127.99 | 118.80 |
| 1 | 1 | 2568 | C | N1-C2-O2 | 8.35 | 123.91 | 118.90 |
| 1 | 5 | 1437 | C | C6-N1-C2 | -8.35 | 116.96 | 120.30 |
| 1 | 1 | 3076 | C | N3-C4-C5 | -8.32 | 118.57 | 121.90 |
| 2 | 6 | 234 | G | N3-C4-C5 | -8.31 | 124.44 | 128.60 |
| 1 | 1 | 424 | G | O5'-P-OP2 | -8.31 | 98.22 | 105.70 |
| 1 | 1 | 675 | C | C6-N1-C2 | -8.30 | 116.98 | 120.30 |
| 1 | 5 | 1592 | G | C4-C5-N7 | 8.30 | 114.12 | 110.80 |
| 1 | 5 | 2881 | C | C6-N1-C2 | 8.30 | 123.62 | 120.30 |
| 1 | 5 | 2160 | G | C8-N9-C4 | 8.28 | 109.71 | 106.40 |
| 1 | 1 | 2212 | C | C4-C5-C6 | -8.27 | 113.27 | 117.40 |
| 1 | 5 | 1220 | U | C5-C6-N1 | 8.27 | 126.83 | 122.70 |
| 1 | 5 | 1633 | C | C6-N1-C2 | -8.27 | 116.99 | 120.30 |
| 1 | 5 | 2245 | C | C6-N1-C2 | 8.26 | 123.60 | 120.30 |
| 1 | 5 | 2968 | G | C4-C5-N7 | 8.26 | 114.10 | 110.80 |
| 1 | 1 | 648 | C | C6-N1-C2 | -8.25 | 117.00 | 120.30 |
| 1 | 1 | 1495 | U | C4-C5-C6 | 8.25 | 124.65 | 119.70 |
| 1 | 5 | 1412 | G | C5-C6-O6 | -8.25 | 123.65 | 128.60 |
| 1 | 1 | 1609 | C | O5'-P-OP2 | -8.25 | 98.28 | 105.70 |
| 1 | 1 | 3217 | C | C2-N1-C1' | 8.23 | 127.85 | 118.80 |
| 1 | 1 | 379 | C | C6-N1-C2 | 8.21 | 123.59 | 120.30 |
| 1 | 1 | 1385 | C | C6-N1-C2 | 8.21 | 123.58 | 120.30 |
| 26 | E1 | 105 | TYR | C-N-CA | 8.20 | 142.20 | 121.70 |
| 1 | 5 | 979 | U | C6-N1-C2 | -8.20 | 116.08 | 121.00 |
| 1 | 1 | 2937 | G | N1-C6-O6 | 8.19 | 124.81 | 119.90 |
| 2 | 6 | 1173 | C | C6-N1-C2 | -8.19 | 117.03 | 120.30 |
| 1 | 1 | 1306 | G | C5-C6-O6 | -8.19 | 123.69 | 128.60 |
| 1 | 1 | 3319 | U | O5'-P-OP1 | -8.18 | 98.34 | 105.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 5 | 635 | G | N9-C4-C5 | -8.18 | 102.13 | 105.40 |
| 1 | 5 | 3124 | G | C6-C5-N7 | -8.17 | 125.50 | 130.40 |
| 1 | 1 | 1092 | C | C6-N1-C2 | -8.17 | 117.03 | 120.30 |
| 2 | 6 | 1773 | C | C6-N1-C2 | -8.15 | 117.04 | 120.30 |
| 1 | 1 | 1201 | C | C6-N1-C2 | -8.15 | 117.04 | 120.30 |
| 1 | 5 | 925 | A | N1-C6-N6 | 8.14 | 123.49 | 118.60 |
| 1 | 1 | 392 | G | C8-N9-C4 | -8.14 | 103.14 | 106.40 |
| 1 | 1 | 2311 | G | C5-C6-O6 | -8.13 | 123.72 | 128.60 |
| 1 | 5 | 726 | G | C8-N9-C4 | -8.13 | 103.15 | 106.40 |
| 1 | 1 | 981 | U | C5-C6-N1 | 8.11 | 126.75 | 122.70 |
| 1 | 1 | 92 | G | N9-C4-C5 | -8.10 | 102.16 | 105.40 |
| 1 | 1 | 2156 | C | C6-N1-C2 | 8.10 | 123.54 | 120.30 |
| 1 | 1 | 2400 | G | C4-C5-N7 | 8.08 | 114.03 | 110.80 |
| 1 | 5 | 347 | G | C5-C6-O6 | -8.08 | 123.75 | 128.60 |
| 1 | 1 | 1432 | C | N3-C4-C5 | -8.08 | 118.67 | 121.90 |
| 2 | 6 | 501 | U | N1-C2-O2 | 8.07 | 128.45 | 122.80 |
| 1 | 5 | 860 | G | N1-C6-O6 | 8.04 | 124.72 | 119.90 |
| 2 | 6 | 1541 | G | N1-C6-O6 | -8.04 | 115.08 | 119.90 |
| 1 | 1 | 636 | C | C6-N1-C2 | -8.04 | 117.09 | 120.30 |
| 1 | 1 | 693 | A | O5'-P-OP1 | -8.03 | 98.47 | 105.70 |
| 1 | 1 | 2572 | C | C2-N1-C1' | 8.03 | 127.63 | 118.80 |
| 1 | 1 | 3217 | C | N1-C2-O2 | 8.03 | 123.72 | 118.90 |
| 1 | 5 | 860 | G | C5-C6-O6 | -8.03 | 123.78 | 128.60 |
| 2 | 6 | 607 | G | N1-C6-O6 | 8.02 | 124.71 | 119.90 |
| 2 | 2 | 1363 | U | N3-C2-O2 | -8.02 | 116.59 | 122.20 |
| 1 | 5 | 1412 | G | C6-C5-N7 | -8.01 | 125.59 | 130.40 |
| 1 | 1 | 218 | G | O5'-P-OP2 | -8.00 | 98.50 | 105.70 |
| 1 | 1 | 2682 | C | C6-N1-C2 | 8.00 | 123.50 | 120.30 |
| 4 | 8 | 81 | U | N1-C2-O2 | 8.00 | 128.40 | 122.80 |
| 1 | 5 | 1152 | G | C5-N7-C8 | -7.99 | 100.30 | 104.30 |
| 2 | 6 | 1465 | C | C6-N1-C2 | -7.99 | 117.10 | 120.30 |
| 1 | 5 | 353 | G | O5'-P-OP2 | -7.98 | 98.52 | 105.70 |
| 1 | 1 | 2922 | G | N3-C4-N9 | 7.97 | 130.78 | 126.00 |
| 1 | 1 | 2572 | C | C6-N1-C2 | -7.97 | 117.11 | 120.30 |
| 2 | 6 | 742 | U | C6-N1-C2 | -7.97 | 116.22 | 121.00 |
| 1 | 1 | 1015 | U | O5'-P-OP2 | -7.97 | 98.53 | 105.70 |
| 1 | 1 | 2206 | G | C8-N9-C1' | -7.97 | 116.64 | 127.00 |
| 1 | 5 | 2635 | A | C8-N9-C4 | -7.97 | 102.61 | 105.80 |
| 1 | 5 | 2952 | G | N1-C6-O6 | 7.96 | 124.68 | 119.90 |
| 1 | 1 | 1381 | A | C8-N9-C4 | 7.96 | 108.98 | 105.80 |
| 1 | 1 | 1762 | C | P-O3'-C3' | 7.96 | 129.25 | 119.70 |
| 2 | 2 | 1096 | C | C2-N1-C1' | 7.95 | 127.55 | 118.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 5 | 1137 | C | N1-C2-O2 | 7.94 | 123.66 | 118.90 |
| 1 | 5 | 1114 | U | C5-C4-O4 | -7.94 | 121.14 | 125.90 |
| 1 | 5 | 1663 | C | C6-N1-C2 | 7.93 | 123.47 | 120.30 |
| 1 | 5 | 2594 | C | O5'-P-OP1 | -7.93 | 98.56 | 105.70 |
| 1 | 1 | 2612 | U | C6-N1-C2 | -7.92 | 116.25 | 121.00 |
| 1 | 1 | 924 | G | N9-C4-C5 | 7.92 | 108.57 | 105.40 |
| 1 | 5 | 1582 | C | C2-N1-C1' | 7.91 | 127.50 | 118.80 |
| 1 | 1 | 2568 | C | N3-C2-O2 | -7.91 | 116.36 | 121.90 |
| 2 | 2 | 758 | U | N3-C2-O2 | -7.91 | 116.66 | 122.20 |
| 1 | 1 | 3084 | C | C6-N1-C2 | -7.90 | 117.14 | 120.30 |
| 1 | 1 | 953 | G | N1-C6-O6 | -7.89 | 115.16 | 119.90 |
| 1 | 1 | 1495 | U | N1-C2-N3 | 7.89 | 119.63 | 114.90 |
| 2 | 2 | 131 | C | C2-N1-C1' | 7.89 | 127.47 | 118.80 |
| 2 | 2 | 864 | U | C6-N1-C2 | -7.89 | 116.27 | 121.00 |
| 1 | 5 | 1307 | G | P-O3'-C3' | 7.88 | 129.15 | 119.70 |
| 1 | 1 | 2867 | C | C6-N1-C2 | 7.87 | 123.45 | 120.30 |
| 1 | 5 | 54 | C | C6-N1-C2 | 7.87 | 123.45 | 120.30 |
| 2 | 2 | 1363 | U | N1-C2-O2 | 7.86 | 128.30 | 122.80 |
| 1 | 5 | 1913 | A | N1-C6-N6 | 7.86 | 123.31 | 118.60 |
| 1 | 1 | 1319 | G | N1-C6-O6 | -7.86 | 115.19 | 119.90 |
| 1 | 1 | 3266 | G | N9-C4-C5 | 7.86 | 108.54 | 105.40 |
| 1 | 1 | 1408 | G | N1-C6-O6 | 7.84 | 124.61 | 119.90 |
| 1 | 1 | 2183 | A | N1-C6-N6 | 7.84 | 123.31 | 118.60 |
| 2 | 2 | 1096 | C | N3-C2-O2 | -7.84 | 116.41 | 121.90 |
| 1 | 1 | 1548 | C | C6-N1-C2 | -7.84 | 117.17 | 120.30 |
| 2 | 2 | 1011 | G | C8-N9-C4 | -7.83 | 103.27 | 106.40 |
| 1 | 1 | 353 | G | C8-N9-C4 | 7.83 | 109.53 | 106.40 |
| 1 | 1 | 3075 | G | N1-C6-O6 | 7.83 | 124.60 | 119.90 |
| 1 | 5 | 2409 | G | C8-N9-C4 | 7.83 | 109.53 | 106.40 |
| 2 | 6 | 590 | C | C6-N1-C2 | -7.82 | 117.17 | 120.30 |
| 1 | 1 | 1194 | G | C5-C6-O6 | -7.82 | 123.91 | 128.60 |
| 1 | 1 | 2400 | G | N1-C6-O6 | 7.82 | 124.59 | 119.90 |
| 2 | 2 | 1280 | C | N3-C4-C5 | -7.82 | 118.77 | 121.90 |
| 1 | 1 | 1443 | G | N1-C6-O6 | 7.81 | 124.59 | 119.90 |
| 1 | 5 | 2406 | C | C6-N1-C2 | 7.81 | 123.42 | 120.30 |
| 1 | 1 | 780 | A | N1-C6-N6 | -7.80 | 113.92 | 118.60 |
| 1 | 5 | 439 | C | N3-C2-O2 | -7.80 | 116.44 | 121.90 |
| 2 | 2 | 1745 | G | N3-C4-N9 | 7.80 | 130.68 | 126.00 |
| 1 | 1 | 2934 | A | N1-C6-N6 | 7.80 | 123.28 | 118.60 |
| 1 | 1 | 2925 | C | N1-C2-O2 | 7.79 | 123.58 | 118.90 |
| 1 | 1 | 1773 | C | C6-N1-C2 | 7.79 | 123.42 | 120.30 |
| 2 | 6 | 1196 | A | P-O3'-C3' | 7.79 | 129.04 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 1 | 895 | A | C4-C5-N7 | 7.79 | 114.59 | 110.70 |
| 2 | 6 | 499 | U | C5-C6-N1 | 7.78 | 126.59 | 122.70 |
| 1 | 5 | 1413 | G | C6-C5-N7 | -7.78 | 125.73 | 130.40 |
| 1 | 5 | 1581 | C | N1-C2-O2 | 7.77 | 123.56 | 118.90 |
| 1 | 1 | 2996 | U | N3-C2-O2 | -7.77 | 116.76 | 122.20 |
| 1 | 1 | 2809 | C | C6-N1-C2 | -7.76 | 117.19 | 120.30 |
| 4 | 4 | 4 | C | O5'-P-OP2 | -7.76 | 98.71 | 105.70 |
| 1 | 1 | 1507 | G | C5-C6-O6 | -7.76 | 123.94 | 128.60 |
| 1 | 5 | 2871 | G | N1-C6-O6 | 7.76 | 124.56 | 119.90 |
| 1 | 1 | 1306 | G | N1-C6-O6 | 7.76 | 124.56 | 119.90 |
| 1 | 1 | 142 | C | C6-N1-C2 | -7.75 | 117.20 | 120.30 |
| 1 | 1 | 1604 | G | C4-N9-C1' | 7.75 | 136.58 | 126.50 |
| 1 | 1 | 924 | G | C4-C5-N7 | -7.75 | 107.70 | 110.80 |
| 1 | 1 | 1542 | G | C4-C5-N7 | 7.74 | 113.90 | 110.80 |
| 57 | o3 | 88 | ASN | C-N-CA | -7.73 | 102.36 | 121.70 |
| 1 | 1 | 2827 | U | N3-C4-O4 | -7.73 | 113.99 | 119.40 |
| 1 | 1 | 633 | C | C6-N1-C2 | 7.73 | 123.39 | 120.30 |
| 1 | 5 | 1307 | G | O5'-P-OP1 | -7.73 | 98.74 | 105.70 |
| 1 | 5 | 2376 | G | C5-C6-O6 | -7.73 | 123.96 | 128.60 |
| 2 | 2 | 1161 | C | O5'-P-OP2 | -7.73 | 98.74 | 105.70 |
| 1 | 1 | 2767 | U | O5'-P-OP2 | -7.73 | 98.75 | 105.70 |
| 1 | 5 | 1730 | G | N3-C4-C5 | -7.72 | 124.74 | 128.60 |
| 2 | 2 | 1059 | U | N3-C2-O2 | -7.72 | 116.80 | 122.20 |
| 1 | 1 | 2206 | G | N3-C4-N9 | 7.70 | 130.62 | 126.00 |
| 1 | 1 | 2572 | C | N1-C2-O2 | 7.70 | 123.52 | 118.90 |
| 1 | 5 | 2572 | C | N3-C2-O2 | -7.70 | 116.51 | 121.90 |
| 1 | 5 | 3245 | A | N1-C2-N3 | 7.70 | 133.15 | 129.30 |
| 1 | 1 | 3278 | C | N1-C2-O2 | 7.69 | 123.52 | 118.90 |
| 2 | 6 | 794 | U | C6-N1-C1' | -7.69 | 110.43 | 121.20 |
| 1 | 5 | 3245 | A | N7-C8-N9 | 7.69 | 117.64 | 113.80 |
| 1 | 1 | 1156 | C | C5-C4-N4 | -7.66 | 114.84 | 120.20 |
| 1 | 1 | 1389 | G | C8-N9-C4 | 7.66 | 109.46 | 106.40 |
| 1 | 1 | 823 | C | C6-N1-C2 | -7.66 | 117.24 | 120.30 |
| 1 | 5 | 3076 | C | C6-N1-C2 | -7.66 | 117.24 | 120.30 |
| 1 | 1 | 1348 | U | C6-N1-C2 | -7.65 | 116.41 | 121.00 |
| 1 | 1 | 1424 | C | C6-N1-C2 | 7.65 | 123.36 | 120.30 |
| 1 | 1 | 2212 | C | N3-C2-O2 | -7.65 | 116.55 | 121.90 |
| 1 | 1 | 1359 | C | C6-N1-C2 | 7.64 | 123.36 | 120.30 |
| 1 | 1 | 3076 | C | C6-N1-C2 | -7.64 | 117.25 | 120.30 |
| 2 | 2 | 1467 | C | C6-N1-C2 | -7.63 | 117.25 | 120.30 |
| 1 | 1 | 2209 | U | O5'-P-OP2 | -7.63 | 98.83 | 105.70 |
| 1 | 1 | 609 | G | C5-C6-O6 | -7.62 | 124.03 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 5 | 439 | C | C5-C6-N1 | 7.61 | 124.81 | 121.00 |
| 4 | 8 | 44 | A | N1-C6-N6 | 7.61 | 123.16 | 118.60 |
| 1 | 5 | 1592 | G | C6-C5-N7 | -7.61 | 125.84 | 130.40 |
| 2 | 2 | 1157 | A | C8-N9-C4 | -7.60 | 102.76 | 105.80 |
| 1 | 5 | 1861 | G | C8-N9-C4 | -7.60 | 103.36 | 106.40 |
| 1 | 1 | 2612 | U | C5-C6-N1 | 7.60 | 126.50 | 122.70 |
| 1 | 5 | 1412 | G | C4-C5-N7 | 7.59 | 113.84 | 110.80 |
| 1 | 1 | 1444 | G | N1-C6-O6 | 7.58 | 124.45 | 119.90 |
| 2 | 6 | 1491 | U | N3-C2-O2 | -7.58 | 116.89 | 122.20 |
| 2 | 6 | 1582 | U | C6-N1-C2 | 7.58 | 125.55 | 121.00 |
| 2 | 2 | 14 | C | C6-N1-C2 | -7.58 | 117.27 | 120.30 |
| 1 | 1 | 2964 | G | O5'-P-OP1 | -7.58 | 98.88 | 105.70 |
| 1 | 1 | 917 | A | O5'-P-OP2 | -7.57 | 98.88 | 105.70 |
| 1 | 1 | 2208 | A | P-O3'-C3' | 7.57 | 128.79 | 119.70 |
| 4 | 4 | 54 | A | C6-C5-N7 | -7.57 | 127.00 | 132.30 |
| 1 | 1 | 2206 | G | C4-N9-C1' | 7.57 | 136.34 | 126.50 |
| 1 | 1 | 2967 | A | N1-C6-N6 | 7.57 | 123.14 | 118.60 |
| 1 | 5 | 2268 | U | C5-C6-N1 | 7.57 | 126.48 | 122.70 |
| 1 | 5 | 2403 | G | C5-C6-N1 | -7.57 | 107.72 | 111.50 |
| 1 | 1 | 1526 | U | O5'-P-OP2 | -7.57 | 98.89 | 105.70 |
| 1 | 5 | 915 | A | O5'-P-OP1 | -7.56 | 98.90 | 105.70 |
| 1 | 5 | 2816 | G | N1-C6-O6 | 7.56 | 124.44 | 119.90 |
| 1 | 1 | 1546 | A | C8-N9-C4 | -7.56 | 102.78 | 105.80 |
| 2 | 6 | 103 | A | P-O3'-C3' | 7.55 | 128.75 | 119.70 |
| 1 | 5 | 3004 | C | C6-N1-C2 | 7.54 | 123.32 | 120.30 |
| 1 | 5 | 3195 | U | C5-C6-N1 | 7.53 | 126.46 | 122.70 |
| 1 | 5 | 423 | A | N1-C6-N6 | -7.52 | 114.09 | 118.60 |
| 1 | 5 | 2993 | G | N1-C6-O6 | -7.52 | 115.39 | 119.90 |
| 2 | 6 | 501 | U | N3-C2-O2 | -7.52 | 116.94 | 122.20 |
| 1 | 5 | 1145 | G | N3-C4-N9 | 7.52 | 130.51 | 126.00 |
| 2 | 6 | 414 | C | C6-N1-C2 | 7.51 | 123.31 | 120.30 |
| 1 | 5 | 2831 | G | C5-C6-O6 | -7.51 | 124.09 | 128.60 |
| 1 | 1 | 1820 | U | P-O3'-C3' | 7.51 | 128.71 | 119.70 |
| 1 | 1 | 298 | U | N1-C2-O2 | 7.50 | 128.05 | 122.80 |
| 1 | 5 | 2355 | G | C6-C5-N7 | -7.50 | 125.90 | 130.40 |
| 3 | 3 | 104 | A | O5'-P-OP2 | -7.50 | 98.95 | 105.70 |
| 2 | 6 | 558 | U | N3-C2-O2 | -7.50 | 116.95 | 122.20 |
| 1 | 1 | 748 | U | C6-N1-C2 | -7.49 | 116.50 | 121.00 |
| 1 | 1 | 1854 | C | C6-N1-C2 | -7.49 | 117.30 | 120.30 |
| 1 | 1 | 895 | A | C5-C6-N6 | -7.49 | 117.71 | 123.70 |
| 1 | 1 | 1852 | G | N1-C6-O6 | 7.49 | 124.39 | 119.90 |
| 2 | 6 | 13 | C | C6-N1-C2 | -7.49 | 117.30 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 1 | 3194 | C | C2-N1-C1' | 7.49 | 127.03 | 118.80 |
| 2 | 2 | 1562 | G | C8-N9-C4 | 7.49 | 109.39 | 106.40 |
| 1 | 1 | 3226 | A | O5'-P-OP1 | -7.48 | 98.97 | 105.70 |
| 2 | 6 | 577 | G | C6-C5-N7 | -7.47 | 125.92 | 130.40 |
| 3 | 3 | 83 | U | C5-C6-N1 | -7.46 | 118.97 | 122.70 |
| 3 | 3 | 116 | C | C6-N1-C2 | -7.46 | 117.31 | 120.30 |
| 2 | 6 | 781 | U | C2-N1-C1' | 7.46 | 126.66 | 117.70 |
| 1 | 1 | 1413 | G | C5-C6-O6 | -7.46 | 124.12 | 128.60 |
| 1 | 1 | 2711 | C | C6-N1-C2 | -7.46 | 117.31 | 120.30 |
| 1 | 1 | 1000 | C | C6-N1-C2 | 7.46 | 123.28 | 120.30 |
| 1 | 5 | 3260 | G | N3-C4-N9 | 7.46 | 130.48 | 126.00 |
| 1 | 1 | 2355 | G | C6-C5-N7 | -7.45 | 125.93 | 130.40 |
| 1 | 1 | 3382 | U | C2-N1-C1' | 7.45 | 126.64 | 117.70 |
| 1 | 1 | 1028 | U | P-O3'-C3' | 7.44 | 128.63 | 119.70 |
| 1 | 5 | 2831 | G | N1-C6-O6 | 7.44 | 124.37 | 119.90 |
| 1 | 5 | 2572 | C | C2-N1-C1' | 7.44 | 126.98 | 118.80 |
| 2 | 6 | 765 | G | C8-N9-C4 | 7.44 | 109.38 | 106.40 |
| 3 | 3 | 80 | G | C8-N9-C4 | -7.43 | 103.43 | 106.40 |
| 1 | 1 | 1451 | C | N3-C2-O2 | 7.43 | 127.10 | 121.90 |
| 2 | 2 | 1459 | C | C6-N1-C2 | -7.43 | 117.33 | 120.30 |
| 1 | 1 | 1417 | G | C4-C5-N7 | 7.42 | 113.77 | 110.80 |
| 1 | 5 | 3103 | A | C8-N9-C4 | 7.42 | 108.77 | 105.80 |
| 1 | 1 | 3269 | U | N3-C2-O2 | -7.42 | 117.00 | 122.20 |
| 2 | 2 | 131 | C | N1-C2-O2 | 7.42 | 123.35 | 118.90 |
| 2 | 2 | 992 | A | C5-N7-C8 | -7.42 | 100.19 | 103.90 |
| 1 | 5 | 887 | G | N1-C6-O6 | 7.41 | 124.34 | 119.90 |
| 1 | 1 | 1417 | G | N9-C4-C5 | -7.40 | 102.44 | 105.40 |
| 2 | 6 | 794 | U | O5'-P-OP1 | 7.40 | 119.58 | 110.70 |
| 1 | 5 | 980 | A | C8-N9-C4 | -7.37 | 102.85 | 105.80 |
| 2 | 6 | 1458 | G | C4-C5-N7 | 7.36 | 113.75 | 110.80 |
| 1 | 5 | 2430 | A | C5-C6-N1 | -7.36 | 114.02 | 117.70 |
| 1 | 5 | 1056 | U | N3-C2-O2 | -7.36 | 117.05 | 122.20 |
| 1 | 5 | 2715 | A | C8-N9-C4 | 7.36 | 108.74 | 105.80 |
| 1 | 1 | 1016 | C | N1-C2-O2 | 7.35 | 123.31 | 118.90 |
| 1 | 5 | 3266 | G | N9-C4-C5 | 7.33 | 108.33 | 105.40 |
| 2 | 6 | 1028 | C | C6-N1-C2 | 7.33 | 123.23 | 120.30 |
| 1 | 1 | 2354 | C | C6-N1-C2 | -7.32 | 117.37 | 120.30 |
| 2 | 6 | 130 | C | OP1-P-OP2 | 7.32 | 130.58 | 119.60 |
| 1 | 5 | 1303 | A | C8-N9-C4 | 7.32 | 108.73 | 105.80 |
| 1 | 1 | 2623 | G | C6-C5-N7 | -7.31 | 126.01 | 130.40 |
| 1 | 5 | 920 | A | N1-C6-N6 | 7.31 | 122.99 | 118.60 |
| 2 | 2 | 192 | U | C2-N1-C1' | 7.30 | 126.47 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 5 | 3382 | U | N3-C2-O2 | -7.30 | 117.09 | 122.20 |
| 1 | 1 | 2420 | C | C6-N1-C2 | -7.30 | 117.38 | 120.30 |
| 1 | 5 | 1495 | U | C5-C6-N1 | 7.30 | 126.35 | 122.70 |
| 1 | 1 | 1399 | A | C8-N9-C4 | 7.29 | 108.72 | 105.80 |
| 1 | 5 | 2251 | G | N1-C6-O6 | 7.29 | 124.28 | 119.90 |
| 1 | 1 | 895 | A | N1-C6-N6 | 7.29 | 122.97 | 118.60 |
| 1 | 1 | 1929 | G | C4-C5-N7 | 7.29 | 113.72 | 110.80 |
| 1 | 5 | 1607 | U | P-O3'-C3' | 7.29 | 128.45 | 119.70 |
| 1 | 5 | 2325 | G | O5'-P-OP2 | -7.29 | 99.14 | 105.70 |
| 1 | 1 | 1016 | C | C2-N1-C1' | 7.29 | 126.82 | 118.80 |
| 1 | 1 | 1307 | G | P-O3'-C3' | 7.29 | 128.44 | 119.70 |
| 1 | 1 | 145 | G | C8-N9-C4 | -7.28 | 103.49 | 106.40 |
| 1 | 1 | 291 | C | C6-N1-C2 | 7.28 | 123.21 | 120.30 |
| 1 | 1 | 632 | G | N1-C6-O6 | 7.28 | 124.27 | 119.90 |
| 1 | 1 | 1296 | C | C6-N1-C2 | -7.28 | 117.39 | 120.30 |
| 38 | m4 | 135 | LEU | CA-CB-CG | 7.28 | 132.05 | 115.30 |
| 1 | 5 | 2365 | C | N3-C4-C5 | 7.27 | 124.81 | 121.90 |
| 2 | 6 | 234 | G | C8-N9-C4 | -7.27 | 103.49 | 106.40 |
| 1 | 5 | 2620 | G | N1-C6-O6 | 7.27 | 124.26 | 119.90 |
| 1 | 1 | 2996 | U | C2-N1-C1' | 7.27 | 126.42 | 117.70 |
| 1 | 5 | 1356 | U | C2-N1-C1' | 7.26 | 126.41 | 117.70 |
| 1 | 1 | 1507 | G | C6-C5-N7 | -7.25 | 126.05 | 130.40 |
| 2 | 6 | 1118 | G | N1-C6-O6 | 7.25 | 124.25 | 119.90 |
| 1 | 1 | 1852 | G | N3-C4-C5 | 7.25 | 132.22 | 128.60 |
| 1 | 1 | 1146 | C | C6-N1-C2 | 7.25 | 123.20 | 120.30 |
| 1 | 5 | 942 | U | N1-C2-O2 | 7.25 | 127.87 | 122.80 |
| 1 | 5 | 2943 | G | C6-C5-N7 | -7.25 | 126.05 | 130.40 |
| 1 | 1 | 2240 | G | O5'-P-OP1 | -7.24 | 99.18 | 105.70 |
| 1 | 1 | 3198 | U | O5'-P-OP1 | -7.24 | 99.19 | 105.70 |
| 2 | 6 | 781 | U | N1-C2-O2 | 7.24 | 127.87 | 122.80 |
| 26 | e1 | 100 | LEU | CA-CB-CG | 7.24 | 131.94 | 115.30 |
| 2 | 2 | 1572 | G | C5-C6-O6 | -7.23 | 124.26 | 128.60 |
| 2 | 6 | 741 | C | P-O3'-C3' | 7.23 | 128.38 | 119.70 |
| 2 | 6 | 1389 | C | N1-C2-O2 | 7.23 | 123.24 | 118.90 |
| 1 | 1 | 1866 | C | N3-C2-O2 | -7.23 | 116.84 | 121.90 |
| 1 | 1 | 867 | G | N1-C6-O6 | 7.22 | 124.23 | 119.90 |
| 1 | 1 | 1145 | G | N3-C4-N9 | 7.22 | 130.33 | 126.00 |
| 1 | 1 | 1417 | G | C5-C6-O6 | -7.22 | 124.27 | 128.60 |
| 2 | 2 | 639 | U | N1-C2-O2 | 7.22 | 127.86 | 122.80 |
| 1 | 1 | 891 | G | C4-C5-N7 | 7.22 | 113.69 | 110.80 |
| 2 | 2 | 507 | U | N3-C2-O2 | -7.22 | 117.15 | 122.20 |
| 1 | 1 | 2093 | A | N3-C4-C5 | -7.22 | 121.75 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 4 | 4 | 9 | A | C8-N9-C4 | 7.21 | 108.69 | 105.80 |
| 4 | 4 | 14 | C | C6-N1-C2 | 7.21 | 123.19 | 120.30 |
| 2 | 2 | 704 | C | C2-N1-C1' | 7.21 | 126.73 | 118.80 |
| 1 | 1 | 116 | A | N1-C6-N6 | -7.21 | 114.27 | 118.60 |
| 1 | 5 | 1481 | A | C8-N9-C4 | -7.21 | 102.92 | 105.80 |
| 1 | 5 | 2385 | G | N3-C4-C5 | 7.21 | 132.20 | 128.60 |
| 2 | 6 | 1074 | G | N1-C6-O6 | 7.20 | 124.22 | 119.90 |
| 1 | 5 | 2281 | A | O4'-C1'-N9 | 7.19 | 113.95 | 108.20 |
| 1 | 1 | 1103 | A | P-O3'-C3' | 7.19 | 128.32 | 119.70 |
| 1 | 5 | 1450 | G | N1-C6-O6 | 7.19 | 124.21 | 119.90 |
| 1 | 5 | 398 | A | C8-N9-C4 | 7.18 | 108.67 | 105.80 |
| 2 | 2 | 576 | G | C8-N9-C4 | -7.18 | 103.53 | 106.40 |
| 3 | 3 | 100 | C | O5'-P-OP1 | -7.18 | 99.23 | 105.70 |
| 1 | 5 | 953 | G | C5-C6-O6 | 7.18 | 132.91 | 128.60 |
| 2 | 6 | 794 | U | N1-C2-O2 | 7.18 | 127.83 | 122.80 |
| 1 | 1 | 580 | C | C6-N1-C2 | 7.18 | 123.17 | 120.30 |
| 1 | 1 | 2287 | C | O5'-P-OP1 | -7.18 | 99.24 | 105.70 |
| 1 | 1 | 91 | G | N1-C6-O6 | 7.18 | 124.21 | 119.90 |
| 1 | 5 | 2899 | C | C6-N1-C2 | -7.18 | 117.43 | 120.30 |
| 1 | 5 | 216 | G | O5'-P-OP1 | -7.17 | 99.24 | 105.70 |
| 1 | 1 | 1607 | U | P-O3'-C3' | 7.17 | 128.31 | 119.70 |
| 2 | 6 | 996 | U | C5-C6-N1 | 7.17 | 126.29 | 122.70 |
| 4 | 4 | 82 | U | N3-C2-O2 | -7.17 | 117.18 | 122.20 |
| 1 | 1 | 593 | C | C6-N1-C2 | 7.16 | 123.17 | 120.30 |
| 1 | 5 | 106 | A | C8-N9-C4 | 7.16 | 108.67 | 105.80 |
| 1 | 1 | 1855 | U | N3-C2-O2 | -7.16 | 117.19 | 122.20 |
| 2 | 6 | 1686 | C | C6-N1-C2 | -7.16 | 117.44 | 120.30 |
| 2 | 2 | 1059 | U | C2-N1-C1' | 7.16 | 126.29 | 117.70 |
| 1 | 1 | 98 | G | C8-N9-C4 | 7.16 | 109.26 | 106.40 |
| 2 | 2 | 1560 | U | N3-C2-O2 | -7.16 | 117.19 | 122.20 |
| 1 | 5 | 412 | G | N1-C6-O6 | 7.15 | 124.19 | 119.90 |
| 1 | 5 | 966 | U | C6-N1-C2 | -7.15 | 116.71 | 121.00 |
| 1 | 5 | 942 | U | N3-C2-O2 | -7.14 | 117.20 | 122.20 |
| 1 | 5 | 821 | U | C5-C6-N1 | 7.14 | 126.27 | 122.70 |
| 2 | 2 | 939 | A | N1-C6-N6 | 7.13 | 122.88 | 118.60 |
| 1 | 5 | 333 | G | C8-N9-C4 | 7.13 | 109.25 | 106.40 |
| 2 | 2 | 995 | A | C8-N9-C4 | 7.13 | 108.65 | 105.80 |
| 1 | 5 | 1103 | A | O5'-P-OP1 | 7.13 | 119.25 | 110.70 |
| 1 | 1 | 91 | G | C5-C6-O6 | -7.12 | 124.33 | 128.60 |
| 1 | 5 | 379 | C | C6-N1-C2 | 7.12 | 123.15 | 120.30 |
| 1 | 5 | 1779 | C | C2-N1-C1' | 7.12 | 126.64 | 118.80 |
| 1 | 5 | 424 | G | C5-C6-O6 | -7.12 | 124.33 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 1 | 1382 | G | N3-C4-C5 | 7.12 | 132.16 | 128.60 |
| 2 | 2 | 1600 | A | N1-C6-N6 | 7.12 | 122.87 | 118.60 |
| 4 | 8 | 94 | C | C6-N1-C2 | 7.12 | 123.15 | 120.30 |
| 1 | 5 | 400 | G | C8-N9-C4 | -7.12 | 103.55 | 106.40 |
| 1 | 5 | 2400 | G | N3-C4-C5 | 7.11 | 132.16 | 128.60 |
| 1 | 5 | 2355 | G | C5-C6-O6 | -7.11 | 124.34 | 128.60 |
| 1 | 1 | 2827 | U | C2-N3-C4 | -7.11 | 122.74 | 127.00 |
| 1 | 1 | 979 | U | C5-C4-O4 | 7.09 | 130.15 | 125.90 |
| 2 | 2 | 1058 | U | N1-C2-O2 | 7.08 | 127.76 | 122.80 |
| 1 | 1 | 1578 | C | C2-N1-C1' | 7.08 | 126.58 | 118.80 |
| 1 | 5 | 1417 | G | N1-C6-O6 | 7.08 | 124.15 | 119.90 |
| 2 | 6 | 194 | U | C2-N1-C1' | 7.08 | 126.19 | 117.70 |
| 1 | 1 | 315 | C | C6-N1-C2 | -7.07 | 117.47 | 120.30 |
| 12 | C7 | 23 | LYS | C-N-CA | 7.07 | 139.38 | 121.70 |
| 2 | 2 | 1746 | A | C8-N9-C4 | 7.07 | 108.63 | 105.80 |
| 1 | 5 | 1152 | G | C4-C5-C6 | -7.07 | 114.56 | 118.80 |
| 1 | 1 | 1589 | A | N1-C6-N6 | 7.07 | 122.84 | 118.60 |
| 2 | 6 | 1458 | G | N9-C4-C5 | -7.07 | 102.57 | 105.40 |
| 1 | 5 | 1901 | A | N1-C6-N6 | -7.06 | 114.36 | 118.60 |
| 2 | 2 | 1148 | C | C6-N1-C2 | -7.06 | 117.47 | 120.30 |
| 2 | 2 | 1470 | C | C6-N1-C2 | -7.06 | 117.47 | 120.30 |
| 2 | 2 | 1316 | G | O5'-P-OP2 | -7.06 | 99.35 | 105.70 |
| 1 | 5 | 2572 | C | C6-N1-C2 | -7.06 | 117.48 | 120.30 |
| 1 | 5 | 3022 | G | C8-N9-C4 | -7.06 | 103.58 | 106.40 |
| 2 | 6 | 501 | U | C2-N1-C1' | 7.05 | 126.16 | 117.70 |
| 1 | 1 | 1604 | G | N3-C4-N9 | 7.05 | 130.23 | 126.00 |
| 1 | 5 | 2817 | A | C8-N9-C4 | 7.05 | 108.62 | 105.80 |
| 1 | 1 | 1581 | C | P-O3'-C3' | 7.05 | 128.16 | 119.70 |
| 2 | 2 | 1736 | G | N1-C6-O6 | 7.04 | 124.13 | 119.90 |
| 2 | 6 | 1148 | C | C6-N1-C2 | -7.04 | 117.48 | 120.30 |
| 1 | 1 | 2896 | A | N1-C6-N6 | 7.04 | 122.83 | 118.60 |
| 2 | 2 | 1324 | G | N3-C4-N9 | -7.04 | 121.77 | 126.00 |
| 2 | 6 | 750 | U | C6-N1-C2 | 7.04 | 125.22 | 121.00 |
| 2 | 6 | 453 | U | C2-N1-C1' | 7.04 | 126.14 | 117.70 |
| 2 | 6 | 67 | A | C8-N9-C4 | 7.03 | 108.61 | 105.80 |
| 1 | 1 | 1342 | C | C6-N1-C2 | 7.03 | 123.11 | 120.30 |
| 1 | 1 | 2651 | G | C5-C6-O6 | -7.03 | 124.38 | 128.60 |
| 1 | 5 | 347 | G | N1-C6-O6 | 7.03 | 124.12 | 119.90 |
| 1 | 1 | 2606 | G | C6-C5-N7 | -7.02 | 126.19 | 130.40 |
| 1 | 5 | 2624 | G | N1-C6-O6 | 7.02 | 124.11 | 119.90 |
| 1 | 5 | 2816 | G | C5-C6-N1 | -7.02 | 107.99 | 111.50 |
| 1 | 1 | 895 | A | C6-C5-N7 | -7.02 | 127.39 | 132.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 5 | 285 | A | N7-C8-N9 | 7.02 | 117.31 | 113.80 |
| 1 | 5 | 1152 | G | C4-C5-N7 | 7.02 | 113.61 | 110.80 |
| 1 | 1 | 1444 | G | C5-C6-O6 | -7.02 | 124.39 | 128.60 |
| 1 | 1 | 200 | C | N3-C4-C5 | -7.01 | 119.09 | 121.90 |
| 1 | 1 | 510 | G | N1-C6-O6 | 7.01 | 124.11 | 119.90 |
| 1 | 1 | 2278 | C | C6-N1-C2 | -7.01 | 117.50 | 120.30 |
| 1 | 5 | 3124 | G | N1-C6-O6 | 7.01 | 124.11 | 119.90 |
| 2 | 6 | 1481 | C | C6-N1-C2 | -7.01 | 117.50 | 120.30 |
| 2 | 6 | 163 | G | C8-N9-C4 | -7.01 | 103.60 | 106.40 |
| 1 | 5 | 3195 | U | C2-N1-C1' | 7.01 | 126.11 | 117.70 |
| 1 | 1 | 2566 | C | C6-N1-C2 | -7.00 | 117.50 | 120.30 |
| 1 | 5 | 2272 | G | OP1-P-O3' | 7.00 | 120.60 | 105.20 |
| 1 | 5 | 3053 | G | C6-C5-N7 | -7.00 | 126.20 | 130.40 |
| 2 | 6 | 453 | U | N1-C2-O2 | 6.99 | 127.70 | 122.80 |
| 1 | 5 | 3245 | A | C8-N9-C4 | -6.99 | 103.00 | 105.80 |
| 1 | 5 | 1329 | U | P-O3'-C3' | 6.99 | 128.09 | 119.70 |
| 1 | 1 | 2348 | A | N1-C6-N6 | -6.99 | 114.41 | 118.60 |
| 2 | 2 | 1059 | U | C6-N1-C2 | -6.98 | 116.81 | 121.00 |
| 1 | 5 | 3124 | G | C4-C5-N7 | 6.98 | 113.59 | 110.80 |
| 1 | 1 | 1419 | A | N1-C6-N6 | 6.98 | 122.79 | 118.60 |
| 1 | 1 | 637 | C | P-O3'-C3' | 6.98 | 128.07 | 119.70 |
| 1 | 1 | 2935 | U | C5-C6-N1 | 6.96 | 126.18 | 122.70 |
| 1 | 5 | 726 | G | N7-C8-N9 | 6.96 | 116.58 | 113.10 |
| 1 | 1 | 2174 | G | N3-C4-C5 | 6.96 | 132.08 | 128.60 |
| 1 | 5 | 2873 | U | C6-N1-C2 | -6.96 | 116.82 | 121.00 |
| 2 | 2 | 1745 | G | N3-C4-C5 | -6.96 | 125.12 | 128.60 |
| 1 | 5 | 428 | A | C8-N9-C4 | 6.96 | 108.58 | 105.80 |
| 1 | 5 | 2548 | C | C5-C6-N1 | 6.96 | 124.48 | 121.00 |
| 1 | 1 | 1858 | A | N1-C6-N6 | -6.96 | 114.43 | 118.60 |
| 2 | 6 | 1286 | U | C5-C4-O4 | -6.96 | 121.73 | 125.90 |
| 1 | 1 | 2645 | G | N1-C6-O6 | 6.95 | 124.07 | 119.90 |
| 2 | 2 | 1324 | G | N3-C2-N2 | -6.95 | 115.03 | 119.90 |
| 1 | 1 | 830 | A | C8-N9-C4 | 6.95 | 108.58 | 105.80 |
| 2 | 2 | 1759 | C | C6-N1-C2 | 6.95 | 123.08 | 120.30 |
| 1 | 5 | 332 | C | C6-N1-C2 | 6.95 | 123.08 | 120.30 |
| 1 | 1 | 329 | U | N1-C2-O2 | 6.95 | 127.66 | 122.80 |
| 2 | 2 | 369 | A | C8-N9-C4 | -6.94 | 103.02 | 105.80 |
| 1 | 5 | 1312 | C | N3-C4-C5 | -6.93 | 119.13 | 121.90 |
| 2 | 2 | 158 | U | P-O3'-C3' | 6.93 | 128.02 | 119.70 |
| 2 | 2 | 704 | C | C6-N1-C2 | -6.93 | 117.53 | 120.30 |
| 1 | 1 | 1609 | C | C6-N1-C2 | 6.92 | 123.07 | 120.30 |
| 1 | 5 | 1303 | A | N1-C6-N6 | 6.92 | 122.75 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 5 | 200 | C | N3-C4-C5 | -6.92 | 119.13 | 121.90 |
| 1 | 5 | 2288 | G | O5'-P-OP1 | -6.92 | 99.47 | 105.70 |
| 2 | 2 | 1754 | A | C8-N9-C4 | -6.92 | 103.03 | 105.80 |
| 1 | 1 | 1866 | C | C2-N1-C1' | 6.91 | 126.41 | 118.80 |
| 1 | 5 | 2920 | U | O5'-P-OP1 | -6.91 | 99.48 | 105.70 |
| 1 | 5 | 49 | A | N1-C6-N6 | 6.91 | 122.75 | 118.60 |
| 1 | 5 | 1387 | G | C8-N9-C4 | -6.91 | 103.64 | 106.40 |
| 1 | 5 | 3053 | G | N1-C6-O6 | 6.91 | 124.05 | 119.90 |
| 1 | 1 | 1858 | A | N3-C4-C5 | -6.90 | 121.97 | 126.80 |
| 1 | 1 | 1892 | G | C8-N9-C4 | 6.90 | 109.16 | 106.40 |
| 3 | 3 | 7 | G | C5-C6-O6 | 6.90 | 132.74 | 128.60 |
| 1 | 1 | 208 | C | C6-N1-C2 | -6.90 | 117.54 | 120.30 |
| 1 | 1 | 329 | U | N3-C2-O2 | -6.89 | 117.37 | 122.20 |
| 1 | 5 | 2315 | G | N1-C6-O6 | 6.89 | 124.04 | 119.90 |
| 4 | 4 | 73 | U | N3-C2-O2 | -6.89 | 117.38 | 122.20 |
| 1 | 5 | 1459 | C | C6-N1-C2 | -6.89 | 117.54 | 120.30 |
| 1 | 1 | 1589 | A | N9-C4-C5 | -6.89 | 103.05 | 105.80 |
| 1 | 5 | 2139 | A | O5'-P-OP2 | -6.89 | 99.50 | 105.70 |
| 4 | 8 | 115 | C | N3-C4-C5 | 6.89 | 124.66 | 121.90 |
| 1 | 5 | 402 | A | O5'-P-OP1 | -6.89 | 99.50 | 105.70 |
| 2 | 6 | 577 | G | N1-C6-O6 | 6.88 | 124.03 | 119.90 |
| 1 | 1 | 1858 | A | C2-N3-C4 | 6.88 | 114.04 | 110.60 |
| 2 | 2 | 1355 | C | C6-N1-C2 | -6.88 | 117.55 | 120.30 |
| 1 | 5 | 2169 | G | N3-C4-N9 | -6.87 | 121.88 | 126.00 |
| 1 | 1 | 91 | G | C6-C5-N7 | -6.87 | 126.28 | 130.40 |
| 1 | 5 | 3205 | G | C5-C6-O6 | -6.87 | 124.48 | 128.60 |
| 1 | 1 | 2298 | U | O5'-P-OP2 | -6.87 | 99.52 | 105.70 |
| 1 | 1 | 3269 | U | P-O3'-C3' | 6.87 | 127.94 | 119.70 |
| 2 | 2 | 626 | U | C6-N1-C2 | -6.87 | 116.88 | 121.00 |
| 1 | 5 | 2968 | G | C6-C5-N7 | -6.87 | 126.28 | 130.40 |
| 1 | 1 | 2679 | A | C4-C5-N7 | 6.87 | 114.13 | 110.70 |
| 1 | 1 | 935 | U | C6-N1-C2 | -6.86 | 116.88 | 121.00 |
| 1 | 1 | 1348 | U | C5-C6-N1 | 6.86 | 126.13 | 122.70 |
| 1 | 1 | 2568 | C | C6-N1-C2 | -6.85 | 117.56 | 120.30 |
| 2 | 2 | 617 | U | C2-N1-C1' | 6.85 | 125.92 | 117.70 |
| 2 | 6 | 1646 | C | C6-N1-C2 | -6.85 | 117.56 | 120.30 |
| 1 | 1 | 34 | A | O5'-P-OP2 | -6.85 | 99.53 | 105.70 |
| 1 | 1 | 1542 | G | C5-C6-O6 | -6.85 | 124.49 | 128.60 |
| 2 | 2 | 1061 | A | O4'-C1'-N9 | 6.84 | 113.68 | 108.20 |
| 1 | 1 | 1493 | G | C5-C6-O6 | 6.84 | 132.71 | 128.60 |
| 1 | 1 | 2817 | A | C8-N9-C4 | -6.84 | 103.06 | 105.80 |
| 2 | 2 | 704 | C | N1-C2-O2 | 6.84 | 123.00 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 1 | 2967 | A | C5-C6-N6 | -6.83 | 118.23 | 123.70 |
| 2 | 6 | 320 | U | C6-N1-C2 | -6.83 | 116.90 | 121.00 |
| 1 | 5 | 1328 | C | C6-N1-C2 | -6.83 | 117.57 | 120.30 |
| 1 | 5 | 3116 | G | N1-C6-O6 | -6.83 | 115.80 | 119.90 |
| 1 | 5 | 1149 | G | N3-C4-N9 | 6.82 | 130.09 | 126.00 |
| 2 | 2 | 780 | A | C8-N9-C4 | -6.82 | 103.07 | 105.80 |
| 2 | 6 | 308 | C | N3-C4-C5 | 6.82 | 124.63 | 121.90 |
| 1 | 1 | 1497 | C | C6-N1-C2 | 6.81 | 123.03 | 120.30 |
| 1 | 1 | 1855 | U | C6-N1-C2 | -6.81 | 116.91 | 121.00 |
| 1 | 1 | 2965 | U | N3-C4-C5 | 6.81 | 118.69 | 114.60 |
| 2 | 2 | 1083 | G | C8-N9-C4 | 6.81 | 109.12 | 106.40 |
| 1 | 5 | 1531 | C | C6-N1-C2 | 6.80 | 123.02 | 120.30 |
| 1 | 5 | 1000 | C | C6-N1-C2 | 6.80 | 123.02 | 120.30 |
| 2 | 6 | 499 | U | C6-N1-C2 | -6.80 | 116.92 | 121.00 |
| 1 | 1 | 273 | A | N1-C6-N6 | -6.80 | 114.52 | 118.60 |
| 1 | 1 | 1417 | G | N1-C6-O6 | 6.79 | 123.97 | 119.90 |
| 3 | 3 | 7 | G | N1-C6-O6 | -6.79 | 115.83 | 119.90 |
| 1 | 1 | 2606 | G | C4-N9-C1' | 6.79 | 135.32 | 126.50 |
| 1 | 1 | 1838 | G | C4-C5-N7 | 6.79 | 113.51 | 110.80 |
| 1 | 5 | 2872 | A | C2-N3-C4 | 6.79 | 113.99 | 110.60 |
| 1 | 5 | 2772 | C | P-O3'-C3' | 6.78 | 127.84 | 119.70 |
| 1 | 1 | 1888 | U | N3-C2-O2 | -6.78 | 117.45 | 122.20 |
| 1 | 1 | 2553 | U | N3-C2-O2 | -6.78 | 117.45 | 122.20 |
| 1 | 1 | 718 | G | N3-C4-C5 | 6.78 | 131.99 | 128.60 |
| 1 | 5 | 827 | A | O5'-P-OP1 | -6.78 | 99.60 | 105.70 |
| 1 | 5 | 2952 | G | C5-C6-O6 | -6.78 | 124.53 | 128.60 |
| 21 | D6 | 64 | LEU | CA-CB-CG | 6.77 | 130.88 | 115.30 |
| 1 | 1 | 660 | A | C5-C6-N6 | 6.77 | 129.12 | 123.70 |
| 1 | 1 | 2572 | C | N3-C2-O2 | -6.77 | 117.16 | 121.90 |
| 1 | 1 | 1145 | G | C6-C5-N7 | -6.77 | 126.34 | 130.40 |
| 1 | 5 | 1149 | G | C5-C6-O6 | -6.77 | 124.54 | 128.60 |
| 2 | 6 | 131 | C | C2-N1-C1' | 6.76 | 126.24 | 118.80 |
| 1 | 1 | 283 | G | C4-N9-C1' | 6.76 | 135.29 | 126.50 |
| 1 | 1 | 1820 | U | OP2-P-O3' | 6.76 | 120.07 | 105.20 |
| 1 | 1 | 1157 | G | N9-C4-C5 | -6.75 | 102.70 | 105.40 |
| 2 | 6 | 337 | G | C5-N7-C8 | -6.75 | 100.92 | 104.30 |
| 2 | 6 | 1568 | C | P-O3'-C3' | 6.75 | 127.81 | 119.70 |
| 1 | 1 | 1194 | G | N1-C6-O6 | 6.75 | 123.95 | 119.90 |
| 1 | 1 | 2821 | C | N3-C4-C5 | -6.75 | 119.20 | 121.90 |
| 1 | 5 | 2821 | C | N1-C2-O2 | 6.75 | 122.95 | 118.90 |
| 1 | 5 | 1716 | U | P-O3'-C3' | 6.75 | 127.80 | 119.70 |
| 1 | 5 | 2403 | G | C4-N9-C1' | 6.75 | 135.28 | 126.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 5 | 2620 | G | N3-C4-C5 | 6.75 | 131.97 | 128.60 |
| 12 | C7 | 115 | LEU | CA-CB-CG | 6.75 | 130.81 | 115.30 |
| 1 | 1 | 2675 | C | C2-N1-C1' | 6.74 | 126.22 | 118.80 |
| 1 | 5 | 2249 | G | N9-C1'-C2' | -6.74 | 104.58 | 112.00 |
| 1 | 5 | 2315 | G | C6-C5-N7 | -6.74 | 126.35 | 130.40 |
| 1 | 5 | 1145 | G | N9-C4-C5 | -6.74 | 102.70 | 105.40 |
| 1 | 1 | 2679 | A | N9-C4-C5 | -6.74 | 103.10 | 105.80 |
| 1 | 5 | 101 | G | N1-C6-O6 | 6.74 | 123.94 | 119.90 |
| 1 | 5 | 867 | G | N1-C6-O6 | 6.74 | 123.94 | 119.90 |
| 1 | 5 | 2416 | U | O5'-P-OP2 | -6.74 | 99.64 | 105.70 |
| 1 | 5 | 2600 | C | C6-N1-C2 | -6.74 | 117.61 | 120.30 |
| 1 | 5 | 1730 | G | N3-C4-N9 | 6.73 | 130.04 | 126.00 |
| 1 | 1 | 1522 | U | N3-C2-O2 | -6.73 | 117.49 | 122.20 |
| 1 | 1 | 1362 | G | C8-N9-C4 | 6.73 | 109.09 | 106.40 |
| 2 | 6 | 234 | G | C4-N9-C1' | 6.73 | 135.25 | 126.50 |
| 2 | 6 | 1582 | U | C5-C6-N1 | -6.73 | 119.34 | 122.70 |
| 1 | 1 | 1764 | U | C5-C6-N1 | 6.72 | 126.06 | 122.70 |
| 2 | 2 | 794 | U | N1-C2-O2 | 6.72 | 127.51 | 122.80 |
| 2 | 2 | 1600 | A | C6-C5-N7 | -6.72 | 127.59 | 132.30 |
| 1 | 1 | 1716 | U | P-O3'-C3' | 6.72 | 127.77 | 119.70 |
| 1 | 1 | 36 | C | C6-N1-C2 | -6.72 | 117.61 | 120.30 |
| 2 | 6 | 355 | G | O5'-P-OP2 | -6.72 | 99.66 | 105.70 |
| 1 | 5 | 2401 | A | N9-C4-C5 | -6.71 | 103.11 | 105.80 |
| 1 | 1 | 780 | A | C4-C5-N7 | -6.71 | 107.34 | 110.70 |
| 2 | 6 | 1277 | G | N9-C4-C5 | 6.71 | 108.08 | 105.40 |
| 1 | 1 | 1929 | G | C5-C6-O6 | -6.71 | 124.58 | 128.60 |
| 1 | 5 | 1115 | G | C4-N9-C1' | 6.71 | 135.22 | 126.50 |
| 1 | 5 | 2405 | C | C6-N1-C2 | 6.71 | 122.98 | 120.30 |
| 1 | 1 | 1780 | G | C8-N9-C4 | -6.71 | 103.72 | 106.40 |
| 1 | 5 | 2222 | A | O5'-P-OP2 | -6.70 | 99.67 | 105.70 |
| 1 | 5 | 2278 | C | N1-C2-O2 | 6.70 | 122.92 | 118.90 |
| 1 | 1 | 1444 | G | C4-C5-N7 | 6.70 | 113.48 | 110.80 |
| 2 | 6 | 558 | U | C6-N1-C2 | -6.70 | 116.98 | 121.00 |
| 2 | 6 | 1773 | C | N3-C4-C5 | -6.70 | 119.22 | 121.90 |
| 1 | 5 | 2872 | A | C8-N9-C4 | -6.70 | 103.12 | 105.80 |
| 1 | 1 | 1763 | U | C6-N1-C2 | -6.69 | 116.98 | 121.00 |
| 1 | 1 | 1493 | G | C4-C5-N7 | -6.69 | 108.12 | 110.80 |
| 2 | 6 | 338 | C | C6-N1-C2 | 6.69 | 122.98 | 120.30 |
| 1 | 1 | 964 | G | OP2-P-O3' | 6.68 | 119.90 | 105.20 |
| 1 | 1 | 2360 | C | C2-N3-C4 | -6.68 | 116.56 | 119.90 |
| 3 | 3 | 8 | G | C8-N9-C4 | 6.67 | 109.07 | 106.40 |
| 1 | 5 | 2837 | A | C8-N9-C4 | 6.67 | 108.47 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2 | 6 | 558 | U | N1-C2-O2 | 6.67 | 127.47 | 122.80 |
| 1 | 1 | 793 | C | C2-N1-C1' | 6.67 | 126.13 | 118.80 |
| 75 | s7 | 118 | LEU | CA-CB-CG | 6.67 | 130.63 | 115.30 |
| 1 | 1 | 1507 | G | C4-C5-N7 | 6.66 | 113.47 | 110.80 |
| 3 | 3 | 29 | C | C6-N1-C2 | -6.66 | 117.64 | 120.30 |
| 1 | 5 | 94 | G | N3-C4-C5 | 6.66 | 131.93 | 128.60 |
| 1 | 5 | 2251 | G | C5-C6-O6 | -6.66 | 124.61 | 128.60 |
| 1 | 5 | 2866 | U | N3-C2-O2 | -6.65 | 117.54 | 122.20 |
| 1 | 5 | 757 | C | C6-N1-C2 | 6.65 | 122.96 | 120.30 |
| 1 | 1 | 1348 | U | C2-N1-C1' | 6.65 | 125.68 | 117.70 |
| 1 | 5 | 3260 | G | N3-C4-C5 | -6.64 | 125.28 | 128.60 |
| 1 | 1 | 1411 | C | N3-C4-C5 | 6.64 | 124.56 | 121.90 |
| 2 | 2 | 1399 | C | N1-C2-O2 | 6.64 | 122.88 | 118.90 |
| 2 | 6 | 389 | G | N1-C6-O6 | 6.64 | 123.88 | 119.90 |
| 1 | 1 | 920 | A | N1-C6-N6 | 6.64 | 122.58 | 118.60 |
| 1 | 1 | 2212 | C | C6-N1-C2 | -6.64 | 117.65 | 120.30 |
| 1 | 1 | 2944 | U | C5-C6-N1 | 6.63 | 126.02 | 122.70 |
| 1 | 5 | 700 | C | N3-C4-C5 | -6.63 | 119.25 | 121.90 |
| 1 | 5 | 2374 | C | O5'-P-OP1 | -6.63 | 99.73 | 105.70 |
| 1 | 1 | 1663 | C | C6-N1-C2 | 6.63 | 122.95 | 120.30 |
| 1 | 1 | 1586 | G | N3-C4-N9 | -6.62 | 122.03 | 126.00 |
| 1 | 1 | 1838 | G | C5-C6-O6 | -6.62 | 124.62 | 128.60 |
| 1 | 1 | 725 | G | C8-N9-C4 | 6.62 | 109.05 | 106.40 |
| 1 | 1 | 116 | A | N9-C4-C5 | 6.62 | 108.45 | 105.80 |
| 1 | 1 | 2708 | C | C6-N1-C2 | 6.61 | 122.94 | 120.30 |
| 2 | 6 | 858 | G | C6-C5-N7 | -6.61 | 126.44 | 130.40 |
| 1 | 5 | 2965 | U | C5-C4-O4 | -6.60 | 121.94 | 125.90 |
| 1 | 1 | 2256 | A | O4'-C1'-N9 | 6.60 | 113.48 | 108.20 |
| 1 | 5 | 420 | G | C6-C5-N7 | -6.60 | 126.44 | 130.40 |
| 1 | 1 | 2646 | C | C6-N1-C2 | 6.60 | 122.94 | 120.30 |
| 1 | 5 | 282 | G | C8-N9-C4 | -6.60 | 103.76 | 106.40 |
| 1 | 5 | 1161 | G | N1-C6-O6 | 6.60 | 123.86 | 119.90 |
| 1 | 1 | 65 | A | P-O3'-C3' | 6.60 | 127.62 | 119.70 |
| 1 | 1 | 2913 | C | N1-C2-N3 | -6.59 | 114.58 | 119.20 |
| 2 | 6 | 794 | U | O5'-P-OP2 | -6.59 | 99.77 | 105.70 |
| 1 | 1 | 92 | G | C8-N9-C4 | 6.59 | 109.04 | 106.40 |
| 2 | 6 | 652 | G | P-O3'-C3' | 6.59 | 127.61 | 119.70 |
| 78 | SM | 171 | PRO | N-CA-CB | 6.59 | 111.21 | 103.30 |
| 2 | 2 | 852 | C | C6-N1-C2 | 6.58 | 122.93 | 120.30 |
| 4 | 4 | 125 | U | N3-C2-O2 | -6.58 | 117.59 | 122.20 |
| 1 | 5 | 360 | G | N3-C4-C5 | -6.58 | 125.31 | 128.60 |
| 34 | l9 | 161 | LEU | CA-CB-CG | 6.58 | 130.44 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 5 | 3266 | G | C5-C6-O6 | 6.58 | 132.55 | 128.60 |
| 2 | 6 | 151 | G | N3-C4-N9 | -6.58 | 122.05 | 126.00 |
| 1 | 5 | 2284 | C | C2-N1-C1' | 6.58 | 126.04 | 118.80 |
| 1 | 1 | 666 | A | C8-N9-C4 | 6.57 | 108.43 | 105.80 |
| 7 | C2 | 103 | LEU | CA-CB-CG | 6.57 | 130.42 | 115.30 |
| 1 | 1 | 432 | G | C5-C6-N1 | -6.57 | 108.22 | 111.50 |
| 1 | 1 | 886 | C | C6-N1-C2 | 6.57 | 122.93 | 120.30 |
| 1 | 5 | 347 | G | C4-C5-N7 | 6.57 | 113.43 | 110.80 |
| 1 | 1 | 2403 | G | C6-C5-N7 | -6.57 | 126.46 | 130.40 |
| 2 | 6 | 613 | G | N3-C4-C5 | -6.57 | 125.32 | 128.60 |
| 1 | 1 | 2726 | C | N3-C2-O2 | -6.57 | 117.30 | 121.90 |
| 1 | 1 | 645 | A | C8-N9-C4 | -6.56 | 103.17 | 105.80 |
| 1 | 1 | 1120 | A | N1-C6-N6 | -6.56 | 114.67 | 118.60 |
| 1 | 1 | 1202 | A | N1-C6-N6 | 6.56 | 122.53 | 118.60 |
| 1 | 1 | 2311 | G | O5'-P-OP1 | -6.55 | 99.80 | 105.70 |
| 1 | 5 | 81 | C | C6-N1-C2 | -6.55 | 117.68 | 120.30 |
| 2 | 6 | 1059 | U | C2-N1-C1' | 6.55 | 125.57 | 117.70 |
| 1 | 5 | 2550 | U | N3-C2-O2 | -6.55 | 117.61 | 122.20 |
| 2 | 6 | 1762 | A | OP1-P-O3' | -6.55 | 90.80 | 105.20 |
| 1 | 1 | 1327 | C | N3-C4-C5 | -6.55 | 119.28 | 121.90 |
| 2 | 2 | 569 | C | C6-N1-C2 | 6.55 | 122.92 | 120.30 |
| 1 | 1 | 1443 | G | C4-C5-N7 | 6.54 | 113.42 | 110.80 |
| 1 | 5 | 1146 | C | C6-N1-C2 | 6.54 | 122.92 | 120.30 |
| 1 | 5 | 975 | C | C6-N1-C2 | 6.54 | 122.92 | 120.30 |
| 2 | 6 | 377 | G | N1-C6-O6 | 6.54 | 123.82 | 119.90 |
| 1 | 1 | 2965 | U | C5-C4-O4 | -6.54 | 121.98 | 125.90 |
| 1 | 1 | 3370 | A | N1-C6-N6 | 6.54 | 122.52 | 118.60 |
| 28 | 13 | 246 | LEU | CA-CB-CG | 6.54 | 130.34 | 115.30 |
| 1 | 5 | 99 | A | N1-C6-N6 | -6.54 | 114.68 | 118.60 |
| 1 | 5 | 1227 | C | C6-N1-C2 | -6.54 | 117.69 | 120.30 |
| 1 | 5 | 2366 | C | C6-N1-C2 | 6.53 | 122.91 | 120.30 |
| 1 | 5 | 94 | G | N3-C4-N9 | -6.53 | 122.08 | 126.00 |
| 1 | 1 | 2418 | G | C5-N7-C8 | -6.53 | 101.04 | 104.30 |
| 1 | 5 | 1356 | U | C6-N1-C2 | -6.52 | 117.09 | 121.00 |
| 1 | 5 | 2315 | G | C4-C5-N7 | 6.52 | 113.41 | 110.80 |
| 2 | 2 | 192 | U | N3-C2-O2 | -6.52 | 117.63 | 122.20 |
| 1 | 1 | 797 | U | C6-N1-C2 | -6.52 | 117.09 | 121.00 |
| 1 | 1 | 1435 | A | N1-C6-N6 | -6.52 | 114.69 | 118.60 |
| 2 | 2 | 1143 | A | O5'-P-OP2 | -6.52 | 99.83 | 105.70 |
| 2 | 2 | 1751 | C | N3-C4-C5 | 6.52 | 124.51 | 121.90 |
| 1 | 1 | 2222 | A | N1-C6-N6 | -6.52 | 114.69 | 118.60 |
| 1 | 5 | 1930 | A | C8-N9-C4 | -6.52 | 103.19 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2 | 2 | 344 | A | C8-N9-C4 | 6.51 | 108.41 | 105.80 |
| 1 | 5 | 2821 | C | C2-N1-C1' | 6.51 | 125.97 | 118.80 |
| 1 | 1 | 3075 | G | C4-C5-N7 | 6.51 | 113.41 | 110.80 |
| 1 | 5 | 1306 | G | OP2-P-O3' | 6.51 | 119.53 | 105.20 |
| 1 | 1 | 2284 | C | N1-C2-O2 | 6.51 | 122.81 | 118.90 |
| 1 | 5 | 2170 | U | O5'-P-OP1 | -6.51 | 99.84 | 105.70 |
| 1 | 5 | 3311 | C | N3-C4-C5 | 6.51 | 124.50 | 121.90 |
| 2 | 6 | 1041 | G | C8-N9-C4 | -6.51 | 103.80 | 106.40 |
| 1 | 5 | 2881 | C | N3-C4-C5 | 6.51 | 124.50 | 121.90 |
| 1 | 1 | 667 | C | C5-C6-N1 | -6.50 | 117.75 | 121.00 |
| 2 | 2 | 1490 | C | P-O3'-C3' | 6.50 | 127.50 | 119.70 |
| 1 | 5 | 2817 | A | N9-C4-C5 | -6.50 | 103.20 | 105.80 |
| 1 | 5 | 2376 | G | N3-C4-N9 | 6.50 | 129.90 | 126.00 |
| 4 | 4 | 44 | A | O5'-P-OP1 | -6.50 | 99.85 | 105.70 |
| 1 | 1 | 725 | G | C4-N9-C1' | -6.50 | 118.06 | 126.50 |
| 1 | 1 | 2227 | C | P-O3'-C3' | 6.50 | 127.49 | 119.70 |
| 1 | 1 | 283 | G | C8-N9-C1' | -6.49 | 118.56 | 127.00 |
| 1 | 1 | 793 | C | C6-N1-C2 | -6.49 | 117.70 | 120.30 |
| 1 | 1 | 979 | U | P-O3'-C3' | 6.49 | 127.48 | 119.70 |
| 1 | 1 | 2556 | C | N3-C2-O2 | -6.49 | 117.36 | 121.90 |
| 1 | 5 | 247 | C | C6-N1-C2 | -6.49 | 117.71 | 120.30 |
| 1 | 5 | 1161 | G | C6-C5-N7 | -6.48 | 126.51 | 130.40 |
| 2 | 6 | 136 | C | N1-C2-O2 | 6.48 | 122.79 | 118.90 |
| 2 | 2 | 1572 | G | C4-C5-N7 | 6.48 | 113.39 | 110.80 |
| 1 | 1 | 884 | A | C5-C6-N6 | -6.48 | 118.52 | 123.70 |
| 1 | 1 | 2282 | U | O5'-P-OP2 | -6.48 | 99.87 | 105.70 |
| 1 | 5 | 601 | U | C5-C6-N1 | 6.48 | 125.94 | 122.70 |
| 2 | 6 | 1541 | G | C5-C6-O6 | 6.48 | 132.49 | 128.60 |
| 1 | 1 | 915 | A | N7-C8-N9 | 6.48 | 117.04 | 113.80 |
| 1 | 1 | 2606 | G | C8-N9-C1' | -6.48 | 118.58 | 127.00 |
| 1 | 5 | 2877 | G | N3-C4-N9 | 6.48 | 129.88 | 126.00 |
| 4 | 8 | 46 | G | N1-C6-O6 | -6.48 | 116.01 | 119.90 |
| 1 | 1 | 3194 | C | C6-N1-C1' | -6.47 | 113.04 | 120.80 |
| 1 | 5 | 61 | A | C8-N9-C4 | -6.47 | 103.21 | 105.80 |
| 1 | 1 | 145 | G | N3-C4-C5 | -6.47 | 125.37 | 128.60 |
| 1 | 1 | 1403 | C | N3-C4-C5 | 6.47 | 124.49 | 121.90 |
| 1 | 5 | 821 | U | C6-N1-C2 | -6.47 | 117.12 | 121.00 |
| 2 | 6 | 1039 | A | O4'-C1'-N9 | 6.47 | 113.37 | 108.20 |
| 1 | 1 | 545 | U | N3-C2-O2 | -6.46 | 117.67 | 122.20 |
| 1 | 5 | 2598 | G | O5'-P-OP2 | -6.46 | 99.88 | 105.70 |
| 2 | 6 | 541 | A | C8-N9-C4 | -6.46 | 103.21 | 105.80 |
| 1 | 5 | 1103 | A | N3-C4-C5 | -6.46 | 122.28 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2 | 6 | 939 | A | C8-N9-C4 | -6.46 | 103.22 | 105.80 |
| 1 | 1 | 919 | U | N3-C2-O2 | -6.46 | 117.68 | 122.20 |
| 1 | 5 | 1078 | U | N1-C2-N3 | 6.46 | 118.78 | 114.90 |
| 1 | 5 | 1825 | G | N1-C6-O6 | -6.46 | 116.03 | 119.90 |
| 1 | 1 | 3042 | U | C6-N1-C2 | -6.46 | 117.13 | 121.00 |
| 1 | 5 | 384 | A | C8-N9-C4 | 6.46 | 108.38 | 105.80 |
| 1 | 5 | 3043 | C | C6-N1-C2 | -6.46 | 117.72 | 120.30 |
| 1 | 1 | 1145 | G | N9-C4-C5 | -6.46 | 102.82 | 105.40 |
| 1 | 1 | 645 | A | C4-C5-N7 | -6.45 | 107.47 | 110.70 |
| 1 | 5 | 2325 | G | N3-C4-C5 | 6.45 | 131.83 | 128.60 |
| 1 | 1 | 251 | G | C4-N9-C1' | 6.45 | 134.89 | 126.50 |
| 1 | 1 | 1145 | G | C5-C6-O6 | -6.45 | 124.73 | 128.60 |
| 1 | 1 | 2996 | U | C6-N1-C1' | -6.45 | 112.17 | 121.20 |
| 1 | 1 | 966 | U | C6-N1-C2 | -6.45 | 117.13 | 121.00 |
| 1 | 1 | 2616 | C | C6-N1-C2 | 6.45 | 122.88 | 120.30 |
| 1 | 1 | 232 | G | O4'-C1'-N9 | 6.44 | 113.35 | 108.20 |
| 1 | 5 | 1863 | G | C8-N9-C4 | 6.44 | 108.98 | 106.40 |
| 1 | 1 | 1306 | G | C4-C5-N7 | 6.44 | 113.38 | 110.80 |
| 1 | 1 | 1542 | G | C6-C5-N7 | -6.44 | 126.53 | 130.40 |
| 32 | 17 | 229 | PHE | CB-CG-CD1 | 6.44 | 125.31 | 120.80 |
| 1 | 1 | 793 | C | N3-C2-O2 | -6.44 | 117.39 | 121.90 |
| 1 | 5 | 1308 | A | N9-C4-C5 | 6.44 | 108.37 | 105.80 |
| 1 | 1 | 1402 | C | C6-N1-C2 | 6.43 | 122.87 | 120.30 |
| 1 | 1 | 2735 | U | C6-N1-C2 | -6.43 | 117.14 | 121.00 |
| 1 | 1 | 1169 | A | N1-C6-N6 | -6.43 | 114.74 | 118.60 |
| 1 | 1 | 1865 | A | N9-C4-C5 | -6.43 | 103.23 | 105.80 |
| 1 | 5 | 3209 | A | C8-N9-C4 | 6.43 | 108.37 | 105.80 |
| 1 | 1 | 3080 | G | C5-C6-O6 | -6.43 | 124.74 | 128.60 |
| 1 | 1 | 2606 | G | N3-C4-N9 | 6.42 | 129.85 | 126.00 |
| 4 | 4 | 33 | A | O5'-P-OP2 | 6.42 | 118.40 | 110.70 |
| 1 | 1 | 2922 | G | C4-N9-C1' | 6.41 | 134.84 | 126.50 |
| 1 | 5 | 1324 | U | C6-N1-C2 | 6.41 | 124.85 | 121.00 |
| 1 | 5 | 2241 | U | C5-C4-O4 | 6.41 | 129.75 | 125.90 |
| 1 | 1 | 545 | U | N1-C2-O2 | 6.41 | 127.29 | 122.80 |
| 2 | 6 | 163 | G | N9-C4-C5 | 6.41 | 107.96 | 105.40 |
| 1 | 1 | 2867 | C | N3-C2-O2 | 6.41 | 126.39 | 121.90 |
| 1 | 1 | 867 | G | C5-C6-O6 | -6.41 | 124.76 | 128.60 |
| 2 | 6 | 455 | C | C6-N1-C2 | -6.41 | 117.74 | 120.30 |
| 1 | 1 | 924 | G | C8-N9-C4 | -6.40 | 103.84 | 106.40 |
| 1 | 1 | 2645 | G | C6-C5-N7 | -6.40 | 126.56 | 130.40 |
| 1 | 5 | 3039 | C | C6-N1-C2 | 6.40 | 122.86 | 120.30 |
| 1 | 5 | 3382 | U | N1-C2-O2 | 6.40 | 127.28 | 122.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 1 | 1143 | A | C8-N9-C4 | 6.40 | 108.36 | 105.80 |
| 2 | 2 | 507 | U | C2-N1-C1' | 6.40 | 125.38 | 117.70 |
| 1 | 5 | 2824 | G | C6-C5-N7 | -6.40 | 126.56 | 130.40 |
| 1 | 1 | 1516 | C | C6-N1-C2 | 6.40 | 122.86 | 120.30 |
| 1 | 5 | 2651 | G | N1-C6-O6 | 6.39 | 123.74 | 119.90 |
| 1 | 1 | 2209 | U | C5-C6-N1 | 6.39 | 125.90 | 122.70 |
| 1 | 1 | 923 | C | C6-N1-C2 | 6.39 | 122.86 | 120.30 |
| 1 | 5 | 203 | G | N1-C6-O6 | -6.39 | 116.06 | 119.90 |
| 2 | 2 | 320 | U | O5'-P-OP1 | -6.39 | 99.95 | 105.70 |
| 1 | 5 | 2231 | C | C2-N1-C1' | 6.39 | 125.83 | 118.80 |
| 1 | 5 | 1078 | U | N1-C2-O2 | -6.38 | 118.33 | 122.80 |
| 2 | 6 | 577 | G | C4-C5-N7 | 6.38 | 113.35 | 110.80 |
| 1 | 1 | 1604 | G | C6-C5-N7 | -6.38 | 126.57 | 130.40 |
| 1 | 1 | 1148 | G | C8-N9-C4 | 6.38 | 108.95 | 106.40 |
| 1 | 5 | 2727 | A | N1-C6-N6 | -6.38 | 114.77 | 118.60 |
| 1 | 1 | 1443 | G | N3-C2-N2 | -6.38 | 115.43 | 119.90 |
| 1 | 5 | 3278 | C | N3-C2-O2 | -6.38 | 117.44 | 121.90 |
| 2 | 2 | 577 | G | N1-C6-O6 | 6.38 | 123.72 | 119.90 |
| 1 | 1 | 1166 | G | C4-C5-N7 | 6.37 | 113.35 | 110.80 |
| 2 | 2 | 794 | U | C2-N1-C1' | 6.37 | 125.34 | 117.70 |
| 2 | 6 | 266 | A | C8-N9-C4 | 6.37 | 108.35 | 105.80 |
| 40 | m6 | 27 | LEU | CA-CB-CG | -6.37 | 100.65 | 115.30 |
| 2 | 2 | 590 | C | C6-N1-C2 | -6.37 | 117.75 | 120.30 |
| 1 | 5 | 635 | G | C8-N9-C4 | 6.37 | 108.95 | 106.40 |
| 2 | 2 | 1456 | C | C2-N1-C1' | 6.37 | 125.80 | 118.80 |
| 1 | 1 | 2556 | C | N1-C2-O2 | 6.37 | 122.72 | 118.90 |
| 2 | 2 | 553 | G | C6-C5-N7 | -6.37 | 126.58 | 130.40 |
| 2 | 2 | 1572 | G | N1-C6-O6 | 6.37 | 123.72 | 119.90 |
| 1 | 5 | 637 | C | C6-N1-C2 | 6.37 | 122.85 | 120.30 |
| 1 | 1 | 336 | A | N9-C4-C5 | -6.36 | 103.25 | 105.80 |
| 2 | 2 | 1768 | G | N1-C6-O6 | -6.36 | 116.08 | 119.90 |
| 1 | 1 | 2311 | G | N1-C6-O6 | 6.36 | 123.72 | 119.90 |
| 1 | 5 | 2852 | C | N3-C4-C5 | -6.36 | 119.36 | 121.90 |
| 2 | 6 | 1059 | U | O4'-C1'-N1 | 6.36 | 113.29 | 108.20 |
| 1 | 1 | 3053 | G | N1-C6-O6 | 6.36 | 123.72 | 119.90 |
| 2 | 2 | 934 | C | C2-N1-C1' | 6.36 | 125.79 | 118.80 |
| 2 | 6 | 1340 | U | C2-N1-C1' | 6.36 | 125.33 | 117.70 |
| 2 | 2 | 364 | G | C8-N9-C4 | 6.35 | 108.94 | 106.40 |
| 2 | 2 | 1370 | U | P-O3'-C3' | 6.35 | 127.32 | 119.70 |
| 9 | C4 | 137 | LEU | CA-CB-CG | 6.35 | 129.91 | 115.30 |
| 1 | 1 | 1435 | A | C6-N1-C2 | -6.35 | 114.79 | 118.60 |
| 1 | 1 | 657 | A | OP1-P-O3' | 6.35 | 119.17 | 105.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2 | 2 | 614 | C | C6-N1-C2 | -6.35 | 117.76 | 120.30 |
| 1 | 1 | 1028 | U | OP2-P-O3' | 6.35 | 119.17 | 105.20 |
| 2 | 6 | 779 | U | O4'-C1'-N1 | 6.35 | 113.28 | 108.20 |
| 1 | 1 | 914 | A | N9-C4-C5 | 6.35 | 108.34 | 105.80 |
| 1 | 1 | 2608 | G | N7-C8-N9 | -6.35 | 109.93 | 113.10 |
| 1 | 5 | 1581 | C | N3-C4-C5 | 6.34 | 124.44 | 121.90 |
| 1 | 1 | 3218 | A | N1-C6-N6 | 6.34 | 122.41 | 118.60 |
| 1 | 1 | 2913 | C | N3-C2-O2 | 6.34 | 126.34 | 121.90 |
| 1 | 1 | 3217 | C | N3-C2-O2 | -6.34 | 117.46 | 121.90 |
| 1 | 5 | 311 | C | C6-N1-C2 | -6.34 | 117.76 | 120.30 |
| 1 | 1 | 1542 | G | N1-C6-O6 | 6.34 | 123.70 | 119.90 |
| 1 | 1 | 2696 | A | O5'-P-OP2 | -6.34 | 100.00 | 105.70 |
| 1 | 5 | 2381 | G | N1-C6-O6 | 6.34 | 123.70 | 119.90 |
| 2 | 6 | 696 | C | C6-N1-C2 | -6.34 | 117.76 | 120.30 |
| 1 | 5 | 833 | G | N9-C4-C5 | -6.34 | 102.87 | 105.40 |
| 1 | 5 | 2927 | C | N3-C4-C5 | 6.34 | 124.43 | 121.90 |
| 1 | 1 | 2937 | G | C4-C5-N7 | 6.33 | 113.33 | 110.80 |
| 1 | 5 | 979 | U | N3-C2-O2 | -6.33 | 117.77 | 122.20 |
| 1 | 1 | 2828 | G | N1-C6-O6 | -6.33 | 116.10 | 119.90 |
| 2 | 2 | 1082 | C | C2-N1-C1' | 6.33 | 125.76 | 118.80 |
| 1 | 5 | 1701 | C | C6-N1-C2 | -6.33 | 117.77 | 120.30 |
| 1 | 5 | 3344 | A | C8-N9-C4 | 6.33 | 108.33 | 105.80 |
| 2 | 6 | 1398 | U | C2-N1-C1' | 6.33 | 125.29 | 117.70 |
| 1 | 5 | 2957 | G | N3-C4-C5 | 6.33 | 131.76 | 128.60 |
| 2 | 2 | 1399 | C | N3-C2-O2 | -6.32 | 117.47 | 121.90 |
| 1 | 1 | 1206 | G | C8-N9-C4 | -6.32 | 103.87 | 106.40 |
| 3 | 3 | 114 | U | O5'-P-OP2 | -6.32 | 100.01 | 105.70 |
| 1 | 1 | 651 | G | C6-C5-N7 | -6.32 | 126.61 | 130.40 |
| 1 | 1 | 979 | U | N1-C2-N3 | 6.32 | 118.69 | 114.90 |
| 2 | 2 | 577 | G | C4-C5-N7 | 6.31 | 113.33 | 110.80 |
| 2 | 6 | 682 | C | C6-N1-C2 | -6.31 | 117.77 | 120.30 |
| 1 | 1 | 1422 | G | C6-C5-N7 | -6.31 | 126.61 | 130.40 |
| 1 | 1 | 28 | C | C5-C6-N1 | -6.31 | 117.85 | 121.00 |
| 2 | 2 | 1154 | G | N1-C6-O6 | -6.31 | 116.11 | 119.90 |
| 1 | 5 | 1053 | A | N1-C6-N6 | 6.31 | 122.38 | 118.60 |
| 1 | 5 | 2177 | G | C8-N9-C4 | 6.31 | 108.92 | 106.40 |
| 1 | 1 | 1554 | U | N1-C2-O2 | -6.30 | 118.39 | 122.80 |
| 1 | 5 | 2934 | A | N1-C6-N6 | 6.30 | 122.38 | 118.60 |
| 1 | 1 | 2158 | A | N1-C6-N6 | 6.30 | 122.38 | 118.60 |
| 1 | 1 | 2209 | U | C2-N1-C1' | 6.30 | 125.26 | 117.70 |
| 1 | 1 | 2553 | U | N1-C2-O2 | 6.30 | 127.21 | 122.80 |
| 4 | 4 | 82 | U | C2-N1-C1' | 6.30 | 125.26 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 1 | 2873 | U | N3-C2-O2 | -6.30 | 117.79 | 122.20 |
| 1 | 1 | 2263 | C | C6-N1-C2 | 6.30 | 122.82 | 120.30 |
| 1 | 5 | 274 | G | C8-N9-C4 | 6.30 | 108.92 | 106.40 |
| 1 | 1 | 3139 | A | C8-N9-C4 | -6.29 | 103.28 | 105.80 |
| 1 | 1 | 2247 | G | C8-N9-C4 | -6.29 | 103.88 | 106.40 |
| 1 | 5 | 860 | G | N9-C4-C5 | -6.29 | 102.88 | 105.40 |
| 2 | 6 | 192 | U | C2-N1-C1' | 6.29 | 125.25 | 117.70 |
| 1 | 5 | 1779 | C | N3-C4-N4 | 6.29 | 122.40 | 118.00 |
| 1 | 1 | 1413 | G | C6-C5-N7 | -6.28 | 126.63 | 130.40 |
| 1 | 1 | 73 | C | C6-N1-C2 | -6.28 | 117.79 | 120.30 |
| 1 | 1 | 1852 | G | C4-C5-N7 | 6.28 | 113.31 | 110.80 |
| 1 | 1 | 2818 | U | O5'-P-OP1 | -6.28 | 100.05 | 105.70 |
| 1 | 5 | 1188 | U | N3-C2-O2 | -6.28 | 117.80 | 122.20 |
| 1 | 1 | 3098 | G | C5-C6-N1 | 6.28 | 114.64 | 111.50 |
| 1 | 1 | 639 | G | N3-C4-C5 | 6.28 | 131.74 | 128.60 |
| 2 | 2 | 1059 | U | N1-C2-O2 | 6.28 | 127.19 | 122.80 |
| 1 | 5 | 2873 | U | N3-C2-O2 | -6.28 | 117.81 | 122.20 |
| 1 | 1 | 234 | G | O5'-P-OP1 | -6.27 | 100.05 | 105.70 |
| 1 | 1 | 3278 | C | C2-N1-C1' | 6.27 | 125.70 | 118.80 |
| 2 | 2 | 543 | C | C4-C5-C6 | 6.27 | 120.54 | 117.40 |
| 1 | 5 | 366 | A | C8-N9-C4 | 6.27 | 108.31 | 105.80 |
| 1 | 5 | 3245 | A | C2-N3-C4 | -6.27 | 107.47 | 110.60 |
| 2 | 6 | 1560 | U | N3-C2-O2 | -6.27 | 117.81 | 122.20 |
| 1 | 1 | 1400 | G | N1-C6-O6 | -6.27 | 116.14 | 119.90 |
| 1 | 5 | 435 | C | C6-N1-C2 | 6.27 | 122.81 | 120.30 |
| 1 | 5 | 1839 | A | N7-C8-N9 | -6.27 | 110.67 | 113.80 |
| 1 | 1 | 1866 | C | C6-N1-C1' | -6.27 | 113.28 | 120.80 |
| 1 | 5 | 2945 | G | O5'-P-OP2 | -6.27 | 100.06 | 105.70 |
| 1 | 1 | 1114 | U | N3-C4-C5 | -6.26 | 110.84 | 114.60 |
| 1 | 1 | 1815 | U | P-O3'-C3' | 6.26 | 127.22 | 119.70 |
| 1 | 5 | 1495 | U | C6-N1-C2 | -6.26 | 117.24 | 121.00 |
| 1 | 1 | 2651 | G | N1-C6-O6 | 6.26 | 123.66 | 119.90 |
| 2 | 2 | 130 | C | C6-N1-C2 | -6.26 | 117.80 | 120.30 |
| 1 | 5 | 2600 | C | C5-C6-N1 | 6.26 | 124.13 | 121.00 |
| 1 | 1 | 282 | G | P-O3'-C3' | 6.26 | 127.21 | 119.70 |
| 1 | 1 | 1157 | G | C8-N9-C4 | 6.26 | 108.90 | 106.40 |
| 1 | 1 | 1404 | G | N1-C6-O6 | 6.26 | 123.65 | 119.90 |
| 2 | 2 | 1096 | C | C6-N1-C2 | -6.26 | 117.80 | 120.30 |
| 1 | 5 | 3100 | U | C6-N1-C2 | 6.26 | 124.75 | 121.00 |
| 2 | 6 | 653 | C | C5-C6-N1 | 6.26 | 124.13 | 121.00 |
| 1 | 1 | 1482 | A | O5'-P-OP2 | -6.25 | 100.07 | 105.70 |
| 1 | 1 | 1102 | A | C8-N9-C4 | 6.25 | 108.30 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 1 | 2152 | A | C8-N9-C4 | -6.25 | 103.30 | 105.80 |
| 1 | 5 | 359 | U | C6-N1-C2 | -6.25 | 117.25 | 121.00 |
| 1 | 1 | 2730 | G | N3-C4-N9 | -6.25 | 122.25 | 126.00 |
| 34 | L9 | 191 | LEU | CA-CB-CG | 6.25 | 129.67 | 115.30 |
| 1 | 1 | 2818 | U | N3-C2-O2 | 6.25 | 126.57 | 122.20 |
| 1 | 1 | 935 | U | N3-C2-O2 | -6.25 | 117.83 | 122.20 |
| 1 | 1 | 2256 | A | OP1-P-O3' | 6.25 | 118.94 | 105.20 |
| 2 | 6 | 1042 | G | N1-C6-O6 | 6.24 | 123.64 | 119.90 |
| 1 | 1 | 1166 | G | N1-C6-O6 | 6.24 | 123.64 | 119.90 |
| 1 | 1 | 1438 | U | C6-N1-C2 | -6.24 | 117.26 | 121.00 |
| 1 | 1 | 2818 | U | N3-C4-O4 | 6.24 | 123.77 | 119.40 |
| 4 | 4 | 14 | C | C2-N1-C1' | -6.24 | 111.94 | 118.80 |
| 1 | 1 | 1889 | G | C5-C6-O6 | -6.24 | 124.86 | 128.60 |
| 1 | 5 | 2935 | U | C5-C6-N1 | 6.24 | 125.82 | 122.70 |
| 1 | 1 | 1581 | C | C6-N1-C2 | -6.23 | 117.81 | 120.30 |
| 2 | 2 | 864 | U | C2-N1-C1' | 6.23 | 125.18 | 117.70 |
| 1 | 1 | 1157 | G | N1-C6-O6 | 6.23 | 123.64 | 119.90 |
| 1 | 1 | 2933 | A | N1-C6-N6 | -6.23 | 114.86 | 118.60 |
| 1 | 5 | 1413 | G | C4-C5-N7 | 6.23 | 113.29 | 110.80 |
| 2 | 2 | 1490 | C | C6-N1-C2 | -6.23 | 117.81 | 120.30 |
| 1 | 1 | 2603 | G | O5'-P-OP2 | -6.23 | 100.10 | 105.70 |
| 1 | 5 | 809 | G | C5-C6-O6 | -6.23 | 124.86 | 128.60 |
| 1 | 1 | 1480 | G | C4-C5-N7 | 6.22 | 113.29 | 110.80 |
| 2 | 2 | 136 | C | C2-N1-C1' | 6.22 | 125.65 | 118.80 |
| 1 | 5 | 1413 | G | C5-C6-O6 | -6.22 | 124.87 | 128.60 |
| 1 | 1 | 224 | C | C5-C4-N4 | -6.22 | 115.85 | 120.20 |
| 1 | 1 | 1348 | U | N3-C2-O2 | -6.22 | 117.85 | 122.20 |
| 2 | 6 | 638 | U | N1-C2-O2 | 6.22 | 127.15 | 122.80 |
| 1 | 1 | 793 | C | N1-C2-O2 | 6.22 | 122.63 | 118.90 |
| 1 | 1 | 2620 | G | N3-C4-C5 | 6.22 | 131.71 | 128.60 |
| 1 | 5 | 1779 | C | C5-C6-N1 | 6.22 | 124.11 | 121.00 |
| 1 | 5 | 1331 | U | C6-N1-C2 | 6.21 | 124.73 | 121.00 |
| 1 | 5 | 1145 | G | C6-C5-N7 | -6.21 | 126.67 | 130.40 |
| 1 | 5 | 1156 | C | C6-N1-C2 | 6.21 | 122.78 | 120.30 |
| 2 | 6 | 418 | G | C8-N9-C4 | 6.21 | 108.88 | 106.40 |
| 4 | 4 | 54 | A | C5-N7-C8 | -6.21 | 100.80 | 103.90 |
| 2 | 2 | 305 | C | C6-N1-C2 | 6.20 | 122.78 | 120.30 |
| 1 | 5 | 1200 | A | N1-C6-N6 | 6.20 | 122.32 | 118.60 |
| 2 | 2 | 1324 | G | N9-C4-C5 | 6.20 | 107.88 | 105.40 |
| 2 | 6 | 607 | G | C5-C6-O6 | -6.20 | 124.88 | 128.60 |
| 1 | 5 | 2386 | A | C8-N9-C4 | 6.20 | 108.28 | 105.80 |
| 2 | 6 | 302 | U | C5-C6-N1 | 6.20 | 125.80 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 5 | 822 | G | C8-N9-C4 | -6.20 | 103.92 | 106.40 |
| 1 | 5 | 988 | U | C6-N1-C2 | 6.20 | 124.72 | 121.00 |
| 1 | 1 | 3084 | C | N3-C4-C5 | -6.20 | 119.42 | 121.90 |
| 2 | 6 | 171 | A | N1-C2-N3 | 6.20 | 132.40 | 129.30 |
| 1 | 1 | 2862 | U | C5-C6-N1 | -6.19 | 119.60 | 122.70 |
| 1 | 1 | 1437 | C | C6-N1-C2 | -6.19 | 117.82 | 120.30 |
| 2 | 2 | 308 | C | N3-C4-C5 | 6.19 | 124.38 | 121.90 |
| 2 | 6 | 1600 | A | C6-C5-N7 | -6.19 | 127.97 | 132.30 |
| 1 | 5 | 2132 | C | C5-C6-N1 | 6.19 | 124.09 | 121.00 |
| 2 | 2 | 794 | U | P-O3'-C3' | 6.19 | 127.12 | 119.70 |
| 2 | 6 | 741 | C | C6-N1-C2 | 6.18 | 122.77 | 120.30 |
| 1 | 1 | 1016 | C | C6-N1-C2 | -6.18 | 117.83 | 120.30 |
| 1 | 1 | 1508 | C | C6-N1-C2 | -6.18 | 117.83 | 120.30 |
| 2 | 6 | 1097 | U | P-O3'-C3' | 6.18 | 127.12 | 119.70 |
| 1 | 1 | 350 | C | C6-N1-C2 | -6.18 | 117.83 | 120.30 |
| 2 | 2 | 1258 | U | N3-C2-O2 | -6.18 | 117.87 | 122.20 |
| 1 | 1 | 3269 | U | N1-C2-O2 | 6.18 | 127.12 | 122.80 |
| 2 | 2 | 780 | A | N1-C2-N3 | 6.18 | 132.39 | 129.30 |
| 1 | 5 | 1520 | G | C5-C6-O6 | -6.18 | 124.89 | 128.60 |
| 3 | 7 | 82 | G | N1-C6-O6 | -6.18 | 116.19 | 119.90 |
| 1 | 1 | 2860 | U | N1-C2-O2 | 6.18 | 127.12 | 122.80 |
| 1 | 5 | 2715 | A | N9-C4-C5 | -6.18 | 103.33 | 105.80 |
| 2 | 2 | 1597 | A | N1-C6-N6 | 6.18 | 122.31 | 118.60 |
| 1 | 5 | 1858 | A | C8-N9-C4 | -6.17 | 103.33 | 105.80 |
| 2 | 6 | 217 | A | P-O3'-C3' | 6.17 | 127.11 | 119.70 |
| 1 | 1 | 2943 | G | C6-C5-N7 | -6.17 | 126.70 | 130.40 |
| 2 | 6 | 765 | G | C5-N7-C8 | 6.17 | 107.39 | 104.30 |
| 1 | 1 | 2818 | U | C5-C4-O4 | -6.17 | 122.20 | 125.90 |
| 1 | 1 | 1076 | C | O5'-P-OP2 | -6.17 | 100.15 | 105.70 |
| 2 | 2 | 734 | A | P-O3'-C3' | 6.17 | 127.10 | 119.70 |
| 1 | 1 | 1382 | G | C8-N9-C4 | 6.17 | 108.87 | 106.40 |
| 1 | 5 | 1436 | U | N1-C2-O2 | 6.16 | 127.11 | 122.80 |
| 2 | 2 | 261 | U | N3-C2-O2 | -6.16 | 117.89 | 122.20 |
| 1 | 5 | 2612 | U | N3-C4-O4 | 6.16 | 123.71 | 119.40 |
| 1 | 5 | 2892 | A | N1-C6-N6 | 6.16 | 122.30 | 118.60 |
| 4 | 8 | 140 | G | N1-C6-O6 | 6.16 | 123.60 | 119.90 |
| 1 | 1 | 1158 | A | O5'-P-OP2 | -6.16 | 100.16 | 105.70 |
| 1 | 1 | 2256 | A | P-O3'-C3' | 6.16 | 127.09 | 119.70 |
| 1 | 1 | 2257 | C | N1-C2-O2 | 6.16 | 122.59 | 118.90 |
| 1 | 1 | 2554 | A | P-O3'-C3' | 6.16 | 127.09 | 119.70 |
| 1 | 5 | 1633 | C | C2-N1-C1' | 6.16 | 125.57 | 118.80 |
| 1 | 1 | 2263 | C | N3-C4-C5 | 6.16 | 124.36 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 5 | 2376 | G | N1-C6-O6 | 6.16 | 123.59 | 119.90 |
| 1 | 5 | 663 | C | C6-N1-C2 | -6.15 | 117.84 | 120.30 |
| 2 | 6 | 558 | U | P-O3'-C3' | 6.15 | 127.08 | 119.70 |
| 2 | 2 | 704 | C | N3-C2-O2 | -6.15 | 117.59 | 121.90 |
| 1 | 5 | 2872 | A | N3-C4-C5 | -6.15 | 122.49 | 126.80 |
| 1 | 1 | 1578 | C | C5-C6-N1 | 6.15 | 124.08 | 121.00 |
| 1 | 1 | 3333 | G | N1-C6-O6 | -6.15 | 116.21 | 119.90 |
| 1 | 5 | 799 | G | N1-C6-O6 | 6.15 | 123.59 | 119.90 |
| 2 | 6 | 276 | C | C6-N1-C2 | 6.15 | 122.76 | 120.30 |
| 1 | 5 | 1149 | G | C6-C5-N7 | -6.15 | 126.71 | 130.40 |
| 1 | 5 | 2822 | U | C5-C6-N1 | 6.15 | 125.78 | 122.70 |
| 2 | 6 | 765 | G | N7-C8-N9 | -6.15 | 110.03 | 113.10 |
| 1 | 1 | 2568 | C | C2-N1-C1' | 6.15 | 125.56 | 118.80 |
| 5 | c0 | 83 | PRO | N-CA-CB | 6.15 | 110.68 | 103.30 |
| 1 | 1 | 3382 | U | C6-N1-C2 | -6.15 | 117.31 | 121.00 |
| 75 | S7 | 31 | SER | N-CA-C | 6.15 | 127.59 | 111.00 |
| 1 | 5 | 427 | C | C6-N1-C2 | 6.14 | 122.76 | 120.30 |
| 1 | 5 | 2403 | G | C8-N9-C1' | -6.14 | 119.01 | 127.00 |
| 1 | 1 | 302 | U | N3-C2-O2 | -6.14 | 117.90 | 122.20 |
| 1 | 5 | 651 | G | C5-C6-O6 | -6.14 | 124.92 | 128.60 |
| 1 | 1 | 1399 | A | N3-C4-C5 | 6.14 | 131.10 | 126.80 |
| 2 | 2 | 1745 | G | C4-N9-C1' | 6.14 | 134.48 | 126.50 |
| 1 | 1 | 2809 | C | C5-C6-N1 | 6.14 | 124.07 | 121.00 |
| 1 | 1 | 669 | U | C6-N1-C2 | 6.14 | 124.68 | 121.00 |
| 3 | 3 | 26 | C | C6-N1-C2 | -6.14 | 117.84 | 120.30 |
| 1 | 5 | 2606 | G | N3-C2-N2 | 6.14 | 124.20 | 119.90 |
| 1 | 5 | 3089 | C | N3-C2-O2 | -6.14 | 117.61 | 121.90 |
| 17 | D2 | 104 | LEU | CA-CB-CG | 6.14 | 129.41 | 115.30 |
| 1 | 1 | 2820 | A | C4-C5-C6 | -6.13 | 113.93 | 117.00 |
| 1 | 5 | 3089 | C | N1-C2-O2 | 6.13 | 122.58 | 118.90 |
| 3 | 7 | 93 | C | C2-N3-C4 | -6.13 | 116.83 | 119.90 |
| 1 | 1 | 1589 | A | C5-C6-N6 | -6.13 | 118.80 | 123.70 |
| 1 | 1 | 891 | G | N9-C4-C5 | -6.13 | 102.95 | 105.40 |
| 1 | 1 | 2340 | U | C5-C6-N1 | 6.13 | 125.76 | 122.70 |
| 1 | 5 | 2105 | G | C8-N9-C4 | 6.13 | 108.85 | 106.40 |
| 2 | 6 | 460 | A | O5'-P-OP1 | -6.13 | 100.18 | 105.70 |
| 1 | 5 | 2332 | A | N1-C6-N6 | 6.13 | 122.28 | 118.60 |
| 1 | 5 | 2362 | C | N3-C2-O2 | -6.13 | 117.61 | 121.90 |
| 1 | 5 | 2949 | U | C5-C6-N1 | -6.12 | 119.64 | 122.70 |
| 1 | 5 | 405 | U | OP2-P-O3' | 6.12 | 118.67 | 105.20 |
| 1 | 5 | 1303 | A | N9-C4-C5 | -6.12 | 103.35 | 105.80 |
| 1 | 5 | 3069 | G | C5-C6-O6 | 6.12 | 132.27 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 4 | 8 | 105 | A | N1-C6-N6 | 6.12 | 122.27 | 118.60 |
| 1 | 1 | 2825 | C | N1-C2-O2 | 6.12 | 122.57 | 118.90 |
| 1 | 5 | 2837 | A | N9-C4-C5 | -6.12 | 103.35 | 105.80 |
| 1 | 1 | 2899 | C | N3-C2-O2 | -6.12 | 117.62 | 121.90 |
| 2 | 2 | 1739 | C | C6-N1-C2 | 6.12 | 122.75 | 120.30 |
| 2 | 6 | 1490 | C | C5-C6-N1 | 6.12 | 124.06 | 121.00 |
| 2 | 6 | 1211 | A | C8-N9-C4 | -6.12 | 103.35 | 105.80 |
| 1 | 5 | 1417 | G | C4-C5-N7 | 6.12 | 113.25 | 110.80 |
| 2 | 6 | 1286 | U | C5-C6-N1 | 6.12 | 125.76 | 122.70 |
| 1 | 1 | 1677 | G | N1-C6-O6 | 6.11 | 123.57 | 119.90 |
| 2 | 2 | 192 | U | C6-N1-C2 | -6.11 | 117.33 | 121.00 |
| 1 | 1 | 2620 | G | N1-C6-O6 | 6.11 | 123.57 | 119.90 |
| 1 | 1 | 1938 | U | C6-N1-C2 | 6.11 | 124.67 | 121.00 |
| 1 | 5 | 609 | G | O5'-P-OP2 | -6.11 | 100.20 | 105.70 |
| 1 | 5 | 1028 | U | N1-C2-O2 | 6.11 | 127.08 | 122.80 |
| 1 | 5 | 1902 | G | N1-C6-O6 | 6.11 | 123.56 | 119.90 |
| 1 | 5 | 2325 | G | C4-C5-N7 | 6.11 | 113.24 | 110.80 |
| 1 | 1 | 1720 | U | C5-C4-O4 | 6.11 | 129.56 | 125.90 |
| 1 | 5 | 1115 | G | C6-C5-N7 | -6.11 | 126.74 | 130.40 |
| 1 | 1 | 635 | G | O5'-P-OP2 | 6.10 | 118.02 | 110.70 |
| 1 | 1 | 1654 | A | C8-N9-C4 | 6.10 | 108.24 | 105.80 |
| 1 | 1 | 92 | G | C5-C6-O6 | -6.10 | 124.94 | 128.60 |
| 1 | 5 | 1878 | G | C8-N9-C4 | -6.10 | 103.96 | 106.40 |
| 1 | 5 | 1150 | A | C8-N9-C4 | -6.10 | 103.36 | 105.80 |
| 1 | 5 | 2169 | G | C6-C5-N7 | 6.10 | 134.06 | 130.40 |
| 1 | 1 | 200 | C | N1-C2-O2 | -6.10 | 115.24 | 118.90 |
| 1 | 1 | 222 | A | N1-C6-N6 | 6.10 | 122.26 | 118.60 |
| 1 | 1 | 508 | U | C6-N1-C2 | -6.10 | 117.34 | 121.00 |
| 1 | 1 | 3382 | U | N3-C2-O2 | -6.10 | 117.93 | 122.20 |
| 1 | 5 | 297 | G | O4'-C1'-N9 | 6.10 | 113.08 | 108.20 |
| 1 | 5 | 359 | U | N1-C2-N3 | 6.10 | 118.56 | 114.90 |
| 1 | 5 | 639 | G | C8-N9-C4 | 6.10 | 108.84 | 106.40 |
| 1 | 1 | 439 | C | C5-C6-N1 | 6.09 | 124.05 | 121.00 |
| 1 | 1 | 2139 | A | OP1-P-O3' | 6.09 | 118.61 | 105.20 |
| 1 | 5 | 873 | C | P-O3'-C3' | 6.09 | 127.01 | 119.70 |
| 2 | 6 | 306 | U | C6-N1-C2 | 6.09 | 124.66 | 121.00 |
| 2 | 6 | 377 | G | C5-C6-O6 | -6.09 | 124.94 | 128.60 |
| 1 | 5 | 1375 | G | C5-C6-O6 | -6.09 | 124.94 | 128.60 |
| 1 | 1 | 3370 | A | O5'-P-OP2 | -6.09 | 100.22 | 105.70 |
| 1 | 1 | 2794 | G | N3-C4-C5 | 6.09 | 131.64 | 128.60 |
| 1 | 1 | 63 | A | C4-C5-C6 | 6.08 | 120.04 | 117.00 |
| 1 | 5 | 1196 | C | C5-C4-N4 | 6.08 | 124.46 | 120.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 5 | 61 | A | N9-C4-C5 | 6.08 | 108.23 | 105.80 |
| 1 | 5 | 2433 | U | C6-N1-C2 | 6.08 | 124.65 | 121.00 |
| 2 | 2 | 507 | U | N1-C2-O2 | 6.08 | 127.06 | 122.80 |
| 1 | 5 | 776 | U | N3-C2-O2 | -6.08 | 117.94 | 122.20 |
| 1 | 5 | 1906 | G | N1-C6-O6 | 6.08 | 123.55 | 119.90 |
| 1 | 1 | 2147 | A | C8-N9-C4 | 6.08 | 108.23 | 105.80 |
| 1 | 5 | 2246 | G | N1-C6-O6 | 6.08 | 123.55 | 119.90 |
| 2 | 6 | 1489 | U | C5-C6-N1 | 6.08 | 125.74 | 122.70 |
| 1 | 1 | 2381 | G | C5-C6-O6 | -6.08 | 124.95 | 128.60 |
| 1 | 5 | 3269 | U | C6-N1-C2 | -6.08 | 117.35 | 121.00 |
| 4 | 4 | 140 | G | C5-C6-O6 | -6.07 | 124.96 | 128.60 |
| 1 | 5 | 525 | C | C6-N1-C2 | -6.07 | 117.87 | 120.30 |
| 1 | 1 | 827 | A | C8-N9-C4 | 6.07 | 108.23 | 105.80 |
| 1 | 5 | 2872 | A | P-O3'-C3' | 6.07 | 126.98 | 119.70 |
| 44 | N0 | 24 | LEU | CA-CB-CG | 6.07 | 129.26 | 115.30 |
| 1 | 1 | 1764 | U | C6-N1-C2 | -6.07 | 117.36 | 121.00 |
| 17 | d2 | 93 | LEU | CA-CB-CG | 6.07 | 129.26 | 115.30 |
| 1 | 1 | 1306 | G | C8-N9-C1' | -6.07 | 119.11 | 127.00 |
| 1 | 1 | 2922 | G | C8-N9-C1' | -6.06 | 119.12 | 127.00 |
| 1 | 1 | 370 | U | O5'-P-OP2 | -6.06 | 100.24 | 105.70 |
| 1 | 5 | 3022 | G | N9-C4-C5 | 6.06 | 107.83 | 105.40 |
| 1 | 5 | 291 | C | C6-N1-C2 | 6.06 | 122.72 | 120.30 |
| 2 | 6 | 321 | C | N1-C2-O2 | 6.06 | 122.54 | 118.90 |
| 1 | 1 | 1495 | U | C2-N1-C1' | -6.06 | 110.43 | 117.70 |
| 1 | 1 | 2612 | U | C2-N1-C1' | 6.06 | 124.97 | 117.70 |
| 1 | 1 | 2613 | U | C6-N1-C2 | -6.06 | 117.36 | 121.00 |
| 1 | 1 | 1943 | C | C6-N1-C2 | -6.06 | 117.88 | 120.30 |
| 1 | 5 | 2809 | C | N3-C4-C5 | -6.06 | 119.48 | 121.90 |
| 2 | 6 | 302 | U | C2-N1-C1' | 6.06 | 124.97 | 117.70 |
| 1 | 1 | 352 | A | C8-N9-C4 | 6.05 | 108.22 | 105.80 |
| 1 | 1 | 1819 | U | C5-C6-N1 | 6.05 | 125.73 | 122.70 |
| 2 | 2 | 1782 | A | C5-C6-N1 | -6.05 | 114.67 | 117.70 |
| 1 | 5 | 3076 | C | C5-C6-N1 | 6.05 | 124.03 | 121.00 |
| 1 | 1 | 1365 | G | C8-N9-C4 | -6.05 | 103.98 | 106.40 |
| 1 | 5 | 638 | C | C6-N1-C2 | -6.05 | 117.88 | 120.30 |
| 2 | 2 | 1291 | G | C5-N7-C8 | -6.05 | 101.27 | 104.30 |
| 2 | 2 | 1745 | G | C8-N9-C1' | -6.05 | 119.14 | 127.00 |
| 1 | 5 | 1520 | G | N1-C6-O6 | 6.05 | 123.53 | 119.90 |
| 1 | 5 | 2606 | G | C8-N9-C1' | -6.05 | 119.14 | 127.00 |
| 1 | 5 | 3180 | A | C8-N9-C4 | 6.05 | 108.22 | 105.80 |
| 2 | 2 | 1339 | C | P-O3'-C3' | 6.05 | 126.96 | 119.70 |
| 2 | 2 | 1465 | C | C6-N1-C2 | -6.05 | 117.88 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 5 | 3362 | A | O4'-C1'-N9 | 6.05 | 113.04 | 108.20 |
| 1 | 1 | 2987 | A | N1-C6-N6 | 6.04 | 122.23 | 118.60 |
| 4 | 4 | 11 | C | C6-N1-C2 | -6.04 | 117.88 | 120.30 |
| 1 | 5 | 409 | A | O5'-P-OP1 | -6.04 | 100.26 | 105.70 |
| 1 | 1 | 1095 | U | C6-N1-C2 | -6.04 | 117.38 | 121.00 |
| 2 | 2 | 782 | U | P-O3'-C3' | 6.04 | 126.95 | 119.70 |
| 2 | 2 | 497 | G | P-O3'-C3' | 6.04 | 126.94 | 119.70 |
| 1 | 1 | 901 | G | O5'-P-OP1 | -6.04 | 100.27 | 105.70 |
| 1 | 5 | 3092 | C | O5'-P-OP2 | 6.04 | 117.94 | 110.70 |
| 3 | 7 | 92 | A | O5'-P-OP1 | -6.04 | 100.27 | 105.70 |
| 1 | 1 | 1003 | A | O5'-P-OP1 | -6.03 | 100.27 | 105.70 |
| 2 | 2 | 1757 | G | C8-N9-C4 | -6.03 | 103.99 | 106.40 |
| 2 | 2 | 1611 | A | N1-C2-N3 | 6.03 | 132.31 | 129.30 |
| 1 | 5 | 1211 | U | C5-C6-N1 | -6.03 | 119.69 | 122.70 |
| 2 | 6 | 1457 | C | N1-C2-O2 | 6.03 | 122.52 | 118.90 |
| 2 | 6 | 1511 | U | C6-N1-C2 | -6.03 | 117.38 | 121.00 |
| 1 | 5 | 420 | G | N1-C6-O6 | 6.02 | 123.51 | 119.90 |
| 1 | 1 | 115 | A | C8-N9-C4 | 6.02 | 108.21 | 105.80 |
| 1 | 5 | 2381 | G | C5-C6-O6 | -6.02 | 124.99 | 128.60 |
| 1 | 1 | 1930 | A | C8-N9-C4 | -6.02 | 103.39 | 105.80 |
| 1 | 5 | 1793 | C | N3-C4-C5 | 6.02 | 124.31 | 121.90 |
| 2 | 6 | 992 | A | C8-N9-C4 | 6.02 | 108.21 | 105.80 |
| 1 | 1 | 1404 | G | N3-C4-C5 | 6.02 | 131.61 | 128.60 |
| 1 | 1 | 1865 | A | C8-N9-C4 | 6.02 | 108.21 | 105.80 |
| 1 | 1 | 2613 | U | N1-C2-N3 | 6.02 | 118.51 | 114.90 |
| 1 | 1 | 3012 | A | C2-N3-C4 | -6.02 | 107.59 | 110.60 |
| 1 | 5 | 2507 | C | C6-N1-C2 | -6.02 | 117.89 | 120.30 |
| 1 | 1 | 1454 | A | N9-C4-C5 | -6.01 | 103.39 | 105.80 |
| 1 | 1 | 817 | A | O5'-P-OP1 | -6.01 | 100.29 | 105.70 |
| 1 | 1 | 2355 | G | C5-C6-O6 | -6.01 | 124.99 | 128.60 |
| 2 | 2 | 1399 | C | C2-N1-C1' | 6.01 | 125.41 | 118.80 |
| 1 | 5 | 2326 | A | N1-C6-N6 | 6.01 | 122.21 | 118.60 |
| 1 | 1 | 2139 | A | N1-C6-N6 | -6.01 | 114.99 | 118.60 |
| 2 | 2 | 1032 | G | C8-N9-C4 | 6.01 | 108.80 | 106.40 |
| 1 | 5 | 1081 | U | P-O3'-C3' | 6.01 | 126.91 | 119.70 |
| 1 | 5 | 2779 | A | O5'-P-OP1 | -6.01 | 100.29 | 105.70 |
| 2 | 6 | 639 | U | N3-C2-O2 | -6.01 | 117.99 | 122.20 |
| 2 | 2 | 1572 | G | N9-C4-C5 | -6.01 | 103.00 | 105.40 |
| 1 | 1 | 2967 | A | N9-C4-C5 | -6.01 | 103.40 | 105.80 |
| 1 | 5 | 3286 | G | N1-C6-O6 | -6.01 | 116.30 | 119.90 |
| 2 | 6 | 542 | A | P-O3'-C3' | 6.01 | 126.91 | 119.70 |
| 2 | 2 | 321 | C | N1-C2-O2 | 6.00 | 122.50 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2 | 2 | 1733 | C | C6-N1-C2 | 6.00 | 122.70 | 120.30 |
| 1 | 5 | 1183 | C | C6-N1-C2 | 6.00 | 122.70 | 120.30 |
| 1 | 5 | 31 | C | N3-C4-C5 | 6.00 | 124.30 | 121.90 |
| 1 | 5 | 1196 | C | N3-C2-O2 | -6.00 | 117.70 | 121.90 |
| 1 | 5 | 2156 | C | C5-C6-N1 | -6.00 | 118.00 | 121.00 |
| 2 | 6 | 576 | G | N1-C6-O6 | 6.00 | 123.50 | 119.90 |
| 1 | 5 | 227 | G | N3-C4-N9 | 6.00 | 129.60 | 126.00 |
| 1 | 5 | 432 | G | N1-C6-O6 | 6.00 | 123.50 | 119.90 |
| 1 | 5 | 644 | G | N9-C4-C5 | 6.00 | 107.80 | 105.40 |
| 2 | 6 | 433 | C | O5'-P-OP1 | -5.99 | 100.31 | 105.70 |
| 1 | 1 | 2735 | U | C2-N1-C1' | 5.99 | 124.89 | 117.70 |
| 1 | 1 | 3217 | C | C6-N1-C1' | -5.99 | 113.61 | 120.80 |
| 1 | 5 | 227 | G | N3-C4-C5 | -5.99 | 125.61 | 128.60 |
| 1 | 5 | 3101 | G | N1-C6-O6 | 5.99 | 123.49 | 119.90 |
| 2 | 6 | 1426 | C | C6-N1-C2 | 5.99 | 122.69 | 120.30 |
| 1 | 1 | 1353 | U | C6-N1-C2 | -5.99 | 117.41 | 121.00 |
| 2 | 6 | 1568 | C | C6-N1-C2 | -5.99 | 117.91 | 120.30 |
| 1 | 5 | 1849 | C | C2-N3-C4 | -5.98 | 116.91 | 119.90 |
| 1 | 5 | 2403 | G | N3-C4-N9 | 5.98 | 129.59 | 126.00 |
| 1 | 5 | 3135 | U | N3-C4-O4 | 5.98 | 123.59 | 119.40 |
| 1 | 5 | 2313 | A | C4-C5-N7 | -5.98 | 107.71 | 110.70 |
| 1 | 1 | 966 | U | C5-C6-N1 | 5.98 | 125.69 | 122.70 |
| 1 | 5 | 2651 | G | C5-C6-O6 | -5.98 | 125.01 | 128.60 |
| 1 | 5 | 1483 | G | O4'-C1'-N9 | 5.98 | 112.98 | 108.20 |
| 1 | 1 | 291 | C | C2-N1-C1' | -5.97 | 112.23 | 118.80 |
| 1 | 1 | 2142 | A | O5'-P-OP2 | -5.97 | 100.32 | 105.70 |
| 2 | 6 | 163 | G | N3-C4-N9 | -5.97 | 122.42 | 126.00 |
| 2 | 6 | 1607 | G | C6-C5-N7 | -5.97 | 126.81 | 130.40 |
| 1 | 1 | 73 | C | N3-C4-C5 | -5.97 | 119.51 | 121.90 |
| 1 | 1 | 570 | A | N1-C6-N6 | 5.97 | 122.18 | 118.60 |
| 2 | 2 | 863 | A | O4'-C1'-N9 | 5.97 | 112.98 | 108.20 |
| 1 | 5 | 2860 | U | N1-C2-O2 | 5.97 | 126.98 | 122.80 |
| 1 | 1 | 798 | G | C8-N9-C4 | -5.97 | 104.01 | 106.40 |
| 1 | 1 | 2360 | C | N3-C4-C5 | 5.97 | 124.29 | 121.90 |
| 3 | 3 | 58 | C | C6-N1-C2 | -5.97 | 117.91 | 120.30 |
| 1 | 5 | 2911 | A | O5'-P-OP2 | -5.97 | 100.33 | 105.70 |
| 50 | N6 | 126 | LEU | CA-CB-CG | 5.97 | 129.03 | 115.30 |
| 1 | 1 | 2893 | C | O5'-P-OP1 | -5.97 | 100.33 | 105.70 |
| 2 | 2 | 73 | U | OP1-P-O3' | 5.97 | 118.33 | 105.20 |
| 1 | 5 | 1775 | G | C5-C6-O6 | -5.97 | 125.02 | 128.60 |
| 1 | 1 | 28 | C | C2-N3-C4 | -5.96 | 116.92 | 119.90 |
| 1 | 1 | 3195 | U | C5-C6-N1 | 5.96 | 125.68 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 5 | 809 | G | C4-C5-N7 | 5.96 | 113.18 | 110.80 |
| 1 | 5 | 2878 | G | N1-C6-O6 | 5.96 | 123.47 | 119.90 |
| 1 | 1 | 2801 | A | N1-C6-N6 | 5.96 | 122.17 | 118.60 |
| 1 | 5 | 2968 | G | OP2-P-O3' | 5.96 | 118.31 | 105.20 |
| 2 | 6 | 337 | G | C5-C6-O6 | -5.96 | 125.03 | 128.60 |
| 1 | 5 | 3209 | A | N9-C4-C5 | -5.95 | 103.42 | 105.80 |
| 1 | 1 | 924 | G | O4'-C1'-N9 | -5.95 | 103.44 | 108.20 |
| 1 | 1 | 3129 | A | C8-N9-C4 | 5.95 | 108.18 | 105.80 |
| 1 | 1 | 3317 | U | N3-C2-O2 | -5.95 | 118.03 | 122.20 |
| 1 | 5 | 635 | G | C4-C5-N7 | 5.95 | 113.18 | 110.80 |
| 1 | 5 | 1196 | C | N3-C4-C5 | -5.95 | 119.52 | 121.90 |
| 1 | 5 | 3266 | G | C4-C5-N7 | -5.95 | 108.42 | 110.80 |
| 1 | 1 | 835 | G | O4'-C1'-N9 | 5.95 | 112.96 | 108.20 |
| 1 | 1 | 1355 | A | P-O3'-C3' | 5.95 | 126.84 | 119.70 |
| 1 | 1 | 2380 | U | C6-N1-C2 | 5.95 | 124.57 | 121.00 |
| 3 | 3 | 67 | G | N1-C6-O6 | 5.95 | 123.47 | 119.90 |
| 2 | 6 | 320 | U | N3-C4-O4 | 5.95 | 123.56 | 119.40 |
| 1 | 1 | 116 | A | C8-N9-C4 | -5.94 | 103.42 | 105.80 |
| 1 | 1 | 764 | U | OP2-P-O3' | 5.94 | 118.28 | 105.20 |
| 1 | 1 | 1604 | G | C8-N9-C1' | -5.94 | 119.27 | 127.00 |
| 2 | 6 | 1197 | C | C6-N1-C2 | -5.94 | 117.92 | 120.30 |
| 1 | 1 | 895 | A | C5-N7-C8 | -5.94 | 100.93 | 103.90 |
| 1 | 1 | 2363 | A | N1-C6-N6 | -5.94 | 115.03 | 118.60 |
| 2 | 2 | 1563 | C | C6-N1-C2 | 5.94 | 122.68 | 120.30 |
| 1 | 5 | 1420 | C | C6-N1-C2 | -5.94 | 117.92 | 120.30 |
| 1 | 1 | 284 | A | C4-C5-C6 | 5.94 | 119.97 | 117.00 |
| 1 | 1 | 3389 | U | OP2-P-O3' | 5.94 | 118.27 | 105.20 |
| 1 | 5 | 1633 | C | C5-C6-N1 | 5.94 | 123.97 | 121.00 |
| 1 | 5 | 2395 | G | N1-C6-O6 | 5.94 | 123.47 | 119.90 |
| 1 | 1 | 2403 | G | N1-C6-O6 | 5.94 | 123.46 | 119.90 |
| 2 | 2 | 720 | G | OP1-P-O3' | 5.94 | 118.26 | 105.20 |
| 1 | 1 | 1484 | U | P-O3'-C3' | 5.94 | 126.82 | 119.70 |
| 1 | 5 | 101 | G | C5-C6-O6 | -5.94 | 125.04 | 128.60 |
| 1 | 5 | 2206 | G | P-O3'-C3' | 5.94 | 126.82 | 119.70 |
| 1 | 5 | 2954 | U | N1-C2-O2 | 5.94 | 126.95 | 122.80 |
| 1 | 1 | 2192 | C | N3-C2-O2 | -5.93 | 117.75 | 121.90 |
| 1 | 1 | 2418 | G | C4-C5-N7 | 5.93 | 113.17 | 110.80 |
| 2 | 2 | 934 | C | N1-C2-O2 | 5.93 | 122.46 | 118.90 |
| 1 | 5 | 1844 | C | N1-C2-O2 | -5.93 | 115.34 | 118.90 |
| 1 | 1 | 639 | G | C2-N3-C4 | -5.93 | 108.93 | 111.90 |
| 1 | 1 | 2632 | G | O5'-P-OP1 | -5.93 | 100.36 | 105.70 |
| 1 | 1 | 2874 | G | C5-C6-N1 | -5.93 | 108.53 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 5 | 2873 | U | N1-C2-N3 | 5.93 | 118.46 | 114.90 |
| 1 | 5 | 953 | G | N1-C6-O6 | -5.93 | 116.34 | 119.90 |
| 1 | 5 | 2606 | G | N9-C4-C5 | -5.92 | 103.03 | 105.40 |
| 1 | 1 | 2860 | U | N3-C2-O2 | -5.92 | 118.05 | 122.20 |
| 2 | 2 | 797 | G | C8-N9-C4 | 5.92 | 108.77 | 106.40 |
| 1 | 5 | 1417 | G | C5-C6-O6 | -5.92 | 125.05 | 128.60 |
| 1 | 1 | 1306 | G | N9-C4-C5 | -5.92 | 103.03 | 105.40 |
| 2 | 2 | 278 | U | N1-C2-O2 | 5.92 | 126.94 | 122.80 |
| 1 | 1 | 953 | G | N3-C2-N2 | 5.92 | 124.04 | 119.90 |
| 2 | 2 | 1644 | C | C6-N1-C2 | -5.92 | 117.93 | 120.30 |
| 1 | 5 | 1152 | G | C5-C6-O6 | -5.92 | 125.05 | 128.60 |
| 1 | 5 | 1284 | C | P-O3'-C3' | 5.92 | 126.80 | 119.70 |
| 1 | 5 | 3337 | G | N3-C4-C5 | 5.92 | 131.56 | 128.60 |
| 1 | 1 | 803 | C | C2-N1-C1' | 5.92 | 125.31 | 118.80 |
| 1 | 1 | 2741 | C | N3-C4-C5 | -5.92 | 119.53 | 121.90 |
| 1 | 1 | 2950 | G | N1-C6-O6 | -5.92 | 116.35 | 119.90 |
| 1 | 5 | 1841 | A | O5'-P-OP1 | -5.92 | 100.38 | 105.70 |
| 1 | 1 | 1763 | U | C5-C6-N1 | 5.92 | 125.66 | 122.70 |
| 1 | 5 | 3099 | C | C5-C4-N4 | -5.92 | 116.06 | 120.20 |
| 1 | 1 | 63 | A | C8-N9-C4 | -5.91 | 103.44 | 105.80 |
| 1 | 1 | 1865 | A | N1-C6-N6 | 5.91 | 122.15 | 118.60 |
| 1 | 5 | 227 | G | C4-N9-C1' | 5.91 | 134.18 | 126.50 |
| 2 | 2 | 966 | A | C8-N9-C4 | 5.91 | 108.16 | 105.80 |
| 4 | 8 | 31 | G | C8-N9-C4 | 5.91 | 108.76 | 106.40 |
| 2 | 6 | 378 | A | N9-C4-C5 | -5.91 | 103.44 | 105.80 |
| 1 | 1 | 543 | C | N1-C2-O2 | 5.91 | 122.44 | 118.90 |
| 1 | 1 | 1385 | C | C5-C6-N1 | -5.91 | 118.05 | 121.00 |
| 1 | 1 | 3012 | A | C8-N9-C4 | 5.91 | 108.16 | 105.80 |
| 2 | 2 | 332 | U | N1-C2-O2 | 5.91 | 126.93 | 122.80 |
| 1 | 5 | 868 | C | C6-N1-C2 | 5.91 | 122.66 | 120.30 |
| 1 | 5 | 3175 | U | O5'-P-OP2 | -5.90 | 100.39 | 105.70 |
| 1 | 1 | 397 | A | N1-C6-N6 | -5.90 | 115.06 | 118.60 |
| 1 | 1 | 601 | U | C5-C6-N1 | 5.90 | 125.65 | 122.70 |
| 4 | 4 | 104 | A | N1-C6-N6 | 5.90 | 122.14 | 118.60 |
| 1 | 5 | 347 | G | N9-C4-C5 | -5.90 | 103.04 | 105.40 |
| 1 | 5 | 2372 | A | OP2-P-O3' | -5.90 | 92.22 | 105.20 |
| 1 | 5 | 2390 | A | N1-C6-N6 | -5.90 | 115.06 | 118.60 |
| 1 | 5 | 3216 | G | N1-C6-O6 | 5.90 | 123.44 | 119.90 |
| 1 | 5 | 2315 | G | C5-C6-O6 | -5.90 | 125.06 | 128.60 |
| 1 | 1 | 2608 | G | N9-C4-C5 | -5.89 | 103.04 | 105.40 |
| 2 | 2 | 895 | G | N9-C4-C5 | 5.89 | 107.76 | 105.40 |
| 1 | 5 | 215 | G | N1-C6-O6 | 5.89 | 123.44 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 5 | 2144 | A | C5-C6-N1 | 5.89 | 120.65 | 117.70 |
| 1 | 1 | 651 | G | C4-C5-C6 | 5.89 | 122.33 | 118.80 |
| 1 | 1 | 2719 | U | C6-N1-C2 | 5.89 | 124.53 | 121.00 |
| 1 | 1 | 1169 | A | N9-C4-C5 | 5.89 | 108.16 | 105.80 |
| 1 | 5 | 2719 | U | C6-N1-C2 | 5.89 | 124.53 | 121.00 |
| 1 | 1 | 3189 | G | O5'-P-OP1 | -5.89 | 100.40 | 105.70 |
| 1 | 1 | 189 | G | O5'-P-OP1 | -5.89 | 100.40 | 105.70 |
| 2 | 2 | 728 | U | C2-N1-C1' | 5.89 | 124.76 | 117.70 |
| 2 | 2 | 1075 | C | C6-N1-C2 | -5.89 | 117.94 | 120.30 |
| 1 | 1 | 264 | G | C8-N9-C4 | -5.88 | 104.05 | 106.40 |
| 1 | 1 | 1356 | U | C2-N1-C1' | -5.88 | 110.64 | 117.70 |
| 1 | 1 | 1166 | G | N3-C4-C5 | 5.88 | 131.54 | 128.60 |
| 1 | 1 | 1909 | A | N9-C4-C5 | -5.88 | 103.45 | 105.80 |
| 2 | 2 | 192 | U | N1-C2-O2 | 5.88 | 126.92 | 122.80 |
| 1 | 1 | 116 | A | C2-N3-C4 | 5.88 | 113.54 | 110.60 |
| 1 | 1 | 1451 | C | C5-C4-N4 | -5.88 | 116.08 | 120.20 |
| 1 | 1 | 1773 | C | N3-C4-C5 | 5.88 | 124.25 | 121.90 |
| 3 | 3 | 89 | G | C8-N9-C4 | 5.88 | 108.75 | 106.40 |
| 1 | 5 | 2869 | U | O5'-P-OP1 | -5.88 | 100.41 | 105.70 |
| 2 | 2 | 1729 | C | C6-N1-C2 | 5.88 | 122.65 | 120.30 |
| 2 | 6 | 417 | A | P-O3'-C3' | 5.88 | 126.76 | 119.70 |
| 2 | 2 | 1061 | A | C8-N9-C4 | -5.88 | 103.45 | 105.80 |
| 2 | 6 | 639 | U | C2-N1-C1' | 5.88 | 124.75 | 117.70 |
| 1 | 5 | 1197 | A | C8-N9-C4 | 5.88 | 108.15 | 105.80 |
| 1 | 5 | 358 | G | N3-C4-N9 | -5.88 | 122.47 | 126.00 |
| 2 | 6 | 1620 | C | C6-N1-C2 | -5.88 | 117.95 | 120.30 |
| 1 | 1 | 729 | C | C6-N1-C2 | -5.87 | 117.95 | 120.30 |
| 1 | 1 | 2969 | A | O5'-P-OP1 | -5.87 | 100.41 | 105.70 |
| 1 | 1 | 2101 | C | OP1-P-O3' | 5.87 | 118.11 | 105.20 |
| 2 | 2 | 1658 | G | N3-C4-C5 | 5.87 | 131.54 | 128.60 |
| 1 | 5 | 835 | G | N3-C4-C5 | 5.87 | 131.54 | 128.60 |
| 1 | 5 | 939 | U | N3-C2-O2 | -5.87 | 118.09 | 122.20 |
| 1 | 1 | 1115 | G | C5-N7-C8 | -5.87 | 101.36 | 104.30 |
| 2 | 2 | 278 | U | P-O3'-C3' | 5.87 | 126.74 | 119.70 |
| 1 | 1 | 3080 | G | N1-C6-O6 | 5.87 | 123.42 | 119.90 |
| 1 | 1 | 251 | G | C8-N9-C1' | -5.87 | 119.37 | 127.00 |
| 1 | 5 | 517 | G | C6-C5-N7 | -5.87 | 126.88 | 130.40 |
| 1 | 5 | 3269 | U | P-O3'-C3' | 5.87 | 126.74 | 119.70 |
| 1 | 1 | 1399 | A | C2-N3-C4 | -5.87 | 107.67 | 110.60 |
| 1 | 1 | 1497 | C | N3-C4-C5 | 5.87 | 124.25 | 121.90 |
| 2 | 2 | 427 | C | C6-N1-C2 | 5.87 | 122.65 | 120.30 |
| 1 | 1 | 124 | U | N3-C2-O2 | -5.86 | 118.09 | 122.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 1 | 2355 | G | C4-C5-N7 | 5.86 | 113.14 | 110.80 |
| 1 | 5 | 1149 | G | C4-C5-N7 | 5.86 | 113.15 | 110.80 |
| 1 | 5 | 732 | C | C6-N1-C2 | -5.86 | 117.95 | 120.30 |
| 1 | 5 | 2169 | G | C8-N9-C1' | 5.86 | 134.62 | 127.00 |
| 1 | 1 | 2730 | G | N9-C4-C5 | 5.86 | 107.74 | 105.40 |
| 2 | 6 | 1 | U | C6-N1-C2 | -5.86 | 117.48 | 121.00 |
| 1 | 1 | 2208 | A | C8-N9-C4 | -5.86 | 103.46 | 105.80 |
| 1 | 5 | 652 | G | N3-C4-C5 | -5.86 | 125.67 | 128.60 |
| 2 | 6 | 192 | U | N1-C2-O2 | 5.86 | 126.90 | 122.80 |
| 4 | 8 | 2 | A | C2-N3-C4 | -5.86 | 107.67 | 110.60 |
| 1 | 1 | 632 | G | C4-C5-N7 | 5.85 | 113.14 | 110.80 |
| 1 | 1 | 671 | U | O5'-P-OP2 | -5.85 | 100.43 | 105.70 |
| 1 | 5 | 2871 | G | C5-N7-C8 | -5.85 | 101.37 | 104.30 |
| 2 | 6 | 1277 | G | C8-N9-C4 | -5.85 | 104.06 | 106.40 |
| 5 | c0 | 88 | PRO | N-CA-CB | 5.85 | 110.32 | 103.30 |
| 1 | 1 | 510 | G | N3-C4-C5 | 5.85 | 131.53 | 128.60 |
| 1 | 5 | 1080 | A | O4'-C1'-N9 | 5.85 | 112.88 | 108.20 |
| 1 | 5 | 384 | A | N9-C4-C5 | -5.85 | 103.46 | 105.80 |
| 1 | 5 | 3261 | C | C6-N1-C2 | 5.85 | 122.64 | 120.30 |
| 1 | 1 | 2873 | U | C5-C4-O4 | 5.85 | 129.41 | 125.90 |
| 2 | 2 | 1052 | U | C2-N1-C1' | 5.85 | 124.72 | 117.70 |
| 1 | 5 | 324 | A | OP2-P-O3' | 5.85 | 118.06 | 105.20 |
| 1 | 1 | 900 | G | C8-N9-C4 | -5.84 | 104.06 | 106.40 |
| 1 | 1 | 1380 | G | C8-N9-C4 | 5.84 | 108.74 | 106.40 |
| 1 | 1 | 1838 | G | C6-C5-N7 | -5.84 | 126.89 | 130.40 |
| 1 | 1 | 1940 | G | C8-N9-C4 | 5.84 | 108.74 | 106.40 |
| 1 | 1 | 2137 | U | O4'-C1'-N1 | 5.84 | 112.88 | 108.20 |
| 1 | 1 | 2593 | A | P-O3'-C3' | 5.84 | 126.71 | 119.70 |
| 4 | 4 | 125 | U | C2-N1-C1' | 5.84 | 124.71 | 117.70 |
| 2 | 6 | 864 | U | N3-C2-O2 | -5.84 | 118.11 | 122.20 |
| 2 | 6 | 1340 | U | C5-C6-N1 | 5.84 | 125.62 | 122.70 |
| 1 | 1 | 2600 | C | C6-N1-C2 | -5.84 | 117.96 | 120.30 |
| 2 | 2 | 1523 | G | N3-C4-C5 | -5.84 | 125.68 | 128.60 |
| 1 | 5 | 2385 | G | N3-C4-N9 | -5.84 | 122.50 | 126.00 |
| 2 | 6 | 802 | G | N3-C4-C5 | -5.84 | 125.68 | 128.60 |
| 1 | 1 | 2741 | C | C6-N1-C2 | -5.84 | 117.97 | 120.30 |
| 1 | 5 | 869 | G | C6-C5-N7 | 5.84 | 133.90 | 130.40 |
| 2 | 6 | 1442 | U | C6-N1-C2 | -5.84 | 117.50 | 121.00 |
| 1 | 1 | 1300 | G | C4-C5-N7 | 5.83 | 113.13 | 110.80 |
| 1 | 5 | 1201 | C | C5-C6-N1 | 5.83 | 123.92 | 121.00 |
| 1 | 5 | 1846 | C | C6-N1-C2 | 5.83 | 122.63 | 120.30 |
| 1 | 1 | 1178 | G | N1-C6-O6 | -5.83 | 116.40 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 1 | 1495 | U | N1-C2-O2 | -5.83 | 118.72 | 122.80 |
| 2 | 2 | 488 | G | O5'-P-OP1 | 5.83 | 117.70 | 110.70 |
| 1 | 5 | 3063 | C | C6-N1-C2 | 5.83 | 122.63 | 120.30 |
| 2 | 2 | 131 | C | N3-C2-O2 | -5.83 | 117.82 | 121.90 |
| 1 | 1 | 2871 | G | C4-C5-N7 | 5.82 | 113.13 | 110.80 |
| 1 | 1 | 3221 | C | C6-N1-C2 | -5.82 | 117.97 | 120.30 |
| 1 | 5 | 980 | A | N9-C4-C5 | 5.82 | 108.13 | 105.80 |
| 2 | 2 | 1472 | C | C6-N1-C2 | 5.82 | 122.63 | 120.30 |
| 1 | 1 | 424 | G | N1-C6-O6 | 5.82 | 123.39 | 119.90 |
| 1 | 1 | 1175 | C | C6-N1-C2 | -5.82 | 117.97 | 120.30 |
| 1 | 1 | 1300 | G | C6-C5-N7 | -5.82 | 126.91 | 130.40 |
| 1 | 1 | 2237 | C | C2-N1-C1' | -5.82 | 112.40 | 118.80 |
| 1 | 1 | 3382 | U | C5-C6-N1 | 5.82 | 125.61 | 122.70 |
| 1 | 5 | 1145 | G | C8-N9-C1' | -5.82 | 119.43 | 127.00 |
| 1 | 5 | 2647 | A | N1-C6-N6 | 5.82 | 122.09 | 118.60 |
| 1 | 1 | 651 | G | C8-N9-C4 | -5.82 | 104.07 | 106.40 |
| 1 | 1 | 1838 | G | N3-C4-N9 | 5.82 | 129.49 | 126.00 |
| 1 | 1 | 2882 | U | C2-N3-C4 | -5.82 | 123.51 | 127.00 |
| 2 | 2 | 1491 | U | P-O3'-C3' | 5.81 | 126.68 | 119.70 |
| 1 | 5 | 2625 | C | C6-N1-C2 | 5.81 | 122.63 | 120.30 |
| 1 | 1 | 2362 | C | C6-N1-C2 | -5.81 | 117.97 | 120.30 |
| 1 | 1 | 2868 | U | C6-N1-C2 | -5.81 | 117.51 | 121.00 |
| 2 | 2 | 1 | U | P-O3'-C3' | 5.81 | 126.68 | 119.70 |
| 1 | 1 | 1892 | G | O5'-P-OP2 | -5.81 | 100.47 | 105.70 |
| 1 | 1 | 2625 | C | N3-C4-C5 | 5.81 | 124.22 | 121.90 |
| 2 | 2 | 864 | U | C5-C6-N1 | 5.81 | 125.61 | 122.70 |
| 1 | 1 | 945 | C | N3-C4-C5 | -5.81 | 119.58 | 121.90 |
| 1 | 5 | 2949 | U | C2-N1-C1' | -5.81 | 110.73 | 117.70 |
| 1 | 5 | 2612 | U | C5-C6-N1 | 5.80 | 125.60 | 122.70 |
| 4 | 8 | 58 | G | OP1-P-OP2 | -5.80 | 110.89 | 119.60 |
| 2 | 2 | 187 | G | P-O3'-C3' | 5.80 | 126.66 | 119.70 |
| 2 | 2 | 453 | U | C6-N1-C1' | -5.80 | 113.08 | 121.20 |
| 1 | 5 | 1779 | C | C6-N1-C2 | -5.80 | 117.98 | 120.30 |
| 1 | 5 | 282 | G | N7-C8-N9 | 5.80 | 116.00 | 113.10 |
| 1 | 1 | 2353 | G | C8-N9-C4 | -5.80 | 104.08 | 106.40 |
| 1 | 5 | 356 | C | C6-N1-C2 | 5.80 | 122.62 | 120.30 |
| 1 | 1 | 1417 | G | C8-N9-C4 | 5.79 | 108.72 | 106.40 |
| 1 | 1 | 3362 | A | N1-C6-N6 | 5.79 | 122.08 | 118.60 |
| 1 | 1 | 3370 | A | C5-C6-N6 | -5.79 | 119.06 | 123.70 |
| 2 | 2 | 1134 | C | C6-N1-C2 | 5.79 | 122.62 | 120.30 |
| 1 | 5 | 2881 | C | OP2-P-O3' | 5.79 | 117.95 | 105.20 |
| 2 | 6 | 993 | A | N3-C4-C5 | -5.79 | 122.74 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 4 | 8 | 39 | G | C8-N9-C4 | -5.79 | 104.08 | 106.40 |
| 36 | M1 | 112 | LEU | CA-CB-CG | 5.79 | 128.62 | 115.30 |
| 1 | 1 | 1174 | G | C4-N9-C1' | 5.79 | 134.03 | 126.50 |
| 1 | 5 | 628 | A | N1-C6-N6 | 5.79 | 122.08 | 118.60 |
| 1 | 5 | 2245 | C | C5-C6-N1 | -5.79 | 118.10 | 121.00 |
| 2 | 6 | 1139 | A | C8-N9-C4 | 5.79 | 108.12 | 105.80 |
| 78 | sM | 166 | PRO | N-CA-CB | 5.79 | 110.25 | 103.30 |
| 1 | 5 | 937 | G | N1-C6-O6 | -5.79 | 116.43 | 119.90 |
| 1 | 5 | 2612 | U | C6-N1-C2 | -5.79 | 117.53 | 121.00 |
| 1 | 1 | 1016 | C | N3-C2-O2 | -5.79 | 117.85 | 121.90 |
| 1 | 1 | 184 | U | O5'-P-OP2 | -5.79 | 100.49 | 105.70 |
| 1 | 1 | 2209 | U | C6-N1-C2 | -5.79 | 117.53 | 121.00 |
| 1 | 1 | 2241 | U | N1-C2-N3 | 5.79 | 118.37 | 114.90 |
| 1 | 5 | 368 | G | C8-N9-C4 | 5.79 | 108.71 | 106.40 |
| 4 | 8 | 70 | G | N9-C4-C5 | -5.79 | 103.08 | 105.40 |
| 1 | 1 | 1145 | G | C4-C5-N7 | 5.78 | 113.11 | 110.80 |
| 1 | 1 | 1913 | A | N1-C6-N6 | 5.78 | 122.07 | 118.60 |
| 2 | 6 | 319 | U | OP1-P-O3' | 5.78 | 117.92 | 105.20 |
| 1 | 5 | 860 | G | C6-C5-N7 | -5.78 | 126.93 | 130.40 |
| 1 | 1 | 1083 | G | C8-N9-C4 | 5.78 | 108.71 | 106.40 |
| 4 | 4 | 17 | A | N1-C6-N6 | 5.78 | 122.07 | 118.60 |
| 1 | 5 | 2355 | G | C4-C5-N7 | 5.78 | 113.11 | 110.80 |
| 2 | 2 | 29 | U | C6-N1-C2 | 5.78 | 124.47 | 121.00 |
| 1 | 5 | 207 | U | C6-N1-C2 | -5.78 | 117.53 | 121.00 |
| 1 | 1 | 55 | G | N9-C4-C5 | -5.78 | 103.09 | 105.40 |
| 1 | 5 | 1329 | U | N1-C2-N3 | 5.78 | 118.36 | 114.90 |
| 1 | 1 | 1174 | G | C6-C5-N7 | -5.77 | 126.94 | 130.40 |
| 1 | 1 | 3181 | C | N3-C2-O2 | -5.77 | 117.86 | 121.90 |
| 2 | 2 | 992 | A | N7-C8-N9 | 5.77 | 116.69 | 113.80 |
| 1 | 5 | 2726 | C | N3-C2-O2 | -5.77 | 117.86 | 121.90 |
| 1 | 1 | 3317 | U | P-O3'-C3' | 5.77 | 126.63 | 119.70 |
| 1 | 5 | 3275 | U | P-O3'-C3' | 5.77 | 126.62 | 119.70 |
| 1 | 1 | 1428 | A | C8-N9-C4 | 5.77 | 108.11 | 105.80 |
| 1 | 1 | 1345 | G | C5-C6-O6 | -5.77 | 125.14 | 128.60 |
| 1 | 1 | 2925 | C | N3-C4-C5 | 5.77 | 124.21 | 121.90 |
| 1 | 1 | 1495 | U | C5-C4-O4 | 5.76 | 129.36 | 125.90 |
| 2 | 6 | 802 | G | C8-N9-C4 | -5.76 | 104.09 | 106.40 |
| 4 | 8 | 121 | U | C6-N1-C2 | -5.76 | 117.54 | 121.00 |
| 1 | 1 | 91 | G | C4-C5-N7 | 5.76 | 113.11 | 110.80 |
| 2 | 6 | 864 | U | C6-N1-C2 | -5.76 | 117.54 | 121.00 |
| 47 | N3 | 15 | LEU | CA-CB-CG | -5.76 | 102.05 | 115.30 |
| 1 | 1 | 1413 | G | N3-C2-N2 | -5.76 | 115.87 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 1 | 2606 | G | N3-C4-C5 | -5.76 | 125.72 | 128.60 |
| 4 | 4 | 16 | G | N1-C6-O6 | 5.76 | 123.36 | 119.90 |
| 2 | 6 | 55 | A | N1-C6-N6 | 5.76 | 122.06 | 118.60 |
| 1 | 1 | 890 | C | N3-C4-C5 | 5.76 | 124.20 | 121.90 |
| 1 | 1 | 980 | A | C8-N9-C4 | -5.76 | 103.50 | 105.80 |
| 1 | 1 | 1411 | C | C2-N3-C4 | -5.76 | 117.02 | 119.90 |
| 2 | 2 | 124 | A | C8-N9-C4 | -5.76 | 103.50 | 105.80 |
| 1 | 5 | 1176 | C | C6-N1-C2 | 5.76 | 122.60 | 120.30 |
| 1 | 1 | 212 | G | C8-N9-C4 | -5.76 | 104.10 | 106.40 |
| 1 | 1 | 2768 | U | O5'-P-OP2 | -5.75 | 100.52 | 105.70 |
| 1 | 5 | 21 | G | O5'-P-OP2 | -5.75 | 100.52 | 105.70 |
| 2 | 6 | 555 | A | C8-N9-C4 | -5.75 | 103.50 | 105.80 |
| 1 | 1 | 660 | A | C2-N3-C4 | -5.75 | 107.72 | 110.60 |
| 1 | 1 | 1382 | G | N1-C6-O6 | 5.75 | 123.35 | 119.90 |
| 1 | 1 | 3390 | G | O5'-P-OP2 | -5.75 | 100.52 | 105.70 |
| 2 | 2 | 794 | U | C5-C6-N1 | 5.75 | 125.58 | 122.70 |
| 1 | 5 | 406 | G | O4'-C1'-N9 | 5.75 | 112.80 | 108.20 |
| 2 | 2 | 577 | G | C6-C5-N7 | -5.75 | 126.95 | 130.40 |
| 1 | 5 | 2332 | A | N9-C4-C5 | -5.75 | 103.50 | 105.80 |
| 2 | 2 | 412 | A | C8-N9-C4 | 5.75 | 108.10 | 105.80 |
| 3 | 3 | 99 | G | N1-C6-O6 | 5.75 | 123.35 | 119.90 |
| 2 | 6 | 958 | U | C6-N1-C2 | -5.75 | 117.55 | 121.00 |
| 1 | 1 | 883 | A | O5'-P-OP1 | 5.75 | 117.60 | 110.70 |
| 2 | 6 | 1762 | A | OP2-P-O3' | 5.75 | 117.84 | 105.20 |
| 1 | 1 | 3053 | G | C6-C5-N7 | -5.74 | 126.95 | 130.40 |
| 1 | 5 | 437 | G | N1-C6-O6 | 5.74 | 123.35 | 119.90 |
| 1 | 5 | 2376 | G | N3-C4-C5 | -5.74 | 125.73 | 128.60 |
| 1 | 1 | 3075 | G | C5-C6-O6 | -5.74 | 125.16 | 128.60 |
| 1 | 1 | 1819 | U | C6-N1-C2 | -5.74 | 117.56 | 121.00 |
| 1 | 1 | 2403 | G | C5-C6-O6 | -5.74 | 125.16 | 128.60 |
| 2 | 2 | 278 | U | N3-C2-O2 | -5.74 | 118.18 | 122.20 |
| 1 | 5 | 966 | U | C5-C6-N1 | 5.74 | 125.57 | 122.70 |
| 2 | 6 | 1493 | A | P-O3'-C3' | 5.74 | 126.59 | 119.70 |
| 3 | 7 | 90 | U | N3-C2-O2 | -5.74 | 118.18 | 122.20 |
| 1 | 1 | 355 | A | O5'-P-OP1 | -5.74 | 100.53 | 105.70 |
| 1 | 1 | 2375 | G | O5'-P-OP1 | -5.74 | 100.54 | 105.70 |
| 4 | 4 | 72 | A | O5'-P-OP1 | -5.74 | 100.53 | 105.70 |
| 2 | 6 | 45 | U | C2-N1-C1' | -5.74 | 110.81 | 117.70 |
| 1 | 5 | 196 | G | N3-C4-C5 | -5.74 | 125.73 | 128.60 |
| 13 | c8 | 15 | LEU | CA-CB-CG | 5.74 | 128.50 | 115.30 |
| 1 | 1 | 2352 | A | C5-C6-N6 | -5.74 | 119.11 | 123.70 |
| 2 | 2 | 306 | U | C6-N1-C2 | 5.74 | 124.44 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 1 | 2978 | U | N1-C2-N3 | 5.73 | 118.34 | 114.90 |
| 1 | 5 | 1137 | C | N3-C2-O2 | -5.73 | 117.89 | 121.90 |
| 1 | 1 | 923 | C | N3-C4-C5 | 5.73 | 124.19 | 121.90 |
| 1 | 1 | 1003 | A | N1-C6-N6 | 5.73 | 122.04 | 118.60 |
| 1 | 1 | 1440 | G | OP1-P-O3' | 5.73 | 117.81 | 105.20 |
| 1 | 1 | 2171 | G | C4-C5-N7 | -5.73 | 108.51 | 110.80 |
| 2 | 6 | 163 | G | N3-C2-N2 | -5.73 | 115.89 | 119.90 |
| 1 | 1 | 658 | G | C4-N9-C1' | 5.73 | 133.95 | 126.50 |
| 1 | 1 | 2922 | G | C4-C5-N7 | 5.73 | 113.09 | 110.80 |
| 1 | 5 | 1380 | G | C8-N9-C4 | 5.73 | 108.69 | 106.40 |
| 1 | 5 | 2305 | G | C8-N9-C4 | -5.73 | 104.11 | 106.40 |
| 1 | 1 | 1435 | A | N1-C2-N3 | 5.73 | 132.16 | 129.30 |
| 1 | 1 | 3120 | C | C6-N1-C2 | -5.73 | 118.01 | 120.30 |
| 2 | 6 | 1274 | C | N1-C2-O2 | 5.73 | 122.34 | 118.90 |
| 1 | 1 | 585 | A | N1-C6-N6 | -5.72 | 115.17 | 118.60 |
| 1 | 1 | 2273 | G | O5'-P-OP1 | 5.72 | 117.57 | 110.70 |
| 1 | 1 | 2690 | G | O5'-P-OP1 | -5.72 | 100.55 | 105.70 |
| 1 | 1 | 2809 | C | N1-C2-O2 | -5.72 | 115.47 | 118.90 |
| 2 | 2 | 1277 | G | C8-N9-C4 | -5.72 | 104.11 | 106.40 |
| 1 | 5 | 652 | G | N3-C4-N9 | 5.72 | 129.44 | 126.00 |
| 1 | 5 | 925 | A | N9-C4-C5 | -5.72 | 103.51 | 105.80 |
| 1 | 5 | 2374 | C | C6-N1-C1' | -5.72 | 113.93 | 120.80 |
| 4 | 4 | 47 | C | N3-C4-N4 | -5.72 | 113.99 | 118.00 |
| 1 | 5 | 37 | U | N3-C2-O2 | -5.72 | 118.19 | 122.20 |
| 4 | 8 | 8 | C | N1-C2-O2 | -5.72 | 115.47 | 118.90 |
| 1 | 1 | 517 | G | C8-N9-C4 | -5.72 | 104.11 | 106.40 |
| 1 | 1 | 1614 | C | C6-N1-C2 | -5.72 | 118.01 | 120.30 |
| 2 | 6 | 1006 | C | C6-N1-C2 | -5.72 | 118.01 | 120.30 |
| 1 | 1 | 2153 | U | C6-N1-C2 | -5.72 | 117.57 | 121.00 |
| 1 | 5 | 22 | G | O5'-P-OP2 | -5.72 | 100.55 | 105.70 |
| 27 | L2 | 191 | LEU | CA-CB-CG | -5.72 | 102.15 | 115.30 |
| 1 | 5 | 2204 | C | N1-C1'-C2' | -5.72 | 105.71 | 112.00 |
| 1 | 1 | 1662 | G | C8-N9-C4 | 5.71 | 108.69 | 106.40 |
| 1 | 1 | 2905 | U | C2-N1-C1' | -5.71 | 110.84 | 117.70 |
| 1 | 1 | 1699 | A | C8-N9-C4 | 5.71 | 108.08 | 105.80 |
| 1 | 5 | 2144 | A | O4'-C1'-N9 | 5.71 | 112.77 | 108.20 |
| 2 | 6 | 590 | C | C5-C6-N1 | 5.71 | 123.86 | 121.00 |
| 1 | 1 | 780 | A | C5-C6-N6 | 5.71 | 128.27 | 123.70 |
| 1 | 5 | 18 | G | N3-C4-N9 | -5.71 | 122.58 | 126.00 |
| 1 | 5 | 691 | A | OP1-P-O3' | 5.71 | 117.76 | 105.20 |
| 1 | 5 | 1878 | G | N9-C4-C5 | 5.71 | 107.68 | 105.40 |
| 1 | 1 | 239 | G | C8-N9-C4 | -5.71 | 104.12 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 1 | 2358 | A | O5'-P-OP2 | -5.71 | 100.56 | 105.70 |
| 2 | 2 | 696 | C | C6-N1-C2 | -5.71 | 118.02 | 120.30 |
| 2 | 2 | 1033 | C | C6-N1-C2 | 5.71 | 122.58 | 120.30 |
| 1 | 1 | 1554 | U | C2-N1-C1' | -5.71 | 110.85 | 117.70 |
| 1 | 5 | 3022 | G | O4'-C1'-N9 | 5.71 | 112.76 | 108.20 |
| 1 | 1 | 2337 | C | C6-N1-C2 | -5.70 | 118.02 | 120.30 |
| 2 | 2 | 326 | G | C8-N9-C4 | -5.70 | 104.12 | 106.40 |
| 1 | 5 | 1496 | C | C2-N1-C1' | 5.70 | 125.07 | 118.80 |
| 1 | 5 | 1931 | U | N1-C2-O2 | 5.70 | 126.79 | 122.80 |
| 2 | 6 | 1458 | G | N3-C4-N9 | 5.70 | 129.42 | 126.00 |
| 2 | 2 | 316 | A | O5'-P-OP1 | -5.70 | 100.57 | 105.70 |
| 2 | 2 | 1568 | C | P-O3'-C3' | 5.70 | 126.54 | 119.70 |
| 1 | 1 | 42 | C | C6-N1-C2 | 5.70 | 122.58 | 120.30 |
| 1 | 1 | 890 | C | OP2-P-O3' | 5.70 | 117.73 | 105.20 |
| 1 | 1 | 1017 | C | C2-N1-C1' | 5.70 | 125.06 | 118.80 |
| 2 | 2 | 992 | A | N1-C6-N6 | 5.70 | 122.02 | 118.60 |
| 1 | 5 | 3231 | U | C5-C6-N1 | -5.70 | 119.85 | 122.70 |
| 2 | 6 | 1602 | C | C6-N1-C2 | 5.70 | 122.58 | 120.30 |
| 1 | 1 | 2870 | C | C6-N1-C2 | 5.69 | 122.58 | 120.30 |
| 1 | 5 | 2856 | G | N1-C6-O6 | 5.69 | 123.32 | 119.90 |
| 1 | 1 | 917 | A | O5'-P-OP1 | 5.69 | 117.53 | 110.70 |
| 1 | 5 | 3216 | G | C5-C6-O6 | -5.69 | 125.19 | 128.60 |
| 1 | 1 | 715 | A | P-O3'-C3' | 5.69 | 126.53 | 119.70 |
| 1 | 1 | 1604 | G | C8-N9-C4 | -5.69 | 104.12 | 106.40 |
| 1 | 1 | 2355 | G | N9-C4-C5 | -5.69 | 103.12 | 105.40 |
| 1 | 5 | 1582 | C | C5-C6-N1 | 5.69 | 123.84 | 121.00 |
| 1 | 5 | 2952 | G | C4-C5-N7 | 5.69 | 113.08 | 110.80 |
| 2 | 6 | 361 | C | C5-C6-N1 | 5.69 | 123.84 | 121.00 |
| 2 | 6 | 1279 | C | C6-N1-C2 | -5.69 | 118.03 | 120.30 |
| 1 | 5 | 1437 | C | C5-C6-N1 | 5.68 | 123.84 | 121.00 |
| 1 | 1 | 2620 | G | C4-C5-N7 | 5.68 | 113.07 | 110.80 |
| 1 | 5 | 330 | G | N1-C6-O6 | 5.68 | 123.31 | 119.90 |
| 1 | 1 | 339 | C | O5'-P-OP1 | -5.68 | 100.59 | 105.70 |
| 2 | 2 | 1059 | U | C5-C6-N1 | 5.68 | 125.54 | 122.70 |
| 1 | 5 | 3217 | C | C5-C6-N1 | -5.68 | 118.16 | 121.00 |
| 26 | E1 | 86 | THR | C-N-CA | 5.68 | 135.90 | 121.70 |
| 1 | 1 | 660 | A | N1-C6-N6 | -5.68 | 115.19 | 118.60 |
| 1 | 1 | 283 | G | O4'-C1'-N9 | -5.68 | 103.66 | 108.20 |
| 1 | 1 | 2973 | G | N7-C8-N9 | -5.68 | 110.26 | 113.10 |
| 2 | 2 | 25 | C | P-O3'-C3' | 5.68 | 126.51 | 119.70 |
| 2 | 2 | 1511 | U | C6-N1-C2 | -5.68 | 117.59 | 121.00 |
| 2 | 6 | 239 | C | C6-N1-C2 | -5.68 | 118.03 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | 6 | 453 | U | N3-C2-O2 | -5.68 | 118.23 | 122.20 |
| 1 | 1 | 3109 | G | N1-C6-O6 | 5.67 | 123.31 | 119.90 |
| 1 | 5 | 1442 | U | C2-N1-C1' | -5.67 | 110.89 | 117.70 |
| 2 | 6 | 158 | U | P-O3'-C3' | 5.67 | 126.51 | 119.70 |
| 2 | 6 | 623 | A | N1-C6-N6 | 5.67 | 122.00 | 118.60 |
| 2 | 2 | 565 | C | C6-N1-C2 | 5.67 | 122.57 | 120.30 |
| 2 | 6 | 747 | C | C6-N1-C2 | -5.67 | 118.03 | 120.30 |
| 1 | 1 | 1383 | G | N3-C4-C5 | 5.67 | 131.43 | 128.60 |
| 1 | 1 | 2679 | A | C5-C6-N6 | -5.67 | 119.17 | 123.70 |
| 2 | 2 | 1534 | G | C8-N9-C4 | 5.67 | 108.67 | 106.40 |
| 1 | 5 | 1329 | U | N3-C2-O2 | -5.67 | 118.23 | 122.20 |
| 1 | 1 | 1556 | C | C6-N1-C2 | -5.67 | 118.03 | 120.30 |
| 1 | 5 | 1481 | A | N7-C8-N9 | 5.67 | 116.63 | 113.80 |
| 1 | 5 | 1834 | U | N3-C4-O4 | 5.67 | 123.37 | 119.40 |
| 4 | 4 | 14 | C | C5-C6-N1 | -5.67 | 118.17 | 121.00 |
| 1 | 5 | 1552 | G | C4-C5-N7 | 5.67 | 113.07 | 110.80 |
| 1 | 5 | 2871 | G | N3-C4-C5 | 5.67 | 131.43 | 128.60 |
| 1 | 1 | 2875 | U | N3-C2-O2 | -5.66 | 118.24 | 122.20 |
| 1 | 5 | 32 | U | C6-N1-C2 | -5.66 | 117.60 | 121.00 |
| 1 | 1 | 2917 | G | N1-C6-O6 | 5.66 | 123.30 | 119.90 |
| 1 | 1 | 1495 | U | C2-N3-C4 | -5.66 | 123.61 | 127.00 |
| 2 | 2 | 610 | G | C8-N9-C1' | -5.66 | 119.64 | 127.00 |
| 1 | 5 | 2112 | U | P-O3'-C3' | 5.66 | 126.49 | 119.70 |
| 1 | 1 | 3318 | G | C8-N9-C4 | -5.66 | 104.14 | 106.40 |
| 3 | 3 | 7 | G | N9-C4-C5 | 5.66 | 107.66 | 105.40 |
| 1 | 5 | 1482 | A | O5'-P-OP2 | -5.66 | 100.61 | 105.70 |
| 4 | 8 | 110 | C | OP2-P-O3' | 5.66 | 117.64 | 105.20 |
| 1 | 5 | 139 | G | C8-N9-C4 | 5.65 | 108.66 | 106.40 |
| 1 | 5 | 3216 | G | O5'-P-OP2 | -5.65 | 100.61 | 105.70 |
| 1 | 1 | 350 | C | N3-C2-O2 | -5.65 | 117.94 | 121.90 |
| 1 | 1 | 1076 | C | N1-C2-O2 | 5.65 | 122.29 | 118.90 |
| 4 | 4 | 8 | C | OP2-P-O3' | 5.65 | 117.63 | 105.20 |
| 1 | 5 | 92 | G | C5-C6-O6 | -5.65 | 125.21 | 128.60 |
| 1 | 5 | 2348 | A | N1-C6-N6 | -5.65 | 115.21 | 118.60 |
| 4 | 8 | 17 | A | N1-C6-N6 | 5.65 | 121.99 | 118.60 |
| 1 | 1 | 1113 | G | N3-C2-N2 | -5.65 | 115.94 | 119.90 |
| 1 | 1 | 1819 | U | C2-N1-C1' | 5.65 | 124.48 | 117.70 |
| 1 | 5 | 1751 | G | C8-N9-C4 | 5.65 | 108.66 | 106.40 |
| 1 | 1 | 1104 | G | O5'-P-OP1 | -5.65 | 100.62 | 105.70 |
| 1 | 1 | 839 | C | C5-C6-N1 | -5.65 | 118.18 | 121.00 |
| 1 | 1 | 3267 | A | N1-C6-N6 | -5.65 | 115.21 | 118.60 |
| 4 | 4 | 90 | U | C6-N1-C2 | 5.65 | 124.39 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 5 | 1056 | U | C6-N1-C2 | -5.65 | 117.61 | 121.00 |
| 2 | 6 | 1467 | C | C5-C6-N1 | 5.65 | 123.82 | 121.00 |
| 2 | 6 | 1301 | U | O5'-P-OP2 | -5.65 | 100.62 | 105.70 |
| 1 | 1 | 510 | G | C5-C6-O6 | -5.64 | 125.21 | 128.60 |
| 1 | 1 | 1319 | G | C5-C6-O6 | 5.64 | 131.99 | 128.60 |
| 1 | 1 | 1838 | G | N9-C4-C5 | -5.64 | 103.14 | 105.40 |
| 2 | 2 | 1782 | A | C8-N9-C4 | -5.64 | 103.54 | 105.80 |
| 2 | 6 | 1658 | G | C4-C5-N7 | 5.64 | 113.06 | 110.80 |
| 1 | 1 | 968 | G | C4-C5-N7 | 5.64 | 113.06 | 110.80 |
| 1 | 1 | 1306 | G | C4-N9-C1' | 5.64 | 133.83 | 126.50 |
| 1 | 5 | 644 | G | N3-C4-N9 | -5.64 | 122.61 | 126.00 |
| 1 | 1 | 88 | A | C8-N9-C4 | 5.64 | 108.06 | 105.80 |
| 1 | 1 | 884 | A | N9-C4-C5 | -5.64 | 103.54 | 105.80 |
| 1 | 1 | 935 | U | N1-C2-N3 | 5.64 | 118.28 | 114.90 |
| 1 | 5 | 1436 | U | N3-C2-O2 | -5.64 | 118.25 | 122.20 |
| 1 | 1 | 703 | G | O5'-P-OP1 | -5.64 | 100.63 | 105.70 |
| 1 | 1 | 2120 | A | O5'-P-OP2 | -5.64 | 100.63 | 105.70 |
| 1 | 5 | 36 | C | C6-N1-C2 | -5.64 | 118.05 | 120.30 |
| 1 | 5 | 2719 | U | N3-C2-O2 | 5.64 | 126.15 | 122.20 |
| 2 | 6 | 779 | U | N1-C2-O2 | 5.64 | 126.75 | 122.80 |
| 1 | 1 | 577 | C | C6-N1-C2 | 5.64 | 122.55 | 120.30 |
| 1 | 1 | 2208 | A | OP1-P-O3' | 5.64 | 117.60 | 105.20 |
| 2 | 2 | 192 | U | C5-C6-N1 | 5.64 | 125.52 | 122.70 |
| 1 | 5 | 1625 | A | C8-N9-C4 | 5.64 | 108.05 | 105.80 |
| 1 | 5 | 3195 | U | N1-C2-O2 | 5.64 | 126.75 | 122.80 |
| 1 | 1 | 961 | C | O5'-P-OP1 | -5.63 | 100.63 | 105.70 |
| 1 | 5 | 2321 | A | C8-N9-C4 | 5.63 | 108.05 | 105.80 |
| 1 | 5 | 3134 | A | C4-C5-N7 | 5.63 | 113.52 | 110.70 |
| 1 | 1 | 884 | A | O5'-P-OP1 | -5.63 | 100.63 | 105.70 |
| 1 | 1 | 1156 | C | N3-C4-N4 | 5.63 | 121.94 | 118.00 |
| 1 | 5 | 2979 | U | O5'-P-OP1 | -5.63 | 100.63 | 105.70 |
| 1 | 1 | 63 | A | N1-C6-N6 | 5.63 | 121.98 | 118.60 |
| 1 | 1 | 966 | U | N3-C4-C5 | -5.63 | 111.22 | 114.60 |
| 1 | 1 | 1480 | G | C5-C6-O6 | -5.63 | 125.22 | 128.60 |
| 1 | 5 | 1581 | C | P-O3'-C3' | 5.63 | 126.46 | 119.70 |
| 1 | 5 | 1581 | C | C6-N1-C1' | -5.63 | 114.04 | 120.80 |
| 1 | 5 | 2524 | A | O4'-C1'-N9 | 5.63 | 112.70 | 108.20 |
| 1 | 5 | 1805 | C | C6-N1-C2 | 5.63 | 122.55 | 120.30 |
| 1 | 1 | 1897 | G | C5-C6-O6 | -5.63 | 125.22 | 128.60 |
| 1 | 1 | 2679 | A | C6-C5-N7 | -5.63 | 128.36 | 132.30 |
| 1 | 5 | 1588 | A | N1-C6-N6 | 5.63 | 121.98 | 118.60 |
| 1 | 1 | 251 | G | N3-C4-N9 | 5.63 | 129.38 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 1 | 806 | A | O4'-C1'-N9 | -5.63 | 103.70 | 108.20 |
| 1 | 1 | 2645 | G | C4-C5-N7 | 5.63 | 113.05 | 110.80 |
| 1 | 5 | 1115 | G | C8-N9-C1' | -5.63 | 119.69 | 127.00 |
| 1 | 5 | 669 | U | C6-N1-C2 | 5.62 | 124.38 | 121.00 |
| 1 | 5 | 2379 | U | N1-C2-O2 | -5.62 | 118.86 | 122.80 |
| 1 | 1 | 62 | A | C8-N9-C4 | 5.62 | 108.05 | 105.80 |
| 1 | 1 | 2896 | A | C6-C5-N7 | -5.62 | 128.36 | 132.30 |
| 1 | 1 | 3016 | A | O5'-P-OP2 | -5.62 | 100.64 | 105.70 |
| 2 | 6 | 194 | U | N1-C2-O2 | 5.62 | 126.74 | 122.80 |
| 1 | 1 | 551 | A | O4'-C1'-N9 | 5.62 | 112.70 | 108.20 |
| 1 | 1 | 1392 | G | N1-C6-O6 | -5.62 | 116.53 | 119.90 |
| 1 | 1 | 1432 | C | N1-C2-O2 | -5.62 | 115.53 | 118.90 |
| 1 | 1 | 1493 | G | C2-N3-C4 | 5.62 | 114.71 | 111.90 |
| 2 | 2 | 1792 | G | C8-N9-C4 | -5.62 | 104.15 | 106.40 |
| 1 | 5 | 2933 | A | O5'-P-OP2 | -5.62 | 100.64 | 105.70 |
| 1 | 1 | 38 | U | C6-N1-C2 | 5.62 | 124.37 | 121.00 |
| 1 | 1 | 2853 | A | N1-C6-N6 | 5.62 | 121.97 | 118.60 |
| 2 | 2 | 130 | C | N1-C2-O2 | 5.62 | 122.27 | 118.90 |
| 1 | 5 | 934 | G | C4-N9-C1' | 5.62 | 133.80 | 126.50 |
| 2 | 2 | 1060 | U | C5-C6-N1 | 5.62 | 125.51 | 122.70 |
| 2 | 6 | 781 | U | C6-N1-C1' | -5.62 | 113.34 | 121.20 |
| 1 | 5 | 1772 | U | C5-C6-N1 | -5.62 | 119.89 | 122.70 |
| 2 | 2 | 734 | A | OP1-P-O3' | 5.61 | 117.55 | 105.20 |
| 2 | 6 | 95 | G | N1-C6-O6 | -5.61 | 116.53 | 119.90 |
| 1 | 1 | 2171 | G | C6-C5-N7 | 5.61 | 133.77 | 130.40 |
| 1 | 1 | 2422 | C | N3-C4-C5 | 5.61 | 124.14 | 121.90 |
| 1 | 1 | 2978 | U | C6-N1-C2 | -5.61 | 117.63 | 121.00 |
| 1 | 1 | 3370 | A | O5'-P-OP1 | 5.61 | 117.43 | 110.70 |
| 1 | 5 | 1095 | U | C2-N1-C1' | 5.61 | 124.43 | 117.70 |
| 1 | 1 | 884 | A | C4-C5-N7 | 5.61 | 113.50 | 110.70 |
| 2 | 2 | 1052 | U | N3-C2-O2 | -5.61 | 118.28 | 122.20 |
| 1 | 5 | 1224 | C | C6-N1-C2 | 5.61 | 122.54 | 120.30 |
| 1 | 5 | 1582 | C | C6-N1-C2 | -5.61 | 118.06 | 120.30 |
| 1 | 5 | 2971 | A | N7-C8-N9 | 5.61 | 116.60 | 113.80 |
| 2 | 6 | 377 | G | N9-C4-C5 | -5.61 | 103.16 | 105.40 |
| 5 | C0 | 76 | LEU | CA-CB-CG | 5.61 | 128.20 | 115.30 |
| 9 | C4 | 124 | ASP | N-CA-C | 5.61 | 126.14 | 111.00 |
| 1 | 1 | 1196 | C | O4'-C1'-N1 | 5.61 | 112.68 | 108.20 |
| 1 | 1 | 2183 | A | C5-C6-N6 | -5.61 | 119.22 | 123.70 |
| 1 | 5 | 2400 | G | C6-C5-N7 | -5.60 | 127.04 | 130.40 |
| 1 | 1 | 1370 | G | C4-C5-N7 | 5.60 | 113.04 | 110.80 |
| 2 | 2 | 1058 | U | N3-C2-O2 | -5.60 | 118.28 | 122.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | 2 | 1768 | G | C5-C6-O6 | 5.60 | 131.96 | 128.60 |
| 1 | 5 | 88 | A | C8-N9-C4 | 5.60 | 108.04 | 105.80 |
| 4 | 8 | 151 | C | N1-C2-O2 | 5.60 | 122.26 | 118.90 |
| 37 | m3 | 51 | LEU | CA-CB-CG | 5.60 | 128.18 | 115.30 |
| 2 | 2 | 1667 | A | N1-C6-N6 | -5.60 | 115.24 | 118.60 |
| 1 | 5 | 1581 | C | C4-C5-C6 | -5.60 | 114.60 | 117.40 |
| 1 | 5 | 2858 | U | O5'-P-OP1 | -5.60 | 100.66 | 105.70 |
| 2 | 2 | 1011 | G | N9-C4-C5 | 5.60 | 107.64 | 105.40 |
| 4 | 4 | 102 | U | O5'-P-OP2 | -5.60 | 100.66 | 105.70 |
| 1 | 1 | 3246 | G | N3-C4-C5 | -5.59 | 125.80 | 128.60 |
| 2 | 6 | 866 | G | C8-N9-C4 | 5.59 | 108.64 | 106.40 |
| 1 | 1 | 968 | G | C5-C6-O6 | -5.59 | 125.24 | 128.60 |
| 1 | 1 | 2794 | G | C5-C6-O6 | -5.59 | 125.24 | 128.60 |
| 1 | 1 | 2874 | G | C5-C6-O6 | 5.59 | 131.96 | 128.60 |
| 2 | 2 | 1761 | U | P-O3'-C3' | 5.59 | 126.41 | 119.70 |
| 4 | 4 | 73 | U | N1-C2-O2 | 5.59 | 126.72 | 122.80 |
| 1 | 5 | 1609 | C | C6-N1-C2 | 5.59 | 122.54 | 120.30 |
| 1 | 1 | 234 | G | C8-N9-C4 | -5.59 | 104.16 | 106.40 |
| 1 | 1 | 1586 | G | N9-C4-C5 | 5.59 | 107.64 | 105.40 |
| 1 | 1 | 2610 | G | N3-C4-C5 | 5.59 | 131.40 | 128.60 |
| 2 | 2 | 1761 | U | OP2-P-O3' | 5.59 | 117.50 | 105.20 |
| 2 | 6 | 1458 | G | C6-C5-N7 | -5.59 | 127.05 | 130.40 |
| 4 | 8 | 32 | C | C6-N1-C2 | 5.59 | 122.54 | 120.30 |
| 4 | 4 | 54 | A | N7-C8-N9 | 5.59 | 116.59 | 113.80 |
| 2 | 6 | 1089 | U | C6-N1-C2 | 5.59 | 124.35 | 121.00 |
| 1 | 1 | 620 | U | C2-N1-C1' | -5.59 | 110.99 | 117.70 |
| 1 | 1 | 879 | U | N3-C2-O2 | 5.59 | 126.11 | 122.20 |
| 4 | 4 | 107 | G | N1-C6-O6 | -5.59 | 116.55 | 119.90 |
| 1 | 5 | 94 | G | C2-N3-C4 | -5.59 | 109.11 | 111.90 |
| 1 | 5 | 2313 | A | N1-C6-N6 | -5.59 | 115.25 | 118.60 |
| 1 | 1 | 300 | G | C8-N9-C4 | -5.59 | 104.17 | 106.40 |
| 1 | 1 | 1852 | G | C2-N3-C4 | -5.59 | 109.11 | 111.90 |
| 1 | 1 | 2922 | G | N3-C4-C5 | -5.59 | 125.81 | 128.60 |
| 1 | 1 | 2984 | C | C2-N1-C1' | -5.59 | 112.66 | 118.80 |
| 2 | 2 | 5 | U | C6-N1-C2 | -5.59 | 117.65 | 121.00 |
| 2 | 2 | 204 | G | C5-N7-C8 | -5.59 | 101.51 | 104.30 |
| 1 | 5 | 1443 | G | C4-C5-N7 | 5.59 | 113.03 | 110.80 |
| 2 | 6 | 425 | A | C8-N9-C4 | -5.59 | 103.56 | 105.80 |
| 2 | 6 | 131 | C | C5-C6-N1 | 5.58 | 123.79 | 121.00 |
| 1 | 1 | 834 | U | C6-N1-C2 | 5.58 | 124.35 | 121.00 |
| 1 | 5 | 284 | A | C8-N9-C4 | -5.58 | 103.57 | 105.80 |
| 1 | 5 | 912 | G | C8-N9-C4 | 5.58 | 108.63 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 5 | 2279 | A | C8-N9-C4 | -5.58 | 103.57 | 105.80 |
| 2 | 6 | 1280 | C | C6-N1-C2 | -5.58 | 118.07 | 120.30 |
| 1 | 1 | 1889 | G | C6-C5-N7 | -5.58 | 127.05 | 130.40 |
| 1 | 5 | 3093 | C | N3-C2-O2 | 5.58 | 125.81 | 121.90 |
| 1 | 1 | 940 | G | N1-C6-O6 | 5.58 | 123.25 | 119.90 |
| 2 | 2 | 1768 | G | C4-C5-N7 | -5.58 | 108.57 | 110.80 |
| 1 | 5 | 2866 | U | C5-C4-O4 | 5.58 | 129.25 | 125.90 |
| 1 | 1 | 1897 | G | N1-C6-O6 | 5.58 | 123.25 | 119.90 |
| 2 | 2 | 242 | U | C2-N1-C1' | 5.58 | 124.39 | 117.70 |
| 1 | 5 | 3205 | G | C6-C5-N7 | -5.58 | 127.05 | 130.40 |
| 1 | 1 | 2732 | G | O5'-P-OP2 | -5.58 | 100.68 | 105.70 |
| 2 | 2 | 1473 | U | N3-C2-O2 | -5.58 | 118.30 | 122.20 |
| 1 | 1 | 142 | C | C5-C6-N1 | 5.57 | 123.79 | 121.00 |
| 1 | 5 | 1145 | G | C5-C6-O6 | -5.57 | 125.26 | 128.60 |
| 1 | 5 | 2976 | A | O5'-P-OP2 | -5.57 | 100.69 | 105.70 |
| 2 | 6 | 1785 | U | O5'-P-OP1 | -5.57 | 100.68 | 105.70 |
| 2 | 6 | 604 | A | N1-C6-N6 | -5.57 | 115.26 | 118.60 |
| 1 | 5 | 2726 | C | C6-N1-C2 | -5.57 | 118.07 | 120.30 |
| 1 | 1 | 2985 | C | N3-C4-N4 | 5.57 | 121.90 | 118.00 |
| 1 | 1 | 2256 | A | O5'-P-OP1 | -5.57 | 100.69 | 105.70 |
| 1 | 5 | 2990 | G | N3-C2-N2 | -5.57 | 116.00 | 119.90 |
| 56 | o2 | 128 | LEU | CA-CB-CG | 5.57 | 128.11 | 115.30 |
| 4 | 4 | 94 | C | C6-N1-C2 | 5.57 | 122.53 | 120.30 |
| 1 | 1 | 2281 | A | O4'-C1'-N9 | 5.56 | 112.65 | 108.20 |
| 1 | 1 | 2422 | C | C2-N3-C4 | -5.56 | 117.12 | 119.90 |
| 1 | 1 | 3012 | A | N3-C4-C5 | 5.56 | 130.69 | 126.80 |
| 1 | 1 | 611 | A | C4-C5-C6 | 5.56 | 119.78 | 117.00 |
| 1 | 1 | 1604 | G | C4-C5-C6 | 5.56 | 122.14 | 118.80 |
| 1 | 5 | 285 | A | C5-N7-C8 | -5.56 | 101.12 | 103.90 |
| 2 | 6 | 1200 | G | N3-C4-C5 | 5.56 | 131.38 | 128.60 |
| 2 | 2 | 1456 | C | N3-C2-O2 | -5.56 | 118.01 | 121.90 |
| 2 | 2 | 1707 | A | C8-N9-C4 | -5.56 | 103.58 | 105.80 |
| 2 | 6 | 360 | A | C8-N9-C4 | 5.56 | 108.02 | 105.80 |
| 1 | 1 | 2651 | G | N3-C4-C5 | 5.56 | 131.38 | 128.60 |
| 1 | 5 | 18 | G | N3-C4-C5 | 5.56 | 131.38 | 128.60 |
| 1 | 5 | 196 | G | C8-N9-C4 | -5.56 | 104.18 | 106.40 |
| 1 | 5 | 1145 | G | C4-C5-N7 | 5.56 | 113.02 | 110.80 |
| 1 | 1 | 92 | G | C5-N7-C8 | -5.56 | 101.52 | 104.30 |
| 1 | 1 | 264 | G | N3-C4-C5 | -5.56 | 125.82 | 128.60 |
| 1 | 5 | 1861 | G | O5'-P-OP1 | -5.56 | 100.70 | 105.70 |
| 2 | 6 | 391 | A | C8-N9-C4 | 5.56 | 108.02 | 105.80 |
| 1 | 5 | 2376 | G | C6-C5-N7 | -5.56 | 127.07 | 130.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 1 | 2770 | G | C8-N9-C4 | -5.55 | 104.18 | 106.40 |
| 1 | 1 | 2842 | U | N3-C2-O2 | -5.55 | 118.31 | 122.20 |
| 1 | 1 | 2320 | A | C8-N9-C4 | 5.55 | 108.02 | 105.80 |
| 1 | 5 | 1332 | A | C8-N9-C4 | -5.55 | 103.58 | 105.80 |
| 1 | 5 | 1449 | A | N1-C6-N6 | 5.55 | 121.93 | 118.60 |
| 1 | 1 | 951 | A | C8-N9-C4 | 5.55 | 108.02 | 105.80 |
| 1 | 5 | 1152 | G | C2-N3-C4 | -5.55 | 109.12 | 111.90 |
| 1 | 5 | 1442 | U | C6-N1-C2 | 5.55 | 124.33 | 121.00 |
| 2 | 2 | 131 | C | C6-N1-C1' | -5.55 | 114.14 | 120.80 |
| 1 | 5 | 890 | C | OP2-P-O3' | 5.55 | 117.40 | 105.20 |
| 1 | 5 | 2363 | A | N1-C6-N6 | -5.55 | 115.27 | 118.60 |
| 2 | 6 | 1457 | C | N3-C2-O2 | -5.55 | 118.02 | 121.90 |
| 1 | 1 | 3070 | A | C8-N9-C4 | 5.54 | 108.02 | 105.80 |
| 1 | 5 | 1375 | G | C4-C5-N7 | 5.54 | 113.02 | 110.80 |
| 1 | 5 | 1481 | A | P-O3'-C3' | 5.54 | 126.35 | 119.70 |
| 1 | 1 | 3362 | A | C4-C5-N7 | 5.54 | 113.47 | 110.70 |
| 2 | 2 | 261 | U | C6-N1-C2 | -5.54 | 117.68 | 121.00 |
| 1 | 5 | 639 | G | N9-C1'-C2' | -5.54 | 105.91 | 112.00 |
| 1 | 5 | 835 | G | N3-C2-N2 | -5.54 | 116.02 | 119.90 |
| 2 | 6 | 136 | C | N3-C2-O2 | -5.54 | 118.02 | 121.90 |
| 4 | 8 | 72 | A | N1-C6-N6 | 5.54 | 121.92 | 118.60 |
| 1 | 1 | 790 | U | C6-N1-C2 | 5.54 | 124.32 | 121.00 |
| 1 | 1 | 2400 | G | C6-C5-N7 | -5.54 | 127.08 | 130.40 |
| 1 | 5 | 809 | G | N1-C6-O6 | 5.54 | 123.22 | 119.90 |
| 1 | 5 | 3260 | G | C8-N9-C1' | -5.54 | 119.80 | 127.00 |
| 2 | 6 | 389 | G | C6-C5-N7 | -5.54 | 127.08 | 130.40 |
| 1 | 1 | 2378 | C | C5-C4-N4 | -5.54 | 116.33 | 120.20 |
| 1 | 1 | 2382 | G | C5-C6-O6 | -5.54 | 125.28 | 128.60 |
| 4 | 8 | 151 | C | C6-N1-C2 | -5.53 | 118.09 | 120.30 |
| 1 | 1 | 3273 | A | O5'-P-OP2 | -5.53 | 100.72 | 105.70 |
| 4 | 4 | 54 | A | C4-C5-N7 | 5.53 | 113.47 | 110.70 |
| 1 | 5 | 339 | C | O5'-P-OP1 | -5.53 | 100.72 | 105.70 |
| 1 | 5 | 1419 | A | N1-C6-N6 | 5.53 | 121.92 | 118.60 |
| 1 | 5 | 517 | G | N1-C6-O6 | 5.53 | 123.22 | 119.90 |
| 2 | 2 | 166 | C | C6-N1-C2 | -5.53 | 118.09 | 120.30 |
| 1 | 5 | 1672 | U | C6-N1-C1' | 5.53 | 128.94 | 121.20 |
| 1 | 5 | 2719 | U | C2-N1-C1' | -5.53 | 111.07 | 117.70 |
| 2 | 6 | 802 | G | C2-N3-C4 | 5.53 | 114.66 | 111.90 |
| 1 | 1 | 3382 | U | N1-C2-O2 | 5.53 | 126.67 | 122.80 |
| 2 | 2 | 1600 | A | C2-N3-C4 | -5.53 | 107.84 | 110.60 |
| 1 | 1 | 2257 | C | O5'-P-OP1 | -5.52 | 100.73 | 105.70 |
| 1 | 5 | 282 | G | P-O3'-C3' | 5.52 | 126.33 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 1 | 2171 | G | C5-C6-O6 | 5.52 | 131.91 | 128.60 |
| 1 | 1 | 2978 | U | O4'-C1'-N1 | 5.52 | 112.62 | 108.20 |
| 3 | 3 | 116 | C | C5-C6-N1 | 5.52 | 123.76 | 121.00 |
| 1 | 5 | 1527 | C | N1-C2-O2 | 5.52 | 122.21 | 118.90 |
| 1 | 1 | 3390 | G | C4-C5-N7 | 5.52 | 113.01 | 110.80 |
| 1 | 5 | 1615 | C | N3-C2-O2 | -5.52 | 118.03 | 121.90 |
| 1 | 1 | 353 | G | C4-N9-C1' | -5.52 | 119.32 | 126.50 |
| 1 | 1 | 2835 | U | C6-N1-C2 | 5.52 | 124.31 | 121.00 |
| 1 | 5 | 2169 | G | C4-N9-C1' | -5.52 | 119.33 | 126.50 |
| 77 | s9 | 99 | LEU | CA-CB-CG | 5.52 | 128.00 | 115.30 |
| 2 | 2 | 1291 | G | N7-C8-N9 | 5.52 | 115.86 | 113.10 |
| 1 | 5 | 1896 | A | OP2-P-O3' | 5.52 | 117.34 | 105.20 |
| 1 | 1 | 1014 | U | C5-C6-N1 | 5.52 | 125.46 | 122.70 |
| 1 | 1 | 1166 | G | C8-N9-C4 | 5.52 | 108.61 | 106.40 |
| 1 | 5 | 408 | A | N7-C8-N9 | 5.52 | 116.56 | 113.80 |
| 1 | 5 | 1450 | G | C5-C6-O6 | -5.52 | 125.29 | 128.60 |
| 1 | 1 | 1391 | C | N3-C4-N4 | 5.51 | 121.86 | 118.00 |
| 1 | 1 | 1432 | C | C5-C6-N1 | 5.51 | 123.76 | 121.00 |
| 1 | 1 | 2922 | G | C4-C5-C6 | 5.51 | 122.11 | 118.80 |
| 1 | 5 | 521 | A | C8-N9-C4 | -5.51 | 103.59 | 105.80 |
| 2 | 6 | 109 | G | N3-C4-C5 | 5.51 | 131.36 | 128.60 |
| 2 | 6 | 1194 | A | N1-C6-N6 | 5.51 | 121.91 | 118.60 |
| 2 | 6 | 1600 | A | N7-C8-N9 | 5.51 | 116.56 | 113.80 |
| 1 | 1 | 2973 | G | C8-N9-C4 | 5.51 | 108.61 | 106.40 |
| 2 | 2 | 405 | C | N3-C4-C5 | 5.51 | 124.11 | 121.90 |
| 1 | 1 | 821 | U | C2-N1-C1' | -5.51 | 111.09 | 117.70 |
| 1 | 1 | 1417 | G | C6-C5-N7 | -5.51 | 127.09 | 130.40 |
| 1 | 1 | 2661 | G | N1-C6-O6 | 5.51 | 123.21 | 119.90 |
| 1 | 5 | 1308 | A | N7-C8-N9 | 5.51 | 116.56 | 113.80 |
| 2 | 6 | 272 | U | P-O3'-C3' | 5.51 | 126.31 | 119.70 |
| 2 | 6 | 1512 | G | C4-C5-N7 | 5.51 | 113.00 | 110.80 |
| 1 | 1 | 1443 | G | C5-N7-C8 | -5.51 | 101.55 | 104.30 |
| 1 | 5 | 1582 | C | N1-C2-O2 | 5.51 | 122.20 | 118.90 |
| 1 | 5 | 3076 | C | N3-C4-C5 | -5.51 | 119.70 | 121.90 |
| 1 | 1 | 120 | G | N3-C4-C5 | -5.50 | 125.85 | 128.60 |
| 1 | 1 | 1512 | U | C6-N1-C2 | -5.50 | 117.70 | 121.00 |
| 1 | 1 | 3276 | G | N3-C4-C5 | 5.50 | 131.35 | 128.60 |
| 1 | 1 | 669 | U | C5-C6-N1 | -5.50 | 119.95 | 122.70 |
| 4 | 8 | 17 | A | N9-C4-C5 | -5.50 | 103.60 | 105.80 |
| 2 | 2 | 941 | A | N1-C6-N6 | -5.50 | 115.30 | 118.60 |
| 2 | 2 | 1600 | A | C4-C5-N7 | 5.50 | 113.45 | 110.70 |
| 1 | 5 | 1429 | G | C8-N9-C1' | -5.50 | 119.85 | 127.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 5 | 2842 | U | N1-C2-O2 | 5.50 | 126.65 | 122.80 |
| 2 | 6 | 858 | G | N1-C6-O6 | 5.50 | 123.20 | 119.90 |
| 1 | 5 | 2809 | C | C6-N1-C2 | -5.50 | 118.10 | 120.30 |
| 4 | 8 | 70 | G | C4-C5-N7 | 5.50 | 113.00 | 110.80 |
| 1 | 1 | 636 | C | N3-C4-C5 | -5.50 | 119.70 | 121.90 |
| 1 | 1 | 1338 | C | N3-C2-O2 | -5.50 | 118.05 | 121.90 |
| 1 | 1 | 2694 | A | N1-C6-N6 | -5.50 | 115.30 | 118.60 |
| 2 | 2 | 577 | G | C5-N7-C8 | -5.50 | 101.55 | 104.30 |
| 1 | 1 | 2093 | A | C8-N9-C4 | -5.50 | 103.60 | 105.80 |
| 1 | 1 | 2163 | C | C6-N1-C2 | -5.50 | 118.10 | 120.30 |
| 1 | 1 | 2186 | U | O5'-P-OP2 | -5.50 | 100.75 | 105.70 |
| 1 | 1 | 2984 | C | N1-C2-O2 | -5.50 | 115.60 | 118.90 |
| 1 | 1 | 2654 | C | C6-N1-C2 | -5.50 | 118.10 | 120.30 |
| 1 | 5 | 1853 | U | C6-N1-C2 | -5.50 | 117.70 | 121.00 |
| 1 | 5 | 1188 | U | N1-C2-N3 | 5.49 | 118.20 | 114.90 |
| 4 | 4 | 17 | A | C2-N3-C4 | -5.49 | 107.85 | 110.60 |
| 1 | 5 | 868 | C | C2-N1-C1' | -5.49 | 112.76 | 118.80 |
| 1 | 1 | 920 | A | C6-C5-N7 | -5.49 | 128.46 | 132.30 |
| 3 | 3 | 100 | C | O5'-P-OP2 | 5.49 | 117.29 | 110.70 |
| 1 | 5 | 1408 | G | N3-C4-C5 | 5.49 | 131.34 | 128.60 |
| 30 | l5 | 110 | LEU | CA-CB-CG | 5.49 | 127.93 | 115.30 |
| 1 | 1 | 1166 | G | C5-C6-O6 | -5.49 | 125.31 | 128.60 |
| 1 | 1 | 2363 | A | N9-C4-C5 | 5.49 | 108.00 | 105.80 |
| 2 | 2 | 1137 | A | C8-N9-C4 | 5.49 | 108.00 | 105.80 |
| 1 | 5 | 835 | G | N9-C4-C5 | 5.49 | 107.59 | 105.40 |
| 2 | 2 | 1768 | G | N9-C4-C5 | 5.49 | 107.59 | 105.40 |
| 1 | 5 | 2132 | C | N3-C4-N4 | 5.49 | 121.84 | 118.00 |
| 1 | 1 | 2932 | U | N3-C4-O4 | -5.49 | 115.56 | 119.40 |
| 2 | 2 | 610 | G | C4-N9-C1' | 5.49 | 133.63 | 126.50 |
| 2 | 2 | 959 | U | N3-C2-O2 | -5.49 | 118.36 | 122.20 |
| 2 | 6 | 1338 | C | C6-N1-C2 | -5.49 | 118.11 | 120.30 |
| 23 | d8 | 66 | LEU | CA-CB-CG | 5.49 | 127.92 | 115.30 |
| 1 | 1 | 2826 | U | N3-C4-O4 | -5.48 | 115.56 | 119.40 |
| 1 | 1 | 3246 | G | N3-C4-N9 | 5.48 | 129.29 | 126.00 |
| 2 | 2 | 1195 | C | O5'-P-OP1 | -5.48 | 100.76 | 105.70 |
| 1 | 1 | 2628 | A | C8-N9-C4 | -5.48 | 103.61 | 105.80 |
| 1 | 5 | 2240 | G | C8-N9-C4 | -5.48 | 104.21 | 106.40 |
| 1 | 5 | 3090 | U | C6-N1-C2 | -5.48 | 117.71 | 121.00 |
| 1 | 5 | 3099 | C | C6-N1-C2 | 5.48 | 122.49 | 120.30 |
| 1 | 1 | 637 | C | C5-C6-N1 | 5.48 | 123.74 | 121.00 |
| 1 | 1 | 1554 | U | P-O3'-C3' | 5.48 | 126.28 | 119.70 |
| 2 | 2 | 1189 | A | C8-N9-C4 | 5.48 | 107.99 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2 | 2 | 1035 | G | C8-N9-C4 | 5.48 | 108.59 | 106.40 |
| 2 | 6 | 429 | G | N1-C6-O6 | 5.48 | 123.19 | 119.90 |
| 2 | 6 | 781 | U | O4'-C1'-N1 | -5.48 | 103.82 | 108.20 |
| 1 | 1 | 2114 | C | N3-C2-O2 | -5.48 | 118.06 | 121.90 |
| 1 | 5 | 3176 | G | N1-C6-O6 | 5.48 | 123.19 | 119.90 |
| 1 | 5 | 2310 | U | C5-C6-N1 | 5.48 | 125.44 | 122.70 |
| 1 | 1 | 632 | G | N9-C4-C5 | -5.47 | 103.21 | 105.40 |
| 1 | 5 | 1825 | G | C5-C6-O6 | 5.47 | 131.88 | 128.60 |
| 1 | 5 | 2093 | A | C8-N9-C4 | 5.47 | 107.99 | 105.80 |
| 1 | 1 | 1664 | G | C8-N9-C4 | 5.47 | 108.59 | 106.40 |
| 2 | 2 | 1001 | A | O5'-P-OP1 | -5.47 | 100.78 | 105.70 |
| 1 | 5 | 1102 | A | C8-N9-C4 | 5.47 | 107.99 | 105.80 |
| 1 | 5 | 1306 | G | N3-C4-N9 | 5.47 | 129.28 | 126.00 |
| 1 | 5 | 2606 | G | C4-N9-C1' | 5.47 | 133.62 | 126.50 |
| 1 | 1 | 221 | A | N9-C4-C5 | 5.47 | 107.99 | 105.80 |
| 1 | 1 | 1359 | C | N3-C4-C5 | 5.47 | 124.09 | 121.90 |
| 1 | 1 | 2257 | C | C2-N1-C1' | 5.47 | 124.82 | 118.80 |
| 2 | 2 | 386 | G | O5'-P-OP2 | -5.47 | 100.78 | 105.70 |
| 2 | 6 | 1600 | A | C4-N9-C1' | 5.47 | 136.15 | 126.30 |
| 1 | 1 | 2572 | C | C5-C6-N1 | 5.47 | 123.73 | 121.00 |
| 2 | 2 | 1058 | U | C2-N1-C1' | 5.47 | 124.26 | 117.70 |
| 1 | 1 | 639 | G | N3-C2-N2 | -5.47 | 116.07 | 119.90 |
| 1 | 1 | 2986 | U | N3-C4-O4 | 5.47 | 123.23 | 119.40 |
| 2 | 2 | 961 | U | C6-N1-C2 | -5.47 | 117.72 | 121.00 |
| 2 | 2 | 1491 | U | C2-N1-C1' | 5.47 | 124.26 | 117.70 |
| 1 | 5 | 3039 | C | N3-C4-C5 | 5.47 | 124.09 | 121.90 |
| 1 | 1 | 199 | A | O4'-C1'-N9 | 5.47 | 112.57 | 108.20 |
| 1 | 1 | 424 | G | C5-C6-O6 | -5.47 | 125.32 | 128.60 |
| 1 | 1 | 1452 | A | C5-N7-C8 | -5.47 | 101.17 | 103.90 |
| 1 | 1 | 2206 | G | N9-C4-C5 | -5.47 | 103.21 | 105.40 |
| 2 | 2 | 378 | A | N9-C4-C5 | -5.47 | 103.61 | 105.80 |
| 4 | 8 | 126 | A | P-O3'-C3' | 5.47 | 126.26 | 119.70 |
| 1 | 1 | 2110 | G | N3-C4-C5 | -5.46 | 125.87 | 128.60 |
| 1 | 1 | 2796 | G | OP1-P-OP2 | 5.46 | 127.80 | 119.60 |
| 1 | 1 | 2871 | G | C6-C5-N7 | -5.46 | 127.12 | 130.40 |
| 2 | 2 | 719 | U | C2-N1-C1' | 5.46 | 124.26 | 117.70 |
| 2 | 2 | 992 | A | C4-C5-N7 | 5.46 | 113.43 | 110.70 |
| 1 | 5 | 1340 | G | N3-C4-N9 | -5.46 | 122.72 | 126.00 |
| 1 | 5 | 2359 | C | C6-N1-C2 | -5.46 | 118.11 | 120.30 |
| 1 | 5 | 2932 | U | C5-C4-O4 | 5.46 | 129.18 | 125.90 |
| 1 | 1 | 2389 | C | N1-C2-O2 | -5.46 | 115.62 | 118.90 |
| 4 | 8 | 83 | C | C6-N1-C2 | -5.46 | 118.11 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 1 | 2541 | U | P-O3'-C3' | 5.46 | 126.25 | 119.70 |
| 1 | 5 | 1745 | C | C6-N1-C2 | 5.46 | 122.48 | 120.30 |
| 1 | 5 | 1851 | G | C8-N9-C4 | -5.46 | 104.22 | 106.40 |
| 1 | 5 | 2149 | A | OP2-P-O3' | 5.46 | 117.22 | 105.20 |
| 2 | 6 | 1794 | A | N1-C6-N6 | -5.46 | 115.32 | 118.60 |
| 1 | 1 | 953 | G | C5-C6-O6 | 5.46 | 131.88 | 128.60 |
| 1 | 1 | 1161 | G | C6-C5-N7 | -5.46 | 127.12 | 130.40 |
| 3 | 3 | 7 | G | C4-C5-N7 | -5.46 | 108.62 | 110.80 |
| 1 | 1 | 2725 | U | C6-N1-C2 | 5.46 | 124.27 | 121.00 |
| 1 | 1 | 2922 | G | N3-C2-N2 | 5.46 | 123.72 | 119.90 |
| 1 | 1 | 3044 | G | N3-C4-C5 | 5.46 | 131.33 | 128.60 |
| 1 | 1 | 3276 | G | C6-N1-C2 | 5.46 | 128.37 | 125.10 |
| 1 | 5 | 2110 | G | N3-C4-N9 | 5.46 | 129.27 | 126.00 |
| 2 | 2 | 1389 | C | C6-N1-C2 | -5.46 | 118.12 | 120.30 |
| 2 | 2 | 136 | C | C5-C6-N1 | 5.45 | 123.73 | 121.00 |
| 2 | 2 | 1611 | A | C2-N3-C4 | -5.45 | 107.87 | 110.60 |
| 1 | 5 | 883 | A | C5-N7-C8 | -5.45 | 101.17 | 103.90 |
| 1 | 5 | 2363 | A | N9-C4-C5 | 5.45 | 107.98 | 105.80 |
| 1 | 5 | 2817 | A | C5-C6-N6 | -5.45 | 119.34 | 123.70 |
| 1 | 1 | 2101 | C | P-O3'-C3' | 5.45 | 126.24 | 119.70 |
| 1 | 1 | 2183 | A | C6-C5-N7 | -5.45 | 128.48 | 132.30 |
| 1 | 1 | 1028 | U | C2-N1-C1' | 5.45 | 124.24 | 117.70 |
| 1 | 1 | 3020 | U | N3-C2-O2 | -5.45 | 118.38 | 122.20 |
| 2 | 6 | 1033 | C | C6-N1-C2 | 5.45 | 122.48 | 120.30 |
| 2 | 6 | 1399 | C | C6-N1-C2 | -5.45 | 118.12 | 120.30 |
| 1 | 1 | 224 | C | N3-C4-N4 | 5.45 | 121.81 | 118.00 |
| 1 | 1 | 609 | G | N1-C6-O6 | 5.45 | 123.17 | 119.90 |
| 1 | 5 | 358 | G | N3-C2-N2 | -5.45 | 116.09 | 119.90 |
| 1 | 5 | 2268 | U | C4-C5-C6 | -5.45 | 116.43 | 119.70 |
| 1 | 5 | 2286 | U | O5'-P-OP2 | -5.45 | 100.80 | 105.70 |
| 2 | 6 | 1189 | A | C8-N9-C4 | 5.45 | 107.98 | 105.80 |
| 2 | 6 | 1596 | C | N3-C2-O2 | -5.45 | 118.08 | 121.90 |
| 1 | 5 | 2993 | G | N3-C2-N2 | 5.45 | 123.71 | 119.90 |
| 72 | S4 | 193 | GLY | N-CA-C | 5.45 | 126.72 | 113.10 |
| 1 | 1 | 1376 | C | N1-C2-O2 | -5.45 | 115.63 | 118.90 |
| 1 | 1 | 2923 | U | C5-C6-N1 | 5.45 | 125.42 | 122.70 |
| 2 | 2 | 653 | C | C6-N1-C2 | -5.45 | 118.12 | 120.30 |
| 1 | 5 | 1450 | G | N3-C4-C5 | 5.45 | 131.32 | 128.60 |
| 2 | 6 | 623 | A | N9-C4-C5 | -5.45 | 103.62 | 105.80 |
| 19 | D4 | 50 | ALA | C-N-CA | 5.45 | 135.31 | 121.70 |
| 1 | 5 | 1901 | A | N9-C4-C5 | 5.44 | 107.98 | 105.80 |
| 2 | 6 | 31 | C | C6-N1-C2 | -5.44 | 118.12 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2 | 6 | 138 | A | C2-N3-C4 | 5.44 | 113.32 | 110.60 |
| 2 | 6 | 250 | C | C6-N1-C2 | -5.44 | 118.12 | 120.30 |
| 1 | 1 | 91 | G | N9-C4-C5 | -5.44 | 103.22 | 105.40 |
| 1 | 1 | 725 | G | N3-C4-C5 | 5.44 | 131.32 | 128.60 |
| 1 | 1 | 2246 | G | O5'-P-OP1 | -5.44 | 100.80 | 105.70 |
| 1 | 1 | 3078 | U | P-O3'-C3' | 5.44 | 126.23 | 119.70 |
| 1 | 5 | 915 | A | OP1-P-OP2 | 5.44 | 127.76 | 119.60 |
| 1 | 5 | 3052 | G | N1-C6-O6 | 5.44 | 123.17 | 119.90 |
| 2 | 6 | 136 | C | C2-N1-C1' | 5.44 | 124.78 | 118.80 |
| 2 | 6 | 385 | A | C8-N9-C4 | -5.44 | 103.62 | 105.80 |
| 1 | 5 | 1343 | A | N1-C6-N6 | 5.44 | 121.86 | 118.60 |
| 1 | 1 | 770 | G | O4'-C1'-N9 | 5.44 | 112.55 | 108.20 |
| 1 | 5 | 1194 | G | N3-C4-C5 | -5.44 | 125.88 | 128.60 |
| 1 | 5 | 2187 | G | N3-C4-C5 | -5.44 | 125.88 | 128.60 |
| 1 | 5 | 2268 | U | N1-C2-N3 | -5.44 | 111.64 | 114.90 |
| 1 | 5 | 580 | C | N3-C4-N4 | -5.44 | 114.19 | 118.00 |
| 1 | 1 | 389 | A | C8-N9-C4 | -5.43 | 103.63 | 105.80 |
| 1 | 1 | 3242 | G | C5-C6-O6 | -5.43 | 125.34 | 128.60 |
| 2 | 2 | 1277 | G | N9-C4-C5 | 5.43 | 107.57 | 105.40 |
| 2 | 2 | 1456 | C | C6-N1-C2 | -5.43 | 118.13 | 120.30 |
| 1 | 1 | 1542 | G | C5-N7-C8 | -5.43 | 101.58 | 104.30 |
| 1 | 1 | 2174 | G | N3-C4-N9 | -5.43 | 122.74 | 126.00 |
| 1 | 1 | 2858 | U | N1-C2-N3 | 5.43 | 118.16 | 114.90 |
| 1 | 5 | 669 | U | C5-C6-N1 | -5.43 | 119.98 | 122.70 |
| 2 | 6 | 369 | A | C8-N9-C4 | -5.43 | 103.63 | 105.80 |
| 1 | 1 | 1525 | G | C8-N9-C4 | -5.43 | 104.23 | 106.40 |
| 2 | 2 | 1198 | G | N3-C4-C5 | 5.43 | 131.31 | 128.60 |
| 1 | 5 | 2431 | C | C6-N1-C2 | -5.43 | 118.13 | 120.30 |
| 1 | 1 | 2094 | C | N1-C2-O2 | 5.43 | 122.16 | 118.90 |
| 1 | 1 | 2400 | G | N9-C4-C5 | -5.43 | 103.23 | 105.40 |
| 1 | 1 | 2719 | U | N3-C2-O2 | 5.43 | 126.00 | 122.20 |
| 2 | 2 | 498 | G | N3-C4-C5 | -5.43 | 125.89 | 128.60 |
| 1 | 5 | 1665 | C | C2-N1-C1' | -5.43 | 112.83 | 118.80 |
| 1 | 1 | 212 | G | N3-C4-C5 | -5.42 | 125.89 | 128.60 |
| 1 | 1 | 274 | G | N1-C6-O6 | -5.42 | 116.64 | 119.90 |
| 1 | 5 | 282 | G | C2'-C3'-O3' | 5.42 | 122.38 | 113.70 |
| 2 | 6 | 1285 | U | C6-N1-C2 | -5.42 | 117.75 | 121.00 |
| 2 | 6 | 1610 | G | N3-C4-N9 | 5.42 | 129.25 | 126.00 |
| 2 | 2 | 807 | A | O5'-P-OP2 | -5.42 | 100.82 | 105.70 |
| 1 | 1 | 2373 | A | O5'-P-OP1 | -5.42 | 100.82 | 105.70 |
| 1 | 1 | 3393 | U | C5-C6-N1 | -5.42 | 119.99 | 122.70 |
| 2 | 2 | 230 | C | N1-C2-O2 | 5.42 | 122.15 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 5 | 1911 | A | N9-C4-C5 | 5.42 | 107.97 | 105.80 |
| 1 | 5 | 2858 | U | N1-C2-N3 | 5.42 | 118.15 | 114.90 |
| 3 | 7 | 6 | C | C6-N1-C2 | 5.42 | 122.47 | 120.30 |
| 1 | 1 | 278 | U | C2-N1-C1' | -5.42 | 111.20 | 117.70 |
| 1 | 1 | 2667 | A | C8-N9-C4 | 5.42 | 107.97 | 105.80 |
| 1 | 1 | 3276 | G | N1-C2-N3 | -5.42 | 120.65 | 123.90 |
| 3 | 3 | 93 | C | C6-N1-C2 | -5.42 | 118.13 | 120.30 |
| 4 | 4 | 82 | U | C6-N1-C2 | -5.42 | 117.75 | 121.00 |
| 1 | 5 | 2138 | A | OP1-P-OP2 | 5.42 | 127.73 | 119.60 |
| 1 | 1 | 559 | A | O5'-P-OP2 | -5.42 | 100.82 | 105.70 |
| 1 | 1 | 1361 | U | OP2-P-O3' | 5.42 | 117.12 | 105.20 |
| 1 | 1 | 2809 | C | N3-C4-C5 | -5.42 | 119.73 | 121.90 |
| 1 | 5 | 94 | G | C5-C6-N1 | -5.42 | 108.79 | 111.50 |
| 1 | 5 | 926 | A | OP2-P-O3' | 5.42 | 117.12 | 105.20 |
| 1 | 5 | 2362 | C | N1-C2-O2 | 5.42 | 122.15 | 118.90 |
| 1 | 5 | 2846 | U | N3-C4-O4 | -5.42 | 115.61 | 119.40 |
| 33 | 18 | 69 | LEU | CA-CB-CG | 5.42 | 127.75 | 115.30 |
| 1 | 1 | 2212 | C | C6-N1-C1' | -5.41 | 114.30 | 120.80 |
| 2 | 2 | 1751 | C | C5-C6-N1 | -5.41 | 118.29 | 121.00 |
| 1 | 5 | 1582 | C | P-O3'-C3' | 5.41 | 126.20 | 119.70 |
| 1 | 5 | 2840 | C | O5'-P-OP1 | -5.41 | 100.83 | 105.70 |
| 2 | 6 | 993 | A | C8-N9-C4 | -5.41 | 103.64 | 105.80 |
| 1 | 1 | 659 | G | N3-C2-N2 | 5.41 | 123.69 | 119.90 |
| 1 | 1 | 1665 | C | N3-C4-C5 | 5.41 | 124.06 | 121.90 |
| 1 | 1 | 16 | A | C8-N9-C4 | 5.41 | 107.96 | 105.80 |
| 1 | 1 | 1543 | G | OP1-P-O3' | 5.41 | 117.10 | 105.20 |
| 2 | 2 | 308 | C | N3-C4-N4 | -5.41 | 114.21 | 118.00 |
| 2 | 2 | 1562 | G | N9-C4-C5 | -5.41 | 103.24 | 105.40 |
| 2 | 6 | 437 | A | C8-N9-C4 | 5.41 | 107.97 | 105.80 |
| 1 | 1 | 908 | G | C5-C6-O6 | 5.41 | 131.84 | 128.60 |
| 1 | 1 | 1353 | U | N3-C2-O2 | -5.41 | 118.41 | 122.20 |
| 1 | 5 | 288 | C | C6-N1-C2 | -5.41 | 118.14 | 120.30 |
| 1 | 5 | 1085 | A | C8-N9-C4 | -5.41 | 103.64 | 105.80 |
| 1 | 5 | 1759 | C | N1-C2-O2 | 5.41 | 122.14 | 118.90 |
| 1 | 5 | 2330 | C | C2-N1-C1' | 5.41 | 124.75 | 118.80 |
| 1 | 5 | 3260 | G | C4-N9-C1' | 5.41 | 133.53 | 126.50 |
| 2 | 6 | 36 | C | C6-N1-C2 | 5.41 | 122.46 | 120.30 |
| 15 | D0 | 16 | GLN | C-N-CA | 5.41 | 135.22 | 121.70 |
| 1 | 1 | 675 | C | N3-C4-C5 | -5.41 | 119.74 | 121.90 |
| 1 | 1 | 1137 | C | OP2-P-O3' | 5.41 | 117.09 | 105.20 |
| 1 | 1 | 1395 | G | N1-C6-O6 | 5.41 | 123.14 | 119.90 |
| 1 | 1 | 1940 | G | N1-C6-O6 | 5.41 | 123.14 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 1 | 2858 | U | C2-N1-C1' | -5.41 | 111.21 | 117.70 |
| 2 | 2 | 956 | C | C6-N1-C2 | -5.41 | 118.14 | 120.30 |
| 1 | 5 | 644 | G | C5-C6-O6 | 5.41 | 131.84 | 128.60 |
| 1 | 5 | 1160 | C | C6-N1-C2 | 5.41 | 122.46 | 120.30 |
| 1 | 5 | 2169 | G | N9-C4-C5 | 5.41 | 107.56 | 105.40 |
| 1 | 5 | 3062 | G | C8-N9-C4 | 5.41 | 108.56 | 106.40 |
| 1 | 1 | 1635 | G | N3-C4-C5 | 5.40 | 131.30 | 128.60 |
| 1 | 5 | 2624 | G | C5-C6-O6 | -5.40 | 125.36 | 128.60 |
| 1 | 5 | 2871 | G | O5'-P-OP2 | -5.40 | 100.84 | 105.70 |
| 1 | 1 | 1364 | C | OP2-P-O3' | 5.40 | 117.09 | 105.20 |
| 2 | 2 | 704 | C | O4'-C1'-N1 | 5.40 | 112.52 | 108.20 |
| 1 | 1 | 1639 | C | C6-N1-C2 | -5.40 | 118.14 | 120.30 |
| 1 | 1 | 2150 | G | N3-C2-N2 | -5.40 | 116.12 | 119.90 |
| 1 | 1 | 790 | U | C5-C6-N1 | -5.40 | 120.00 | 122.70 |
| 1 | 5 | 2397 | A | O4'-C1'-N9 | -5.40 | 103.88 | 108.20 |
| 2 | 2 | 1277 | G | C5-C6-O6 | 5.40 | 131.84 | 128.60 |
| 1 | 5 | 1148 | G | C2-N3-C4 | -5.40 | 109.20 | 111.90 |
| 1 | 5 | 2400 | G | C5-N7-C8 | -5.40 | 101.60 | 104.30 |
| 1 | 5 | 2890 | A | C8-N9-C4 | -5.40 | 103.64 | 105.80 |
| 1 | 1 | 1157 | G | C4-C5-N7 | 5.39 | 112.96 | 110.80 |
| 2 | 2 | 1081 | A | P-O3'-C3' | 5.39 | 126.17 | 119.70 |
| 1 | 5 | 212 | G | N3-C4-C5 | -5.39 | 125.90 | 128.60 |
| 1 | 5 | 379 | C | C2-N1-C1' | -5.39 | 112.87 | 118.80 |
| 1 | 5 | 398 | A | N9-C4-C5 | -5.39 | 103.64 | 105.80 |
| 1 | 5 | 427 | C | C5-C4-N4 | -5.39 | 116.42 | 120.20 |
| 1 | 1 | 116 | A | C4-C5-N7 | -5.39 | 108.00 | 110.70 |
| 1 | 1 | 639 | G | N9-C1'-C2' | -5.39 | 106.07 | 112.00 |
| 1 | 1 | 1858 | A | C8-N9-C4 | -5.39 | 103.64 | 105.80 |
| 1 | 5 | 410 | U | N1-C2-O2 | -5.39 | 119.03 | 122.80 |
| 1 | 1 | 1062 | A | C8-N9-C4 | 5.39 | 107.96 | 105.80 |
| 1 | 1 | 1166 | G | N9-C4-C5 | -5.39 | 103.24 | 105.40 |
| 1 | 5 | 943 | U | C5-C6-N1 | -5.39 | 120.01 | 122.70 |
| 2 | 6 | 1389 | C | C2-N1-C1' | 5.39 | 124.73 | 118.80 |
| 1 | 5 | 3075 | G | N1-C6-O6 | 5.39 | 123.13 | 119.90 |
| 2 | 2 | 309 | C | C2-N1-C1' | 5.39 | 124.72 | 118.80 |
| 1 | 1 | 1442 | U | C5-C4-O4 | -5.38 | 122.67 | 125.90 |
| 1 | 1 | 1444 | G | C5-N7-C8 | -5.38 | 101.61 | 104.30 |
| 1 | 1 | 2376 | G | N3-C2-N2 | -5.38 | 116.13 | 119.90 |
| 2 | 2 | 1181 | U | C6-N1-C2 | -5.38 | 117.77 | 121.00 |
| 1 | 5 | 1150 | A | N7-C8-N9 | 5.38 | 116.49 | 113.80 |
| 1 | 5 | 3286 | G | C6-C5-N7 | 5.38 | 133.63 | 130.40 |
| 2 | 2 | 547 | U | O5'-P-OP2 | -5.38 | 100.86 | 105.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 5 | 1846 | C | O5'-P-OP1 | 5.38 | 117.16 | 110.70 |
| 2 | 6 | 20 | G | N1-C6-O6 | 5.38 | 123.13 | 119.90 |
| 21 | D6 | 86 | VAL | N-CA-C | -5.38 | 96.47 | 111.00 |
| 1 | 1 | 1773 | C | C5-C6-N1 | -5.38 | 118.31 | 121.00 |
| 1 | 1 | 2714 | G | N3-C4-C5 | 5.38 | 131.29 | 128.60 |
| 1 | 1 | 2144 | A | C5-C6-N1 | 5.38 | 120.39 | 117.70 |
| 1 | 1 | 2885 | C | O5'-P-OP2 | -5.38 | 100.86 | 105.70 |
| 2 | 2 | 309 | C | C5-C6-N1 | 5.38 | 123.69 | 121.00 |
| 2 | 2 | 1370 | U | OP2-P-O3' | 5.38 | 117.03 | 105.20 |
| 2 | 2 | 888 | U | C6-N1-C2 | -5.38 | 117.78 | 121.00 |
| 1 | 5 | 637 | C | N3-C4-C5 | 5.38 | 124.05 | 121.90 |
| 1 | 5 | 2574 | G | N9-C4-C5 | -5.38 | 103.25 | 105.40 |
| 1 | 5 | 2609 | A | C8-N9-C4 | 5.38 | 107.95 | 105.80 |
| 1 | 5 | 1527 | C | N3-C2-O2 | -5.38 | 118.14 | 121.90 |
| 2 | 6 | 496 | G | O4'-C1'-N9 | -5.38 | 103.90 | 108.20 |
| 1 | 5 | 927 | C | C2-N1-C1' | 5.37 | 124.71 | 118.80 |
| 1 | 5 | 3134 | A | N1-C6-N6 | 5.37 | 121.82 | 118.60 |
| 1 | 1 | 836 | A | C4-C5-C6 | -5.37 | 114.31 | 117.00 |
| 1 | 1 | 1551 | C | N3-C4-C5 | 5.37 | 124.05 | 121.90 |
| 1 | 1 | 2853 | A | C4-C5-N7 | 5.37 | 113.39 | 110.70 |
| 2 | 2 | 1600 | A | C5-N7-C8 | -5.37 | 101.21 | 103.90 |
| 1 | 5 | 1017 | C | C6-N1-C2 | -5.37 | 118.15 | 120.30 |
| 1 | 1 | 1194 | G | C4-C5-N7 | 5.37 | 112.95 | 110.80 |
| 1 | 1 | 1600 | U | C6-N1-C2 | 5.37 | 124.22 | 121.00 |
| 1 | 1 | 2924 | U | N3-C2-O2 | -5.37 | 118.44 | 122.20 |
| 2 | 2 | 61 | A | O4'-C1'-N9 | 5.37 | 112.49 | 108.20 |
| 1 | 5 | 838 | G | OP2-P-O3' | 5.37 | 117.01 | 105.20 |
| 2 | 6 | 153 | G | N3-C4-C5 | 5.37 | 131.28 | 128.60 |
| 2 | 6 | 1340 | U | C6-N1-C2 | -5.37 | 117.78 | 121.00 |
| 1 | 1 | 2794 | G | C4-N9-C1' | -5.37 | 119.52 | 126.50 |
| 2 | 2 | 327 | U | C5-C6-N1 | 5.37 | 125.38 | 122.70 |
| 2 | 2 | 1320 | U | O5'-P-OP2 | -5.37 | 100.87 | 105.70 |
| 1 | 5 | 2873 | U | C2-N1-C1' | 5.37 | 124.14 | 117.70 |
| 1 | 5 | 2928 | C | N1-C2-O2 | 5.37 | 122.12 | 118.90 |
| 1 | 5 | 3195 | U | C6-N1-C1' | -5.37 | 113.69 | 121.20 |
| 2 | 6 | 1539 | G | N1-C6-O6 | 5.37 | 123.12 | 119.90 |
| 1 | 5 | 2606 | G | N3-C4-C5 | -5.36 | 125.92 | 128.60 |
| 1 | 5 | 2877 | G | N3-C4-C5 | -5.36 | 125.92 | 128.60 |
| 1 | 5 | 2935 | U | C6-N1-C2 | -5.36 | 117.78 | 121.00 |
| 2 | 6 | 927 | C | C6-N1-C2 | -5.36 | 118.16 | 120.30 |
| 1 | 1 | 75 | G | O5'-P-OP2 | -5.36 | 100.87 | 105.70 |
| 1 | 5 | 1464 | G | N3-C4-N9 | -5.36 | 122.78 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 5 | 2772 | C | OP2-P-O3' | 5.36 | 117.00 | 105.20 |
| 1 | 1 | 903 | U | C2-N1-C1' | -5.36 | 111.27 | 117.70 |
| 1 | 1 | 1574 | C | C6-N1-C2 | -5.36 | 118.16 | 120.30 |
| 1 | 5 | 1460 | A | C8-N9-C4 | 5.36 | 107.94 | 105.80 |
| 1 | 5 | 1832 | C | OP2-P-O3' | 5.36 | 116.99 | 105.20 |
| 1 | 5 | 3388 | C | C6-N1-C2 | 5.36 | 122.44 | 120.30 |
| 1 | 1 | 2748 | A | C8-N9-C4 | 5.36 | 107.94 | 105.80 |
| 1 | 1 | 2278 | C | O5'-P-OP2 | -5.36 | 100.88 | 105.70 |
| 1 | 1 | 2423 | U | C2-N1-C1' | 5.36 | 124.13 | 117.70 |
| 1 | 1 | 2943 | G | C4-N9-C1' | 5.36 | 133.47 | 126.50 |
| 1 | 5 | 1343 | A | C8-N9-C4 | 5.36 | 107.94 | 105.80 |
| 1 | 5 | 1674 | G | C8-N9-C4 | 5.36 | 108.54 | 106.40 |
| 2 | 6 | 163 | G | N7-C8-N9 | 5.36 | 115.78 | 113.10 |
| 1 | 1 | 890 | C | C5-C6-N1 | -5.36 | 118.32 | 121.00 |
| 1 | 1 | 1338 | C | C2-N1-C1' | 5.36 | 124.69 | 118.80 |
| 2 | 2 | 948 | G | N3-C4-C5 | 5.36 | 131.28 | 128.60 |
| 1 | 1 | 645 | A | C6-C5-N7 | 5.35 | 136.05 | 132.30 |
| 1 | 1 | 2702 | A | N1-C6-N6 | 5.35 | 121.81 | 118.60 |
| 2 | 2 | 1324 | G | N1-C2-N2 | 5.35 | 121.02 | 116.20 |
| 1 | 5 | 860 | G | C5-N7-C8 | -5.35 | 101.62 | 104.30 |
| 1 | 5 | 2812 | C | N3-C4-C5 | 5.35 | 124.04 | 121.90 |
| 3 | 3 | 81 | U | C2-N1-C1' | -5.35 | 111.28 | 117.70 |
| 1 | 5 | 1375 | G | N1-C6-O6 | 5.35 | 123.11 | 119.90 |
| 1 | 5 | 1220 | U | C2-N1-C1' | 5.35 | 124.12 | 117.70 |
| 1 | 5 | 1906 | G | O4'-C1'-N9 | -5.35 | 103.92 | 108.20 |
| 1 | 1 | 1775 | G | C5-C6-O6 | -5.35 | 125.39 | 128.60 |
| 1 | 5 | 3278 | C | C2-N1-C1' | 5.35 | 124.68 | 118.80 |
| 1 | 1 | 3246 | G | C6-C5-N7 | -5.34 | 127.19 | 130.40 |
| 2 | 2 | 1062 | A | O4'-C1'-N9 | 5.34 | 112.48 | 108.20 |
| 2 | 6 | 576 | G | C5-C6-O6 | -5.34 | 125.39 | 128.60 |
| 1 | 1 | 3075 | G | C6-C5-N7 | -5.34 | 127.19 | 130.40 |
| 2 | 2 | 913 | G | OP1-P-O3' | 5.34 | 116.96 | 105.20 |
| 2 | 2 | 1794 | A | N9-C4-C5 | 5.34 | 107.94 | 105.80 |
| 1 | 5 | 221 | A | N9-C4-C5 | 5.34 | 107.94 | 105.80 |
| 1 | 5 | 619 | A | OP1-P-O3' | 5.34 | 116.95 | 105.20 |
| 1 | 5 | 1199 | C | O5'-P-OP1 | -5.34 | 100.89 | 105.70 |
| 1 | 5 | 1228 | C | C6-N1-C2 | -5.34 | 118.16 | 120.30 |
| 2 | 6 | 1100 | G | C2-N3-C4 | -5.34 | 109.23 | 111.90 |
| 1 | 1 | 315 | C | C5-C6-N1 | 5.34 | 123.67 | 121.00 |
| 1 | 1 | 1403 | C | N3-C2-O2 | 5.34 | 125.64 | 121.90 |
| 1 | 5 | 864 | G | N3-C4-N9 | 5.34 | 129.20 | 126.00 |
| 1 | 5 | 1582 | C | C6-N1-C1' | -5.34 | 114.39 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 5 | 3195 | U | O4'-C1'-N1 | -5.34 | 103.93 | 108.20 |
| 2 | 6 | 378 | A | N1-C6-N6 | 5.34 | 121.80 | 118.60 |
| 1 | 1 | 2425 | G | N3-C2-N2 | -5.34 | 116.16 | 119.90 |
| 1 | 1 | 803 | C | C6-N1-C2 | -5.34 | 118.17 | 120.30 |
| 1 | 1 | 1556 | C | C5-C6-N1 | 5.34 | 123.67 | 121.00 |
| 1 | 1 | 3362 | A | C5-N7-C8 | -5.34 | 101.23 | 103.90 |
| 2 | 2 | 639 | U | N3-C2-O2 | -5.34 | 118.46 | 122.20 |
| 2 | 2 | 1075 | C | C5-C6-N1 | 5.34 | 123.67 | 121.00 |
| 69 | S1 | 218 | LEU | CA-CB-CG | 5.34 | 127.57 | 115.30 |
| 1 | 5 | 352 | A | C8-N9-C4 | 5.33 | 107.93 | 105.80 |
| 1 | 5 | 2572 | C | C5-C6-N1 | 5.33 | 123.67 | 121.00 |
| 1 | 1 | 44 | U | C6-N1-C2 | 5.33 | 124.20 | 121.00 |
| 1 | 1 | 2247 | G | O5'-P-OP1 | -5.33 | 100.90 | 105.70 |
| 4 | 4 | 14 | C | N3-C4-C5 | 5.33 | 124.03 | 121.90 |
| 1 | 5 | 356 | C | C5-C6-N1 | -5.33 | 118.33 | 121.00 |
| 1 | 1 | 187 | A | C8-N9-C4 | -5.33 | 103.67 | 105.80 |
| 4 | 4 | 113 | U | N3-C4-O4 | -5.33 | 115.67 | 119.40 |
| 1 | 1 | 1582 | C | C2-N1-C1' | -5.33 | 112.94 | 118.80 |
| 2 | 2 | 1196 | A | P-O3'-C3' | 5.33 | 126.10 | 119.70 |
| 1 | 5 | 424 | G | C6-C5-N7 | -5.33 | 127.20 | 130.40 |
| 17 | D2 | 28 | ARG | C-N-CD | -5.33 | 108.87 | 120.60 |
| 1 | 1 | 2201 | G | N3-C4-C5 | -5.33 | 125.94 | 128.60 |
| 1 | 5 | 511 | G | C5-C6-O6 | -5.33 | 125.40 | 128.60 |
| 1 | 5 | 656 | A | C5-N7-C8 | -5.33 | 101.24 | 103.90 |
| 1 | 5 | 1161 | G | C5-C6-O6 | -5.33 | 125.40 | 128.60 |
| 1 | 5 | 2987 | A | C2-N3-C4 | 5.33 | 113.26 | 110.60 |
| 2 | 6 | 576 | G | C6-C5-N7 | -5.33 | 127.20 | 130.40 |
| 2 | 6 | 1671 | A | N1-C6-N6 | -5.33 | 115.40 | 118.60 |
| 11 | C6 | 28 | LEU | CA-CB-CG | 5.33 | 127.55 | 115.30 |
| 1 | 1 | 41 | G | N1-C6-O6 | -5.33 | 116.70 | 119.90 |
| 1 | 1 | 1929 | G | N1-C6-O6 | 5.33 | 123.10 | 119.90 |
| 1 | 1 | 2514 | U | O5'-P-OP1 | -5.33 | 100.91 | 105.70 |
| 1 | 5 | 291 | C | N3-C4-C5 | 5.33 | 124.03 | 121.90 |
| 1 | 5 | 3047 | U | N1-C2-O2 | -5.33 | 119.07 | 122.80 |
| 1 | 1 | 2651 | G | C4-C5-N7 | 5.33 | 112.93 | 110.80 |
| 1 | 1 | 226 | C | C6-N1-C2 | -5.32 | 118.17 | 120.30 |
| 1 | 1 | 287 | G | N1-C6-O6 | 5.32 | 123.09 | 119.90 |
| 1 | 1 | 1446 | A | C8-N9-C4 | -5.32 | 103.67 | 105.80 |
| 1 | 5 | 2201 | G | C6-C5-N7 | -5.32 | 127.21 | 130.40 |
| 2 | 6 | 78 | A | C8-N9-C4 | -5.32 | 103.67 | 105.80 |
| 1 | 1 | 1306 | G | N3-C4-C5 | -5.32 | 125.94 | 128.60 |
| 1 | 1 | 3122 | A | N1-C6-N6 | -5.32 | 115.41 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 5 | 2320 | A | C8-N9-C4 | 5.32 | 107.93 | 105.80 |
| 1 | 5 | 3211 | C | C6-N1-C2 | 5.32 | 122.43 | 120.30 |
| 1 | 1 | 864 | G | OP2-P-O3' | 5.32 | 116.90 | 105.20 |
| 2 | 2 | 947 | U | C5-C6-N1 | 5.32 | 125.36 | 122.70 |
| 1 | 1 | 2603 | G | N9-C4-C5 | -5.32 | 103.27 | 105.40 |
| 4 | 4 | 135 | G | C4-C5-N7 | -5.32 | 108.67 | 110.80 |
| 1 | 1 | 667 | C | N1-C2-O2 | 5.32 | 122.09 | 118.90 |
| 1 | 1 | 1024 | G | P-O3'-C3' | 5.32 | 126.08 | 119.70 |
| 1 | 1 | 2311 | G | C4-C5-N7 | 5.32 | 112.93 | 110.80 |
| 1 | 1 | 3056 | U | C6-N1-C2 | 5.32 | 124.19 | 121.00 |
| 1 | 5 | 1355 | A | P-O3'-C3' | 5.32 | 126.08 | 119.70 |
| 1 | 1 | 1544 | G | N9-C4-C5 | -5.32 | 103.27 | 105.40 |
| 2 | 2 | 1607 | G | N3-C4-C5 | -5.32 | 125.94 | 128.60 |
| 2 | 6 | 487 | G | N3-C4-N9 | 5.32 | 129.19 | 126.00 |
| 2 | 2 | 433 | C | C6-N1-C2 | 5.31 | 122.42 | 120.30 |
| 1 | 5 | 384 | A | N1-C6-N6 | 5.31 | 121.79 | 118.60 |
| 1 | 1 | 1853 | U | N1-C2-O2 | -5.31 | 119.08 | 122.80 |
| 1 | 1 | 1915 | A | C8-N9-C4 | 5.31 | 107.92 | 105.80 |
| 2 | 2 | 1600 | A | C5-C6-N1 | -5.31 | 115.04 | 117.70 |
| 36 | m1 | 112 | LEU | CA-CB-CG | 5.31 | 127.52 | 115.30 |
| 1 | 1 | 1482 | A | N7-C8-N9 | 5.31 | 116.46 | 113.80 |
| 1 | 1 | 3310 | A | N1-C6-N6 | 5.31 | 121.79 | 118.60 |
| 1 | 1 | 668 | G | C8-N9-C4 | 5.31 | 108.52 | 106.40 |
| 2 | 2 | 1097 | U | O4'-C1'-N1 | 5.31 | 112.45 | 108.20 |
| 2 | 2 | 238 | U | C5-C6-N1 | 5.31 | 125.35 | 122.70 |
| 1 | 5 | 2574 | G | C4-C5-N7 | 5.31 | 112.92 | 110.80 |
| 1 | 1 | 837 | A | C2-N3-C4 | -5.31 | 107.95 | 110.60 |
| 2 | 2 | 1778 | G | C8-N9-C4 | -5.31 | 104.28 | 106.40 |
| 1 | 5 | 227 | G | C8-N9-C1' | -5.31 | 120.10 | 127.00 |
| 1 | 1 | 1169 | A | C5-C6-N6 | 5.30 | 127.94 | 123.70 |
| 1 | 1 | 3316 | A | P-O3'-C3' | 5.30 | 126.06 | 119.70 |
| 2 | 2 | 1343 | U | C6-N1-C2 | -5.30 | 117.82 | 121.00 |
| 1 | 5 | 824 | C | N3-C4-C5 | -5.30 | 119.78 | 121.90 |
| 1 | 5 | 2849 | C | O5'-P-OP2 | -5.30 | 100.93 | 105.70 |
| 2 | 6 | 1607 | G | N1-C6-O6 | 5.30 | 123.08 | 119.90 |
| 17 | D2 | 65 | LEU | CA-CB-CG | 5.30 | 127.50 | 115.30 |
| 1 | 1 | 1356 | U | N3-C2-O2 | 5.30 | 125.91 | 122.20 |
| 2 | 2 | 1794 | A | N1-C6-N6 | -5.30 | 115.42 | 118.60 |
| 1 | 5 | 26 | A | N1-C6-N6 | 5.30 | 121.78 | 118.60 |
| 1 | 5 | 1115 | G | N7-C8-N9 | 5.30 | 115.75 | 113.10 |
| 1 | 1 | 3268 | A | C8-N9-C4 | -5.30 | 103.68 | 105.80 |
| 2 | 2 | 939 | A | C5-C6-N6 | -5.30 | 119.46 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | 5 | 2606 | G | C6-C5-N7 | -5.30 | 127.22 | 130.40 |
| 2 | 2 | 895 | G | C4-C5-N7 | -5.30 | 108.68 | 110.80 |
| 1 | 1 | 2110 | G | N3-C4-N9 | 5.30 | 129.18 | 126.00 |
| 2 | 2 | 622 | A | OP1-P-O3' | 5.30 | 116.85 | 105.20 |
| 1 | 5 | 1004 | U | N3-C4-O4 | 5.30 | 123.11 | 119.40 |
| 1 | 5 | 1149 | G | N3-C4-C5 | -5.30 | 125.95 | 128.60 |
| 1 | 1 | 229 | G | C8-N9-C4 | -5.29 | 104.28 | 106.40 |
| 1 | 1 | 1702 | U | C6-N1-C2 | -5.29 | 117.82 | 121.00 |
| 1 | 1 | 195 | U | OP1-P-O3' | 5.29 | 116.84 | 105.20 |
| 2 | 2 | 1427 | A | N9-C4-C5 | 5.29 | 107.92 | 105.80 |
| 1 | 5 | 1913 | A | C5-C6-N6 | -5.29 | 119.47 | 123.70 |
| 2 | 6 | 391 | A | O5'-P-OP2 | -5.29 | 100.94 | 105.70 |
| 2 | 6 | 466 | U | C6-N1-C2 | -5.29 | 117.82 | 121.00 |
| 1 | 1 | 2946 | A | OP2-P-O3' | 5.29 | 116.84 | 105.20 |
| 1 | 5 | 880 | G | N1-C6-O6 | -5.29 | 116.72 | 119.90 |
| 1 | 5 | 2977 | G | N1-C2-N2 | -5.29 | 111.44 | 116.20 |
| 1 | 5 | 953 | G | N3-C2-N2 | 5.29 | 123.60 | 119.90 |
| 2 | 2 | 1332 | C | C6-N1-C2 | -5.29 | 118.18 | 120.30 |
| 1 | 5 | 3307 | A | C5-C6-N6 | -5.29 | 119.47 | 123.70 |
| 1 | 1 | 3278 | C | N3-C2-O2 | -5.29 | 118.20 | 121.90 |
| 2 | 6 | 1060 | U | C2-N1-C1' | 5.29 | 124.04 | 117.70 |
| 1 | 1 | 2401 | A | O4'-C1'-N9 | 5.29 | 112.43 | 108.20 |
| 1 | 5 | 1775 | G | N1-C6-O6 | 5.29 | 123.07 | 119.90 |
| 1 | 1 | 929 | A | OP1-P-O3' | 5.28 | 116.82 | 105.20 |
| 1 | 1 | 964 | G | C8-N9-C4 | -5.28 | 104.29 | 106.40 |
| 1 | 1 | 1218 | U | C2-N1-C1' | 5.28 | 124.04 | 117.70 |
| 1 | 1 | 2112 | U | P-O3'-C3' | 5.28 | 126.04 | 119.70 |
| 2 | 2 | 498 | G | C8-N9-C4 | -5.28 | 104.29 | 106.40 |
| 1 | 5 | 2137 | U | C2-N1-C1' | 5.28 | 124.04 | 117.70 |
| 2 | 6 | 1059 | U | C5-C6-N1 | 5.28 | 125.34 | 122.70 |
| 2 | 6 | 1657 | U | C3'-C2'-C1' | 5.28 | 105.73 | 101.50 |
| 1 | 1 | 632 | G | C5-C6-O6 | -5.28 | 125.43 | 128.60 |
| 1 | 1 | 2761 | G | N1-C6-O6 | -5.28 | 116.73 | 119.90 |
| 1 | 1 | 3303 | G | C8-N9-C4 | 5.28 | 108.51 | 106.40 |
| 1 | 5 | 1878 | G | C5-C6-O6 | 5.28 | 131.77 | 128.60 |
| 1 | 1 | 753 | C | N3-C4-C5 | 5.28 | 124.01 | 121.90 |
| 1 | 1 | 915 | A | C8-N9-C4 | -5.28 | 103.69 | 105.80 |
| 1 | 5 | 3266 | G | N1-C6-O6 | -5.28 | 116.73 | 119.90 |
| 1 | 1 | 216 | G | N1-C6-O6 | 5.28 | 123.07 | 119.90 |
| 1 | 1 | 273 | A | C6-C5-N7 | 5.28 | 136.00 | 132.30 |
| 1 | 1 | 1581 | C | OP2-P-O3' | 5.28 | 116.81 | 105.20 |
| 1 | 1 | 2372 | A | C8-N9-C4 | 5.28 | 107.91 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 1 | 193 | C | C6-N1-C2 | -5.28 | 118.19 | 120.30 |
| 1 | 1 | 966 | U | C5-C4-O4 | -5.28 | 122.73 | 125.90 |
| 1 | 1 | 1047 | A | O5'-P-OP2 | -5.28 | 100.95 | 105.70 |
| 1 | 1 | 2764 | C | C6-N1-C2 | -5.28 | 118.19 | 120.30 |
| 1 | 1 | 2794 | G | N1-C6-O6 | 5.28 | 123.07 | 119.90 |
| 2 | 2 | 1649 | G | C8-N9-C4 | 5.28 | 108.51 | 106.40 |
| 1 | 5 | 2824 | G | N3-C4-N9 | 5.28 | 129.17 | 126.00 |
| 1 | 1 | 1610 | G | C6-C5-N7 | -5.28 | 127.23 | 130.40 |
| 1 | 1 | 1614 | C | N3-C2-O2 | -5.28 | 118.21 | 121.90 |
| 3 | 3 | 113 | C | C6-N1-C2 | 5.28 | 122.41 | 120.30 |
| 1 | 5 | 1078 | U | C6-N1-C1' | 5.28 | 128.59 | 121.20 |
| 3 | 7 | 85 | G | N3-C4-C5 | 5.28 | 131.24 | 128.60 |
| 14 | C9 | 28 | LEU | CA-CB-CG | 5.28 | 127.43 | 115.30 |
| 2 | 2 | 1420 | C | N3-C4-C5 | 5.27 | 124.01 | 121.90 |
| 1 | 5 | 2837 | A | N1-C6-N6 | 5.27 | 121.76 | 118.60 |
| 1 | 5 | 1146 | C | C5-C6-N1 | -5.27 | 118.36 | 121.00 |
| 1 | 5 | 1370 | G | N1-C6-O6 | 5.27 | 123.06 | 119.90 |
| 1 | 5 | 1429 | G | C6-C5-N7 | -5.27 | 127.24 | 130.40 |
| 1 | 5 | 2983 | C | O5'-P-OP2 | 5.27 | 117.03 | 110.70 |
| 1 | 1 | 1610 | G | N1-C6-O6 | 5.27 | 123.06 | 119.90 |
| 1 | 1 | 2846 | U | N3-C2-O2 | -5.27 | 118.51 | 122.20 |
| 50 | N6 | 111 | LEU | CA-CB-CG | -5.27 | 103.18 | 115.30 |
| 1 | 1 | 1202 | A | C5-C6-N6 | -5.27 | 119.48 | 123.70 |
| 1 | 1 | 2857 | C | N3-C4-C5 | -5.27 | 119.79 | 121.90 |
| 4 | 4 | 136 | G | C8-N9-C4 | 5.27 | 108.51 | 106.40 |
| 1 | 5 | 3245 | A | C4-C5-C6 | 5.27 | 119.64 | 117.00 |
| 3 | 7 | 91 | G | N3-C2-N2 | -5.27 | 116.21 | 119.90 |
| 1 | 5 | 2246 | G | C5-C6-O6 | -5.27 | 125.44 | 128.60 |
| 1 | 5 | 1000 | C | N3-C4-C5 | 5.27 | 124.01 | 121.90 |
| 2 | 6 | 1736 | G | N1-C6-O6 | 5.27 | 123.06 | 119.90 |
| 1 | 1 | 869 | G | C5-C6-N1 | 5.26 | 114.13 | 111.50 |
| 1 | 1 | 1886 | A | N1-C6-N6 | -5.26 | 115.44 | 118.60 |
| 1 | 5 | 826 | G | N1-C6-O6 | 5.26 | 123.06 | 119.90 |
| 1 | 5 | 2260 | U | C6-N1-C2 | -5.26 | 117.84 | 121.00 |
| 1 | 1 | 919 | U | N1-C2-O2 | 5.26 | 126.48 | 122.80 |
| 2 | 2 | 130 | C | N3-C2-O2 | -5.26 | 118.22 | 121.90 |
| 2 | 2 | 926 | A | N1-C2-N3 | 5.26 | 131.93 | 129.30 |
| 1 | 5 | 920 | A | C2-N3-C4 | -5.26 | 107.97 | 110.60 |
| 1 | 5 | 1825 | G | C4-C5-N7 | -5.26 | 108.70 | 110.80 |
| 1 | 5 | 2382 | G | C5-C6-O6 | -5.26 | 125.44 | 128.60 |
| 2 | 6 | 779 | U | C2-N1-C1' | 5.26 | 124.01 | 117.70 |
| 1 | 1 | 1316 | C | C6-N1-C2 | 5.26 | 122.40 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 1 | 2961 | G | C8-N9-C4 | -5.26 | 104.30 | 106.40 |
| 4 | 4 | 140 | G | C6-C5-N7 | -5.26 | 127.24 | 130.40 |
| 1 | 5 | 3245 | A | C6-C5-N7 | -5.26 | 128.62 | 132.30 |
| 1 | 1 | 2150 | G | N1-C6-O6 | 5.26 | 123.05 | 119.90 |
| 1 | 1 | 3217 | C | C5-C6-N1 | 5.26 | 123.63 | 121.00 |
| 1 | 1 | 3318 | G | C4-N9-C1' | 5.26 | 133.33 | 126.50 |
| 1 | 5 | 287 | G | N9-C4-C5 | -5.26 | 103.30 | 105.40 |
| 1 | 5 | 562 | C | C6-N1-C2 | -5.26 | 118.20 | 120.30 |
| 1 | 5 | 917 | A | O5'-P-OP2 | -5.26 | 100.97 | 105.70 |
| 1 | 5 | 3338 | C | N3-C4-C5 | 5.26 | 124.00 | 121.90 |
| 2 | 6 | 9 | U | C5-C6-N1 | 5.26 | 125.33 | 122.70 |
| 1 | 1 | 3068 | U | C2-N1-C1' | -5.25 | 111.40 | 117.70 |
| 1 | 5 | 1855 | U | C5-C4-O4 | 5.25 | 129.05 | 125.90 |
| 1 | 5 | 2413 | A | C2-N3-C4 | -5.25 | 107.97 | 110.60 |
| 2 | 6 | 858 | G | C4-N9-C1' | 5.25 | 133.33 | 126.50 |
| 1 | 1 | 584 | G | O5'-P-OP2 | -5.25 | 100.97 | 105.70 |
| 1 | 1 | 1161 | G | C8-N9-C4 | -5.25 | 104.30 | 106.40 |
| 1 | 5 | 1878 | G | N1-C6-O6 | -5.25 | 116.75 | 119.90 |
| 1 | 5 | 2240 | G | C6-C5-N7 | -5.25 | 127.25 | 130.40 |
| 2 | 6 | 75 | U | P-O3'-C3' | 5.25 | 126.00 | 119.70 |
| 2 | 6 | 548 | G | N1-C6-O6 | 5.25 | 123.05 | 119.90 |
| 1 | 1 | 2174 | G | N3-C2-N2 | -5.25 | 116.23 | 119.90 |
| 2 | 2 | 204 | G | C4-C5-N7 | 5.25 | 112.90 | 110.80 |
| 2 | 2 | 1736 | G | C5-C6-O6 | -5.25 | 125.45 | 128.60 |
| 1 | 5 | 422 | A | C8-N9-C4 | -5.25 | 103.70 | 105.80 |
| 2 | 6 | 1491 | U | C6-N1-C2 | -5.25 | 117.85 | 121.00 |
| 1 | 5 | 2827 | U | C5-C6-N1 | -5.25 | 120.08 | 122.70 |
| 1 | 5 | 3049 | A | N1-C6-N6 | 5.25 | 121.75 | 118.60 |
| 1 | 1 | 1174 | G | C8-N9-C1' | -5.25 | 120.18 | 127.00 |
| 3 | 3 | 83 | U | C6-N1-C2 | 5.25 | 124.15 | 121.00 |
| 1 | 1 | 782 | U | OP2-P-O3' | 5.24 | 116.74 | 105.20 |
| 1 | 5 | 1155 | C | O5'-P-OP1 | -5.24 | 100.98 | 105.70 |
| 1 | 5 | 1581 | C | C2-N1-C1' | 5.24 | 124.57 | 118.80 |
| 1 | 5 | 3205 | G | C4-C5-N7 | 5.24 | 112.90 | 110.80 |
| 2 | 6 | 1625 | C | C6-N1-C2 | 5.24 | 122.40 | 120.30 |
| 1 | 1 | 2420 | C | C5-C6-N1 | 5.24 | 123.62 | 121.00 |
| 1 | 1 | 2645 | G | C5-C6-O6 | -5.24 | 125.45 | 128.60 |
| 1 | 1 | 2940 | A | C5-C6-N1 | 5.24 | 120.32 | 117.70 |
| 2 | 2 | 1760 | G | N1-C6-O6 | 5.24 | 123.04 | 119.90 |
| 1 | 5 | 283 | G | C4-N9-C1' | 5.24 | 133.31 | 126.50 |
| 1 | 5 | 1657 | C | C6-N1-C2 | -5.24 | 118.20 | 120.30 |
| 1 | 5 | 799 | G | C6-C5-N7 | -5.24 | 127.26 | 130.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 5 | 2951 | G | C4-C5-N7 | 5.24 | 112.90 | 110.80 |
| 1 | 1 | 63 | A | O5'-P-OP1 | -5.24 | 100.99 | 105.70 |
| 1 | 1 | 350 | C | N1-C2-O2 | 5.24 | 122.04 | 118.90 |
| 1 | 1 | 891 | G | C6-C5-N7 | -5.24 | 127.26 | 130.40 |
| 2 | 2 | 1154 | G | C5-C6-O6 | 5.24 | 131.74 | 128.60 |
| 1 | 5 | 1730 | G | C8-N9-C4 | -5.24 | 104.31 | 106.40 |
| 1 | 5 | 2619 | G | C6-C5-N7 | -5.24 | 127.26 | 130.40 |
| 2 | 6 | 1495 | C | C6-N1-C2 | -5.24 | 118.21 | 120.30 |
| 1 | 1 | 2817 | A | C2-N3-C4 | 5.23 | 113.22 | 110.60 |
| 1 | 5 | 1437 | C | N3-C4-N4 | 5.23 | 121.66 | 118.00 |
| 2 | 6 | 176 | C | N1-C2-O2 | 5.23 | 122.04 | 118.90 |
| 1 | 1 | 96 | G | N3-C4-C5 | 5.23 | 131.22 | 128.60 |
| 1 | 1 | 2541 | U | C2-N1-C1' | 5.23 | 123.98 | 117.70 |
| 1 | 5 | 1465 | A | N1-C6-N6 | -5.23 | 115.46 | 118.60 |
| 2 | 6 | 151 | G | C6-C5-N7 | 5.23 | 133.54 | 130.40 |
| 2 | 6 | 320 | U | O5'-P-OP1 | -5.23 | 100.99 | 105.70 |
| 1 | 1 | 1571 | A | P-O3'-C3' | 5.23 | 125.98 | 119.70 |
| 1 | 1 | 2617 | U | N1-C2-O2 | -5.23 | 119.14 | 122.80 |
| 4 | 4 | 104 | A | C5-C6-N6 | -5.23 | 119.52 | 123.70 |
| 1 | 5 | 3243 | A | O4'-C1'-N9 | -5.23 | 104.02 | 108.20 |
| 1 | 1 | 2180 | G | N3-C4-C5 | 5.23 | 131.22 | 128.60 |
| 1 | 1 | 2425 | G | N1-C6-O6 | 5.23 | 123.04 | 119.90 |
| 1 | 5 | 2404 | A | N3-C4-C5 | 5.23 | 130.46 | 126.80 |
| 1 | 1 | 1602 | A | N1-C6-N6 | -5.23 | 115.46 | 118.60 |
| 1 | 5 | 1715 | A | OP1-P-O3' | 5.23 | 116.70 | 105.20 |
| 1 | 5 | 2651 | G | C8-N9-C4 | 5.23 | 108.49 | 106.40 |
| 2 | 6 | 192 | U | C5-C6-N1 | 5.23 | 125.31 | 122.70 |
| 1 | 1 | 94 | G | O5'-P-OP1 | -5.23 | 101.00 | 105.70 |
| 1 | 5 | 2830 | G | C2-N3-C4 | -5.23 | 109.29 | 111.90 |
| 2 | 6 | 581 | U | C2-N1-C1' | -5.23 | 111.43 | 117.70 |
| 2 | 2 | 294 | C | C6-N1-C2 | 5.22 | 122.39 | 120.30 |
| 2 | 2 | 616 | G | N9-C4-C5 | 5.22 | 107.49 | 105.40 |
| 4 | 4 | 51 | G | N1-C6-O6 | 5.22 | 123.03 | 119.90 |
| 1 | 1 | 1450 | G | OP1-P-OP2 | -5.22 | 111.77 | 119.60 |
| 1 | 5 | 601 | U | C2-N1-C1' | 5.22 | 123.97 | 117.70 |
| 4 | 8 | 118 | C | C6-N1-C2 | -5.22 | 118.21 | 120.30 |
| 1 | 1 | 780 | A | N9-C4-C5 | 5.22 | 107.89 | 105.80 |
| 1 | 1 | 928 | C | N3-C4-C5 | 5.22 | 123.99 | 121.90 |
| 1 | 5 | 439 | C | C6-N1-C1' | -5.22 | 114.53 | 120.80 |
| 2 | 6 | 624 | G | N1-C6-O6 | 5.22 | 123.03 | 119.90 |
| 1 | 1 | 1322 | U | N3-C4-C5 | -5.22 | 111.47 | 114.60 |
| 3 | 3 | 8 | G | N3-C4-C5 | 5.22 | 131.21 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 5 | 913 | A | N1-C6-N6 | 5.22 | 121.73 | 118.60 |
| 1 | 5 | 925 | A | C2-N3-C4 | -5.22 | 107.99 | 110.60 |
| 2 | 6 | 176 | C | N3-C2-O2 | -5.22 | 118.25 | 121.90 |
| 2 | 6 | 1458 | G | C8-N9-C1' | -5.22 | 120.21 | 127.00 |
| 1 | 1 | 1211 | U | C6-N1-C2 | 5.22 | 124.13 | 121.00 |
| 1 | 1 | 2836 | C | C6-N1-C2 | -5.22 | 118.21 | 120.30 |
| 1 | 5 | 2366 | C | N3-C4-C5 | 5.22 | 123.99 | 121.90 |
| 1 | 1 | 2403 | G | O5'-P-OP2 | -5.22 | 101.00 | 105.70 |
| 1 | 1 | 3220 | G | N1-C6-O6 | 5.22 | 123.03 | 119.90 |
| 1 | 5 | 718 | G | O4'-C1'-N9 | 5.22 | 112.37 | 108.20 |
| 1 | 5 | 2628 | A | N1-C6-N6 | 5.22 | 121.73 | 118.60 |
| 1 | 1 | 611 | A | C6-C5-N7 | -5.21 | 128.65 | 132.30 |
| 1 | 1 | 1399 | A | N1-C6-N6 | 5.21 | 121.73 | 118.60 |
| 1 | 1 | 1413 | G | C2-N3-C4 | -5.21 | 109.29 | 111.90 |
| 2 | 2 | 209 | U | O5'-P-OP1 | -5.21 | 101.01 | 105.70 |
| 1 | 5 | 909 | G | N1-C6-O6 | -5.21 | 116.77 | 119.90 |
| 1 | 5 | 2942 | C | C6-N1-C2 | -5.21 | 118.21 | 120.30 |
| 1 | 5 | 2964 | G | OP1-P-O3' | 5.21 | 116.67 | 105.20 |
| 3 | 7 | 79 | A | N1-C6-N6 | -5.21 | 115.47 | 118.60 |
| 4 | 8 | 121 | U | N3-C2-O2 | -5.21 | 118.55 | 122.20 |
| 1 | 5 | 2181 | C | N3-C4-C5 | 5.21 | 123.98 | 121.90 |
| 2 | 6 | 1453 | G | C8-N9-C4 | 5.21 | 108.48 | 106.40 |
| 50 | N6 | 57 | LEU | CA-CB-CG | 5.21 | 127.29 | 115.30 |
| 1 | 1 | 1000 | C | N3-C4-C5 | 5.21 | 123.98 | 121.90 |
| 1 | 1 | 1422 | G | C5-C6-O6 | -5.21 | 125.47 | 128.60 |
| 1 | 1 | 2934 | A | C2-N3-C4 | -5.21 | 108.00 | 110.60 |
| 1 | 1 | 3373 | U | C6-N1-C2 | 5.21 | 124.13 | 121.00 |
| 2 | 2 | 306 | U | C5-C6-N1 | -5.21 | 120.10 | 122.70 |
| 4 | 8 | 46 | G | C5-C6-O6 | 5.21 | 131.72 | 128.60 |
| 2 | 6 | 1686 | C | C5-C6-N1 | 5.21 | 123.60 | 121.00 |
| 79 | sR | 165 | ASP | C-N-CA | 5.21 | 134.72 | 121.70 |
| 1 | 1 | 3216 | G | N3-C4-C5 | 5.21 | 131.20 | 128.60 |
| 1 | 5 | 601 | U | C6-N1-C2 | -5.21 | 117.88 | 121.00 |
| 3 | 3 | 51 | A | C8-N9-C4 | -5.20 | 103.72 | 105.80 |
| 3 | 3 | 77 | G | C8-N9-C4 | 5.20 | 108.48 | 106.40 |
| 1 | 5 | 1672 | U | O4'-C1'-N1 | 5.20 | 112.36 | 108.20 |
| 1 | 5 | 2204 | C | P-O3'-C3' | 5.20 | 125.94 | 119.70 |
| 2 | 6 | 1003 | A | C8-N9-C4 | 5.20 | 107.88 | 105.80 |
| 1 | 1 | 1941 | C | C5-C6-N1 | 5.20 | 123.60 | 121.00 |
| 1 | 5 | 3252 | G | N3-C4-C5 | 5.20 | 131.20 | 128.60 |
| 4 | 8 | 82 | U | P-O3'-C3' | 5.20 | 125.94 | 119.70 |
| 1 | 1 | 359 | U | N1-C2-N3 | 5.20 | 118.02 | 114.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 1 | 1086 | C | C6-N1-C2 | -5.20 | 118.22 | 120.30 |
| 1 | 1 | 3220 | G | C5-C6-O6 | -5.20 | 125.48 | 128.60 |
| 2 | 2 | 91 | G | C8-N9-C4 | 5.20 | 108.48 | 106.40 |
| 1 | 5 | 1075 | A | C8-N9-C4 | 5.20 | 107.88 | 105.80 |
| 17 | D2 | 93 | LEU | CA-CB-CG | 5.20 | 127.26 | 115.30 |
| 1 | 1 | 645 | A | C5-C6-N6 | 5.20 | 127.86 | 123.70 |
| 1 | 1 | 1078 | U | C6-N1-C2 | -5.20 | 117.88 | 121.00 |
| 1 | 1 | 2206 | G | O4'-C1'-N9 | -5.20 | 104.04 | 108.20 |
| 1 | 1 | 211 | A | O5'-P-OP1 | -5.20 | 101.03 | 105.70 |
| 1 | 5 | 2332 | A | C8-N9-C4 | 5.20 | 107.88 | 105.80 |
| 4 | 8 | 100 | U | C2-N1-C1' | 5.20 | 123.93 | 117.70 |
| 2 | 2 | 1760 | G | C5-C6-O6 | -5.19 | 125.48 | 128.60 |
| 1 | 5 | 1592 | G | N3-C4-N9 | 5.19 | 129.12 | 126.00 |
| 1 | 5 | 3008 | A | N1-C6-N6 | -5.19 | 115.48 | 118.60 |
| 1 | 1 | 260 | C | C6-N1-C2 | 5.19 | 122.38 | 120.30 |
| 1 | 1 | 839 | C | C6-N1-C2 | 5.19 | 122.38 | 120.30 |
| 1 | 1 | 2960 | C | OP2-P-O3' | 5.19 | 116.62 | 105.20 |
| 3 | 3 | 31 | U | C6-N1-C2 | -5.19 | 117.89 | 121.00 |
| 1 | 5 | 368 | G | N9-C4-C5 | -5.19 | 103.32 | 105.40 |
| 1 | 5 | 2286 | U | C2-N1-C1' | -5.19 | 111.47 | 117.70 |
| 1 | 1 | 620 | U | N1-C2-N3 | 5.19 | 118.01 | 114.90 |
| 1 | 1 | 2186 | U | O5'-P-OP1 | 5.19 | 116.93 | 110.70 |
| 1 | 1 | 2372 | A | N7-C8-N9 | -5.19 | 111.20 | 113.80 |
| 1 | 1 | 62 | A | N9-C4-C5 | -5.19 | 103.72 | 105.80 |
| 2 | 2 | 39 | A | O4'-C1'-N9 | 5.19 | 112.35 | 108.20 |
| 2 | 2 | 1473 | U | N1-C2-O2 | 5.19 | 126.43 | 122.80 |
| 1 | 5 | 711 | A | N1-C6-N6 | -5.19 | 115.49 | 118.60 |
| 2 | 6 | 789 | A | N1-C6-N6 | -5.19 | 115.49 | 118.60 |
| 1 | 1 | 637 | C | C4-C5-C6 | -5.19 | 114.81 | 117.40 |
| 2 | 2 | 1729 | C | N3-C4-C5 | 5.18 | 123.97 | 121.90 |
| 1 | 5 | 423 | A | N9-C4-C5 | 5.18 | 107.87 | 105.80 |
| 1 | 5 | 529 | A | C8-N9-C4 | -5.18 | 103.73 | 105.80 |
| 2 | 6 | 42 | G | N1-C6-O6 | 5.18 | 123.01 | 119.90 |
| 2 | 6 | 553 | G | N1-C6-O6 | 5.18 | 123.01 | 119.90 |
| 1 | 1 | 1871 | U | N3-C2-O2 | -5.18 | 118.57 | 122.20 |
| 1 | 5 | 2430 | A | N1-C6-N6 | 5.18 | 121.71 | 118.60 |
| 1 | 1 | 1028 | U | C5-C6-N1 | 5.18 | 125.29 | 122.70 |
| 2 | 6 | 639 | U | N1-C2-O2 | 5.18 | 126.43 | 122.80 |
| 1 | 1 | 54 | C | C6-N1-C2 | 5.18 | 122.37 | 120.30 |
| 1 | 1 | 632 | G | C6-C5-N7 | -5.18 | 127.29 | 130.40 |
| 1 | 1 | 808 | A | C8-N9-C4 | -5.18 | 103.73 | 105.80 |
| 1 | 1 | 2654 | C | C5-C6-N1 | 5.18 | 123.59 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | 1 | 2817 | A | N9-C4-C5 | 5.18 | 107.87 | 105.80 |
| 1 | 1 | 2937 | G | C6-C5-N7 | -5.18 | 127.29 | 130.40 |
| 1 | 5 | 280 | U | O5'-P-OP2 | -5.18 | 101.04 | 105.70 |
| 1 | 5 | 1858 | A | N9-C4-C5 | 5.18 | 107.87 | 105.80 |
| 1 | 5 | 2625 | C | N3-C2-O2 | 5.18 | 125.53 | 121.90 |
| 2 | 6 | 765 | G | C4-C5-N7 | -5.18 | 108.73 | 110.80 |
| 78 | sM | 134 | ASP | CB-CG-OD2 | 5.18 | 122.96 | 118.30 |
| 1 | 1 | 2209 | U | P-O3'-C3' | 5.18 | 125.91 | 119.70 |
| 1 | 1 | 2620 | G | C2-N3-C4 | -5.18 | 109.31 | 111.90 |
| 1 | 5 | 2892 | A | N9-C4-C5 | -5.18 | 103.73 | 105.80 |
| 1 | 5 | 2987 | A | N1-C2-N3 | -5.18 | 126.71 | 129.30 |
| 2 | 2 | 499 | U | C3'-C2'-C1' | 5.17 | 105.64 | 101.50 |
| 1 | 5 | 1552 | G | N9-C4-C5 | -5.17 | 103.33 | 105.40 |
| 2 | 6 | 393 | C | C6-N1-C2 | 5.17 | 122.37 | 120.30 |
| 2 | 6 | 565 | C | C2-N1-C1' | 5.17 | 124.49 | 118.80 |
| 2 | 6 | 810 | G | N1-C6-O6 | 5.17 | 123.00 | 119.90 |
| 1 | 1 | 869 | G | O5'-P-OP1 | 5.17 | 116.91 | 110.70 |
| 1 | 1 | 1206 | G | N3-C4-C5 | -5.17 | 126.01 | 128.60 |
| 1 | 1 | 353 | G | O4'-C1'-N9 | -5.17 | 104.06 | 108.20 |
| 1 | 1 | 2383 | C | C6-N1-C2 | 5.17 | 122.37 | 120.30 |
| 1 | 1 | 2868 | U | C2-N1-C1' | 5.17 | 123.91 | 117.70 |
| 1 | 1 | 2901 | G | N1-C6-O6 | 5.17 | 123.00 | 119.90 |
| 2 | 2 | 1093 | A | N1-C6-N6 | 5.17 | 121.70 | 118.60 |
| 1 | 5 | 32 | U | N3-C2-O2 | -5.17 | 118.58 | 122.20 |
| 1 | 5 | 887 | G | C5-C6-O6 | -5.17 | 125.50 | 128.60 |
| 1 | 5 | 1858 | A | N1-C6-N6 | -5.17 | 115.50 | 118.60 |
| 1 | 5 | 2240 | G | N7-C8-N9 | 5.17 | 115.69 | 113.10 |
| 2 | 6 | 302 | U | C6-N1-C2 | -5.17 | 117.90 | 121.00 |
| 76 | S8 | 121 | LEU | CA-CB-CG | 5.17 | 127.19 | 115.30 |
| 1 | 1 | 1197 | A | N1-C6-N6 | 5.17 | 121.70 | 118.60 |
| 1 | 1 | 336 | A | N1-C6-N6 | 5.17 | 121.70 | 118.60 |
| 2 | 2 | 75 | U | N3-C2-O2 | -5.17 | 118.58 | 122.20 |
| 1 | 5 | 216 | G | N1-C6-O6 | 5.17 | 123.00 | 119.90 |
| 2 | 6 | 1591 | C | C6-N1-C2 | -5.17 | 118.23 | 120.30 |
| 1 | 1 | 2150 | G | N3-C4-C5 | 5.17 | 131.18 | 128.60 |
| 1 | 5 | 1481 | A | C4-N9-C1' | 5.17 | 135.60 | 126.30 |
| 1 | 5 | 1776 | G | C8-N9-C4 | -5.17 | 104.33 | 106.40 |
| 1 | 5 | 2954 | U | N3-C2-O2 | -5.17 | 118.58 | 122.20 |
| 1 | 1 | 1521 | G | N3-C4-N9 | -5.17 | 122.90 | 126.00 |
| 1 | 5 | 18 | G | N3-C2-N2 | -5.17 | 116.28 | 119.90 |
| 78 | SM | 134 | ASP | CB-CG-OD2 | 5.17 | 122.95 | 118.30 |
| 1 | 1 | 756 | U | C6-N1-C2 | 5.16 | 124.10 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 1 | 2354 | C | N3-C4-C5 | -5.16 | 119.83 | 121.90 |
| 1 | 1 | 2870 | C | P-O3'-C3' | 5.16 | 125.90 | 119.70 |
| 1 | 5 | 68 | C | N1-C2-O2 | 5.16 | 122.00 | 118.90 |
| 1 | 5 | 2371 | G | N3-C4-N9 | 5.16 | 129.10 | 126.00 |
| 2 | 6 | 558 | U | C5-C6-N1 | 5.16 | 125.28 | 122.70 |
| 2 | 6 | 1524 | A | C8-N9-C4 | -5.16 | 103.73 | 105.80 |
| 1 | 1 | 1508 | C | OP1-P-O3' | 5.16 | 116.56 | 105.20 |
| 2 | 2 | 75 | U | C2-N1-C1' | 5.16 | 123.89 | 117.70 |
| 1 | 5 | 2620 | G | C2-N3-C4 | -5.16 | 109.32 | 111.90 |
| 1 | 1 | 339 | C | N3-C4-C5 | 5.16 | 123.96 | 121.90 |
| 1 | 1 | 1381 | A | N9-C4-C5 | -5.16 | 103.74 | 105.80 |
| 1 | 1 | 2180 | G | C8-N9-C4 | 5.16 | 108.46 | 106.40 |
| 2 | 2 | 881 | A | C8-N9-C4 | 5.16 | 107.86 | 105.80 |
| 2 | 2 | 1052 | U | O4'-C1'-N1 | 5.16 | 112.33 | 108.20 |
| 1 | 5 | 2831 | G | C4-C5-N7 | 5.16 | 112.86 | 110.80 |
| 1 | 1 | 2646 | C | C5-C6-N1 | -5.16 | 118.42 | 121.00 |
| 2 | 2 | 1783 | C | C2-N1-C1' | 5.16 | 124.47 | 118.80 |
| 1 | 5 | 1006 | A | C8-N9-C4 | 5.16 | 107.86 | 105.80 |
| 1 | 5 | 1338 | C | N3-C4-N4 | 5.16 | 121.61 | 118.00 |
| 1 | 5 | 1913 | A | C6-C5-N7 | -5.16 | 128.69 | 132.30 |
| 1 | 5 | 2401 | A | N3-C4-N9 | 5.16 | 131.53 | 127.40 |
| 1 | 5 | 2848 | G | N9-C4-C5 | 5.16 | 107.46 | 105.40 |
| 2 | 6 | 1060 | U | C5-C6-N1 | 5.16 | 125.28 | 122.70 |
| 4 | 8 | 84 | C | N1-C2-O2 | -5.16 | 115.80 | 118.90 |
| 1 | 1 | 949 | C | N3-C4-C5 | 5.16 | 123.96 | 121.90 |
| 1 | 1 | 3280 | U | N3-C2-O2 | 5.16 | 125.81 | 122.20 |
| 3 | 3 | 45 | A | C8-N9-C4 | -5.16 | 103.74 | 105.80 |
| 1 | 1 | 2348 | A | N9-C4-C5 | 5.16 | 107.86 | 105.80 |
| 1 | 1 | 3056 | U | N3-C2-O2 | 5.16 | 125.81 | 122.20 |
| 1 | 5 | 106 | A | N9-C4-C5 | -5.16 | 103.74 | 105.80 |
| 1 | 5 | 924 | G | O5'-P-OP1 | -5.16 | 101.06 | 105.70 |
| 1 | 5 | 3090 | U | N3-C4-C5 | -5.16 | 111.51 | 114.60 |
| 1 | 1 | 3110 | C | C6-N1-C2 | -5.15 | 118.24 | 120.30 |
| 1 | 1 | 2853 | A | C5-C6-N6 | -5.15 | 119.58 | 123.70 |
| 1 | 5 | 48 | A | C5-C6-N6 | 5.15 | 127.82 | 123.70 |
| 1 | 5 | 877 | C | C6-N1-C2 | 5.15 | 122.36 | 120.30 |
| 1 | 5 | 2574 | G | O4'-C1'-N9 | -5.15 | 104.08 | 108.20 |
| 1 | 1 | 1437 | C | C5-C6-N1 | 5.15 | 123.58 | 121.00 |
| 1 | 1 | 1582 | C | C6-N1-C1' | 5.15 | 126.98 | 120.80 |
| 1 | 5 | 1437 | C | N3-C4-C5 | -5.15 | 119.84 | 121.90 |
| 1 | 5 | 2298 | U | N3-C2-O2 | -5.15 | 118.59 | 122.20 |
| 1 | 1 | 2385 | G | N1-C6-O6 | 5.15 | 122.99 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 5 | 1531 | C | C5-C4-N4 | -5.15 | 116.60 | 120.20 |
| 2 | 6 | 1458 | G | C5-C6-O6 | -5.15 | 125.51 | 128.60 |
| 1 | 1 | 1940 | G | N9-C4-C5 | -5.15 | 103.34 | 105.40 |
| 2 | 2 | 1096 | C | C6-N1-C1' | -5.15 | 114.62 | 120.80 |
| 76 | s8 | 29 | LEU | CA-CB-CG | 5.15 | 127.14 | 115.30 |
| 1 | 1 | 251 | G | N3-C4-C5 | -5.14 | 126.03 | 128.60 |
| 2 | 2 | 29 | U | C2-N1-C1' | -5.14 | 111.53 | 117.70 |
| 1 | 5 | 1229 | G | N3-C4-C5 | -5.14 | 126.03 | 128.60 |
| 1 | 5 | 2611 | U | O5'-P-OP1 | 5.14 | 116.88 | 110.70 |
| 2 | 6 | 163 | G | C2-N3-C4 | -5.14 | 109.33 | 111.90 |
| 2 | 6 | 1034 | C | C6-N1-C2 | 5.14 | 122.36 | 120.30 |
| 1 | 1 | 2613 | U | O5'-P-OP2 | -5.14 | 101.07 | 105.70 |
| 1 | 1 | 2748 | A | N9-C4-C5 | -5.14 | 103.74 | 105.80 |
| 1 | 1 | 3318 | G | C6-C5-N7 | -5.14 | 127.31 | 130.40 |
| 1 | 5 | 439 | C | C2-N3-C4 | 5.14 | 122.47 | 119.90 |
| 1 | 5 | 1024 | G | N3-C4-C5 | -5.14 | 126.03 | 128.60 |
| 1 | 5 | 3100 | U | N3-C2-O2 | 5.14 | 125.80 | 122.20 |
| 2 | 6 | 45 | U | O4'-C1'-N1 | 5.14 | 112.31 | 108.20 |
| 1 | 1 | 1625 | A | C8-N9-C4 | 5.14 | 107.86 | 105.80 |
| 1 | 5 | 813 | G | C5-C6-O6 | -5.14 | 125.52 | 128.60 |
| 2 | 6 | 1422 | A | N9-C4-C5 | -5.14 | 103.74 | 105.80 |
| 1 | 1 | 2961 | G | OP1-P-O3' | 5.14 | 116.51 | 105.20 |
| 2 | 2 | 1486 | G | C4-C5-N7 | 5.14 | 112.86 | 110.80 |
| 1 | 5 | 701 | G | C8-N9-C4 | -5.14 | 104.34 | 106.40 |
| 1 | 5 | 1205 | A | N1-C6-N6 | 5.14 | 121.68 | 118.60 |
| 1 | 5 | 1400 | G | N1-C6-O6 | -5.14 | 116.82 | 119.90 |
| 2 | 6 | 1323 | C | C6-N1-C2 | -5.14 | 118.24 | 120.30 |
| 1 | 1 | 227 | G | N3-C4-N9 | 5.14 | 129.08 | 126.00 |
| 1 | 1 | 992 | A | C8-N9-C4 | 5.14 | 107.86 | 105.80 |
| 1 | 5 | 609 | G | C5-C6-O6 | -5.14 | 125.52 | 128.60 |
| 2 | 6 | 434 | G | O5'-P-OP2 | -5.14 | 101.08 | 105.70 |
| 4 | 8 | 72 | A | C5-C6-N6 | -5.14 | 119.59 | 123.70 |
| 1 | 1 | 1454 | A | N7-C8-N9 | -5.14 | 111.23 | 113.80 |
| 2 | 2 | 1798 | U | N3-C2-O2 | -5.14 | 118.61 | 122.20 |
| 4 | 4 | 47 | C | N3-C4-C5 | 5.14 | 123.95 | 121.90 |
| 1 | 5 | 894 | G | N3-C4-N9 | 5.14 | 129.08 | 126.00 |
| 1 | 5 | 1343 | A | C2-N3-C4 | -5.13 | 108.03 | 110.60 |
| 1 | 5 | 1590 | G | C8-N9-C4 | 5.13 | 108.45 | 106.40 |
| 1 | 5 | 1782 | U | C2-N1-C1' | 5.13 | 123.86 | 117.70 |
| 2 | 6 | 767 | U | C2-N1-C1' | 5.13 | 123.86 | 117.70 |
| 1 | 1 | 1085 | A | N1-C6-N6 | 5.13 | 121.68 | 118.60 |
| 1 | 5 | 912 | G | N9-C4-C5 | -5.13 | 103.35 | 105.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | 5 | 1609 | C | N3-C4-C5 | 5.13 | 123.95 | 121.90 |
| 1 | 1 | 1204 | A | N1-C6-N6 | 5.13 | 121.68 | 118.60 |
| 1 | 1 | 2943 | G | C8-N9-C4 | -5.13 | 104.35 | 106.40 |
| 2 | 2 | 497 | G | C3'-C2'-C1' | 5.13 | 105.61 | 101.50 |
| 54 | o0 | 104 | LEU | CA-CB-CG | 5.13 | 127.10 | 115.30 |
| 1 | 1 | 968 | G | N9-C4-C5 | -5.13 | 103.35 | 105.40 |
| 1 | 5 | 3158 | G | C8-N9-C4 | -5.13 | 104.35 | 106.40 |
| 1 | 1 | 96 | G | C2-N3-C4 | -5.13 | 109.34 | 111.90 |
| 1 | 1 | 884 | A | C6-C5-N7 | -5.13 | 128.71 | 132.30 |
| 2 | 2 | 1389 | C | C2-N1-C1' | 5.13 | 124.44 | 118.80 |
| 4 | 4 | 140 | G | N9-C4-C5 | -5.13 | 103.35 | 105.40 |
| 1 | 5 | 1495 | U | C2-N1-C1' | 5.13 | 123.85 | 117.70 |
| 1 | 1 | 3216 | G | C8-N9-C4 | 5.13 | 108.45 | 106.40 |
| 1 | 5 | 970 | A | N9-C1'-C2' | -5.13 | 106.36 | 112.00 |
| 1 | 5 | 2726 | C | C5-C4-N4 | 5.13 | 123.79 | 120.20 |
| 2 | 6 | 1605 | G | C8-N9-C4 | -5.13 | 104.35 | 106.40 |
| 1 | 5 | 1323 | G | C5-C6-O6 | -5.12 | 125.53 | 128.60 |
| 1 | 5 | 1606 | U | OP2-P-O3' | 5.12 | 116.47 | 105.20 |
| 1 | 5 | 3195 | U | N1-C2-N3 | -5.12 | 111.83 | 114.90 |
| 2 | 6 | 557 | G | C4-N9-C1' | 5.12 | 133.16 | 126.50 |
| 1 | 1 | 1473 | G | C8-N9-C4 | 5.12 | 108.45 | 106.40 |
| 2 | 2 | 1324 | G | C8-N9-C1' | 5.12 | 133.66 | 127.00 |
| 1 | 5 | 506 | U | C6-N1-C2 | -5.12 | 117.93 | 121.00 |
| 1 | 5 | 2817 | A | C4-C5-C6 | -5.12 | 114.44 | 117.00 |
| 1 | 1 | 758 | C | C6-N1-C2 | -5.12 | 118.25 | 120.30 |
| 2 | 2 | 1331 | A | N1-C6-N6 | -5.12 | 115.53 | 118.60 |
| 1 | 5 | 2403 | G | C5-C6-O6 | -5.12 | 125.53 | 128.60 |
| 2 | 6 | 1773 | C | C5-C6-N1 | 5.12 | 123.56 | 121.00 |
| 24 | d9 | 36 | LEU | CA-CB-CG | 5.12 | 127.08 | 115.30 |
| 1 | 1 | 1113 | G | C8-N9-C4 | -5.12 | 104.35 | 106.40 |
| 1 | 1 | 2857 | C | O5'-P-OP1 | -5.12 | 101.09 | 105.70 |
| 2 | 2 | 1162 | C | C6-N1-C2 | -5.12 | 118.25 | 120.30 |
| 1 | 5 | 1672 | U | C2-N1-C1' | -5.12 | 111.56 | 117.70 |
| 1 | 1 | 141 | C | C6-N1-C2 | -5.12 | 118.25 | 120.30 |
| 2 | 2 | 15 | U | OP2-P-O3' | 5.12 | 116.46 | 105.20 |
| 1 | 5 | 2404 | A | C8-N9-C4 | 5.12 | 107.85 | 105.80 |
| 1 | 1 | 63 | A | C6-C5-N7 | -5.12 | 128.72 | 132.30 |
| 1 | 1 | 651 | G | N3-C4-C5 | -5.12 | 126.04 | 128.60 |
| 1 | 1 | 1842 | A | O4'-C1'-N9 | -5.12 | 104.11 | 108.20 |
| 1 | 1 | 2376 | G | N1-C6-O6 | 5.12 | 122.97 | 119.90 |
| 1 | 1 | 3390 | G | N1-C6-O6 | 5.12 | 122.97 | 119.90 |
| 2 | 2 | 1490 | C | OP1-P-O3' | 5.12 | 116.45 | 105.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3 | 3 | 9 | C | C6-N1-C2 | 5.12 | 122.35 | 120.30 |
| 1 | 5 | 228 | U | C6-N1-C2 | -5.12 | 117.93 | 121.00 |
| 1 | 5 | 1851 | G | N7-C8-N9 | 5.12 | 115.66 | 113.10 |
| 1 | 1 | 3050 | U | N1-C2-O2 | 5.11 | 126.38 | 122.80 |
| 2 | 2 | 1286 | U | C6-N1-C1' | 5.11 | 128.36 | 121.20 |
| 1 | 5 | 1303 | A | C4-C5-N7 | 5.11 | 113.26 | 110.70 |
| 2 | 6 | 163 | G | N1-C2-N3 | 5.11 | 126.97 | 123.90 |
| 2 | 6 | 577 | G | N7-C8-N9 | 5.11 | 115.66 | 113.10 |
| 2 | 2 | 1473 | U | C5-C4-O4 | 5.11 | 128.97 | 125.90 |
| 1 | 5 | 2105 | G | C4-N9-C1' | -5.11 | 119.86 | 126.50 |
| 1 | 5 | 2225 | U | C6-N1-C2 | -5.11 | 117.93 | 121.00 |
| 1 | 1 | 2973 | G | C5-N7-C8 | 5.11 | 106.86 | 104.30 |
| 1 | 1 | 3128 | G | OP2-P-O3' | 5.11 | 116.44 | 105.20 |
| 1 | 1 | 3194 | C | C5-C6-N1 | 5.11 | 123.56 | 121.00 |
| 1 | 5 | 1931 | U | N3-C2-O2 | -5.11 | 118.62 | 122.20 |
| 2 | 6 | 238 | U | P-O3'-C3' | 5.11 | 125.83 | 119.70 |
| 1 | 1 | 3128 | G | N3-C4-C5 | -5.11 | 126.05 | 128.60 |
| 26 | E1 | 84 | VAL | C-N-CA | 5.11 | 134.47 | 121.70 |
| 1 | 1 | 1487 | G | C6-C5-N7 | -5.11 | 127.34 | 130.40 |
| 2 | 2 | 1726 | G | O5'-P-OP1 | -5.11 | 101.10 | 105.70 |
| 1 | 5 | 251 | G | N3-C4-C5 | -5.11 | 126.05 | 128.60 |
| 1 | 1 | 3109 | G | C5-C6-O6 | -5.11 | 125.54 | 128.60 |
| 1 | 5 | 1831 | U | OP2-P-O3' | 5.11 | 116.43 | 105.20 |
| 1 | 5 | 3320 | A | C8-N9-C4 | 5.11 | 107.84 | 105.80 |
| 1 | 1 | 3033 | A | C8-N9-C4 | -5.10 | 103.76 | 105.80 |
| 1 | 5 | 641 | C | C5-C6-N1 | 5.10 | 123.55 | 121.00 |
| 1 | 1 | 1157 | G | C5-C6-O6 | -5.10 | 125.54 | 128.60 |
| 1 | 1 | 1197 | A | N9-C4-C5 | -5.10 | 103.76 | 105.80 |
| 2 | 2 | 1150 | G | C3'-C2'-C1' | 5.10 | 105.58 | 101.50 |
| 2 | 2 | 1536 | G | C4-N9-C1' | 5.10 | 133.13 | 126.50 |
| 3 | 3 | 7 | G | N3-C4-C5 | -5.10 | 126.05 | 128.60 |
| 1 | 1 | 120 | G | N3-C4-N9 | 5.10 | 129.06 | 126.00 |
| 1 | 1 | 1178 | G | C5-C6-O6 | 5.10 | 131.66 | 128.60 |
| 2 | 2 | 1241 | G | O4'-C1'-N9 | 5.10 | 112.28 | 108.20 |
| 1 | 1 | 1086 | C | C5-C6-N1 | 5.10 | 123.55 | 121.00 |
| 1 | 1 | 2415 | C | N3-C4-C5 | 5.10 | 123.94 | 121.90 |
| 1 | 5 | 2971 | A | C8-N9-C4 | -5.10 | 103.76 | 105.80 |
| 1 | 1 | 2617 | U | N1-C2-N3 | 5.10 | 117.96 | 114.90 |
| 1 | 5 | 48 | A | N9-C4-C5 | 5.10 | 107.84 | 105.80 |
| 2 | 6 | 577 | G | C5-N7-C8 | -5.10 | 101.75 | 104.30 |
| 2 | 6 | 1187 | U | C6-N1-C2 | -5.10 | 117.94 | 121.00 |
| 4 | 8 | 2 | A | C8-N9-C4 | -5.10 | 103.76 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 1 | 2366 | C | C4-C5-C6 | -5.09 | 114.85 | 117.40 |
| 1 | 5 | 1775 | G | C4-C5-N7 | 5.09 | 112.84 | 110.80 |
| 1 | 5 | 1920 | U | C5-C4-O4 | 5.09 | 128.96 | 125.90 |
| 20 | d5 | 69 | LEU | CA-CB-CG | 5.09 | 127.02 | 115.30 |
| 69 | S1 | 73 | LEU | CA-CB-CG | 5.09 | 127.02 | 115.30 |
| 1 | 1 | 639 | G | C8-N9-C4 | 5.09 | 108.44 | 106.40 |
| 1 | 1 | 1888 | U | N1-C2-O2 | 5.09 | 126.36 | 122.80 |
| 1 | 1 | 1493 | G | C5-N7-C8 | 5.09 | 106.84 | 104.30 |
| 1 | 5 | 1594 | A | C8-N9-C4 | 5.09 | 107.84 | 105.80 |
| 1 | 5 | 2980 | U | C2-N1-C1' | 5.09 | 123.81 | 117.70 |
| 1 | 1 | 1496 | C | O5'-P-OP2 | -5.09 | 101.12 | 105.70 |
| 1 | 1 | 1554 | U | N3-C2-O2 | 5.09 | 125.76 | 122.20 |
| 1 | 1 | 2984 | C | C6-N1-C1' | 5.09 | 126.91 | 120.80 |
| 1 | 5 | 1450 | G | C4-C5-N7 | 5.09 | 112.84 | 110.80 |
| 1 | 5 | 2817 | A | C4-C5-N7 | 5.09 | 113.25 | 110.70 |
| 1 | 5 | 3043 | C | N3-C4-C5 | -5.09 | 119.86 | 121.90 |
| 2 | 6 | 864 | U | C2-N1-C1' | 5.09 | 123.81 | 117.70 |
| 2 | 6 | 1491 | U | N1-C2-O2 | 5.09 | 126.36 | 122.80 |
| 1 | 1 | 353 | G | N7-C8-N9 | -5.09 | 110.56 | 113.10 |
| 1 | 1 | 648 | C | N3-C4-C5 | -5.09 | 119.86 | 121.90 |
| 1 | 1 | 1145 | G | N1-C6-O6 | 5.09 | 122.95 | 119.90 |
| 1 | 5 | 511 | G | N3-C2-N2 | -5.09 | 116.34 | 119.90 |
| 1 | 5 | 2651 | G | C4-C5-N7 | 5.09 | 112.83 | 110.80 |
| 1 | 1 | 1075 | A | N1-C6-N6 | -5.09 | 115.55 | 118.60 |
| 1 | 1 | 1404 | G | C5-C6-O6 | -5.09 | 125.55 | 128.60 |
| 1 | 1 | 2137 | U | C2-N1-C1' | 5.09 | 123.80 | 117.70 |
| 1 | 5 | 1538 | G | C8-N9-C4 | -5.09 | 104.36 | 106.40 |
| 1 | 5 | 2651 | G | N9-C4-C5 | -5.09 | 103.36 | 105.40 |
| 1 | 5 | 3144 | G | C5-C6-O6 | -5.09 | 125.55 | 128.60 |
| 2 | 6 | 417 | A | N3-C4-C5 | -5.09 | 123.24 | 126.80 |
| 2 | 6 | 1246 | C | C2-N1-C1' | 5.09 | 124.39 | 118.80 |
| 1 | 1 | 1764 | U | C2-N1-C1' | 5.08 | 123.80 | 117.70 |
| 1 | 1 | 876 | A | C2-N3-C4 | -5.08 | 108.06 | 110.60 |
| 1 | 1 | 1801 | U | O5'-P-OP2 | -5.08 | 101.12 | 105.70 |
| 1 | 1 | 1908 | A | C8-N9-C4 | 5.08 | 107.83 | 105.80 |
| 1 | 5 | 2619 | G | C4-C5-N7 | 5.08 | 112.83 | 110.80 |
| 1 | 1 | 60 | A | C2-N3-C4 | -5.08 | 108.06 | 110.60 |
| 1 | 1 | 116 | A | N3-C4-C5 | -5.08 | 123.24 | 126.80 |
| 1 | 1 | 1556 | C | C2-N1-C1' | 5.08 | 124.39 | 118.80 |
| 1 | 1 | 1655 | G | N1-C2-N2 | -5.08 | 111.63 | 116.20 |
| 1 | 1 | 1720 | U | C6-N1-C2 | -5.08 | 117.95 | 121.00 |
| 1 | 1 | 3044 | G | OP2-P-O3' | 5.08 | 116.38 | 105.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 5 | 580 | C | N3-C4-C5 | 5.08 | 123.93 | 121.90 |
| 2 | 6 | 1286 | U | N3-C4-O4 | 5.08 | 122.96 | 119.40 |
| 2 | 2 | 1798 | U | C2-N1-C1' | 5.08 | 123.80 | 117.70 |
| 1 | 1 | 966 | U | C2-N1-C1' | 5.08 | 123.80 | 117.70 |
| 1 | 1 | 2633 | U | O5'-P-OP2 | 5.08 | 116.79 | 110.70 |
| 2 | 2 | 1573 | A | OP2-P-O3' | 5.08 | 116.37 | 105.20 |
| 1 | 5 | 1548 | C | C6-N1-C2 | -5.08 | 118.27 | 120.30 |
| 1 | 5 | 2617 | U | C6-N1-C2 | -5.08 | 117.95 | 121.00 |
| 1 | 5 | 3394 | U | C6-N1-C2 | 5.08 | 124.05 | 121.00 |
| 2 | 6 | 501 | U | C6-N1-C1' | -5.08 | 114.09 | 121.20 |
| 1 | 1 | 2507 | C | C6-N1-C2 | -5.08 | 118.27 | 120.30 |
| 1 | 1 | 2675 | C | C6-N1-C1' | -5.08 | 114.71 | 120.80 |
| 1 | 5 | 1588 | A | O5'-P-OP1 | -5.08 | 101.13 | 105.70 |
| 2 | 6 | 1114 | G | O4'-C1'-N9 | 5.08 | 112.26 | 108.20 |
| 1 | 1 | 336 | A | C4-C5-N7 | 5.08 | 113.24 | 110.70 |
| 1 | 1 | 1899 | G | O5'-P-OP1 | -5.08 | 101.13 | 105.70 |
| 2 | 2 | 111 | U | C2-N1-C1' | 5.08 | 123.79 | 117.70 |
| 2 | 2 | 380 | U | C2-N1-C1' | 5.08 | 123.79 | 117.70 |
| 2 | 2 | 453 | U | N3-C2-O2 | -5.08 | 118.65 | 122.20 |
| 1 | 5 | 2240 | G | N1-C6-O6 | 5.08 | 122.94 | 119.90 |
| 2 | 6 | 76 | A | P-O3'-C3' | 5.08 | 125.79 | 119.70 |
| 2 | 6 | 687 | G | N9-C4-C5 | 5.08 | 107.43 | 105.40 |
| 1 | 1 | 1024 | G | OP1-P-O3' | 5.07 | 116.36 | 105.20 |
| 2 | 6 | 1462 | G | N1-C6-O6 | -5.07 | 116.86 | 119.90 |
| 2 | 2 | 61 | A | C8-N9-C4 | -5.07 | 103.77 | 105.80 |
| 2 | 2 | 1560 | U | N1-C2-O2 | 5.07 | 126.35 | 122.80 |
| 1 | 1 | 666 | A | N7-C8-N9 | -5.07 | 111.27 | 113.80 |
| 1 | 1 | 2097 | U | C6-N1-C2 | -5.07 | 117.96 | 121.00 |
| 1 | 1 | 2623 | G | N1-C6-O6 | 5.07 | 122.94 | 119.90 |
| 1 | 1 | 3059 | G | C8-N9-C4 | 5.07 | 108.43 | 106.40 |
| 1 | 1 | 3158 | G | N1-C6-O6 | -5.07 | 116.86 | 119.90 |
| 2 | 2 | 1363 | U | C2-N1-C1' | 5.07 | 123.78 | 117.70 |
| 1 | 5 | 770 | G | C8-N9-C4 | -5.07 | 104.37 | 106.40 |
| 2 | 6 | 234 | G | N3-C4-N9 | 5.07 | 129.04 | 126.00 |
| 2 | 6 | 794 | U | N1-C2-N3 | -5.07 | 111.86 | 114.90 |
| 1 | 1 | 48 | A | N9-C4-C5 | 5.07 | 107.83 | 105.80 |
| 2 | 2 | 1 | U | OP2-P-O3' | 5.07 | 116.35 | 105.20 |
| 2 | 2 | 1414 | U | C6-N1-C2 | -5.07 | 117.96 | 121.00 |
| 2 | 2 | 1535 | U | O5'-P-OP1 | 5.07 | 116.78 | 110.70 |
| 1 | 5 | 1321 | G | N3-C4-C5 | 5.07 | 131.13 | 128.60 |
| 46 | n2 | 28 | PHE | C-N-CA | 5.07 | 134.37 | 121.70 |
| 2 | 2 | 553 | G | N1-C6-O6 | 5.07 | 122.94 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2 | 2 | 1082 | C | N1-C2-O2 | 5.07 | 121.94 | 118.90 |
| 4 | 8 | 112 | U | N1-C2-O2 | -5.07 | 119.25 | 122.80 |
| 4 | 8 | 126 | A | OP1-P-O3' | 5.07 | 116.34 | 105.20 |
| 2 | 2 | 1601 | G | O5'-P-OP2 | -5.06 | 101.14 | 105.70 |
| 1 | 1 | 798 | G | N7-C8-N9 | 5.06 | 115.63 | 113.10 |
| 1 | 1 | 1490 | A | C8-N9-C4 | 5.06 | 107.83 | 105.80 |
| 1 | 1 | 2381 | G | N9-C4-C5 | -5.06 | 103.38 | 105.40 |
| 4 | 4 | 134 | G | O5'-P-OP2 | 5.06 | 116.78 | 110.70 |
| 4 | 4 | 144 | G | C8-N9-C4 | 5.06 | 108.42 | 106.40 |
| 1 | 1 | 391 | A | N1-C6-N6 | 5.06 | 121.64 | 118.60 |
| 1 | 1 | 2943 | G | N7-C8-N9 | 5.06 | 115.63 | 113.10 |
| 2 | 6 | 806 | A | O5'-P-OP2 | -5.06 | 101.14 | 105.70 |
| 1 | 1 | 298 | U | C6-N1-C1' | -5.06 | 114.12 | 121.20 |
| 1 | 1 | 1118 | C | C6-N1-C2 | -5.06 | 118.28 | 120.30 |
| 1 | 1 | 2779 | A | C8-N9-C4 | 5.06 | 107.82 | 105.80 |
| 1 | 1 | 3290 | G | C8-N9-C4 | -5.06 | 104.38 | 106.40 |
| 4 | 4 | 2 | A | C2-N3-C4 | -5.06 | 108.07 | 110.60 |
| 4 | 4 | 81 | U | O4'-C1'-N1 | 5.06 | 112.25 | 108.20 |
| 1 | 5 | 2797 | C | C6-N1-C2 | 5.06 | 122.32 | 120.30 |
| 2 | 6 | 646 | C | C6-N1-C2 | -5.06 | 118.28 | 120.30 |
| 2 | 6 | 1060 | U | C6-N1-C2 | -5.06 | 117.96 | 121.00 |
| 1 | 1 | 611 | A | N1-C6-N6 | 5.06 | 121.64 | 118.60 |
| 1 | 1 | 1448 | U | C6-N1-C2 | 5.06 | 124.03 | 121.00 |
| 1 | 1 | 1663 | C | C5-C6-N1 | -5.06 | 118.47 | 121.00 |
| 1 | 1 | 2888 | U | C5-C4-O4 | -5.06 | 122.86 | 125.90 |
| 1 | 5 | 2288 | G | C4-N9-C1' | 5.06 | 133.07 | 126.50 |
| 2 | 6 | 453 | U | C6-N1-C1' | -5.06 | 114.12 | 121.20 |
| 1 | 1 | 591 | G | C4-C5-N7 | 5.06 | 112.82 | 110.80 |
| 1 | 1 | 1434 | G | C8-N9-C4 | 5.05 | 108.42 | 106.40 |
| 1 | 1 | 1446 | A | N9-C4-C5 | 5.05 | 107.82 | 105.80 |
| 4 | 4 | 54 | A | C4-C5-C6 | 5.05 | 119.53 | 117.00 |
| 1 | 5 | 770 | G | N9-C4-C5 | 5.05 | 107.42 | 105.40 |
| 1 | 5 | 1219 | C | N3-C2-O2 | -5.05 | 118.36 | 121.90 |
| 1 | 5 | 2160 | G | N9-C4-C5 | -5.05 | 103.38 | 105.40 |
| 4 | 8 | 84 | C | N3-C2-O2 | 5.05 | 125.44 | 121.90 |
| 1 | 1 | 1763 | U | N3-C2-O2 | -5.05 | 118.66 | 122.20 |
| 1 | 1 | 2735 | U | C5-C6-N1 | 5.05 | 125.23 | 122.70 |
| 1 | 1 | 3390 | G | C5-C6-O6 | -5.05 | 125.57 | 128.60 |
| 1 | 5 | 898 | U | C6-N1-C2 | -5.05 | 117.97 | 121.00 |
| 1 | 5 | 3124 | G | N9-C4-C5 | -5.05 | 103.38 | 105.40 |
| 1 | 5 | 3126 | C | O5'-P-OP2 | -5.05 | 101.15 | 105.70 |
| 1 | 1 | 2320 | A | C2-N3-C4 | -5.05 | 108.08 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 4 | 4 | 70 | G | C8-N9-C4 | 5.05 | 108.42 | 106.40 |
| 1 | 5 | 1863 | G | N3-C4-C5 | 5.05 | 131.12 | 128.60 |
| 1 | 5 | 2382 | G | N3-C4-C5 | 5.05 | 131.12 | 128.60 |
| 3 | 7 | 89 | G | N1-C6-O6 | 5.05 | 122.93 | 119.90 |
| 1 | 1 | 620 | U | C6-N1-C1' | 5.05 | 128.27 | 121.20 |
| 1 | 1 | 1340 | G | C8-N9-C4 | 5.05 | 108.42 | 106.40 |
| 1 | 1 | 1373 | A | OP2-P-O3' | 5.05 | 116.31 | 105.20 |
| 1 | 1 | 1531 | C | O5'-P-OP1 | 5.05 | 116.76 | 110.70 |
| 1 | 1 | 2381 | G | N1-C6-O6 | 5.05 | 122.93 | 119.90 |
| 1 | 1 | 2896 | A | C5-N7-C8 | -5.05 | 101.38 | 103.90 |
| 1 | 5 | 98 | G | C8-N9-C4 | 5.05 | 108.42 | 106.40 |
| 2 | 2 | 1610 | G | N3-C4-C5 | -5.05 | 126.08 | 128.60 |
| 1 | 5 | 934 | G | C6-C5-N7 | -5.05 | 127.37 | 130.40 |
| 1 | 5 | 1429 | G | N3-C4-N9 | 5.05 | 129.03 | 126.00 |
| 1 | 5 | 2811 | A | O5'-P-OP2 | -5.05 | 101.16 | 105.70 |
| 4 | 8 | 80 | A | C2-N3-C4 | 5.04 | 113.12 | 110.60 |
| 2 | 2 | 453 | U | C5-C6-N1 | 5.04 | 125.22 | 122.70 |
| 1 | 5 | 1442 | U | C5-C6-N1 | -5.04 | 120.18 | 122.70 |
| 2 | 6 | 1074 | G | C4-C5-N7 | 5.04 | 112.82 | 110.80 |
| 2 | 2 | 720 | G | P-O3'-C3' | 5.04 | 125.75 | 119.70 |
| 3 | 3 | 97 | A | N1-C6-N6 | 5.04 | 121.62 | 118.60 |
| 4 | 4 | 36 | G | N1-C6-O6 | 5.04 | 122.92 | 119.90 |
| 1 | 5 | 2421 | U | C5-C6-N1 | -5.04 | 120.18 | 122.70 |
| 1 | 1 | 2616 | C | N3-C2-O2 | 5.04 | 125.43 | 121.90 |
| 1 | 1 | 3242 | G | N1-C6-O6 | 5.04 | 122.92 | 119.90 |
| 2 | 2 | 188 | A | O5'-P-OP1 | -5.04 | 101.17 | 105.70 |
| 1 | 5 | 51 | A | C5-C6-N6 | -5.04 | 119.67 | 123.70 |
| 2 | 6 | 565 | C | C6-N1-C1' | -5.04 | 114.75 | 120.80 |
| 2 | 6 | 687 | G | N3-C4-N9 | -5.04 | 122.98 | 126.00 |
| 2 | 6 | 1524 | A | OP2-P-O3' | 5.04 | 116.28 | 105.20 |
| 1 | 1 | 2934 | A | N9-C4-C5 | -5.04 | 103.78 | 105.80 |
| 2 | 6 | 555 | A | P-O3'-C3' | 5.04 | 125.74 | 119.70 |
| 2 | 6 | 1340 | U | N3-C2-O2 | -5.04 | 118.67 | 122.20 |
| 1 | 1 | 55 | G | N1-C6-O6 | 5.04 | 122.92 | 119.90 |
| 1 | 1 | 2935 | U | C2-N1-C1' | 5.04 | 123.74 | 117.70 |
| 2 | 2 | 256 | A | C8-N9-C4 | -5.04 | 103.79 | 105.80 |
| 1 | 5 | 48 | A | N3-C4-N9 | -5.04 | 123.37 | 127.40 |
| 1 | 5 | 1770 | G | C4-N9-C1' | 5.04 | 133.05 | 126.50 |
| 2 | 6 | 1787 | C | C6-N1-C2 | 5.04 | 122.31 | 120.30 |
| 1 | 1 | 1365 | G | N3-C4-C5 | -5.03 | 126.08 | 128.60 |
| 1 | 1 | 1413 | G | C4-C5-N7 | 5.03 | 112.81 | 110.80 |
| 1 | 1 | 1892 | G | N3-C4-C5 | 5.03 | 131.12 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 1 | 2127 | U | N3-C2-O2 | 5.03 | 125.72 | 122.20 |
| 1 | 1 | 2943 | G | C4-C5-C6 | 5.03 | 121.82 | 118.80 |
| 1 | 1 | 3362 | A | C2-N3-C4 | -5.03 | 108.08 | 110.60 |
| 2 | 2 | 1051 | G | P-O3'-C3' | 5.03 | 125.74 | 119.70 |
| 2 | 6 | 194 | U | N3-C2-O2 | -5.03 | 118.68 | 122.20 |
| 1 | 5 | 2239 | G | N1-C6-O6 | 5.03 | 122.92 | 119.90 |
| 1 | 5 | 2862 | U | C5-C6-N1 | -5.03 | 120.18 | 122.70 |
| 1 | 1 | 619 | A | OP1-P-O3' | 5.03 | 116.27 | 105.20 |
| 1 | 1 | 2571 | U | C2-N1-C1' | 5.03 | 123.74 | 117.70 |
| 1 | 5 | 1303 | A | C5-C6-N6 | -5.03 | 119.67 | 123.70 |
| 1 | 5 | 1413 | G | C2-N3-C4 | -5.03 | 109.38 | 111.90 |
| 1 | 5 | 1795 | U | N1-C2-O2 | 5.03 | 126.32 | 122.80 |
| 1 | 5 | 2986 | U | C6-N1-C2 | -5.03 | 117.98 | 121.00 |
| 1 | 1 | 2833 | A | C5-C6-N1 | 5.03 | 120.21 | 117.70 |
| 1 | 5 | 916 | G | P-O3'-C3' | 5.03 | 125.73 | 119.70 |
| 1 | 5 | 1408 | G | N1-C6-O6 | 5.03 | 122.92 | 119.90 |
| 1 | 5 | 2427 | U | O5'-P-OP1 | 5.03 | 116.73 | 110.70 |
| 1 | 5 | 3049 | A | C5-C6-N6 | -5.03 | 119.68 | 123.70 |
| 1 | 1 | 544 | C | O4'-C1'-N1 | 5.03 | 112.22 | 108.20 |
| 1 | 1 | 639 | G | C5-C6-N1 | -5.03 | 108.99 | 111.50 |
| 1 | 1 | 1897 | G | C4-C5-N7 | 5.03 | 112.81 | 110.80 |
| 1 | 1 | 1911 | A | O5'-P-OP1 | -5.03 | 101.17 | 105.70 |
| 1 | 1 | 3056 | U | N1-C2-O2 | -5.03 | 119.28 | 122.80 |
| 2 | 2 | 23 | G | C8-N9-C4 | -5.03 | 104.39 | 106.40 |
| 1 | 5 | 934 | G | C8-N9-C1' | -5.03 | 120.46 | 127.00 |
| 1 | 5 | 2346 | C | N3-C2-O2 | 5.03 | 125.42 | 121.90 |
| 1 | 5 | 2620 | G | N3-C4-N9 | -5.03 | 122.98 | 126.00 |
| 1 | 1 | 1507 | G | O4'-C1'-N9 | -5.03 | 104.18 | 108.20 |
| 1 | 1 | 1607 | U | N3-C2-O2 | -5.03 | 118.68 | 122.20 |
| 2 | 2 | 139 | C | P-O3'-C3' | 5.03 | 125.73 | 119.70 |
| 2 | 2 | 187 | G | OP1-P-O3' | 5.03 | 116.26 | 105.20 |
| 2 | 2 | 913 | G | P-O3'-C3' | 5.03 | 125.73 | 119.70 |
| 1 | 5 | 412 | G | N3-C2-N2 | -5.03 | 116.38 | 119.90 |
| 1 | 1 | 1595 | U | C2-N1-C1' | -5.02 | 111.67 | 117.70 |
| 2 | 2 | 1559 | A | O4'-C1'-N9 | 5.02 | 112.22 | 108.20 |
| 1 | 5 | 200 | C | C5-C4-N4 | 5.02 | 123.72 | 120.20 |
| 1 | 5 | 278 | U | C6-N1-C2 | -5.02 | 117.98 | 121.00 |
| 1 | 5 | 515 | C | C6-N1-C2 | -5.02 | 118.29 | 120.30 |
| 1 | 5 | 2719 | U | N1-C2-O2 | -5.02 | 119.28 | 122.80 |
| 2 | 2 | 526 | A | C8-N9-C4 | -5.02 | 103.79 | 105.80 |
| 2 | 2 | 1398 | U | C6-N1-C2 | -5.02 | 117.99 | 121.00 |
| 1 | 5 | 2612 | U | N3-C4-C5 | -5.02 | 111.59 | 114.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2 | 6 | 972 | G | C5-C6-O6 | -5.02 | 125.59 | 128.60 |
| 2 | 6 | 1274 | C | N3-C2-O2 | -5.02 | 118.38 | 121.90 |
| 2 | 2 | 1596 | C | N1-C2-O2 | 5.02 | 121.91 | 118.90 |
| 1 | 1 | 2725 | U | C5-C6-N1 | -5.02 | 120.19 | 122.70 |
| 1 | 1 | 3159 | C | C2-N1-C1' | -5.02 | 113.28 | 118.80 |
| 2 | 2 | 1466 | G | C8-N9-C4 | 5.02 | 108.41 | 106.40 |
| 1 | 5 | 110 | G | C8-N9-C4 | 5.02 | 108.41 | 106.40 |
| 1 | 5 | 400 | G | N3-C4-C5 | -5.02 | 126.09 | 128.60 |
| 1 | 5 | 915 | A | N7-C8-N9 | 5.02 | 116.31 | 113.80 |
| 1 | 5 | 1105 | A | C8-N9-C4 | -5.02 | 103.79 | 105.80 |
| 1 | 5 | 2626 | A | N1-C6-N6 | 5.02 | 121.61 | 118.60 |
| 1 | 5 | 3275 | U | OP1-P-O3' | 5.02 | 116.24 | 105.20 |
| 2 | 6 | 1177 | C | C6-N1-C2 | 5.02 | 122.31 | 120.30 |
| 2 | 2 | 915 | A | OP1-P-OP2 | -5.02 | 112.08 | 119.60 |
| 1 | 5 | 1324 | U | C5-C6-N1 | -5.02 | 120.19 | 122.70 |
| 2 | 6 | 17 | C | C6-N1-C2 | -5.02 | 118.29 | 120.30 |
| 4 | 8 | 137 | C | C6-N1-C2 | 5.02 | 122.31 | 120.30 |
| 22 | D7 | 41 | LEU | CA-CB-CG | 5.02 | 126.84 | 115.30 |
| 1 | 1 | 2868 | U | C5-C6-N1 | 5.02 | 125.21 | 122.70 |
| 1 | 5 | 1911 | A | C4-C5-N7 | -5.02 | 108.19 | 110.70 |
| 1 | 1 | 1348 | U | N1-C2-O2 | 5.01 | 126.31 | 122.80 |
| 1 | 1 | 2362 | C | N3-C2-O2 | -5.01 | 118.39 | 121.90 |
| 1 | 1 | 2759 | U | C2-N1-C1' | 5.01 | 123.72 | 117.70 |
| 1 | 1 | 3142 | A | N3-C4-C5 | 5.01 | 130.31 | 126.80 |
| 1 | 1 | 3303 | G | N3-C4-C5 | 5.01 | 131.11 | 128.60 |
| 1 | 5 | 898 | U | C5-C6-N1 | 5.01 | 125.21 | 122.70 |
| 1 | 5 | 2978 | U | OP1-P-O3' | 5.01 | 116.23 | 105.20 |
| 1 | 1 | 2566 | C | N3-C4-C5 | -5.01 | 119.89 | 121.90 |
| 1 | 5 | 1391 | C | C5-C4-N4 | -5.01 | 116.69 | 120.20 |
| 1 | 5 | 1437 | C | N1-C2-O2 | -5.01 | 115.89 | 118.90 |
| 1 | 5 | 3180 | A | N1-C6-N6 | 5.01 | 121.61 | 118.60 |
| 1 | 1 | 1216 | C | C6-N1-C2 | 5.01 | 122.31 | 120.30 |
| 1 | 1 | 2366 | C | N3-C4-C5 | 5.01 | 123.90 | 121.90 |
| 1 | 1 | 3225 | C | C6-N1-C2 | -5.01 | 118.30 | 120.30 |
| 2 | 2 | 453 | U | N1-C2-O2 | 5.01 | 126.31 | 122.80 |
| 2 | 2 | 929 | A | N1-C6-N6 | -5.01 | 115.59 | 118.60 |
| 2 | 2 | 1000 | C | O4'-C1'-N1 | 5.01 | 112.21 | 108.20 |
| 2 | 2 | 1187 | U | C5-C4-O4 | 5.01 | 128.91 | 125.90 |
| 2 | 2 | 1604 | U | C6-N1-C2 | -5.01 | 117.99 | 121.00 |
| 1 | 5 | 1834 | U | C6-N1-C2 | -5.01 | 117.99 | 121.00 |
| 2 | 6 | 1200 | G | N3-C4-N9 | -5.01 | 122.99 | 126.00 |
| 1 | 1 | 435 | C | C6-N1-C2 | 5.01 | 122.30 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 1 | 2858 | U | C6-N1-C1' | 5.01 | 128.21 | 121.20 |
| 2 | 2 | 1215 | C | C6-N1-C2 | -5.01 | 118.30 | 120.30 |
| 1 | 5 | 2345 | A | N1-C6-N6 | 5.01 | 121.61 | 118.60 |
| 2 | 6 | 956 | C | C6-N1-C2 | -5.01 | 118.30 | 120.30 |
| 1 | 1 | 1382 | G | N9-C4-C5 | -5.01 | 103.40 | 105.40 |
| 1 | 1 | 2523 | A | C8-N9-C4 | 5.01 | 107.80 | 105.80 |
| 1 | 1 | 545 | U | C6-N1-C1' | -5.01 | 114.19 | 121.20 |
| 1 | 1 | 1578 | C | C6-N1-C1' | -5.01 | 114.79 | 120.80 |
| 1 | 1 | 2513 | U | OP1-P-O3' | 5.01 | 116.21 | 105.20 |
| 2 | 6 | 1052 | U | C6-N1-C2 | -5.01 | 118.00 | 121.00 |
| 1 | 1 | 3056 | U | C2-N1-C1' | -5.00 | 111.69 | 117.70 |
| 2 | 2 | 1610 | G | N3-C4-N9 | 5.00 | 129.00 | 126.00 |
| 2 | 2 | 1629 | G | N3-C4-C5 | -5.00 | 126.10 | 128.60 |
| 1 | 1 | 1853 | U | N3-C2-O2 | 5.00 | 125.70 | 122.20 |
| 2 | 2 | 1157 | A | N7-C8-N9 | 5.00 | 116.30 | 113.80 |
| 1 | 5 | 3048 | A | C8-N9-C4 | -5.00 | 103.80 | 105.80 |
| 2 | 6 | 773 | C | C6-N1-C2 | -5.00 | 118.30 | 120.30 |
| 3 | 7 | 29 | C | C6-N1-C2 | -5.00 | 118.30 | 120.30 |
| 1 | 1 | 1324 | U | O5'-P-OP1 | -5.00 | 101.20 | 105.70 |
| 1 | 1 | 1370 | G | C5-C6-O6 | -5.00 | 125.60 | 128.60 |
| 1 | 1 | 1544 | G | C4-C5-N7 | 5.00 | 112.80 | 110.80 |
| 1 | 1 | 1936 | A | C8-N9-C4 | 5.00 | 107.80 | 105.80 |
| 1 | 1 | 2351 | U | N3-C4-C5 | 5.00 | 117.60 | 114.60 |
| 2 | 2 | 364 | G | N9-C4-C5 | -5.00 | 103.40 | 105.40 |
| 1 | 5 | 2407 | C | C6-N1-C2 | -5.00 | 118.30 | 120.30 |
| 1 | 5 | 3137 | C | OP1-P-O3' | 5.00 | 116.20 | 105.20 |
| 1 | 5 | 3176 | G | C5-C6-N1 | -5.00 | 109.00 | 111.50 |
| 2 | 6 | 131 | C | N1-C2-O2 | 5.00 | 121.90 | 118.90 |
| 2 | 6 | 1721 | A | N1-C6-N6 | -5.00 | 115.60 | 118.60 |

There are no chirality outliers.

All (137) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 7 | C2 | 102 | GLY | Peptide |
| 7 | C2 | 88 | LEU | Peptide |
| 9 | C4 | 123 | SER | Peptide |
| 9 | C4 | 90 | ARG | Peptide |
| 10 | C5 | 124 | THR | Peptide |
| 11 | C6 | 113 | ASP | Peptide |
| 11 | C6 | 40 | GLU | Peptide |
| 12 | C7 | 22 | PRO | Peptide |

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| Mol | Chain | Res | Type | Group |
|------------|--------------|------------|-------------|--------------|
| 12 | C7 | 24 | LEU | Peptide |
| 12 | C7 | 85 | VAL | Peptide |
| 13 | C8 | 27 | LYS | Peptide |
| 17 | D2 | 54 | ASP | Peptide |
| 18 | D3 | 88 | PRO | Peptide |
| 19 | D4 | 46 | GLU | Peptide |
| 19 | D4 | 50 | ALA | Peptide |
| 20 | D5 | 54 | VAL | Peptide |
| 20 | D5 | 87 | GLY | Peptide |
| 20 | D5 | 94 | LYS | Peptide |
| 21 | D6 | 10 | ARG | Peptide |
| 21 | D6 | 74 | CYS | Peptide |
| 21 | D6 | 97 | PRO | Peptide |
| 22 | D7 | 50 | ALA | Peptide |
| 26 | E1 | 102 | VAL | Peptide |
| 26 | E1 | 138 | ARG | Peptide |
| 26 | E1 | 146 | SER | Peptide |
| 26 | E1 | 147 | VAL | Peptide |
| 28 | L3 | 290 | ASP | Peptide |
| 28 | L3 | 346 | THR | Peptide |
| 28 | L3 | 349 | LYS | Peptide |
| 29 | L4 | 182 | LEU | Peptide |
| 30 | L5 | 258 | LYS | Peptide |
| 33 | L8 | 30 | THR | Peptide |
| 34 | L9 | 49 | ASN | Peptide |
| 37 | M3 | 129 | ASN | Peptide |
| 40 | M6 | 110 | PRO | Peptide |
| 41 | M7 | 157 | VAL | Peptide |
| 41 | M7 | 158 | ALA | Peptide |
| 43 | M9 | 128 | LYS | Peptide |
| 44 | N0 | 12 | ARG | Peptide |
| 44 | N0 | 166 | LYS | Peptide |
| 44 | N0 | 22 | PRO | Peptide |
| 51 | N7 | 102 | GLU | Peptide |
| 51 | N7 | 124 | ALA | Peptide |
| 53 | N9 | 19 | ASN | Peptide |
| 55 | O1 | 83 | GLU | Peptide |
| 59 | O5 | 90 | ARG | Peptide |
| 60 | O6 | 27 | SER | Peptide |
| 66 | Q2 | 99 | GLN | Peptide |
| 68 | S0 | 188 | LEU | Peptide |
| 68 | S0 | 94 | GLY | Peptide |

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| Mol | Chain | Res | Type | Group |
|------------|--------------|------------|-------------|--------------|
| 69 | S1 | 131 | ASP | Peptide |
| 69 | S1 | 81 | PHE | Peptide |
| 70 | S2 | 106 | ASP | Peptide |
| 70 | S2 | 144 | TRP | Peptide |
| 71 | S3 | 221 | SER | Peptide |
| 72 | S4 | 193 | GLY | Peptide |
| 73 | S5 | 44 | ASN | Peptide |
| 73 | S5 | 56 | ALA | Peptide |
| 73 | S5 | 62 | VAL | Peptide |
| 73 | S5 | 65 | ARG | Peptide |
| 75 | S7 | 110 | GLN | Peptide |
| 75 | S7 | 131 | PHE | Peptide |
| 75 | S7 | 30 | SER | Peptide |
| 75 | S7 | 64 | VAL | Peptide |
| 78 | SM | 51 | ARG | Peptide |
| 79 | SR | 96 | THR | Peptide |
| 5 | c0 | 25 | LYS | Peptide |
| 7 | c2 | 102 | GLY | Peptide |
| 9 | c4 | 125 | SER | Peptide |
| 10 | c5 | 124 | THR | Peptide |
| 10 | c5 | 50 | THR | Peptide |
| 10 | c5 | 68 | PRO | Peptide |
| 11 | c6 | 40 | GLU | Peptide |
| 12 | c7 | 111 | LYS | Peptide |
| 12 | c7 | 112 | SER | Peptide |
| 12 | c7 | 94 | SER | Peptide |
| 13 | c8 | 90 | ASN | Peptide |
| 15 | d0 | 51 | VAL | Peptide |
| 15 | d0 | 70 | THR | Peptide |
| 15 | d0 | 96 | PRO | Peptide |
| 17 | d2 | 54 | ASP | Peptide |
| 20 | d5 | 69 | LEU | Peptide |
| 20 | d5 | 87 | GLY | Peptide |
| 24 | d9 | 17 | GLY | Peptide |
| 25 | e0 | 44 | PHE | Peptide |
| 26 | e1 | 135 | HIS | Peptide |
| 26 | e1 | 146 | SER | Peptide |
| 26 | e1 | 147 | VAL | Peptide |
| 26 | e1 | 82 | LYS | Peptide |
| 26 | e1 | 87 | THR | Peptide |
| 26 | e1 | 88 | PRO | Peptide |
| 27 | l2 | 143 | GLU | Peptide |

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| Mol | Chain | Res | Type | Group |
|------------|--------------|------------|-------------|--------------|
| 27 | l2 | 211 | HIS | Peptide |
| 27 | l2 | 213 | GLY | Peptide |
| 28 | l3 | 346 | THR | Peptide |
| 29 | l4 | 300 | ARG | Peptide |
| 29 | l4 | 339 | LEU | Peptide |
| 29 | l4 | 352 | ALA | Peptide |
| 30 | l5 | 270 | LYS | Peptide |
| 30 | l5 | 294 | ALA | Peptide |
| 31 | l6 | 67 | GLY | Peptide |
| 32 | l7 | 158 | LYS | Peptide |
| 32 | l7 | 226 | GLY | Peptide |
| 36 | m1 | 151 | SER | Peptide |
| 36 | m1 | 9 | MET | Peptide |
| 36 | m1 | 94 | ARG | Peptide |
| 37 | m3 | 141 | ALA | Peptide |
| 38 | m4 | 48 | GLY | Peptide |
| 39 | m5 | 184 | LYS | Peptide |
| 39 | m5 | 67 | ARG | Peptide |
| 44 | n0 | 133 | ALA | Peptide |
| 44 | n0 | 170 | THR | Peptide |
| 48 | n4 | 25 | ASP | Peptide |
| 50 | n6 | 75 | ARG | Peptide |
| 51 | n7 | 101 | PHE | Peptide |
| 53 | n9 | 19 | ASN | Peptide |
| 55 | o1 | 6 | ASP | Peptide |
| 55 | o1 | 82 | GLU | Peptide |
| 56 | o2 | 122 | PRO | Peptide |
| 58 | o4 | 80 | ARG | Peptide |
| 58 | o4 | 81 | CYS | Peptide |
| 67 | q3 | 49 | ARG | Peptide |
| 70 | s2 | 106 | ASP | Peptide |
| 70 | s2 | 144 | TRP | Peptide |
| 71 | s3 | 143 | ARG | Peptide |
| 71 | s3 | 215 | GLU | Peptide |
| 71 | s3 | 219 | ALA | Peptide |
| 71 | s3 | 221 | SER | Peptide |
| 73 | s5 | 44 | ASN | Peptide |
| 74 | s6 | 164 | LYS | Peptide |
| 75 | s7 | 115 | SER | Peptide |
| 75 | s7 | 130 | VAL | Peptide |
| 75 | s7 | 31 | SER | Peptide |
| 75 | s7 | 64 | VAL | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 77 | s9 | 88 | GLU | Peptide |
| 77 | s9 | 89 | ASP | Peptide |
| 77 | s9 | 90 | LYS | 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 | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 5 | C0 | 94/105 (90%) | 80 (85%) | 12 (13%) | 2 (2%) | 7 | 38 |
| 5 | c0 | 91/105 (87%) | 68 (75%) | 19 (21%) | 4 (4%) | 2 | 24 |
| 6 | C1 | 152/156 (97%) | 136 (90%) | 14 (9%) | 2 (1%) | 12 | 47 |
| 6 | c1 | 144/156 (92%) | 130 (90%) | 12 (8%) | 2 (1%) | 11 | 45 |
| 7 | C2 | 117/143 (82%) | 87 (74%) | 26 (22%) | 4 (3%) | 3 | 30 |
| 7 | c2 | 122/143 (85%) | 95 (78%) | 22 (18%) | 5 (4%) | 3 | 26 |
| 8 | C3 | 148/150 (99%) | 135 (91%) | 11 (7%) | 2 (1%) | 11 | 45 |
| 8 | c3 | 148/150 (99%) | 134 (90%) | 10 (7%) | 4 (3%) | 5 | 33 |
| 9 | C4 | 125/128 (98%) | 112 (90%) | 11 (9%) | 2 (2%) | 9 | 43 |
| 9 | c4 | 126/128 (98%) | 112 (89%) | 13 (10%) | 1 (1%) | 19 | 56 |
| 10 | C5 | 122/141 (86%) | 102 (84%) | 15 (12%) | 5 (4%) | 3 | 26 |
| 10 | c5 | 123/141 (87%) | 104 (85%) | 16 (13%) | 3 (2%) | 6 | 35 |
| 11 | C6 | 139/141 (99%) | 121 (87%) | 13 (9%) | 5 (4%) | 3 | 29 |
| 11 | c6 | 139/141 (99%) | 128 (92%) | 10 (7%) | 1 (1%) | 22 | 59 |
| 12 | C7 | 116/136 (85%) | 98 (84%) | 14 (12%) | 4 (3%) | 3 | 30 |
| 12 | c7 | 119/136 (88%) | 104 (87%) | 13 (11%) | 2 (2%) | 9 | 42 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 13 | C8 | 143/145 (99%) | 125 (87%) | 15 (10%) | 3 (2%) | 7 | 38 |
| 13 | c8 | 143/145 (99%) | 126 (88%) | 13 (9%) | 4 (3%) | 5 | 33 |
| 14 | C9 | 141/143 (99%) | 127 (90%) | 14 (10%) | 0 | 100 | 100 |
| 14 | c9 | 141/143 (99%) | 129 (92%) | 11 (8%) | 1 (1%) | 22 | 59 |
| 15 | D0 | 103/107 (96%) | 95 (92%) | 7 (7%) | 1 (1%) | 15 | 51 |
| 15 | d0 | 102/107 (95%) | 87 (85%) | 12 (12%) | 3 (3%) | 4 | 32 |
| 16 | D1 | 85/87 (98%) | 70 (82%) | 14 (16%) | 1 (1%) | 13 | 48 |
| 16 | d1 | 85/87 (98%) | 76 (89%) | 8 (9%) | 1 (1%) | 13 | 48 |
| 17 | D2 | 127/129 (98%) | 118 (93%) | 7 (6%) | 2 (2%) | 9 | 43 |
| 17 | d2 | 127/129 (98%) | 118 (93%) | 8 (6%) | 1 (1%) | 19 | 56 |
| 18 | D3 | 142/144 (99%) | 120 (84%) | 18 (13%) | 4 (3%) | 5 | 33 |
| 18 | d3 | 142/144 (99%) | 134 (94%) | 8 (6%) | 0 | 100 | 100 |
| 19 | D4 | 132/134 (98%) | 119 (90%) | 10 (8%) | 3 (2%) | 6 | 36 |
| 19 | d4 | 132/134 (98%) | 115 (87%) | 15 (11%) | 2 (2%) | 10 | 44 |
| 20 | D5 | 68/70 (97%) | 53 (78%) | 14 (21%) | 1 (2%) | 10 | 44 |
| 20 | d5 | 67/70 (96%) | 61 (91%) | 5 (8%) | 1 (2%) | 10 | 44 |
| 21 | D6 | 95/97 (98%) | 66 (70%) | 22 (23%) | 7 (7%) | 1 | 13 |
| 21 | d6 | 95/97 (98%) | 76 (80%) | 17 (18%) | 2 (2%) | 7 | 38 |
| 22 | D7 | 79/81 (98%) | 74 (94%) | 5 (6%) | 0 | 100 | 100 |
| 22 | d7 | 79/81 (98%) | 73 (92%) | 5 (6%) | 1 (1%) | 12 | 47 |
| 23 | D8 | 61/63 (97%) | 53 (87%) | 8 (13%) | 0 | 100 | 100 |
| 23 | d8 | 61/63 (97%) | 53 (87%) | 8 (13%) | 0 | 100 | 100 |
| 24 | D9 | 50/53 (94%) | 47 (94%) | 3 (6%) | 0 | 100 | 100 |
| 24 | d9 | 51/53 (96%) | 46 (90%) | 3 (6%) | 2 (4%) | 3 | 27 |
| 25 | E0 | 58/61 (95%) | 53 (91%) | 4 (7%) | 1 (2%) | 9 | 42 |
| 25 | e0 | 59/61 (97%) | 54 (92%) | 5 (8%) | 0 | 100 | 100 |
| 26 | E1 | 69/73 (94%) | 39 (56%) | 20 (29%) | 10 (14%) | 0 | 3 |
| 26 | e1 | 71/73 (97%) | 43 (61%) | 21 (30%) | 7 (10%) | 0 | 8 |
| 27 | L2 | 250/252 (99%) | 235 (94%) | 15 (6%) | 0 | 100 | 100 |
| 27 | l2 | 250/252 (99%) | 231 (92%) | 18 (7%) | 1 (0%) | 34 | 69 |
| 28 | L3 | 384/386 (100%) | 354 (92%) | 30 (8%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 28 | I3 | 384/386 (100%) | 367 (96%) | 15 (4%) | 2 (0%) | 29 | 66 |
| 29 | L4 | 359/361 (99%) | 321 (89%) | 36 (10%) | 2 (1%) | 25 | 62 |
| 29 | I4 | 359/361 (99%) | 328 (91%) | 27 (8%) | 4 (1%) | 14 | 50 |
| 30 | L5 | 294/296 (99%) | 261 (89%) | 28 (10%) | 5 (2%) | 9 | 42 |
| 30 | I5 | 292/296 (99%) | 280 (96%) | 11 (4%) | 1 (0%) | 41 | 74 |
| 31 | L6 | 153/176 (87%) | 144 (94%) | 5 (3%) | 4 (3%) | 5 | 34 |
| 31 | I6 | 153/176 (87%) | 139 (91%) | 12 (8%) | 2 (1%) | 12 | 47 |
| 32 | L7 | 220/223 (99%) | 206 (94%) | 13 (6%) | 1 (0%) | 29 | 66 |
| 32 | I7 | 221/223 (99%) | 206 (93%) | 11 (5%) | 4 (2%) | 8 | 41 |
| 33 | L8 | 231/233 (99%) | 208 (90%) | 19 (8%) | 4 (2%) | 9 | 42 |
| 33 | I8 | 229/233 (98%) | 201 (88%) | 26 (11%) | 2 (1%) | 17 | 54 |
| 34 | L9 | 189/191 (99%) | 176 (93%) | 12 (6%) | 1 (0%) | 29 | 66 |
| 34 | I9 | 189/191 (99%) | 173 (92%) | 15 (8%) | 1 (0%) | 29 | 66 |
| 35 | M0 | 207/221 (94%) | 195 (94%) | 11 (5%) | 1 (0%) | 29 | 66 |
| 35 | m0 | 205/221 (93%) | 192 (94%) | 12 (6%) | 1 (0%) | 29 | 66 |
| 36 | M1 | 167/169 (99%) | 142 (85%) | 23 (14%) | 2 (1%) | 13 | 48 |
| 36 | m1 | 167/169 (99%) | 147 (88%) | 12 (7%) | 8 (5%) | 2 | 22 |
| 37 | M3 | 191/194 (98%) | 171 (90%) | 18 (9%) | 2 (1%) | 15 | 51 |
| 37 | m3 | 192/194 (99%) | 167 (87%) | 22 (12%) | 3 (2%) | 9 | 43 |
| 38 | M4 | 134/137 (98%) | 124 (92%) | 8 (6%) | 2 (2%) | 10 | 44 |
| 38 | m4 | 135/137 (98%) | 132 (98%) | 3 (2%) | 0 | 100 | 100 |
| 39 | M5 | 201/203 (99%) | 185 (92%) | 14 (7%) | 2 (1%) | 15 | 51 |
| 39 | m5 | 201/203 (99%) | 191 (95%) | 8 (4%) | 2 (1%) | 15 | 51 |
| 40 | M6 | 195/197 (99%) | 187 (96%) | 6 (3%) | 2 (1%) | 15 | 51 |
| 40 | m6 | 195/197 (99%) | 188 (96%) | 7 (4%) | 0 | 100 | 100 |
| 41 | M7 | 181/184 (98%) | 171 (94%) | 9 (5%) | 1 (1%) | 25 | 62 |
| 41 | m7 | 181/184 (98%) | 171 (94%) | 9 (5%) | 1 (1%) | 25 | 62 |
| 42 | M8 | 183/185 (99%) | 171 (93%) | 12 (7%) | 0 | 100 | 100 |
| 42 | m8 | 183/185 (99%) | 172 (94%) | 11 (6%) | 0 | 100 | 100 |
| 43 | M9 | 186/188 (99%) | 177 (95%) | 8 (4%) | 1 (0%) | 29 | 66 |
| 43 | m9 | 182/188 (97%) | 177 (97%) | 4 (2%) | 1 (0%) | 29 | 66 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 44 | N0 | 170/172 (99%) | 157 (92%) | 11 (6%) | 2 (1%) | 13 | 48 |
| 44 | n0 | 169/172 (98%) | 166 (98%) | 3 (2%) | 0 | 100 | 100 |
| 45 | N1 | 157/159 (99%) | 146 (93%) | 10 (6%) | 1 (1%) | 25 | 62 |
| 45 | n1 | 157/159 (99%) | 150 (96%) | 6 (4%) | 1 (1%) | 25 | 62 |
| 46 | N2 | 98/100 (98%) | 87 (89%) | 10 (10%) | 1 (1%) | 15 | 51 |
| 46 | n2 | 96/100 (96%) | 89 (93%) | 7 (7%) | 0 | 100 | 100 |
| 47 | N3 | 134/136 (98%) | 129 (96%) | 5 (4%) | 0 | 100 | 100 |
| 47 | n3 | 133/136 (98%) | 130 (98%) | 2 (2%) | 1 (1%) | 19 | 56 |
| 48 | N4 | 128/155 (83%) | 116 (91%) | 12 (9%) | 0 | 100 | 100 |
| 48 | n4 | 128/155 (83%) | 115 (90%) | 10 (8%) | 3 (2%) | 6 | 36 |
| 49 | N5 | 119/121 (98%) | 113 (95%) | 5 (4%) | 1 (1%) | 19 | 56 |
| 49 | n5 | 118/121 (98%) | 106 (90%) | 10 (8%) | 2 (2%) | 9 | 42 |
| 50 | N6 | 124/126 (98%) | 118 (95%) | 6 (5%) | 0 | 100 | 100 |
| 50 | n6 | 120/126 (95%) | 116 (97%) | 4 (3%) | 0 | 100 | 100 |
| 51 | N7 | 133/135 (98%) | 122 (92%) | 9 (7%) | 2 (2%) | 10 | 44 |
| 51 | n7 | 133/135 (98%) | 114 (86%) | 16 (12%) | 3 (2%) | 6 | 36 |
| 52 | N8 | 146/148 (99%) | 132 (90%) | 13 (9%) | 1 (1%) | 22 | 59 |
| 52 | n8 | 146/148 (99%) | 133 (91%) | 10 (7%) | 3 (2%) | 7 | 38 |
| 53 | N9 | 56/58 (97%) | 52 (93%) | 4 (7%) | 0 | 100 | 100 |
| 53 | n9 | 54/58 (93%) | 46 (85%) | 7 (13%) | 1 (2%) | 8 | 40 |
| 54 | O0 | 95/100 (95%) | 90 (95%) | 5 (5%) | 0 | 100 | 100 |
| 54 | o0 | 98/100 (98%) | 92 (94%) | 6 (6%) | 0 | 100 | 100 |
| 55 | O1 | 107/109 (98%) | 100 (94%) | 4 (4%) | 3 (3%) | 5 | 33 |
| 55 | o1 | 107/109 (98%) | 99 (92%) | 4 (4%) | 4 (4%) | 3 | 28 |
| 56 | O2 | 125/127 (98%) | 116 (93%) | 8 (6%) | 1 (1%) | 19 | 56 |
| 56 | o2 | 125/127 (98%) | 115 (92%) | 9 (7%) | 1 (1%) | 19 | 56 |
| 57 | O3 | 104/106 (98%) | 100 (96%) | 4 (4%) | 0 | 100 | 100 |
| 57 | o3 | 104/106 (98%) | 97 (93%) | 6 (6%) | 1 (1%) | 15 | 51 |
| 58 | O4 | 110/112 (98%) | 105 (96%) | 5 (4%) | 0 | 100 | 100 |
| 58 | o4 | 110/112 (98%) | 104 (94%) | 5 (4%) | 1 (1%) | 17 | 54 |
| 59 | O5 | 117/119 (98%) | 105 (90%) | 11 (9%) | 1 (1%) | 17 | 54 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 59 | o5 | 117/119 (98%) | 106 (91%) | 10 (8%) | 1 (1%) | 17 | 54 |
| 60 | O6 | 97/99 (98%) | 84 (87%) | 12 (12%) | 1 (1%) | 15 | 51 |
| 60 | o6 | 97/99 (98%) | 89 (92%) | 5 (5%) | 3 (3%) | 4 | 32 |
| 61 | O7 | 85/87 (98%) | 78 (92%) | 7 (8%) | 0 | 100 | 100 |
| 61 | o7 | 81/87 (93%) | 74 (91%) | 7 (9%) | 0 | 100 | 100 |
| 62 | O8 | 75/77 (97%) | 69 (92%) | 6 (8%) | 0 | 100 | 100 |
| 62 | o8 | 75/77 (97%) | 68 (91%) | 6 (8%) | 1 (1%) | 12 | 47 |
| 63 | O9 | 48/50 (96%) | 44 (92%) | 3 (6%) | 1 (2%) | 7 | 38 |
| 63 | o9 | 48/50 (96%) | 47 (98%) | 1 (2%) | 0 | 100 | 100 |
| 64 | Q0 | 50/52 (96%) | 47 (94%) | 3 (6%) | 0 | 100 | 100 |
| 64 | q0 | 50/52 (96%) | 46 (92%) | 3 (6%) | 1 (2%) | 7 | 39 |
| 65 | Q1 | 23/25 (92%) | 23 (100%) | 0 | 0 | 100 | 100 |
| 65 | q1 | 23/25 (92%) | 23 (100%) | 0 | 0 | 100 | 100 |
| 66 | Q2 | 103/105 (98%) | 91 (88%) | 12 (12%) | 0 | 100 | 100 |
| 66 | q2 | 102/105 (97%) | 97 (95%) | 5 (5%) | 0 | 100 | 100 |
| 67 | Q3 | 89/91 (98%) | 82 (92%) | 6 (7%) | 1 (1%) | 14 | 50 |
| 67 | q3 | 89/91 (98%) | 81 (91%) | 8 (9%) | 0 | 100 | 100 |
| 68 | S0 | 204/206 (99%) | 172 (84%) | 27 (13%) | 5 (2%) | 5 | 35 |
| 68 | s0 | 204/206 (99%) | 176 (86%) | 21 (10%) | 7 (3%) | 3 | 30 |
| 69 | S1 | 212/216 (98%) | 167 (79%) | 42 (20%) | 3 (1%) | 11 | 45 |
| 69 | s1 | 214/216 (99%) | 190 (89%) | 19 (9%) | 5 (2%) | 6 | 36 |
| 70 | S2 | 215/217 (99%) | 192 (89%) | 19 (9%) | 4 (2%) | 8 | 40 |
| 70 | s2 | 215/217 (99%) | 203 (94%) | 11 (5%) | 1 (0%) | 29 | 66 |
| 71 | S3 | 221/223 (99%) | 201 (91%) | 15 (7%) | 5 (2%) | 6 | 36 |
| 71 | s3 | 221/223 (99%) | 198 (90%) | 15 (7%) | 8 (4%) | 3 | 29 |
| 72 | S4 | 258/260 (99%) | 233 (90%) | 23 (9%) | 2 (1%) | 19 | 56 |
| 72 | s4 | 258/260 (99%) | 232 (90%) | 24 (9%) | 2 (1%) | 19 | 56 |
| 73 | S5 | 204/206 (99%) | 175 (86%) | 26 (13%) | 3 (2%) | 10 | 44 |
| 73 | s5 | 204/206 (99%) | 181 (89%) | 20 (10%) | 3 (2%) | 10 | 44 |
| 74 | S6 | 224/236 (95%) | 208 (93%) | 9 (4%) | 7 (3%) | 4 | 32 |
| 74 | s6 | 216/236 (92%) | 198 (92%) | 15 (7%) | 3 (1%) | 11 | 45 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|-----------|----------|-------------|-----|
| 75 | S7 | 182/184 (99%) | 151 (83%) | 24 (13%) | 7 (4%) | 3 | 27 |
| 75 | s7 | 182/184 (99%) | 153 (84%) | 25 (14%) | 4 (2%) | 6 | 37 |
| 76 | S8 | 184/200 (92%) | 160 (87%) | 22 (12%) | 2 (1%) | 14 | 50 |
| 76 | s8 | 181/200 (90%) | 171 (94%) | 8 (4%) | 2 (1%) | 14 | 50 |
| 77 | S9 | 183/185 (99%) | 159 (87%) | 22 (12%) | 2 (1%) | 14 | 50 |
| 77 | s9 | 183/185 (99%) | 169 (92%) | 13 (7%) | 1 (0%) | 29 | 66 |
| 78 | SM | 155/272 (57%) | 125 (81%) | 27 (17%) | 3 (2%) | 8 | 40 |
| 78 | sM | 125/272 (46%) | 105 (84%) | 17 (14%) | 3 (2%) | 6 | 35 |
| 79 | SR | 316/318 (99%) | 293 (93%) | 23 (7%) | 0 | 100 | 100 |
| 79 | sR | 314/318 (99%) | 290 (92%) | 24 (8%) | 0 | 100 | 100 |
| All | All | 22224/23150 (96%) | 20097 (90%) | 1833 (8%) | 294 (1%) | 12 | 47 |

All (294) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | C0 | 88 | PRO |
| 7 | c2 | 91 | VAL |
| 10 | c5 | 11 | VAL |
| 10 | c5 | 126 | VAL |
| 11 | C6 | 58 | ASP |
| 11 | C6 | 59 | LYS |
| 11 | c6 | 116 | LEU |
| 13 | C8 | 28 | ILE |
| 13 | C8 | 92 | ILE |
| 13 | c8 | 91 | ASP |
| 14 | c9 | 34 | VAL |
| 17 | d2 | 6 | VAL |
| 17 | D2 | 83 | ILE |
| 18 | D3 | 97 | ASP |
| 22 | d7 | 62 | ILE |
| 26 | e1 | 102 | VAL |
| 31 | l6 | 98 | VAL |
| 31 | L6 | 98 | VAL |
| 33 | L8 | 36 | ILE |
| 34 | L9 | 50 | ASN |
| 36 | m1 | 10 | ARG |
| 36 | m1 | 95 | ASN |
| 36 | m1 | 115 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 38 | M4 | 8 | LYS |
| 39 | m5 | 184 | LYS |
| 53 | n9 | 21 | ILE |
| 60 | o6 | 33 | ALA |
| 69 | s1 | 210 | ILE |
| 71 | S3 | 220 | PRO |
| 71 | s3 | 220 | PRO |
| 74 | S6 | 149 | LYS |
| 74 | S6 | 153 | VAL |
| 74 | S6 | 154 | ARG |
| 75 | s7 | 65 | PRO |
| 75 | S7 | 111 | LYS |
| 78 | SM | 171 | PRO |
| 5 | c0 | 82 | LEU |
| 5 | c0 | 92 | ILE |
| 6 | C1 | 8 | GLN |
| 6 | c1 | 7 | VAL |
| 6 | c1 | 133 | LYS |
| 7 | C2 | 91 | VAL |
| 7 | c2 | 63 | VAL |
| 8 | c3 | 66 | ILE |
| 11 | C6 | 39 | VAL |
| 11 | C6 | 138 | PHE |
| 12 | C7 | 88 | VAL |
| 12 | c7 | 88 | VAL |
| 18 | D3 | 89 | ASN |
| 19 | d4 | 52 | LYS |
| 19 | d4 | 123 | LYS |
| 19 | D4 | 4 | ALA |
| 21 | D6 | 45 | VAL |
| 21 | D6 | 46 | GLU |
| 21 | D6 | 75 | VAL |
| 26 | e1 | 98 | VAL |
| 26 | E1 | 84 | VAL |
| 26 | E1 | 98 | VAL |
| 26 | E1 | 103 | LEU |
| 26 | E1 | 128 | ALA |
| 30 | L5 | 276 | LYS |
| 31 | L6 | 5 | LYS |
| 33 | L8 | 37 | GLY |
| 36 | M1 | 165 | GLN |
| 40 | M6 | 111 | PRO |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 43 | M9 | 131 | ALA |
| 45 | N1 | 124 | VAL |
| 48 | n4 | 76 | VAL |
| 51 | n7 | 17 | ARG |
| 51 | n7 | 130 | PHE |
| 51 | N7 | 17 | ARG |
| 55 | o1 | 7 | VAL |
| 60 | o6 | 34 | SER |
| 60 | o6 | 63 | ASN |
| 68 | s0 | 30 | GLN |
| 71 | s3 | 217 | ILE |
| 71 | s3 | 221 | SER |
| 73 | S5 | 58 | LEU |
| 74 | s6 | 153 | VAL |
| 75 | s7 | 64 | VAL |
| 75 | S7 | 112 | ARG |
| 75 | S7 | 133 | THR |
| 75 | S7 | 134 | GLU |
| 78 | sM | 66 | ALA |
| 7 | C2 | 54 | ARG |
| 7 | C2 | 89 | ILE |
| 7 | c2 | 119 | SER |
| 8 | C3 | 28 | LEU |
| 9 | C4 | 124 | ASP |
| 10 | C5 | 81 | ARG |
| 13 | c8 | 26 | ILE |
| 15 | D0 | 18 | GLN |
| 18 | D3 | 114 | LYS |
| 19 | D4 | 5 | VAL |
| 24 | d9 | 7 | TRP |
| 24 | d9 | 19 | ARG |
| 26 | e1 | 88 | PRO |
| 26 | E1 | 102 | VAL |
| 26 | E1 | 137 | ASP |
| 26 | E1 | 148 | TYR |
| 28 | l3 | 129 | ALA |
| 30 | L5 | 20 | PHE |
| 30 | L5 | 261 | THR |
| 31 | L6 | 6 | ALA |
| 32 | l7 | 229 | PHE |
| 35 | m0 | 175 | ASN |
| 36 | m1 | 11 | ASP |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 44 | N0 | 13 | ARG |
| 47 | n3 | 42 | SER |
| 49 | N5 | 24 | LEU |
| 51 | n7 | 129 | TRP |
| 55 | o1 | 83 | GLU |
| 55 | O1 | 82 | GLU |
| 55 | O1 | 83 | GLU |
| 59 | o5 | 40 | SER |
| 59 | O5 | 91 | ALA |
| 62 | o8 | 17 | ARG |
| 63 | O9 | 4 | GLN |
| 68 | s0 | 29 | VAL |
| 69 | S1 | 63 | GLY |
| 69 | s1 | 179 | SER |
| 70 | S2 | 146 | THR |
| 71 | S3 | 221 | SER |
| 71 | s3 | 44 | THR |
| 71 | s3 | 91 | VAL |
| 71 | s3 | 115 | ILE |
| 72 | s4 | 196 | VAL |
| 73 | S5 | 64 | VAL |
| 74 | S6 | 173 | PRO |
| 74 | S6 | 174 | LYS |
| 74 | s6 | 70 | PRO |
| 75 | s7 | 116 | ARG |
| 5 | C0 | 87 | VAL |
| 7 | C2 | 106 | ILE |
| 7 | c2 | 106 | ILE |
| 10 | C5 | 18 | ARG |
| 12 | C7 | 85 | VAL |
| 12 | C7 | 86 | PRO |
| 12 | C7 | 124 | VAL |
| 13 | c8 | 92 | ILE |
| 15 | d0 | 97 | VAL |
| 16 | D1 | 82 | VAL |
| 18 | D3 | 96 | VAL |
| 20 | d5 | 104 | ALA |
| 21 | d6 | 62 | TYR |
| 26 | e1 | 87 | THR |
| 26 | e1 | 136 | LYS |
| 26 | e1 | 148 | TYR |
| 26 | E1 | 86 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 26 | E1 | 104 | SER |
| 29 | l4 | 329 | PRO |
| 29 | l4 | 341 | SER |
| 29 | L4 | 317 | PRO |
| 30 | L5 | 259 | LYS |
| 32 | l7 | 158 | LYS |
| 32 | l7 | 228 | SER |
| 37 | M3 | 77 | LEU |
| 39 | m5 | 183 | THR |
| 39 | M5 | 74 | PRO |
| 40 | M6 | 110 | PRO |
| 41 | m7 | 158 | ALA |
| 48 | n4 | 63 | ILE |
| 49 | n5 | 47 | ALA |
| 58 | o4 | 83 | ASN |
| 68 | S0 | 191 | ARG |
| 69 | s1 | 209 | ASN |
| 70 | S2 | 109 | GLY |
| 71 | S3 | 217 | ILE |
| 71 | s3 | 45 | LYS |
| 73 | s5 | 58 | LEU |
| 73 | s5 | 184 | PHE |
| 76 | S8 | 152 | ILE |
| 78 | sM | 87 | THR |
| 78 | SM | 87 | THR |
| 5 | c0 | 83 | PRO |
| 6 | C1 | 7 | VAL |
| 8 | c3 | 87 | ASP |
| 9 | c4 | 132 | ARG |
| 10 | C5 | 125 | PRO |
| 10 | c5 | 125 | PRO |
| 11 | C6 | 114 | ARG |
| 12 | c7 | 103 | ASP |
| 15 | d0 | 51 | VAL |
| 17 | D2 | 31 | SER |
| 28 | l3 | 187 | SER |
| 29 | l4 | 24 | ALA |
| 29 | l4 | 342 | LYS |
| 32 | l7 | 191 | VAL |
| 32 | L7 | 164 | SER |
| 33 | l8 | 203 | VAL |
| 33 | L8 | 31 | PRO |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | m1 | 8 | PRO |
| 36 | m1 | 12 | LEU |
| 36 | m1 | 94 | ARG |
| 37 | m3 | 140 | SER |
| 41 | M7 | 158 | ALA |
| 43 | m9 | 35 | ALA |
| 44 | N0 | 167 | ARG |
| 48 | n4 | 25 | ASP |
| 49 | n5 | 136 | ALA |
| 52 | n8 | 48 | TYR |
| 52 | n8 | 78 | LEU |
| 52 | N8 | 48 | TYR |
| 55 | o1 | 42 | LEU |
| 57 | o3 | 61 | GLY |
| 64 | q0 | 78 | ILE |
| 67 | Q3 | 58 | SER |
| 68 | S0 | 95 | ALA |
| 68 | s0 | 103 | THR |
| 68 | s0 | 206 | ASP |
| 69 | s1 | 62 | LYS |
| 69 | s1 | 82 | ARG |
| 70 | S2 | 148 | LEU |
| 70 | s2 | 106 | ASP |
| 71 | S3 | 212 | LYS |
| 71 | s3 | 216 | PRO |
| 72 | S4 | 196 | VAL |
| 73 | S5 | 51 | VAL |
| 75 | s7 | 11 | GLN |
| 75 | S7 | 131 | PHE |
| 77 | S9 | 100 | LYS |
| 77 | S9 | 134 | ILE |
| 77 | s9 | 134 | ILE |
| 78 | sM | 48 | ARG |
| 8 | C3 | 22 | ALA |
| 10 | C5 | 126 | VAL |
| 21 | D6 | 64 | LEU |
| 25 | E0 | 47 | VAL |
| 30 | L5 | 116 | ASP |
| 33 | L8 | 157 | VAL |
| 34 | l9 | 144 | ILE |
| 36 | M1 | 114 | ILE |
| 37 | m3 | 141 | ALA |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 37 | M3 | 47 | ALA |
| 39 | M5 | 75 | VAL |
| 45 | n1 | 136 | ARG |
| 51 | N7 | 103 | GLN |
| 52 | n8 | 47 | LYS |
| 55 | O1 | 7 | VAL |
| 56 | O2 | 12 | LYS |
| 68 | s0 | 189 | VAL |
| 69 | S1 | 130 | SER |
| 74 | S6 | 70 | PRO |
| 75 | S7 | 132 | PRO |
| 76 | S8 | 9 | HIS |
| 78 | SM | 12 | VAL |
| 5 | c0 | 35 | ILE |
| 9 | C4 | 42 | VAL |
| 10 | C5 | 53 | PRO |
| 15 | d0 | 118 | VAL |
| 26 | e1 | 84 | VAL |
| 26 | E1 | 87 | THR |
| 31 | L6 | 140 | VAL |
| 68 | S0 | 103 | THR |
| 68 | S0 | 158 | VAL |
| 70 | S2 | 150 | GLN |
| 71 | S3 | 211 | PRO |
| 72 | S4 | 195 | ILE |
| 74 | S6 | 69 | LEU |
| 74 | s6 | 69 | LEU |
| 8 | c3 | 22 | ALA |
| 16 | d1 | 6 | GLY |
| 21 | D6 | 86 | VAL |
| 36 | m1 | 114 | ILE |
| 55 | o1 | 33 | VAL |
| 56 | o2 | 6 | HIS |
| 68 | S0 | 64 | ILE |
| 68 | s0 | 158 | VAL |
| 68 | s0 | 194 | PRO |
| 76 | s8 | 101 | ILE |
| 7 | c2 | 66 | VAL |
| 13 | C8 | 14 | ILE |
| 19 | D4 | 35 | VAL |
| 20 | D5 | 41 | ILE |
| 21 | d6 | 59 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21 | D6 | 36 | ILE |
| 27 | l2 | 56 | ALA |
| 35 | M0 | 70 | ILE |
| 37 | m3 | 47 | ALA |
| 46 | N2 | 11 | ILE |
| 69 | S1 | 210 | ILE |
| 72 | s4 | 90 | ILE |
| 76 | s8 | 78 | ILE |
| 13 | c8 | 14 | ILE |
| 21 | D6 | 19 | LYS |
| 29 | L4 | 131 | VAL |
| 30 | l5 | 125 | VAL |
| 31 | l6 | 10 | TYR |
| 33 | l8 | 237 | ILE |
| 38 | M4 | 6 | ILE |
| 60 | O6 | 9 | ILE |
| 75 | S7 | 98 | ILE |
| 8 | c3 | 60 | VAL |
| 73 | s5 | 29 | ILE |

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 | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 5 | C0 | 77/98 (79%) | 63 (82%) | 14 (18%) | 1 | 11 |
| 5 | c0 | 73/98 (74%) | 57 (78%) | 16 (22%) | 1 | 6 |
| 6 | C1 | 128/137 (93%) | 110 (86%) | 18 (14%) | 3 | 20 |
| 6 | c1 | 129/137 (94%) | 101 (78%) | 28 (22%) | 1 | 7 |
| 7 | C2 | 88/119 (74%) | 61 (69%) | 27 (31%) | 0 | 2 |
| 7 | c2 | 88/119 (74%) | 62 (70%) | 26 (30%) | 0 | 2 |
| 8 | C3 | 127/127 (100%) | 103 (81%) | 24 (19%) | 1 | 9 |
| 8 | c3 | 127/127 (100%) | 105 (83%) | 22 (17%) | 2 | 12 |
| 9 | C4 | 81/97 (84%) | 59 (73%) | 22 (27%) | 0 | 3 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 9 | c4 | 97/97 (100%) | 77 (79%) | 20 (21%) | 1 | 7 |
| 10 | C5 | 101/117 (86%) | 82 (81%) | 19 (19%) | 1 | 10 |
| 10 | c5 | 102/117 (87%) | 85 (83%) | 17 (17%) | 2 | 14 |
| 11 | C6 | 117/117 (100%) | 94 (80%) | 23 (20%) | 1 | 8 |
| 11 | c6 | 117/117 (100%) | 90 (77%) | 27 (23%) | 1 | 6 |
| 12 | C7 | 94/124 (76%) | 75 (80%) | 19 (20%) | 1 | 8 |
| 12 | c7 | 92/124 (74%) | 78 (85%) | 14 (15%) | 3 | 17 |
| 13 | C8 | 128/128 (100%) | 96 (75%) | 32 (25%) | 0 | 4 |
| 13 | c8 | 128/128 (100%) | 104 (81%) | 24 (19%) | 1 | 10 |
| 14 | C9 | 115/115 (100%) | 97 (84%) | 18 (16%) | 2 | 16 |
| 14 | c9 | 115/115 (100%) | 94 (82%) | 21 (18%) | 1 | 10 |
| 15 | D0 | 98/100 (98%) | 75 (76%) | 23 (24%) | 1 | 5 |
| 15 | d0 | 97/100 (97%) | 75 (77%) | 22 (23%) | 1 | 6 |
| 16 | D1 | 74/74 (100%) | 63 (85%) | 11 (15%) | 3 | 18 |
| 16 | d1 | 74/74 (100%) | 64 (86%) | 10 (14%) | 4 | 21 |
| 17 | D2 | 110/110 (100%) | 92 (84%) | 18 (16%) | 2 | 15 |
| 17 | d2 | 110/110 (100%) | 97 (88%) | 13 (12%) | 5 | 26 |
| 18 | D3 | 119/119 (100%) | 100 (84%) | 19 (16%) | 2 | 15 |
| 18 | d3 | 119/119 (100%) | 102 (86%) | 17 (14%) | 3 | 19 |
| 19 | D4 | 112/112 (100%) | 90 (80%) | 22 (20%) | 1 | 9 |
| 19 | d4 | 112/112 (100%) | 93 (83%) | 19 (17%) | 2 | 13 |
| 20 | D5 | 61/61 (100%) | 45 (74%) | 16 (26%) | 0 | 4 |
| 20 | d5 | 61/61 (100%) | 47 (77%) | 14 (23%) | 1 | 6 |
| 21 | D6 | 83/83 (100%) | 63 (76%) | 20 (24%) | 0 | 5 |
| 21 | d6 | 83/83 (100%) | 68 (82%) | 15 (18%) | 1 | 11 |
| 22 | D7 | 70/70 (100%) | 59 (84%) | 11 (16%) | 2 | 16 |
| 22 | d7 | 70/70 (100%) | 59 (84%) | 11 (16%) | 2 | 16 |
| 23 | D8 | 56/56 (100%) | 41 (73%) | 15 (27%) | 0 | 3 |
| 23 | d8 | 56/56 (100%) | 40 (71%) | 16 (29%) | 0 | 2 |
| 24 | D9 | 46/47 (98%) | 39 (85%) | 7 (15%) | 3 | 17 |
| 24 | d9 | 47/47 (100%) | 40 (85%) | 7 (15%) | 3 | 18 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 25 | E0 | 51/52 (98%) | 42 (82%) | 9 (18%) | 2 | 12 |
| 25 | e0 | 52/52 (100%) | 43 (83%) | 9 (17%) | 2 | 12 |
| 26 | E1 | 62/64 (97%) | 46 (74%) | 16 (26%) | 0 | 4 |
| 26 | e1 | 64/64 (100%) | 48 (75%) | 16 (25%) | 0 | 4 |
| 27 | L2 | 193/194 (100%) | 163 (84%) | 30 (16%) | 2 | 17 |
| 27 | l2 | 192/194 (99%) | 157 (82%) | 35 (18%) | 1 | 11 |
| 28 | L3 | 320/322 (99%) | 264 (82%) | 56 (18%) | 2 | 12 |
| 28 | l3 | 319/322 (99%) | 260 (82%) | 59 (18%) | 1 | 10 |
| 29 | L4 | 288/288 (100%) | 239 (83%) | 49 (17%) | 2 | 13 |
| 29 | l4 | 288/288 (100%) | 237 (82%) | 51 (18%) | 2 | 12 |
| 30 | L5 | 244/244 (100%) | 196 (80%) | 48 (20%) | 1 | 8 |
| 30 | l5 | 243/244 (100%) | 212 (87%) | 31 (13%) | 4 | 23 |
| 31 | L6 | 135/153 (88%) | 114 (84%) | 21 (16%) | 2 | 17 |
| 31 | l6 | 135/153 (88%) | 118 (87%) | 17 (13%) | 4 | 23 |
| 32 | L7 | 186/187 (100%) | 168 (90%) | 18 (10%) | 8 | 33 |
| 32 | l7 | 187/187 (100%) | 163 (87%) | 24 (13%) | 4 | 23 |
| 33 | L8 | 187/191 (98%) | 160 (86%) | 27 (14%) | 3 | 19 |
| 33 | l8 | 178/191 (93%) | 150 (84%) | 28 (16%) | 2 | 16 |
| 34 | L9 | 171/171 (100%) | 132 (77%) | 39 (23%) | 1 | 6 |
| 34 | l9 | 171/171 (100%) | 134 (78%) | 37 (22%) | 1 | 7 |
| 35 | M0 | 177/187 (95%) | 154 (87%) | 23 (13%) | 4 | 22 |
| 35 | m0 | 177/187 (95%) | 149 (84%) | 28 (16%) | 2 | 16 |
| 36 | M1 | 147/147 (100%) | 124 (84%) | 23 (16%) | 2 | 17 |
| 36 | m1 | 147/147 (100%) | 124 (84%) | 23 (16%) | 2 | 17 |
| 37 | M3 | 154/154 (100%) | 122 (79%) | 32 (21%) | 1 | 7 |
| 37 | m3 | 154/154 (100%) | 129 (84%) | 25 (16%) | 2 | 15 |
| 38 | M4 | 107/108 (99%) | 93 (87%) | 14 (13%) | 4 | 22 |
| 38 | m4 | 108/108 (100%) | 94 (87%) | 14 (13%) | 4 | 22 |
| 39 | M5 | 175/175 (100%) | 154 (88%) | 21 (12%) | 5 | 25 |
| 39 | m5 | 175/175 (100%) | 148 (85%) | 27 (15%) | 2 | 17 |
| 40 | M6 | 160/160 (100%) | 137 (86%) | 23 (14%) | 3 | 19 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 40 | m6 | 160/160 (100%) | 138 (86%) | 22 (14%) | 3 | 21 |
| 41 | M7 | 140/146 (96%) | 111 (79%) | 29 (21%) | 1 | 7 |
| 41 | m7 | 140/146 (96%) | 115 (82%) | 25 (18%) | 2 | 11 |
| 42 | M8 | 150/150 (100%) | 127 (85%) | 23 (15%) | 2 | 17 |
| 42 | m8 | 150/150 (100%) | 132 (88%) | 18 (12%) | 5 | 25 |
| 43 | M9 | 153/153 (100%) | 132 (86%) | 21 (14%) | 3 | 21 |
| 43 | m9 | 150/153 (98%) | 123 (82%) | 27 (18%) | 1 | 11 |
| 44 | N0 | 156/156 (100%) | 127 (81%) | 29 (19%) | 1 | 10 |
| 44 | n0 | 155/156 (99%) | 132 (85%) | 23 (15%) | 3 | 18 |
| 45 | N1 | 136/136 (100%) | 101 (74%) | 35 (26%) | 0 | 4 |
| 45 | n1 | 136/136 (100%) | 113 (83%) | 23 (17%) | 2 | 13 |
| 46 | N2 | 87/87 (100%) | 70 (80%) | 17 (20%) | 1 | 9 |
| 46 | n2 | 85/87 (98%) | 68 (80%) | 17 (20%) | 1 | 8 |
| 47 | N3 | 104/104 (100%) | 91 (88%) | 13 (12%) | 4 | 23 |
| 47 | n3 | 103/104 (99%) | 95 (92%) | 8 (8%) | 12 | 42 |
| 48 | N4 | 85/129 (66%) | 74 (87%) | 11 (13%) | 4 | 22 |
| 48 | n4 | 97/129 (75%) | 89 (92%) | 8 (8%) | 11 | 41 |
| 49 | N5 | 104/105 (99%) | 85 (82%) | 19 (18%) | 1 | 10 |
| 49 | n5 | 104/105 (99%) | 75 (72%) | 29 (28%) | 0 | 2 |
| 50 | N6 | 109/109 (100%) | 89 (82%) | 20 (18%) | 1 | 10 |
| 50 | n6 | 106/109 (97%) | 87 (82%) | 19 (18%) | 2 | 11 |
| 51 | N7 | 115/115 (100%) | 96 (84%) | 19 (16%) | 2 | 14 |
| 51 | n7 | 115/115 (100%) | 93 (81%) | 22 (19%) | 1 | 9 |
| 52 | N8 | 118/118 (100%) | 102 (86%) | 16 (14%) | 3 | 21 |
| 52 | n8 | 118/118 (100%) | 102 (86%) | 16 (14%) | 3 | 21 |
| 53 | N9 | 46/46 (100%) | 36 (78%) | 10 (22%) | 1 | 7 |
| 53 | n9 | 44/46 (96%) | 40 (91%) | 4 (9%) | 9 | 36 |
| 54 | O0 | 81/84 (96%) | 68 (84%) | 13 (16%) | 2 | 15 |
| 54 | o0 | 84/84 (100%) | 72 (86%) | 12 (14%) | 3 | 19 |
| 55 | O1 | 92/96 (96%) | 77 (84%) | 15 (16%) | 2 | 15 |
| 55 | o1 | 94/96 (98%) | 76 (81%) | 18 (19%) | 1 | 9 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 56 | O2 | 109/109 (100%) | 96 (88%) | 13 (12%) | 5 | 25 |
| 56 | o2 | 109/109 (100%) | 93 (85%) | 16 (15%) | 3 | 18 |
| 57 | O3 | 90/90 (100%) | 79 (88%) | 11 (12%) | 5 | 24 |
| 57 | o3 | 90/90 (100%) | 78 (87%) | 12 (13%) | 4 | 22 |
| 58 | O4 | 95/95 (100%) | 80 (84%) | 15 (16%) | 2 | 16 |
| 58 | o4 | 95/95 (100%) | 83 (87%) | 12 (13%) | 4 | 23 |
| 59 | O5 | 104/104 (100%) | 83 (80%) | 21 (20%) | 1 | 8 |
| 59 | o5 | 103/104 (99%) | 77 (75%) | 26 (25%) | 0 | 4 |
| 60 | O6 | 81/81 (100%) | 62 (76%) | 19 (24%) | 1 | 5 |
| 60 | o6 | 80/81 (99%) | 58 (72%) | 22 (28%) | 0 | 3 |
| 61 | O7 | 70/70 (100%) | 54 (77%) | 16 (23%) | 1 | 6 |
| 61 | o7 | 68/70 (97%) | 59 (87%) | 9 (13%) | 4 | 22 |
| 62 | O8 | 68/68 (100%) | 52 (76%) | 16 (24%) | 1 | 5 |
| 62 | o8 | 67/68 (98%) | 57 (85%) | 10 (15%) | 3 | 18 |
| 63 | O9 | 45/45 (100%) | 37 (82%) | 8 (18%) | 2 | 12 |
| 63 | o9 | 45/45 (100%) | 40 (89%) | 5 (11%) | 6 | 28 |
| 64 | Q0 | 47/47 (100%) | 40 (85%) | 7 (15%) | 3 | 18 |
| 64 | q0 | 47/47 (100%) | 40 (85%) | 7 (15%) | 3 | 18 |
| 65 | Q1 | 23/23 (100%) | 19 (83%) | 4 (17%) | 2 | 12 |
| 65 | q1 | 23/23 (100%) | 19 (83%) | 4 (17%) | 2 | 12 |
| 66 | Q2 | 90/90 (100%) | 71 (79%) | 19 (21%) | 1 | 7 |
| 66 | q2 | 89/90 (99%) | 76 (85%) | 13 (15%) | 3 | 18 |
| 67 | Q3 | 71/71 (100%) | 61 (86%) | 10 (14%) | 3 | 20 |
| 67 | q3 | 71/71 (100%) | 58 (82%) | 13 (18%) | 1 | 10 |
| 68 | S0 | 164/173 (95%) | 134 (82%) | 30 (18%) | 1 | 10 |
| 68 | s0 | 165/173 (95%) | 138 (84%) | 27 (16%) | 2 | 15 |
| 69 | S1 | 191/192 (100%) | 144 (75%) | 47 (25%) | 0 | 5 |
| 69 | s1 | 192/192 (100%) | 156 (81%) | 36 (19%) | 1 | 10 |
| 70 | S2 | 176/176 (100%) | 137 (78%) | 39 (22%) | 1 | 6 |
| 70 | s2 | 176/176 (100%) | 143 (81%) | 33 (19%) | 1 | 10 |
| 71 | S3 | 182/182 (100%) | 149 (82%) | 33 (18%) | 1 | 11 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|------------|-------------|----|
| 71 | s3 | 182/182 (100%) | 148 (81%) | 34 (19%) | 1 | 10 |
| 72 | S4 | 221/221 (100%) | 183 (83%) | 38 (17%) | 2 | 13 |
| 72 | s4 | 221/221 (100%) | 190 (86%) | 31 (14%) | 3 | 20 |
| 73 | S5 | 173/173 (100%) | 148 (86%) | 25 (14%) | 3 | 18 |
| 73 | s5 | 173/173 (100%) | 139 (80%) | 34 (20%) | 1 | 8 |
| 74 | S6 | 188/201 (94%) | 156 (83%) | 32 (17%) | 2 | 13 |
| 74 | s6 | 187/201 (93%) | 157 (84%) | 30 (16%) | 2 | 15 |
| 75 | S7 | 165/165 (100%) | 135 (82%) | 30 (18%) | 1 | 11 |
| 75 | s7 | 165/165 (100%) | 139 (84%) | 26 (16%) | 2 | 16 |
| 76 | S8 | 150/161 (93%) | 130 (87%) | 20 (13%) | 4 | 22 |
| 76 | s8 | 148/161 (92%) | 124 (84%) | 24 (16%) | 2 | 15 |
| 77 | S9 | 158/158 (100%) | 129 (82%) | 29 (18%) | 1 | 10 |
| 77 | s9 | 158/158 (100%) | 135 (85%) | 23 (15%) | 3 | 18 |
| 78 | SM | 97/227 (43%) | 73 (75%) | 24 (25%) | 0 | 5 |
| 78 | sM | 94/227 (41%) | 68 (72%) | 26 (28%) | 0 | 2 |
| 79 | SR | 259/261 (99%) | 226 (87%) | 33 (13%) | 4 | 23 |
| 79 | sR | 258/261 (99%) | 228 (88%) | 30 (12%) | 5 | 27 |
| All | All | 18669/19450 (96%) | 15436 (83%) | 3233 (17%) | 2 | 12 |

All (3233) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | C0 | 1 | MET |
| 5 | C0 | 7 | ASP |
| 5 | C0 | 8 | ARG |
| 5 | C0 | 20 | VAL |
| 5 | C0 | 28 | ASN |
| 5 | C0 | 32 | HIS |
| 5 | C0 | 46 | LEU |
| 5 | C0 | 49 | LEU |
| 5 | C0 | 55 | VAL |
| 5 | C0 | 56 | LYS |
| 5 | C0 | 71 | GLU |
| 5 | C0 | 76 | LEU |
| 5 | C0 | 78 | GLU |
| 5 | C0 | 82 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 5 | c0 | 2 | LEU |
| 5 | c0 | 5 | LYS |
| 5 | c0 | 8 | ARG |
| 5 | c0 | 15 | LEU |
| 5 | c0 | 20 | VAL |
| 5 | c0 | 21 | VAL |
| 5 | c0 | 26 | ASP |
| 5 | c0 | 27 | PHE |
| 5 | c0 | 33 | GLU |
| 5 | c0 | 37 | THR |
| 5 | c0 | 40 | LEU |
| 5 | c0 | 49 | LEU |
| 5 | c0 | 55 | VAL |
| 5 | c0 | 57 | THR |
| 5 | c0 | 71 | GLU |
| 5 | c0 | 77 | ARG |
| 6 | C1 | 5 | LEU |
| 6 | C1 | 8 | GLN |
| 6 | C1 | 10 | GLU |
| 6 | C1 | 21 | ASN |
| 6 | C1 | 27 | THR |
| 6 | C1 | 29 | LYS |
| 6 | C1 | 40 | LEU |
| 6 | C1 | 44 | THR |
| 6 | C1 | 54 | ILE |
| 6 | C1 | 67 | ARG |
| 6 | C1 | 69 | LYS |
| 6 | C1 | 74 | THR |
| 6 | C1 | 83 | THR |
| 6 | C1 | 99 | ARG |
| 6 | C1 | 109 | VAL |
| 6 | C1 | 132 | SER |
| 6 | C1 | 136 | ARG |
| 6 | C1 | 140 | VAL |
| 6 | c1 | 2 | SER |
| 6 | c1 | 5 | LEU |
| 6 | c1 | 10 | GLU |
| 6 | c1 | 21 | ASN |
| 6 | c1 | 26 | LYS |
| 6 | c1 | 27 | THR |
| 6 | c1 | 30 | ARG |
| 6 | c1 | 31 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 6 | c1 | 32 | LYS |
| 6 | c1 | 33 | ARG |
| 6 | c1 | 40 | LEU |
| 6 | c1 | 44 | THR |
| 6 | c1 | 47 | THR |
| 6 | c1 | 50 | GLU |
| 6 | c1 | 56 | LYS |
| 6 | c1 | 60 | PHE |
| 6 | c1 | 67 | ARG |
| 6 | c1 | 72 | THR |
| 6 | c1 | 74 | THR |
| 6 | c1 | 80 | MET |
| 6 | c1 | 83 | THR |
| 6 | c1 | 87 | ARG |
| 6 | c1 | 90 | TYR |
| 6 | c1 | 99 | ARG |
| 6 | c1 | 125 | VAL |
| 6 | c1 | 129 | ARG |
| 6 | c1 | 132 | SER |
| 6 | c1 | 140 | VAL |
| 7 | C2 | 28 | LEU |
| 7 | C2 | 33 | ARG |
| 7 | C2 | 36 | LEU |
| 7 | C2 | 43 | ARG |
| 7 | C2 | 46 | ARG |
| 7 | C2 | 50 | LYS |
| 7 | C2 | 52 | LEU |
| 7 | C2 | 58 | LEU |
| 7 | C2 | 59 | LEU |
| 7 | C2 | 61 | VAL |
| 7 | C2 | 66 | VAL |
| 7 | C2 | 71 | ILE |
| 7 | C2 | 74 | LEU |
| 7 | C2 | 83 | GLU |
| 7 | C2 | 85 | LYS |
| 7 | C2 | 89 | ILE |
| 7 | C2 | 91 | VAL |
| 7 | C2 | 97 | LEU |
| 7 | C2 | 103 | LEU |
| 7 | C2 | 119 | SER |
| 7 | C2 | 121 | VAL |
| 7 | C2 | 126 | TRP |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 7 | C2 | 129 | GLU |
| 7 | C2 | 132 | GLU |
| 7 | C2 | 137 | MET |
| 7 | C2 | 138 | GLU |
| 7 | C2 | 139 | HIS |
| 7 | c2 | 28 | LEU |
| 7 | c2 | 36 | LEU |
| 7 | c2 | 43 | ARG |
| 7 | c2 | 45 | LEU |
| 7 | c2 | 58 | LEU |
| 7 | c2 | 59 | LEU |
| 7 | c2 | 61 | VAL |
| 7 | c2 | 62 | LEU |
| 7 | c2 | 66 | VAL |
| 7 | c2 | 71 | ILE |
| 7 | c2 | 74 | LEU |
| 7 | c2 | 83 | GLU |
| 7 | c2 | 93 | ASP |
| 7 | c2 | 97 | LEU |
| 7 | c2 | 103 | LEU |
| 7 | c2 | 115 | VAL |
| 7 | c2 | 116 | VAL |
| 7 | c2 | 120 | VAL |
| 7 | c2 | 121 | VAL |
| 7 | c2 | 125 | ASN |
| 7 | c2 | 126 | TRP |
| 7 | c2 | 129 | GLU |
| 7 | c2 | 132 | GLU |
| 7 | c2 | 136 | ILE |
| 7 | c2 | 139 | HIS |
| 7 | c2 | 140 | PHE |
| 8 | C3 | 3 | ARG |
| 8 | C3 | 6 | SER |
| 8 | C3 | 9 | LYS |
| 8 | C3 | 16 | ILE |
| 8 | C3 | 27 | LYS |
| 8 | C3 | 31 | GLU |
| 8 | C3 | 39 | LYS |
| 8 | C3 | 42 | ARG |
| 8 | C3 | 45 | LEU |
| 8 | C3 | 56 | ASP |
| 8 | C3 | 58 | HIS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 8 | C3 | 62 | GLN |
| 8 | C3 | 64 | ARG |
| 8 | C3 | 67 | THR |
| 8 | C3 | 76 | LYS |
| 8 | C3 | 88 | LEU |
| 8 | C3 | 102 | LEU |
| 8 | C3 | 105 | ASN |
| 8 | C3 | 115 | LEU |
| 8 | C3 | 120 | SER |
| 8 | C3 | 125 | LEU |
| 8 | C3 | 140 | LYS |
| 8 | C3 | 150 | VAL |
| 8 | C3 | 151 | ASN |
| 8 | c3 | 6 | SER |
| 8 | c3 | 16 | ILE |
| 8 | c3 | 21 | ASN |
| 8 | c3 | 27 | LYS |
| 8 | c3 | 28 | LEU |
| 8 | c3 | 29 | SER |
| 8 | c3 | 64 | ARG |
| 8 | c3 | 66 | ILE |
| 8 | c3 | 70 | LYS |
| 8 | c3 | 84 | ILE |
| 8 | c3 | 86 | GLU |
| 8 | c3 | 87 | ASP |
| 8 | c3 | 94 | LYS |
| 8 | c3 | 104 | ARG |
| 8 | c3 | 105 | ASN |
| 8 | c3 | 115 | LEU |
| 8 | c3 | 125 | LEU |
| 8 | c3 | 138 | ASN |
| 8 | c3 | 139 | TRP |
| 8 | c3 | 141 | TYR |
| 8 | c3 | 143 | SER |
| 8 | c3 | 147 | SER |
| 9 | C4 | 13 | VAL |
| 9 | C4 | 14 | PHE |
| 9 | C4 | 26 | THR |
| 9 | C4 | 29 | HIS |
| 9 | C4 | 31 | THR |
| 9 | C4 | 38 | THR |
| 9 | C4 | 39 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 9 | C4 | 43 | THR |
| 9 | C4 | 51 | ASP |
| 9 | C4 | 52 | ARG |
| 9 | C4 | 79 | VAL |
| 9 | C4 | 81 | VAL |
| 9 | C4 | 89 | THR |
| 9 | C4 | 92 | LYS |
| 9 | C4 | 93 | THR |
| 9 | C4 | 102 | LEU |
| 9 | C4 | 103 | ARG |
| 9 | C4 | 114 | ARG |
| 9 | C4 | 127 | ARG |
| 9 | C4 | 133 | ARG |
| 9 | C4 | 136 | ARG |
| 9 | C4 | 137 | LEU |
| 9 | c4 | 13 | VAL |
| 9 | c4 | 26 | THR |
| 9 | c4 | 31 | THR |
| 9 | c4 | 33 | LEU |
| 9 | c4 | 34 | SER |
| 9 | c4 | 42 | VAL |
| 9 | c4 | 49 | LYS |
| 9 | c4 | 51 | ASP |
| 9 | c4 | 61 | MET |
| 9 | c4 | 66 | ASP |
| 9 | c4 | 79 | VAL |
| 9 | c4 | 81 | VAL |
| 9 | c4 | 91 | THR |
| 9 | c4 | 102 | LEU |
| 9 | c4 | 114 | ARG |
| 9 | c4 | 119 | THR |
| 9 | c4 | 124 | ASP |
| 9 | c4 | 132 | ARG |
| 9 | c4 | 136 | ARG |
| 9 | c4 | 137 | LEU |
| 10 | C5 | 12 | PHE |
| 10 | C5 | 22 | LEU |
| 10 | C5 | 26 | LEU |
| 10 | C5 | 27 | GLU |
| 10 | C5 | 34 | VAL |
| 10 | C5 | 35 | LYS |
| 10 | C5 | 36 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 10 | C5 | 40 | ARG |
| 10 | C5 | 44 | ARG |
| 10 | C5 | 47 | ARG |
| 10 | C5 | 50 | THR |
| 10 | C5 | 51 | SER |
| 10 | C5 | 52 | LYS |
| 10 | C5 | 69 | GLU |
| 10 | C5 | 86 | VAL |
| 10 | C5 | 110 | GLU |
| 10 | C5 | 121 | ILE |
| 10 | C5 | 124 | THR |
| 10 | C5 | 128 | HIS |
| 10 | c5 | 10 | ARG |
| 10 | c5 | 14 | THR |
| 10 | c5 | 15 | HIS |
| 10 | c5 | 21 | ASP |
| 10 | c5 | 24 | LYS |
| 10 | c5 | 27 | GLU |
| 10 | c5 | 36 | LEU |
| 10 | c5 | 44 | ARG |
| 10 | c5 | 69 | GLU |
| 10 | c5 | 77 | ARG |
| 10 | c5 | 107 | ILE |
| 10 | c5 | 110 | GLU |
| 10 | c5 | 121 | ILE |
| 10 | c5 | 122 | THR |
| 10 | c5 | 124 | THR |
| 10 | c5 | 126 | VAL |
| 10 | c5 | 127 | ARG |
| 11 | C6 | 4 | VAL |
| 11 | C6 | 8 | GLN |
| 11 | C6 | 14 | LYS |
| 11 | C6 | 15 | SER |
| 11 | C6 | 17 | THR |
| 11 | C6 | 26 | LYS |
| 11 | C6 | 43 | ILE |
| 11 | C6 | 44 | LEU |
| 11 | C6 | 53 | LEU |
| 11 | C6 | 54 | LEU |
| 11 | C6 | 57 | LEU |
| 11 | C6 | 58 | ASP |
| 11 | C6 | 66 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 11 | C6 | 68 | ARG |
| 11 | C6 | 69 | VAL |
| 11 | C6 | 97 | VAL |
| 11 | C6 | 98 | ASP |
| 11 | C6 | 118 | ILE |
| 11 | C6 | 123 | ARG |
| 11 | C6 | 128 | LYS |
| 11 | C6 | 136 | SER |
| 11 | C6 | 137 | ARG |
| 11 | C6 | 141 | SER |
| 11 | c6 | 17 | THR |
| 11 | c6 | 23 | LYS |
| 11 | c6 | 28 | LEU |
| 11 | c6 | 37 | THR |
| 11 | c6 | 40 | GLU |
| 11 | c6 | 43 | ILE |
| 11 | c6 | 48 | VAL |
| 11 | c6 | 53 | LEU |
| 11 | c6 | 57 | LEU |
| 11 | c6 | 68 | ARG |
| 11 | c6 | 69 | VAL |
| 11 | c6 | 87 | LYS |
| 11 | c6 | 90 | VAL |
| 11 | c6 | 94 | GLN |
| 11 | c6 | 95 | LYS |
| 11 | c6 | 97 | VAL |
| 11 | c6 | 98 | ASP |
| 11 | c6 | 110 | THR |
| 11 | c6 | 113 | ASP |
| 11 | c6 | 115 | THR |
| 11 | c6 | 116 | LEU |
| 11 | c6 | 117 | LEU |
| 11 | c6 | 127 | LYS |
| 11 | c6 | 128 | LYS |
| 11 | c6 | 137 | ARG |
| 11 | c6 | 141 | SER |
| 11 | c6 | 143 | ARG |
| 12 | C7 | 5 | ARG |
| 12 | C7 | 6 | THR |
| 12 | C7 | 7 | LYS |
| 12 | C7 | 19 | ARG |
| 12 | C7 | 24 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 12 | C7 | 25 | THR |
| 12 | C7 | 38 | ILE |
| 12 | C7 | 46 | LEU |
| 12 | C7 | 49 | LYS |
| 12 | C7 | 60 | ARG |
| 12 | C7 | 69 | ILE |
| 12 | C7 | 72 | LYS |
| 12 | C7 | 78 | ARG |
| 12 | C7 | 83 | GLN |
| 12 | C7 | 85 | VAL |
| 12 | C7 | 88 | VAL |
| 12 | C7 | 105 | GLN |
| 12 | C7 | 115 | LEU |
| 12 | C7 | 119 | LEU |
| 12 | c7 | 3 | ARG |
| 12 | c7 | 8 | THR |
| 12 | c7 | 19 | ARG |
| 12 | c7 | 29 | GLN |
| 12 | c7 | 34 | LEU |
| 12 | c7 | 38 | ILE |
| 12 | c7 | 46 | LEU |
| 12 | c7 | 67 | ARG |
| 12 | c7 | 69 | ILE |
| 12 | c7 | 78 | ARG |
| 12 | c7 | 79 | GLU |
| 12 | c7 | 85 | VAL |
| 12 | c7 | 104 | ASN |
| 12 | c7 | 112 | SER |
| 13 | C8 | 3 | LEU |
| 13 | C8 | 8 | GLN |
| 13 | C8 | 11 | PHE |
| 13 | C8 | 14 | ILE |
| 13 | C8 | 15 | LEU |
| 13 | C8 | 17 | LEU |
| 13 | C8 | 21 | ASN |
| 13 | C8 | 26 | ILE |
| 13 | C8 | 28 | ILE |
| 13 | C8 | 32 | LEU |
| 13 | C8 | 38 | VAL |
| 13 | C8 | 46 | VAL |
| 13 | C8 | 55 | HIS |
| 13 | C8 | 60 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 13 | C8 | 61 | LEU |
| 13 | C8 | 68 | ARG |
| 13 | C8 | 70 | VAL |
| 13 | C8 | 71 | GLN |
| 13 | C8 | 74 | GLN |
| 13 | C8 | 92 | ILE |
| 13 | C8 | 93 | THR |
| 13 | C8 | 100 | THR |
| 13 | C8 | 107 | SER |
| 13 | C8 | 108 | LYS |
| 13 | C8 | 110 | ARG |
| 13 | C8 | 116 | LEU |
| 13 | C8 | 132 | ARG |
| 13 | C8 | 133 | VAL |
| 13 | C8 | 136 | GLN |
| 13 | C8 | 138 | THR |
| 13 | C8 | 141 | THR |
| 13 | C8 | 143 | ARG |
| 13 | c8 | 3 | LEU |
| 13 | c8 | 10 | SER |
| 13 | c8 | 13 | HIS |
| 13 | c8 | 15 | LEU |
| 13 | c8 | 17 | LEU |
| 13 | c8 | 23 | ASP |
| 13 | c8 | 26 | ILE |
| 13 | c8 | 28 | ILE |
| 13 | c8 | 36 | LYS |
| 13 | c8 | 40 | ARG |
| 13 | c8 | 43 | SER |
| 13 | c8 | 55 | HIS |
| 13 | c8 | 61 | LEU |
| 13 | c8 | 77 | THR |
| 13 | c8 | 85 | PHE |
| 13 | c8 | 92 | ILE |
| 13 | c8 | 94 | ASP |
| 13 | c8 | 100 | THR |
| 13 | c8 | 105 | VAL |
| 13 | c8 | 116 | LEU |
| 13 | c8 | 119 | ILE |
| 13 | c8 | 136 | GLN |
| 13 | c8 | 138 | THR |
| 13 | c8 | 144 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 14 | C9 | 5 | SER |
| 14 | C9 | 22 | LEU |
| 14 | C9 | 28 | LEU |
| 14 | C9 | 33 | TYR |
| 14 | C9 | 35 | ASP |
| 14 | C9 | 36 | ILE |
| 14 | C9 | 57 | ARG |
| 14 | C9 | 63 | ARG |
| 14 | C9 | 67 | MET |
| 14 | C9 | 75 | LYS |
| 14 | C9 | 84 | LYS |
| 14 | C9 | 86 | ARG |
| 14 | C9 | 89 | ARG |
| 14 | C9 | 94 | ILE |
| 14 | C9 | 126 | GLU |
| 14 | C9 | 130 | ARG |
| 14 | C9 | 131 | ASP |
| 14 | C9 | 134 | ARG |
| 14 | c9 | 6 | VAL |
| 14 | c9 | 20 | SER |
| 14 | c9 | 27 | LYS |
| 14 | c9 | 28 | LEU |
| 14 | c9 | 33 | TYR |
| 14 | c9 | 34 | VAL |
| 14 | c9 | 36 | ILE |
| 14 | c9 | 57 | ARG |
| 14 | c9 | 71 | VAL |
| 14 | c9 | 75 | LYS |
| 14 | c9 | 89 | ARG |
| 14 | c9 | 111 | ILE |
| 14 | c9 | 123 | ARG |
| 14 | c9 | 126 | GLU |
| 14 | c9 | 132 | LEU |
| 14 | c9 | 135 | ILE |
| 14 | c9 | 139 | THR |
| 14 | c9 | 140 | LEU |
| 14 | c9 | 141 | GLU |
| 14 | c9 | 142 | GLU |
| 14 | c9 | 143 | ASP |
| 15 | d0 | 18 | GLN |
| 15 | d0 | 20 | ILE |
| 15 | d0 | 22 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 15 | d0 | 23 | ARG |
| 15 | d0 | 27 | THR |
| 15 | d0 | 31 | VAL |
| 15 | d0 | 34 | LEU |
| 15 | d0 | 44 | ASN |
| 15 | d0 | 47 | GLN |
| 15 | d0 | 51 | VAL |
| 15 | d0 | 57 | ARG |
| 15 | d0 | 60 | THR |
| 15 | d0 | 70 | THR |
| 15 | d0 | 74 | GLU |
| 15 | d0 | 77 | LYS |
| 15 | d0 | 81 | THR |
| 15 | d0 | 99 | ILE |
| 15 | d0 | 102 | ARG |
| 15 | d0 | 103 | ILE |
| 15 | d0 | 105 | GLN |
| 15 | d0 | 115 | GLU |
| 15 | d0 | 120 | SER |
| 15 | D0 | 15 | GLN |
| 15 | D0 | 16 | GLN |
| 15 | D0 | 17 | GLN |
| 15 | D0 | 18 | GLN |
| 15 | D0 | 23 | ARG |
| 15 | D0 | 25 | THR |
| 15 | D0 | 27 | THR |
| 15 | D0 | 30 | LYS |
| 15 | D0 | 31 | VAL |
| 15 | D0 | 34 | LEU |
| 15 | D0 | 35 | GLU |
| 15 | D0 | 47 | GLN |
| 15 | D0 | 48 | HIS |
| 15 | D0 | 51 | VAL |
| 15 | D0 | 57 | ARG |
| 15 | D0 | 61 | LYS |
| 15 | D0 | 70 | THR |
| 15 | D0 | 74 | GLU |
| 15 | D0 | 78 | THR |
| 15 | D0 | 89 | ARG |
| 15 | D0 | 103 | ILE |
| 15 | D0 | 108 | ILE |
| 15 | D0 | 109 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 16 | d1 | 2 | GLU |
| 16 | d1 | 5 | LYS |
| 16 | d1 | 10 | GLU |
| 16 | d1 | 11 | LEU |
| 16 | d1 | 12 | TYR |
| 16 | d1 | 32 | VAL |
| 16 | d1 | 38 | LYS |
| 16 | d1 | 52 | THR |
| 16 | d1 | 56 | SER |
| 16 | d1 | 68 | SER |
| 16 | D1 | 1 | MET |
| 16 | D1 | 2 | GLU |
| 16 | D1 | 3 | ASN |
| 16 | D1 | 5 | LYS |
| 16 | D1 | 7 | GLN |
| 16 | D1 | 11 | LEU |
| 16 | D1 | 41 | GLU |
| 16 | D1 | 52 | THR |
| 16 | D1 | 76 | ASP |
| 16 | D1 | 78 | LEU |
| 16 | D1 | 80 | LYS |
| 17 | d2 | 6 | VAL |
| 17 | d2 | 7 | LEU |
| 17 | d2 | 15 | ASN |
| 17 | d2 | 16 | ASN |
| 17 | d2 | 23 | ARG |
| 17 | d2 | 31 | SER |
| 17 | d2 | 37 | PHE |
| 17 | d2 | 43 | LYS |
| 17 | d2 | 57 | ARG |
| 17 | d2 | 68 | ARG |
| 17 | d2 | 98 | GLN |
| 17 | d2 | 103 | ILE |
| 17 | d2 | 126 | LEU |
| 17 | D2 | 7 | LEU |
| 17 | D2 | 24 | GLN |
| 17 | D2 | 47 | ILE |
| 17 | D2 | 53 | ILE |
| 17 | D2 | 56 | HIS |
| 17 | D2 | 65 | LEU |
| 17 | D2 | 68 | ARG |
| 17 | D2 | 76 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 17 | D2 | 83 | ILE |
| 17 | D2 | 87 | GLU |
| 17 | D2 | 93 | LEU |
| 17 | D2 | 98 | GLN |
| 17 | D2 | 103 | ILE |
| 17 | D2 | 104 | LEU |
| 17 | D2 | 111 | MET |
| 17 | D2 | 121 | VAL |
| 17 | D2 | 122 | SER |
| 17 | D2 | 126 | LEU |
| 18 | d3 | 3 | LYS |
| 18 | d3 | 9 | LEU |
| 18 | d3 | 11 | SER |
| 18 | d3 | 14 | LYS |
| 18 | d3 | 16 | ARG |
| 18 | d3 | 19 | ARG |
| 18 | d3 | 47 | SER |
| 18 | d3 | 56 | LYS |
| 18 | d3 | 73 | ARG |
| 18 | d3 | 79 | ASN |
| 18 | d3 | 84 | THR |
| 18 | d3 | 96 | VAL |
| 18 | d3 | 100 | ASP |
| 18 | d3 | 103 | LEU |
| 18 | d3 | 107 | PHE |
| 18 | d3 | 127 | VAL |
| 18 | d3 | 130 | VAL |
| 18 | D3 | 7 | ARG |
| 18 | D3 | 9 | LEU |
| 18 | D3 | 16 | ARG |
| 18 | D3 | 19 | ARG |
| 18 | D3 | 26 | GLU |
| 18 | D3 | 28 | ASN |
| 18 | D3 | 40 | SER |
| 18 | D3 | 43 | PHE |
| 18 | D3 | 73 | ARG |
| 18 | D3 | 82 | LYS |
| 18 | D3 | 83 | VAL |
| 18 | D3 | 84 | THR |
| 18 | D3 | 94 | ASN |
| 18 | D3 | 100 | ASP |
| 18 | D3 | 103 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 18 | D3 | 107 | PHE |
| 18 | D3 | 110 | LYS |
| 18 | D3 | 140 | LYS |
| 18 | D3 | 144 | ARG |
| 19 | d4 | 6 | THR |
| 19 | d4 | 10 | ARG |
| 19 | d4 | 13 | ILE |
| 19 | d4 | 14 | SER |
| 19 | d4 | 21 | LYS |
| 19 | d4 | 34 | ASN |
| 19 | d4 | 35 | VAL |
| 19 | d4 | 36 | SER |
| 19 | d4 | 43 | LYS |
| 19 | d4 | 47 | VAL |
| 19 | d4 | 49 | LYS |
| 19 | d4 | 58 | PHE |
| 19 | d4 | 62 | THR |
| 19 | d4 | 77 | ASN |
| 19 | d4 | 83 | LYS |
| 19 | d4 | 88 | THR |
| 19 | d4 | 125 | LEU |
| 19 | d4 | 128 | LYS |
| 19 | d4 | 133 | ASN |
| 19 | D4 | 14 | SER |
| 19 | D4 | 17 | LEU |
| 19 | D4 | 21 | LYS |
| 19 | D4 | 32 | ARG |
| 19 | D4 | 34 | ASN |
| 19 | D4 | 35 | VAL |
| 19 | D4 | 46 | GLU |
| 19 | D4 | 47 | VAL |
| 19 | D4 | 49 | LYS |
| 19 | D4 | 51 | GLU |
| 19 | D4 | 57 | VAL |
| 19 | D4 | 61 | ARG |
| 19 | D4 | 62 | THR |
| 19 | D4 | 88 | THR |
| 19 | D4 | 96 | LEU |
| 19 | D4 | 99 | LYS |
| 19 | D4 | 100 | VAL |
| 19 | D4 | 102 | LYS |
| 19 | D4 | 121 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 19 | D4 | 124 | ARG |
| 19 | D4 | 127 | LYS |
| 19 | D4 | 128 | LYS |
| 20 | d5 | 37 | GLN |
| 20 | d5 | 46 | LYS |
| 20 | d5 | 51 | LEU |
| 20 | d5 | 53 | GLU |
| 20 | d5 | 57 | TYR |
| 20 | d5 | 58 | ARG |
| 20 | d5 | 69 | LEU |
| 20 | d5 | 74 | SER |
| 20 | d5 | 81 | ARG |
| 20 | d5 | 85 | LYS |
| 20 | d5 | 88 | ILE |
| 20 | d5 | 93 | SER |
| 20 | d5 | 102 | THR |
| 20 | d5 | 105 | THR |
| 20 | D5 | 38 | HIS |
| 20 | D5 | 40 | VAL |
| 20 | D5 | 42 | LEU |
| 20 | D5 | 44 | GLN |
| 20 | D5 | 59 | TYR |
| 20 | D5 | 67 | ASP |
| 20 | D5 | 68 | ARG |
| 20 | D5 | 69 | LEU |
| 20 | D5 | 70 | LYS |
| 20 | D5 | 71 | ILE |
| 20 | D5 | 75 | LEU |
| 20 | D5 | 85 | LYS |
| 20 | D5 | 88 | ILE |
| 20 | D5 | 92 | ILE |
| 20 | D5 | 95 | HIS |
| 20 | D5 | 102 | THR |
| 21 | d6 | 10 | ARG |
| 21 | d6 | 12 | LYS |
| 21 | d6 | 33 | ASP |
| 21 | d6 | 39 | MET |
| 21 | d6 | 41 | ILE |
| 21 | d6 | 44 | ILE |
| 21 | d6 | 53 | LEU |
| 21 | d6 | 58 | VAL |
| 21 | d6 | 61 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 21 | d6 | 82 | ARG |
| 21 | d6 | 83 | ILE |
| 21 | d6 | 84 | VAL |
| 21 | d6 | 85 | ARG |
| 21 | d6 | 89 | ARG |
| 21 | d6 | 90 | GLU |
| 21 | D6 | 7 | SER |
| 21 | D6 | 12 | LYS |
| 21 | D6 | 18 | VAL |
| 21 | D6 | 36 | ILE |
| 21 | D6 | 39 | MET |
| 21 | D6 | 41 | ILE |
| 21 | D6 | 44 | ILE |
| 21 | D6 | 45 | VAL |
| 21 | D6 | 52 | ASP |
| 21 | D6 | 61 | GLU |
| 21 | D6 | 64 | LEU |
| 21 | D6 | 69 | ASN |
| 21 | D6 | 70 | LYS |
| 21 | D6 | 74 | CYS |
| 21 | D6 | 76 | SER |
| 21 | D6 | 83 | ILE |
| 21 | D6 | 84 | VAL |
| 21 | D6 | 85 | ARG |
| 21 | D6 | 90 | GLU |
| 21 | D6 | 91 | ASP |
| 22 | d7 | 3 | LEU |
| 22 | d7 | 4 | VAL |
| 22 | d7 | 22 | LYS |
| 22 | d7 | 34 | ASP |
| 22 | d7 | 37 | CYS |
| 22 | d7 | 43 | ILE |
| 22 | d7 | 52 | THR |
| 22 | d7 | 57 | GLU |
| 22 | d7 | 77 | THR |
| 22 | d7 | 80 | ARG |
| 22 | d7 | 82 | LYS |
| 22 | D7 | 3 | LEU |
| 22 | D7 | 20 | LYS |
| 22 | D7 | 33 | LEU |
| 22 | D7 | 34 | ASP |
| 22 | D7 | 36 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 22 | D7 | 37 | CYS |
| 22 | D7 | 40 | CYS |
| 22 | D7 | 41 | LEU |
| 22 | D7 | 55 | THR |
| 22 | D7 | 58 | SER |
| 22 | D7 | 62 | ILE |
| 23 | d8 | 5 | THR |
| 23 | d8 | 7 | VAL |
| 23 | d8 | 11 | LYS |
| 23 | d8 | 15 | VAL |
| 23 | d8 | 19 | THR |
| 23 | d8 | 22 | ARG |
| 23 | d8 | 28 | VAL |
| 23 | d8 | 30 | VAL |
| 23 | d8 | 32 | PHE |
| 23 | d8 | 36 | THR |
| 23 | d8 | 39 | THR |
| 23 | d8 | 40 | ILE |
| 23 | d8 | 49 | ARG |
| 23 | d8 | 54 | LEU |
| 23 | d8 | 64 | ARG |
| 23 | d8 | 65 | ARG |
| 23 | D8 | 5 | THR |
| 23 | D8 | 7 | VAL |
| 23 | D8 | 8 | THR |
| 23 | D8 | 13 | ILE |
| 23 | D8 | 14 | LYS |
| 23 | D8 | 19 | THR |
| 23 | D8 | 30 | VAL |
| 23 | D8 | 32 | PHE |
| 23 | D8 | 33 | LEU |
| 23 | D8 | 36 | THR |
| 23 | D8 | 49 | ARG |
| 23 | D8 | 52 | ASP |
| 23 | D8 | 58 | GLU |
| 23 | D8 | 61 | ARG |
| 23 | D8 | 65 | ARG |
| 24 | d9 | 6 | VAL |
| 24 | d9 | 7 | TRP |
| 24 | d9 | 12 | ARG |
| 24 | d9 | 36 | LEU |
| 24 | d9 | 38 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 24 | d9 | 53 | ASN |
| 24 | d9 | 54 | LYS |
| 24 | D9 | 6 | VAL |
| 24 | D9 | 8 | PHE |
| 24 | D9 | 19 | ARG |
| 24 | D9 | 22 | ARG |
| 24 | D9 | 30 | LEU |
| 24 | D9 | 36 | LEU |
| 24 | D9 | 48 | ASN |
| 25 | e0 | 13 | LYS |
| 25 | e0 | 26 | LYS |
| 25 | e0 | 28 | LYS |
| 25 | e0 | 29 | LYS |
| 25 | e0 | 31 | LYS |
| 25 | e0 | 44 | PHE |
| 25 | e0 | 54 | ARG |
| 25 | e0 | 56 | MET |
| 25 | e0 | 62 | VAL |
| 25 | E0 | 20 | LYS |
| 25 | E0 | 28 | LYS |
| 25 | E0 | 29 | LYS |
| 25 | E0 | 42 | ARG |
| 25 | E0 | 45 | VAL |
| 25 | E0 | 47 | VAL |
| 25 | E0 | 50 | VAL |
| 25 | E0 | 54 | ARG |
| 25 | E0 | 56 | MET |
| 26 | e1 | 93 | HIS |
| 26 | e1 | 97 | LYS |
| 26 | e1 | 98 | VAL |
| 26 | e1 | 100 | LEU |
| 26 | e1 | 106 | TYR |
| 26 | e1 | 109 | ASP |
| 26 | e1 | 116 | LYS |
| 26 | e1 | 118 | ARG |
| 26 | e1 | 120 | GLU |
| 26 | e1 | 135 | HIS |
| 26 | e1 | 141 | CYS |
| 26 | e1 | 144 | CYS |
| 26 | e1 | 146 | SER |
| 26 | e1 | 147 | VAL |
| 26 | e1 | 148 | TYR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 26 | e1 | 150 | VAL |
| 26 | E1 | 82 | LYS |
| 26 | E1 | 83 | LYS |
| 26 | E1 | 85 | TYR |
| 26 | E1 | 86 | THR |
| 26 | E1 | 91 | ILE |
| 26 | E1 | 92 | LYS |
| 26 | E1 | 103 | LEU |
| 26 | E1 | 107 | LYS |
| 26 | E1 | 115 | THR |
| 26 | E1 | 119 | ARG |
| 26 | E1 | 120 | GLU |
| 26 | E1 | 140 | TYR |
| 26 | E1 | 146 | SER |
| 26 | E1 | 147 | VAL |
| 26 | E1 | 148 | TYR |
| 26 | E1 | 149 | LYS |
| 27 | l2 | 15 | ILE |
| 27 | l2 | 23 | ARG |
| 27 | l2 | 30 | ARG |
| 27 | l2 | 32 | LEU |
| 27 | l2 | 44 | ILE |
| 27 | l2 | 45 | VAL |
| 27 | l2 | 48 | ILE |
| 27 | l2 | 70 | ARG |
| 27 | l2 | 71 | LEU |
| 27 | l2 | 74 | GLU |
| 27 | l2 | 79 | ASN |
| 27 | l2 | 84 | THR |
| 27 | l2 | 96 | LEU |
| 27 | l2 | 98 | VAL |
| 27 | l2 | 101 | VAL |
| 27 | l2 | 107 | VAL |
| 27 | l2 | 113 | VAL |
| 27 | l2 | 119 | LYS |
| 27 | l2 | 128 | ARG |
| 27 | l2 | 134 | VAL |
| 27 | l2 | 137 | ILE |
| 27 | l2 | 147 | ARG |
| 27 | l2 | 152 | SER |
| 27 | l2 | 155 | LYS |
| 27 | l2 | 157 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 27 | l2 | 165 | VAL |
| 27 | l2 | 179 | LEU |
| 27 | l2 | 180 | LEU |
| 27 | l2 | 181 | LYS |
| 27 | l2 | 190 | ARG |
| 27 | l2 | 193 | ARG |
| 27 | l2 | 202 | VAL |
| 27 | l2 | 224 | THR |
| 27 | l2 | 241 | ARG |
| 27 | l2 | 247 | ARG |
| 27 | L2 | 9 | ARG |
| 27 | L2 | 20 | THR |
| 27 | L2 | 32 | LEU |
| 27 | L2 | 44 | ILE |
| 27 | L2 | 45 | VAL |
| 27 | L2 | 47 | GLN |
| 27 | L2 | 48 | ILE |
| 27 | L2 | 72 | ARG |
| 27 | L2 | 74 | GLU |
| 27 | L2 | 88 | ILE |
| 27 | L2 | 95 | SER |
| 27 | L2 | 98 | VAL |
| 27 | L2 | 101 | VAL |
| 27 | L2 | 104 | LEU |
| 27 | L2 | 113 | VAL |
| 27 | L2 | 119 | LYS |
| 27 | L2 | 134 | VAL |
| 27 | L2 | 157 | VAL |
| 27 | L2 | 158 | ILE |
| 27 | L2 | 169 | ILE |
| 27 | L2 | 179 | LEU |
| 27 | L2 | 180 | LEU |
| 27 | L2 | 191 | LEU |
| 27 | L2 | 193 | ARG |
| 27 | L2 | 202 | VAL |
| 27 | L2 | 204 | MET |
| 27 | L2 | 223 | SER |
| 27 | L2 | 227 | ARG |
| 27 | L2 | 230 | VAL |
| 27 | L2 | 252 | THR |
| 28 | l3 | 3 | HIS |
| 28 | l3 | 4 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 28 | l3 | 10 | ARG |
| 28 | l3 | 17 | LEU |
| 28 | l3 | 19 | ARG |
| 28 | l3 | 37 | ARG |
| 28 | l3 | 39 | LYS |
| 28 | l3 | 41 | VAL |
| 28 | l3 | 47 | LEU |
| 28 | l3 | 50 | LYS |
| 28 | l3 | 54 | THR |
| 28 | l3 | 55 | THR |
| 28 | l3 | 56 | ILE |
| 28 | l3 | 73 | VAL |
| 28 | l3 | 77 | THR |
| 28 | l3 | 81 | THR |
| 28 | l3 | 85 | VAL |
| 28 | l3 | 102 | LEU |
| 28 | l3 | 103 | THR |
| 28 | l3 | 114 | VAL |
| 28 | l3 | 123 | TYR |
| 28 | l3 | 139 | GLN |
| 28 | l3 | 145 | GLU |
| 28 | l3 | 148 | LEU |
| 28 | l3 | 156 | SER |
| 28 | l3 | 168 | LYS |
| 28 | l3 | 169 | THR |
| 28 | l3 | 184 | ASN |
| 28 | l3 | 188 | ILE |
| 28 | l3 | 192 | VAL |
| 28 | l3 | 196 | ARG |
| 28 | l3 | 197 | GLU |
| 28 | l3 | 202 | THR |
| 28 | l3 | 205 | VAL |
| 28 | l3 | 218 | ILE |
| 28 | l3 | 229 | VAL |
| 28 | l3 | 232 | ARG |
| 28 | l3 | 238 | LEU |
| 28 | l3 | 244 | ARG |
| 28 | l3 | 246 | LEU |
| 28 | l3 | 248 | LYS |
| 28 | l3 | 257 | PRO |
| 28 | l3 | 260 | VAL |
| 28 | l3 | 304 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 28 | l3 | 316 | GLU |
| 28 | l3 | 319 | ASN |
| 28 | l3 | 324 | VAL |
| 28 | l3 | 328 | ILE |
| 28 | l3 | 332 | ARG |
| 28 | l3 | 338 | LEU |
| 28 | l3 | 340 | LYS |
| 28 | l3 | 347 | SER |
| 28 | l3 | 348 | ARG |
| 28 | l3 | 355 | SER |
| 28 | l3 | 365 | PHE |
| 28 | l3 | 367 | LYS |
| 28 | l3 | 369 | ARG |
| 28 | l3 | 382 | THR |
| 28 | l3 | 385 | LYS |
| 28 | L3 | 5 | LYS |
| 28 | L3 | 7 | GLU |
| 28 | L3 | 10 | ARG |
| 28 | L3 | 19 | ARG |
| 28 | L3 | 20 | LYS |
| 28 | L3 | 25 | ILE |
| 28 | L3 | 37 | ARG |
| 28 | L3 | 39 | LYS |
| 28 | L3 | 41 | VAL |
| 28 | L3 | 44 | THR |
| 28 | L3 | 47 | LEU |
| 28 | L3 | 55 | THR |
| 28 | L3 | 56 | ILE |
| 28 | L3 | 73 | VAL |
| 28 | L3 | 85 | VAL |
| 28 | L3 | 101 | SER |
| 28 | L3 | 102 | LEU |
| 28 | L3 | 103 | THR |
| 28 | L3 | 110 | LEU |
| 28 | L3 | 114 | VAL |
| 28 | L3 | 144 | ILE |
| 28 | L3 | 156 | SER |
| 28 | L3 | 166 | ILE |
| 28 | L3 | 169 | THR |
| 28 | L3 | 173 | GLN |
| 28 | L3 | 188 | ILE |
| 28 | L3 | 192 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 28 | L3 | 196 | ARG |
| 28 | L3 | 202 | THR |
| 28 | L3 | 205 | VAL |
| 28 | L3 | 206 | ASP |
| 28 | L3 | 211 | GLN |
| 28 | L3 | 235 | THR |
| 28 | L3 | 236 | LYS |
| 28 | L3 | 238 | LEU |
| 28 | L3 | 241 | LYS |
| 28 | L3 | 244 | ARG |
| 28 | L3 | 246 | LEU |
| 28 | L3 | 252 | ILE |
| 28 | L3 | 261 | MET |
| 28 | L3 | 284 | ARG |
| 28 | L3 | 302 | LYS |
| 28 | L3 | 305 | ILE |
| 28 | L3 | 319 | ASN |
| 28 | L3 | 320 | ASP |
| 28 | L3 | 328 | ILE |
| 28 | L3 | 332 | ARG |
| 28 | L3 | 338 | LEU |
| 28 | L3 | 344 | THR |
| 28 | L3 | 361 | THR |
| 28 | L3 | 365 | PHE |
| 28 | L3 | 367 | LYS |
| 28 | L3 | 372 | THR |
| 28 | L3 | 380 | MET |
| 28 | L3 | 386 | ASP |
| 28 | L3 | 387 | LEU |
| 29 | 14 | 3 | ARG |
| 29 | 14 | 14 | GLU |
| 29 | 14 | 18 | ASN |
| 29 | 14 | 22 | LEU |
| 29 | 14 | 73 | ARG |
| 29 | 14 | 85 | SER |
| 29 | 14 | 93 | MET |
| 29 | 14 | 98 | ARG |
| 29 | 14 | 99 | MET |
| 29 | 14 | 103 | THR |
| 29 | 14 | 120 | TYR |
| 29 | 14 | 122 | THR |
| 29 | 14 | 138 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 29 | 14 | 142 | VAL |
| 29 | 14 | 145 | ILE |
| 29 | 14 | 148 | ILE |
| 29 | 14 | 150 | LEU |
| 29 | 14 | 153 | SER |
| 29 | 14 | 156 | LEU |
| 29 | 14 | 170 | LYS |
| 29 | 14 | 172 | VAL |
| 29 | 14 | 177 | ASP |
| 29 | 14 | 179 | LEU |
| 29 | 14 | 186 | LYS |
| 29 | 14 | 187 | LEU |
| 29 | 14 | 193 | LYS |
| 29 | 14 | 194 | TYR |
| 29 | 14 | 203 | ARG |
| 29 | 14 | 206 | LEU |
| 29 | 14 | 217 | LYS |
| 29 | 14 | 220 | ARG |
| 29 | 14 | 230 | VAL |
| 29 | 14 | 246 | ARG |
| 29 | 14 | 256 | THR |
| 29 | 14 | 258 | LEU |
| 29 | 14 | 259 | ASP |
| 29 | 14 | 261 | VAL |
| 29 | 14 | 265 | GLU |
| 29 | 14 | 267 | VAL |
| 29 | 14 | 270 | SER |
| 29 | 14 | 307 | GLN |
| 29 | 14 | 310 | THR |
| 29 | 14 | 313 | LEU |
| 29 | 14 | 319 | LYS |
| 29 | 14 | 327 | LEU |
| 29 | 14 | 342 | LYS |
| 29 | 14 | 343 | LYS |
| 29 | 14 | 346 | LYS |
| 29 | 14 | 347 | THR |
| 29 | 14 | 357 | GLU |
| 29 | 14 | 359 | LEU |
| 29 | L4 | 14 | GLU |
| 29 | L4 | 47 | ARG |
| 29 | L4 | 54 | GLU |
| 29 | L4 | 69 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 29 | L4 | 82 | THR |
| 29 | L4 | 93 | MET |
| 29 | L4 | 98 | ARG |
| 29 | L4 | 112 | LYS |
| 29 | L4 | 120 | TYR |
| 29 | L4 | 124 | SER |
| 29 | L4 | 136 | LEU |
| 29 | L4 | 138 | ARG |
| 29 | L4 | 141 | ARG |
| 29 | L4 | 148 | ILE |
| 29 | L4 | 153 | SER |
| 29 | L4 | 156 | LEU |
| 29 | L4 | 170 | LYS |
| 29 | L4 | 179 | LEU |
| 29 | L4 | 182 | LEU |
| 29 | L4 | 187 | LEU |
| 29 | L4 | 193 | LYS |
| 29 | L4 | 203 | ARG |
| 29 | L4 | 206 | LEU |
| 29 | L4 | 213 | ASN |
| 29 | L4 | 220 | ARG |
| 29 | L4 | 222 | VAL |
| 29 | L4 | 230 | VAL |
| 29 | L4 | 232 | SER |
| 29 | L4 | 246 | ARG |
| 29 | L4 | 258 | LEU |
| 29 | L4 | 259 | ASP |
| 29 | L4 | 261 | VAL |
| 29 | L4 | 267 | VAL |
| 29 | L4 | 270 | SER |
| 29 | L4 | 278 | SER |
| 29 | L4 | 283 | THR |
| 29 | L4 | 287 | THR |
| 29 | L4 | 297 | SER |
| 29 | L4 | 306 | THR |
| 29 | L4 | 307 | GLN |
| 29 | L4 | 310 | THR |
| 29 | L4 | 313 | LEU |
| 29 | L4 | 319 | LYS |
| 29 | L4 | 323 | VAL |
| 29 | L4 | 327 | LEU |
| 29 | L4 | 345 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 29 | L4 | 346 | LYS |
| 29 | L4 | 347 | THR |
| 29 | L4 | 354 | VAL |
| 30 | l5 | 4 | GLN |
| 30 | l5 | 5 | LYS |
| 30 | l5 | 13 | SER |
| 30 | l5 | 18 | THR |
| 30 | l5 | 34 | LYS |
| 30 | l5 | 35 | ARG |
| 30 | l5 | 51 | LEU |
| 30 | l5 | 68 | THR |
| 30 | l5 | 70 | THR |
| 30 | l5 | 74 | VAL |
| 30 | l5 | 89 | THR |
| 30 | l5 | 110 | LEU |
| 30 | l5 | 112 | LYS |
| 30 | l5 | 113 | LEU |
| 30 | l5 | 118 | THR |
| 30 | l5 | 133 | GLU |
| 30 | l5 | 144 | VAL |
| 30 | l5 | 146 | LEU |
| 30 | l5 | 148 | ILE |
| 30 | l5 | 152 | ARG |
| 30 | l5 | 155 | THR |
| 30 | l5 | 178 | ASN |
| 30 | l5 | 187 | THR |
| 30 | l5 | 194 | LEU |
| 30 | l5 | 211 | LEU |
| 30 | l5 | 230 | ASP |
| 30 | l5 | 254 | LYS |
| 30 | l5 | 258 | LYS |
| 30 | l5 | 259 | LYS |
| 30 | l5 | 268 | GLU |
| 30 | l5 | 273 | ARG |
| 30 | L5 | 5 | LYS |
| 30 | L5 | 10 | SER |
| 30 | L5 | 13 | SER |
| 30 | L5 | 22 | ARG |
| 30 | L5 | 23 | ARG |
| 30 | L5 | 35 | ARG |
| 30 | L5 | 41 | LYS |
| 30 | L5 | 45 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 30 | L5 | 46 | THR |
| 30 | L5 | 50 | ARG |
| 30 | L5 | 56 | THR |
| 30 | L5 | 69 | ILE |
| 30 | L5 | 70 | THR |
| 30 | L5 | 75 | LEU |
| 30 | L5 | 85 | ARG |
| 30 | L5 | 90 | HIS |
| 30 | L5 | 92 | LEU |
| 30 | L5 | 93 | THR |
| 30 | L5 | 95 | TRP |
| 30 | L5 | 105 | ILE |
| 30 | L5 | 107 | ARG |
| 30 | L5 | 109 | THR |
| 30 | L5 | 113 | LEU |
| 30 | L5 | 118 | THR |
| 30 | L5 | 128 | GLU |
| 30 | L5 | 131 | LEU |
| 30 | L5 | 144 | VAL |
| 30 | L5 | 146 | LEU |
| 30 | L5 | 148 | ILE |
| 30 | L5 | 150 | LEU |
| 30 | L5 | 151 | GLN |
| 30 | L5 | 152 | ARG |
| 30 | L5 | 155 | THR |
| 30 | L5 | 159 | VAL |
| 30 | L5 | 163 | LEU |
| 30 | L5 | 177 | GLU |
| 30 | L5 | 185 | PHE |
| 30 | L5 | 187 | THR |
| 30 | L5 | 188 | GLU |
| 30 | L5 | 194 | LEU |
| 30 | L5 | 211 | LEU |
| 30 | L5 | 222 | LEU |
| 30 | L5 | 231 | ILE |
| 30 | L5 | 261 | THR |
| 30 | L5 | 263 | GLU |
| 30 | L5 | 264 | GLN |
| 30 | L5 | 273 | ARG |
| 30 | L5 | 277 | LEU |
| 31 | 16 | 8 | LYS |
| 31 | 16 | 20 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 31 | l6 | 21 | THR |
| 31 | l6 | 46 | ARG |
| 31 | l6 | 50 | LYS |
| 31 | l6 | 52 | VAL |
| 31 | l6 | 62 | THR |
| 31 | l6 | 64 | LEU |
| 31 | l6 | 65 | ILE |
| 31 | l6 | 76 | LEU |
| 31 | l6 | 79 | VAL |
| 31 | l6 | 82 | ARG |
| 31 | l6 | 98 | VAL |
| 31 | l6 | 108 | LYS |
| 31 | l6 | 128 | LYS |
| 31 | l6 | 152 | THR |
| 31 | l6 | 155 | LEU |
| 31 | L6 | 5 | LYS |
| 31 | L6 | 15 | VAL |
| 31 | L6 | 21 | THR |
| 31 | L6 | 31 | ARG |
| 31 | L6 | 48 | ARG |
| 31 | L6 | 52 | VAL |
| 31 | L6 | 56 | LYS |
| 31 | L6 | 59 | GLU |
| 31 | L6 | 64 | LEU |
| 31 | L6 | 65 | ILE |
| 31 | L6 | 79 | VAL |
| 31 | L6 | 84 | VAL |
| 31 | L6 | 89 | THR |
| 31 | L6 | 91 | VAL |
| 31 | L6 | 96 | VAL |
| 31 | L6 | 98 | VAL |
| 31 | L6 | 129 | GLU |
| 31 | L6 | 134 | ARG |
| 31 | L6 | 146 | ILE |
| 31 | L6 | 152 | THR |
| 31 | L6 | 167 | ASN |
| 32 | l7 | 22 | THR |
| 32 | l7 | 41 | ARG |
| 32 | l7 | 60 | ARG |
| 32 | l7 | 77 | VAL |
| 32 | l7 | 78 | GLU |
| 32 | l7 | 84 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 32 | 17 | 87 | VAL |
| 32 | 17 | 88 | ARG |
| 32 | 17 | 101 | LYS |
| 32 | 17 | 108 | LEU |
| 32 | 17 | 110 | ARG |
| 32 | 17 | 121 | LYS |
| 32 | 17 | 124 | LEU |
| 32 | 17 | 151 | ARG |
| 32 | 17 | 158 | LYS |
| 32 | 17 | 164 | SER |
| 32 | 17 | 173 | LEU |
| 32 | 17 | 175 | LYS |
| 32 | 17 | 179 | LEU |
| 32 | 17 | 184 | LEU |
| 32 | 17 | 216 | VAL |
| 32 | 17 | 225 | GLN |
| 32 | 17 | 229 | PHE |
| 32 | 17 | 239 | LEU |
| 32 | L7 | 25 | GLN |
| 32 | L7 | 26 | VAL |
| 32 | L7 | 60 | ARG |
| 32 | L7 | 82 | LYS |
| 32 | L7 | 84 | VAL |
| 32 | L7 | 87 | VAL |
| 32 | L7 | 92 | ILE |
| 32 | L7 | 93 | ASN |
| 32 | L7 | 98 | LYS |
| 32 | L7 | 101 | LYS |
| 32 | L7 | 124 | LEU |
| 32 | L7 | 173 | LEU |
| 32 | L7 | 179 | LEU |
| 32 | L7 | 181 | ILE |
| 32 | L7 | 184 | LEU |
| 32 | L7 | 208 | SER |
| 32 | L7 | 216 | VAL |
| 32 | L7 | 239 | LEU |
| 33 | 18 | 27 | THR |
| 33 | 18 | 41 | GLN |
| 33 | 18 | 68 | ARG |
| 33 | 18 | 79 | GLN |
| 33 | 18 | 81 | THR |
| 33 | 18 | 83 | ASP |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 33 | 18 | 89 | GLU |
| 33 | 18 | 95 | ASN |
| 33 | 18 | 126 | SER |
| 33 | 18 | 136 | LEU |
| 33 | 18 | 146 | LYS |
| 33 | 18 | 156 | ASP |
| 33 | 18 | 160 | ILE |
| 33 | 18 | 163 | VAL |
| 33 | 18 | 169 | LEU |
| 33 | 18 | 172 | LYS |
| 33 | 18 | 180 | VAL |
| 33 | 18 | 185 | ARG |
| 33 | 18 | 200 | LEU |
| 33 | 18 | 208 | GLU |
| 33 | 18 | 213 | LYS |
| 33 | 18 | 214 | LEU |
| 33 | 18 | 217 | THR |
| 33 | 18 | 219 | ASP |
| 33 | 18 | 230 | LYS |
| 33 | 18 | 241 | LYS |
| 33 | 18 | 245 | LYS |
| 33 | 18 | 248 | LYS |
| 33 | L8 | 26 | LEU |
| 33 | L8 | 27 | THR |
| 33 | L8 | 41 | GLN |
| 33 | L8 | 63 | LYS |
| 33 | L8 | 74 | THR |
| 33 | L8 | 79 | GLN |
| 33 | L8 | 83 | ASP |
| 33 | L8 | 84 | ARG |
| 33 | L8 | 90 | THR |
| 33 | L8 | 92 | LYS |
| 33 | L8 | 95 | ASN |
| 33 | L8 | 132 | VAL |
| 33 | L8 | 136 | LEU |
| 33 | L8 | 150 | LEU |
| 33 | L8 | 163 | VAL |
| 33 | L8 | 169 | LEU |
| 33 | L8 | 180 | VAL |
| 33 | L8 | 181 | LYS |
| 33 | L8 | 185 | ARG |
| 33 | L8 | 189 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 33 | L8 | 197 | VAL |
| 33 | L8 | 203 | VAL |
| 33 | L8 | 208 | GLU |
| 33 | L8 | 214 | LEU |
| 33 | L8 | 216 | SER |
| 33 | L8 | 232 | HIS |
| 33 | L8 | 246 | MET |
| 34 | 19 | 1 | MET |
| 34 | 19 | 4 | ILE |
| 34 | 19 | 5 | GLN |
| 34 | 19 | 6 | THR |
| 34 | 19 | 17 | THR |
| 34 | 19 | 18 | VAL |
| 34 | 19 | 19 | SER |
| 34 | 19 | 33 | THR |
| 34 | 19 | 48 | VAL |
| 34 | 19 | 55 | VAL |
| 34 | 19 | 62 | ARG |
| 34 | 19 | 68 | LEU |
| 34 | 19 | 69 | ARG |
| 34 | 19 | 70 | THR |
| 34 | 19 | 80 | THR |
| 34 | 19 | 82 | VAL |
| 34 | 19 | 92 | TYR |
| 34 | 19 | 105 | GLU |
| 34 | 19 | 106 | LYS |
| 34 | 19 | 107 | ASP |
| 34 | 19 | 123 | ILE |
| 34 | 19 | 129 | ARG |
| 34 | 19 | 132 | VAL |
| 34 | 19 | 138 | THR |
| 34 | 19 | 140 | VAL |
| 34 | 19 | 143 | GLU |
| 34 | 19 | 144 | ILE |
| 34 | 19 | 151 | VAL |
| 34 | 19 | 152 | GLU |
| 34 | 19 | 157 | ASN |
| 34 | 19 | 161 | LEU |
| 34 | 19 | 162 | GLN |
| 34 | 19 | 164 | ILE |
| 34 | 19 | 165 | CYS |
| 34 | 19 | 177 | ASP |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 34 | l9 | 179 | ILE |
| 34 | l9 | 190 | ASP |
| 34 | L9 | 1 | MET |
| 34 | L9 | 3 | TYR |
| 34 | L9 | 5 | GLN |
| 34 | L9 | 9 | GLN |
| 34 | L9 | 18 | VAL |
| 34 | L9 | 20 | ILE |
| 34 | L9 | 22 | SER |
| 34 | L9 | 33 | THR |
| 34 | L9 | 41 | ILE |
| 34 | L9 | 48 | VAL |
| 34 | L9 | 52 | LEU |
| 34 | L9 | 62 | ARG |
| 34 | L9 | 68 | LEU |
| 34 | L9 | 69 | ARG |
| 34 | L9 | 70 | THR |
| 34 | L9 | 82 | VAL |
| 34 | L9 | 92 | TYR |
| 34 | L9 | 104 | VAL |
| 34 | L9 | 130 | ASP |
| 34 | L9 | 132 | VAL |
| 34 | L9 | 137 | SER |
| 34 | L9 | 138 | THR |
| 34 | L9 | 139 | ASN |
| 34 | L9 | 140 | VAL |
| 34 | L9 | 141 | LYS |
| 34 | L9 | 146 | LEU |
| 34 | L9 | 147 | SER |
| 34 | L9 | 149 | ASN |
| 34 | L9 | 150 | SER |
| 34 | L9 | 151 | VAL |
| 34 | L9 | 157 | ASN |
| 34 | L9 | 161 | LEU |
| 34 | L9 | 162 | GLN |
| 34 | L9 | 164 | ILE |
| 34 | L9 | 172 | ILE |
| 34 | L9 | 173 | ARG |
| 34 | L9 | 177 | ASP |
| 34 | L9 | 189 | GLU |
| 34 | L9 | 190 | ASP |
| 35 | m0 | 4 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 35 | m0 | 7 | ARG |
| 35 | m0 | 24 | ARG |
| 35 | m0 | 26 | VAL |
| 35 | m0 | 36 | LEU |
| 35 | m0 | 48 | LEU |
| 35 | m0 | 52 | LEU |
| 35 | m0 | 63 | GLU |
| 35 | m0 | 74 | LYS |
| 35 | m0 | 76 | MET |
| 35 | m0 | 87 | LEU |
| 35 | m0 | 91 | VAL |
| 35 | m0 | 129 | VAL |
| 35 | m0 | 144 | ASN |
| 35 | m0 | 156 | ARG |
| 35 | m0 | 163 | GLN |
| 35 | m0 | 168 | SER |
| 35 | m0 | 169 | LYS |
| 35 | m0 | 174 | THR |
| 35 | m0 | 175 | ASN |
| 35 | m0 | 177 | ASP |
| 35 | m0 | 178 | ARG |
| 35 | m0 | 186 | GLU |
| 35 | m0 | 200 | LEU |
| 35 | m0 | 205 | SER |
| 35 | m0 | 215 | GLU |
| 35 | m0 | 216 | TYR |
| 35 | m0 | 217 | PHE |
| 35 | M0 | 3 | ARG |
| 35 | M0 | 30 | LYS |
| 35 | M0 | 33 | ILE |
| 35 | M0 | 40 | LYS |
| 35 | M0 | 42 | THR |
| 35 | M0 | 48 | LEU |
| 35 | M0 | 52 | LEU |
| 35 | M0 | 63 | GLU |
| 35 | M0 | 74 | LYS |
| 35 | M0 | 87 | LEU |
| 35 | M0 | 91 | VAL |
| 35 | M0 | 116 | ARG |
| 35 | M0 | 129 | VAL |
| 35 | M0 | 130 | ASP |
| 35 | M0 | 139 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 35 | M0 | 143 | SER |
| 35 | M0 | 146 | ASP |
| 35 | M0 | 156 | ARG |
| 35 | M0 | 163 | GLN |
| 35 | M0 | 165 | ILE |
| 35 | M0 | 174 | THR |
| 35 | M0 | 191 | LYS |
| 35 | M0 | 203 | LYS |
| 36 | m1 | 9 | MET |
| 36 | m1 | 10 | ARG |
| 36 | m1 | 12 | LEU |
| 36 | m1 | 30 | LEU |
| 36 | m1 | 31 | THR |
| 36 | m1 | 34 | SER |
| 36 | m1 | 44 | THR |
| 36 | m1 | 54 | VAL |
| 36 | m1 | 80 | LEU |
| 36 | m1 | 87 | LYS |
| 36 | m1 | 94 | ARG |
| 36 | m1 | 106 | ILE |
| 36 | m1 | 107 | ASP |
| 36 | m1 | 112 | LEU |
| 36 | m1 | 129 | VAL |
| 36 | m1 | 130 | VAL |
| 36 | m1 | 140 | ARG |
| 36 | m1 | 145 | LYS |
| 36 | m1 | 147 | THR |
| 36 | m1 | 152 | HIS |
| 36 | m1 | 158 | ASP |
| 36 | m1 | 161 | SER |
| 36 | m1 | 172 | LEU |
| 36 | M1 | 10 | ARG |
| 36 | M1 | 12 | LEU |
| 36 | M1 | 13 | LYS |
| 36 | M1 | 17 | LEU |
| 36 | M1 | 19 | LEU |
| 36 | M1 | 23 | VAL |
| 36 | M1 | 34 | SER |
| 36 | M1 | 44 | THR |
| 36 | M1 | 65 | ILE |
| 36 | M1 | 80 | LEU |
| 36 | M1 | 85 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | M1 | 94 | ARG |
| 36 | M1 | 106 | ILE |
| 36 | M1 | 107 | ASP |
| 36 | M1 | 112 | LEU |
| 36 | M1 | 115 | LYS |
| 36 | M1 | 137 | ARG |
| 36 | M1 | 138 | VAL |
| 36 | M1 | 140 | ARG |
| 36 | M1 | 165 | GLN |
| 36 | M1 | 166 | LYS |
| 36 | M1 | 173 | ASP |
| 36 | M1 | 174 | LYS |
| 37 | m3 | 13 | HIS |
| 37 | m3 | 16 | LYS |
| 37 | m3 | 46 | ILE |
| 37 | m3 | 55 | ARG |
| 37 | m3 | 63 | VAL |
| 37 | m3 | 67 | ARG |
| 37 | m3 | 68 | LYS |
| 37 | m3 | 69 | VAL |
| 37 | m3 | 73 | ARG |
| 37 | m3 | 75 | PHE |
| 37 | m3 | 76 | THR |
| 37 | m3 | 85 | LEU |
| 37 | m3 | 100 | ARG |
| 37 | m3 | 107 | GLU |
| 37 | m3 | 122 | LYS |
| 37 | m3 | 123 | ILE |
| 37 | m3 | 128 | ARG |
| 37 | m3 | 131 | LYS |
| 37 | m3 | 149 | GLN |
| 37 | m3 | 164 | GLU |
| 37 | m3 | 171 | ARG |
| 37 | m3 | 176 | GLU |
| 37 | m3 | 184 | GLU |
| 37 | m3 | 189 | GLU |
| 37 | m3 | 194 | GLU |
| 37 | M3 | 4 | SER |
| 37 | M3 | 5 | LYS |
| 37 | M3 | 10 | LEU |
| 37 | M3 | 13 | HIS |
| 37 | M3 | 23 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 37 | M3 | 46 | ILE |
| 37 | M3 | 54 | LEU |
| 37 | M3 | 55 | ARG |
| 37 | M3 | 57 | VAL |
| 37 | M3 | 58 | VAL |
| 37 | M3 | 59 | ARG |
| 37 | M3 | 62 | THR |
| 37 | M3 | 67 | ARG |
| 37 | M3 | 69 | VAL |
| 37 | M3 | 77 | LEU |
| 37 | M3 | 85 | LEU |
| 37 | M3 | 91 | ARG |
| 37 | M3 | 100 | ARG |
| 37 | M3 | 107 | GLU |
| 37 | M3 | 108 | ILE |
| 37 | M3 | 114 | GLN |
| 37 | M3 | 124 | ILE |
| 37 | M3 | 131 | LYS |
| 37 | M3 | 136 | GLU |
| 37 | M3 | 137 | GLN |
| 37 | M3 | 144 | THR |
| 37 | M3 | 147 | ILE |
| 37 | M3 | 164 | GLU |
| 37 | M3 | 168 | ARG |
| 37 | M3 | 171 | ARG |
| 37 | M3 | 190 | LYS |
| 37 | M3 | 194 | GLU |
| 38 | m4 | 2 | SER |
| 38 | m4 | 4 | ASP |
| 38 | m4 | 10 | SER |
| 38 | m4 | 27 | GLN |
| 38 | m4 | 41 | GLN |
| 38 | m4 | 55 | ARG |
| 38 | m4 | 62 | GLN |
| 38 | m4 | 64 | VAL |
| 38 | m4 | 72 | LEU |
| 38 | m4 | 90 | VAL |
| 38 | m4 | 98 | SER |
| 38 | m4 | 107 | GLU |
| 38 | m4 | 108 | ARG |
| 38 | m4 | 135 | LEU |
| 38 | M4 | 4 | ASP |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 38 | M4 | 5 | SER |
| 38 | M4 | 10 | SER |
| 38 | M4 | 20 | VAL |
| 38 | M4 | 42 | LYS |
| 38 | M4 | 47 | ASP |
| 38 | M4 | 58 | ILE |
| 38 | M4 | 64 | VAL |
| 38 | M4 | 102 | LYS |
| 38 | M4 | 108 | ARG |
| 38 | M4 | 113 | THR |
| 38 | M4 | 126 | GLN |
| 38 | M4 | 129 | TYR |
| 38 | M4 | 133 | LYS |
| 39 | m5 | 5 | LYS |
| 39 | m5 | 10 | LEU |
| 39 | m5 | 12 | ARG |
| 39 | m5 | 15 | GLN |
| 39 | m5 | 18 | VAL |
| 39 | m5 | 22 | LEU |
| 39 | m5 | 49 | ARG |
| 39 | m5 | 75 | VAL |
| 39 | m5 | 85 | THR |
| 39 | m5 | 91 | GLU |
| 39 | m5 | 96 | ARG |
| 39 | m5 | 97 | SER |
| 39 | m5 | 98 | LEU |
| 39 | m5 | 106 | VAL |
| 39 | m5 | 117 | ASN |
| 39 | m5 | 138 | GLN |
| 39 | m5 | 155 | VAL |
| 39 | m5 | 167 | THR |
| 39 | m5 | 172 | ARG |
| 39 | m5 | 176 | LYS |
| 39 | m5 | 183 | THR |
| 39 | m5 | 184 | LYS |
| 39 | m5 | 188 | ARG |
| 39 | m5 | 190 | THR |
| 39 | m5 | 194 | GLN |
| 39 | m5 | 201 | ARG |
| 39 | m5 | 204 | LYS |
| 39 | M5 | 15 | GLN |
| 39 | M5 | 22 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 39 | M5 | 38 | ARG |
| 39 | M5 | 50 | ARG |
| 39 | M5 | 62 | TYR |
| 39 | M5 | 80 | THR |
| 39 | M5 | 83 | LYS |
| 39 | M5 | 91 | GLU |
| 39 | M5 | 92 | LEU |
| 39 | M5 | 96 | ARG |
| 39 | M5 | 98 | LEU |
| 39 | M5 | 104 | GLU |
| 39 | M5 | 105 | ARG |
| 39 | M5 | 109 | ARG |
| 39 | M5 | 133 | ILE |
| 39 | M5 | 138 | GLN |
| 39 | M5 | 151 | ILE |
| 39 | M5 | 159 | ARG |
| 39 | M5 | 183 | THR |
| 39 | M5 | 194 | GLN |
| 39 | M5 | 204 | LYS |
| 40 | m6 | 34 | VAL |
| 40 | m6 | 40 | GLU |
| 40 | m6 | 44 | SER |
| 40 | m6 | 58 | LEU |
| 40 | m6 | 60 | LYS |
| 40 | m6 | 74 | ARG |
| 40 | m6 | 78 | ARG |
| 40 | m6 | 85 | ARG |
| 40 | m6 | 100 | GLU |
| 40 | m6 | 106 | GLU |
| 40 | m6 | 115 | LYS |
| 40 | m6 | 117 | ARG |
| 40 | m6 | 119 | VAL |
| 40 | m6 | 126 | VAL |
| 40 | m6 | 143 | THR |
| 40 | m6 | 160 | ARG |
| 40 | m6 | 171 | LYS |
| 40 | m6 | 172 | ARG |
| 40 | m6 | 175 | THR |
| 40 | m6 | 182 | ASN |
| 40 | m6 | 184 | THR |
| 40 | m6 | 197 | LEU |
| 40 | M6 | 16 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 40 | M6 | 41 | LEU |
| 40 | M6 | 44 | SER |
| 40 | M6 | 58 | LEU |
| 40 | M6 | 59 | ARG |
| 40 | M6 | 67 | THR |
| 40 | M6 | 78 | ARG |
| 40 | M6 | 85 | ARG |
| 40 | M6 | 102 | LEU |
| 40 | M6 | 106 | GLU |
| 40 | M6 | 108 | ILE |
| 40 | M6 | 110 | PRO |
| 40 | M6 | 116 | LYS |
| 40 | M6 | 117 | ARG |
| 40 | M6 | 119 | VAL |
| 40 | M6 | 122 | GLN |
| 40 | M6 | 124 | LEU |
| 40 | M6 | 128 | ARG |
| 40 | M6 | 143 | THR |
| 40 | M6 | 148 | LYS |
| 40 | M6 | 160 | ARG |
| 40 | M6 | 182 | ASN |
| 40 | M6 | 190 | VAL |
| 41 | m7 | 7 | THR |
| 41 | m7 | 23 | ARG |
| 41 | m7 | 24 | VAL |
| 41 | m7 | 32 | THR |
| 41 | m7 | 41 | LEU |
| 41 | m7 | 49 | GLU |
| 41 | m7 | 52 | LEU |
| 41 | m7 | 56 | ARG |
| 41 | m7 | 61 | ARG |
| 41 | m7 | 65 | SER |
| 41 | m7 | 67 | ILE |
| 41 | m7 | 69 | ARG |
| 41 | m7 | 74 | LYS |
| 41 | m7 | 79 | THR |
| 41 | m7 | 80 | LYS |
| 41 | m7 | 89 | LYS |
| 41 | m7 | 94 | LEU |
| 41 | m7 | 114 | VAL |
| 41 | m7 | 136 | ILE |
| 41 | m7 | 144 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 41 | m7 | 154 | GLU |
| 41 | m7 | 165 | VAL |
| 41 | m7 | 169 | THR |
| 41 | m7 | 180 | LYS |
| 41 | m7 | 181 | ARG |
| 41 | M7 | 3 | ARG |
| 41 | M7 | 7 | THR |
| 41 | M7 | 9 | THR |
| 41 | M7 | 24 | VAL |
| 41 | M7 | 32 | THR |
| 41 | M7 | 36 | ILE |
| 41 | M7 | 42 | THR |
| 41 | M7 | 52 | LEU |
| 41 | M7 | 53 | ASP |
| 41 | M7 | 56 | ARG |
| 41 | M7 | 61 | ARG |
| 41 | M7 | 67 | ILE |
| 41 | M7 | 69 | ARG |
| 41 | M7 | 70 | THR |
| 41 | M7 | 75 | GLU |
| 41 | M7 | 111 | LYS |
| 41 | M7 | 112 | LEU |
| 41 | M7 | 114 | VAL |
| 41 | M7 | 124 | LYS |
| 41 | M7 | 127 | ARG |
| 41 | M7 | 128 | ARG |
| 41 | M7 | 142 | SER |
| 41 | M7 | 153 | LYS |
| 41 | M7 | 154 | GLU |
| 41 | M7 | 165 | VAL |
| 41 | M7 | 168 | LEU |
| 41 | M7 | 180 | LYS |
| 41 | M7 | 181 | ARG |
| 41 | M7 | 182 | ILE |
| 42 | m8 | 7 | SER |
| 42 | m8 | 13 | SER |
| 42 | m8 | 17 | THR |
| 42 | m8 | 26 | LEU |
| 42 | m8 | 32 | LEU |
| 42 | m8 | 49 | LEU |
| 42 | m8 | 57 | ILE |
| 42 | m8 | 64 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 42 | m8 | 80 | THR |
| 42 | m8 | 81 | VAL |
| 42 | m8 | 86 | THR |
| 42 | m8 | 105 | ARG |
| 42 | m8 | 135 | GLN |
| 42 | m8 | 138 | LEU |
| 42 | m8 | 161 | LYS |
| 42 | m8 | 165 | ILE |
| 42 | m8 | 171 | LYS |
| 42 | m8 | 180 | ARG |
| 42 | M8 | 3 | ILE |
| 42 | M8 | 8 | LYS |
| 42 | M8 | 17 | THR |
| 42 | M8 | 21 | SER |
| 42 | M8 | 24 | VAL |
| 42 | M8 | 26 | LEU |
| 42 | M8 | 32 | LEU |
| 42 | M8 | 41 | ASP |
| 42 | M8 | 49 | LEU |
| 42 | M8 | 61 | PRO |
| 42 | M8 | 63 | SER |
| 42 | M8 | 64 | VAL |
| 42 | M8 | 69 | ARG |
| 42 | M8 | 86 | THR |
| 42 | M8 | 93 | ILE |
| 42 | M8 | 122 | ILE |
| 42 | M8 | 135 | GLN |
| 42 | M8 | 138 | LEU |
| 42 | M8 | 140 | LEU |
| 42 | M8 | 165 | ILE |
| 42 | M8 | 178 | ARG |
| 42 | M8 | 179 | ARG |
| 42 | M8 | 185 | LYS |
| 43 | m9 | 7 | GLN |
| 43 | m9 | 9 | ARG |
| 43 | m9 | 10 | LEU |
| 43 | m9 | 20 | ARG |
| 43 | m9 | 36 | ASN |
| 43 | m9 | 37 | SER |
| 43 | m9 | 43 | LYS |
| 43 | m9 | 55 | VAL |
| 43 | m9 | 56 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 43 | m9 | 63 | THR |
| 43 | m9 | 70 | LYS |
| 43 | m9 | 74 | ARG |
| 43 | m9 | 84 | THR |
| 43 | m9 | 88 | ARG |
| 43 | m9 | 98 | ARG |
| 43 | m9 | 99 | LEU |
| 43 | m9 | 105 | LEU |
| 43 | m9 | 106 | LEU |
| 43 | m9 | 126 | GLU |
| 43 | m9 | 128 | LYS |
| 43 | m9 | 133 | LYS |
| 43 | m9 | 138 | LEU |
| 43 | m9 | 152 | GLU |
| 43 | m9 | 153 | LYS |
| 43 | m9 | 162 | ARG |
| 43 | m9 | 164 | LEU |
| 43 | m9 | 173 | ARG |
| 43 | M9 | 5 | ARG |
| 43 | M9 | 10 | LEU |
| 43 | M9 | 31 | GLU |
| 43 | M9 | 41 | ILE |
| 43 | M9 | 42 | ARG |
| 43 | M9 | 46 | LYS |
| 43 | M9 | 57 | VAL |
| 43 | M9 | 74 | ARG |
| 43 | M9 | 81 | ARG |
| 43 | M9 | 86 | GLU |
| 43 | M9 | 98 | ARG |
| 43 | M9 | 103 | ARG |
| 43 | M9 | 110 | ARG |
| 43 | M9 | 120 | TYR |
| 43 | M9 | 138 | LEU |
| 43 | M9 | 164 | LEU |
| 43 | M9 | 165 | LYS |
| 43 | M9 | 175 | GLN |
| 43 | M9 | 182 | ASP |
| 43 | M9 | 185 | LEU |
| 43 | M9 | 186 | LYS |
| 44 | n0 | 17 | GLU |
| 44 | n0 | 32 | SER |
| 44 | n0 | 45 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 44 | n0 | 50 | LYS |
| 44 | n0 | 51 | VAL |
| 44 | n0 | 73 | LYS |
| 44 | n0 | 80 | ARG |
| 44 | n0 | 85 | SER |
| 44 | n0 | 87 | THR |
| 44 | n0 | 97 | VAL |
| 44 | n0 | 100 | VAL |
| 44 | n0 | 104 | GLU |
| 44 | n0 | 136 | LYS |
| 44 | n0 | 137 | ARG |
| 44 | n0 | 139 | TYR |
| 44 | n0 | 148 | LEU |
| 44 | n0 | 149 | LYS |
| 44 | n0 | 155 | ARG |
| 44 | n0 | 160 | THR |
| 44 | n0 | 162 | THR |
| 44 | n0 | 164 | SER |
| 44 | n0 | 167 | ARG |
| 44 | n0 | 172 | TYR |
| 44 | N0 | 1 | MET |
| 44 | N0 | 12 | ARG |
| 44 | N0 | 13 | ARG |
| 44 | N0 | 16 | THR |
| 44 | N0 | 17 | GLU |
| 44 | N0 | 21 | GLU |
| 44 | N0 | 40 | ARG |
| 44 | N0 | 45 | LEU |
| 44 | N0 | 49 | HIS |
| 44 | N0 | 51 | VAL |
| 44 | N0 | 59 | VAL |
| 44 | N0 | 61 | ILE |
| 44 | N0 | 71 | LYS |
| 44 | N0 | 80 | ARG |
| 44 | N0 | 87 | THR |
| 44 | N0 | 97 | VAL |
| 44 | N0 | 113 | ARG |
| 44 | N0 | 117 | ARG |
| 44 | N0 | 130 | GLU |
| 44 | N0 | 136 | LYS |
| 44 | N0 | 137 | ARG |
| 44 | N0 | 138 | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 44 | N0 | 142 | GLN |
| 44 | N0 | 145 | THR |
| 44 | N0 | 155 | ARG |
| 44 | N0 | 160 | THR |
| 44 | N0 | 164 | SER |
| 44 | N0 | 167 | ARG |
| 44 | N0 | 172 | TYR |
| 45 | n1 | 16 | GLN |
| 45 | n1 | 25 | VAL |
| 45 | n1 | 26 | HIS |
| 45 | n1 | 27 | LEU |
| 45 | n1 | 35 | LYS |
| 45 | n1 | 55 | LYS |
| 45 | n1 | 64 | VAL |
| 45 | n1 | 71 | SER |
| 45 | n1 | 78 | LYS |
| 45 | n1 | 80 | VAL |
| 45 | n1 | 83 | ARG |
| 45 | n1 | 88 | ARG |
| 45 | n1 | 102 | ARG |
| 45 | n1 | 103 | GLN |
| 45 | n1 | 104 | GLU |
| 45 | n1 | 118 | GLU |
| 45 | n1 | 124 | VAL |
| 45 | n1 | 128 | LEU |
| 45 | n1 | 131 | GLN |
| 45 | n1 | 139 | ARG |
| 45 | n1 | 143 | THR |
| 45 | n1 | 149 | GLN |
| 45 | n1 | 150 | THR |
| 45 | N1 | 12 | ARG |
| 45 | N1 | 17 | ARG |
| 45 | N1 | 18 | ASP |
| 45 | N1 | 25 | VAL |
| 45 | N1 | 26 | HIS |
| 45 | N1 | 27 | LEU |
| 45 | N1 | 35 | LYS |
| 45 | N1 | 36 | VAL |
| 45 | N1 | 55 | LYS |
| 45 | N1 | 64 | VAL |
| 45 | N1 | 71 | SER |
| 45 | N1 | 75 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 45 | N1 | 76 | ILE |
| 45 | N1 | 78 | LYS |
| 45 | N1 | 79 | MET |
| 45 | N1 | 80 | VAL |
| 45 | N1 | 83 | ARG |
| 45 | N1 | 88 | ARG |
| 45 | N1 | 89 | LEU |
| 45 | N1 | 93 | VAL |
| 45 | N1 | 96 | ILE |
| 45 | N1 | 102 | ARG |
| 45 | N1 | 103 | GLN |
| 45 | N1 | 104 | GLU |
| 45 | N1 | 106 | LEU |
| 45 | N1 | 126 | VAL |
| 45 | N1 | 127 | GLN |
| 45 | N1 | 128 | LEU |
| 45 | N1 | 131 | GLN |
| 45 | N1 | 136 | ARG |
| 45 | N1 | 139 | ARG |
| 45 | N1 | 143 | THR |
| 45 | N1 | 158 | THR |
| 45 | N1 | 159 | PHE |
| 45 | N1 | 160 | ILE |
| 46 | n2 | 11 | ILE |
| 46 | n2 | 14 | THR |
| 46 | n2 | 21 | SER |
| 46 | n2 | 28 | PHE |
| 46 | n2 | 29 | ASP |
| 46 | n2 | 37 | LEU |
| 46 | n2 | 43 | VAL |
| 46 | n2 | 50 | LEU |
| 46 | n2 | 52 | ASN |
| 46 | n2 | 54 | VAL |
| 46 | n2 | 55 | THR |
| 46 | n2 | 58 | GLU |
| 46 | n2 | 62 | VAL |
| 46 | n2 | 63 | VAL |
| 46 | n2 | 68 | THR |
| 46 | n2 | 98 | THR |
| 46 | n2 | 100 | THR |
| 46 | N2 | 9 | GLN |
| 46 | N2 | 27 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 46 | N2 | 29 | ASP |
| 46 | N2 | 38 | ILE |
| 46 | N2 | 39 | ASP |
| 46 | N2 | 43 | VAL |
| 46 | N2 | 44 | GLU |
| 46 | N2 | 52 | ASN |
| 46 | N2 | 57 | THR |
| 46 | N2 | 59 | ASP |
| 46 | N2 | 61 | THR |
| 46 | N2 | 66 | VAL |
| 46 | N2 | 72 | SER |
| 46 | N2 | 88 | GLN |
| 46 | N2 | 90 | ARG |
| 46 | N2 | 93 | ILE |
| 46 | N2 | 100 | THR |
| 47 | n3 | 4 | ASN |
| 47 | n3 | 13 | ILE |
| 47 | n3 | 44 | SER |
| 47 | n3 | 58 | VAL |
| 47 | n3 | 70 | ARG |
| 47 | n3 | 84 | SER |
| 47 | n3 | 88 | ARG |
| 47 | n3 | 91 | VAL |
| 47 | N3 | 4 | ASN |
| 47 | N3 | 7 | GLN |
| 47 | N3 | 13 | ILE |
| 47 | N3 | 23 | MET |
| 47 | N3 | 64 | LYS |
| 47 | N3 | 69 | LEU |
| 47 | N3 | 72 | LYS |
| 47 | N3 | 83 | LYS |
| 47 | N3 | 91 | VAL |
| 47 | N3 | 102 | ILE |
| 47 | N3 | 120 | LYS |
| 47 | N3 | 125 | LEU |
| 47 | N3 | 135 | VAL |
| 48 | n4 | 7 | SER |
| 48 | n4 | 39 | LEU |
| 48 | n4 | 57 | LYS |
| 48 | n4 | 63 | ILE |
| 48 | n4 | 100 | VAL |
| 48 | n4 | 105 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 48 | n4 | 126 | GLU |
| 48 | n4 | 127 | LYS |
| 48 | N4 | 1 | MET |
| 48 | N4 | 4 | GLU |
| 48 | N4 | 5 | ILE |
| 48 | N4 | 19 | THR |
| 48 | N4 | 39 | LEU |
| 48 | N4 | 43 | ARG |
| 48 | N4 | 54 | LEU |
| 48 | N4 | 96 | LEU |
| 48 | N4 | 105 | ARG |
| 48 | N4 | 126 | GLU |
| 48 | N4 | 127 | LYS |
| 49 | n5 | 24 | LEU |
| 49 | n5 | 27 | ARG |
| 49 | n5 | 28 | THR |
| 49 | n5 | 29 | SER |
| 49 | n5 | 34 | LEU |
| 49 | n5 | 38 | LEU |
| 49 | n5 | 39 | LYS |
| 49 | n5 | 40 | LEU |
| 49 | n5 | 45 | LYS |
| 49 | n5 | 46 | TYR |
| 49 | n5 | 51 | VAL |
| 49 | n5 | 56 | ARG |
| 49 | n5 | 57 | LEU |
| 49 | n5 | 59 | SER |
| 49 | n5 | 63 | ILE |
| 49 | n5 | 68 | THR |
| 49 | n5 | 71 | THR |
| 49 | n5 | 73 | MET |
| 49 | n5 | 74 | LYS |
| 49 | n5 | 86 | VAL |
| 49 | n5 | 108 | LEU |
| 49 | n5 | 109 | LYS |
| 49 | n5 | 115 | ARG |
| 49 | n5 | 125 | ARG |
| 49 | n5 | 133 | LEU |
| 49 | n5 | 134 | ASP |
| 49 | n5 | 135 | ILE |
| 49 | n5 | 137 | ASN |
| 49 | n5 | 142 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 49 | N5 | 24 | LEU |
| 49 | N5 | 27 | ARG |
| 49 | N5 | 38 | LEU |
| 49 | N5 | 39 | LYS |
| 49 | N5 | 40 | LEU |
| 49 | N5 | 45 | LYS |
| 49 | N5 | 49 | LYS |
| 49 | N5 | 51 | VAL |
| 49 | N5 | 58 | ASP |
| 49 | N5 | 63 | ILE |
| 49 | N5 | 73 | MET |
| 49 | N5 | 86 | VAL |
| 49 | N5 | 92 | LYS |
| 49 | N5 | 108 | LEU |
| 49 | N5 | 115 | ARG |
| 49 | N5 | 125 | ARG |
| 49 | N5 | 135 | ILE |
| 49 | N5 | 139 | ILE |
| 49 | N5 | 142 | ILE |
| 50 | n6 | 4 | GLN |
| 50 | n6 | 13 | ARG |
| 50 | n6 | 17 | LYS |
| 50 | n6 | 25 | SER |
| 50 | n6 | 37 | LYS |
| 50 | n6 | 39 | LEU |
| 50 | n6 | 50 | ILE |
| 50 | n6 | 51 | ARG |
| 50 | n6 | 56 | VAL |
| 50 | n6 | 57 | LEU |
| 50 | n6 | 74 | TYR |
| 50 | n6 | 76 | LEU |
| 50 | n6 | 94 | SER |
| 50 | n6 | 95 | VAL |
| 50 | n6 | 97 | ILE |
| 50 | n6 | 103 | LYS |
| 50 | n6 | 112 | ASP |
| 50 | n6 | 115 | ARG |
| 50 | n6 | 120 | GLN |
| 50 | N6 | 13 | ARG |
| 50 | N6 | 17 | LYS |
| 50 | N6 | 32 | SER |
| 50 | N6 | 37 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 50 | N6 | 42 | GLN |
| 50 | N6 | 45 | ILE |
| 50 | N6 | 50 | ILE |
| 50 | N6 | 51 | ARG |
| 50 | N6 | 56 | VAL |
| 50 | N6 | 57 | LEU |
| 50 | N6 | 70 | ILE |
| 50 | N6 | 74 | TYR |
| 50 | N6 | 76 | LEU |
| 50 | N6 | 80 | VAL |
| 50 | N6 | 87 | LYS |
| 50 | N6 | 94 | SER |
| 50 | N6 | 105 | VAL |
| 50 | N6 | 111 | LEU |
| 50 | N6 | 115 | ARG |
| 50 | N6 | 126 | LEU |
| 51 | n7 | 3 | LYS |
| 51 | n7 | 14 | VAL |
| 51 | n7 | 15 | ARG |
| 51 | n7 | 17 | ARG |
| 51 | n7 | 30 | ASP |
| 51 | n7 | 31 | GLU |
| 51 | n7 | 34 | LYS |
| 51 | n7 | 36 | HIS |
| 51 | n7 | 46 | ILE |
| 51 | n7 | 52 | LYS |
| 51 | n7 | 72 | ILE |
| 51 | n7 | 81 | LEU |
| 51 | n7 | 83 | THR |
| 51 | n7 | 95 | VAL |
| 51 | n7 | 99 | GLU |
| 51 | n7 | 100 | THR |
| 51 | n7 | 102 | GLU |
| 51 | n7 | 121 | ARG |
| 51 | n7 | 126 | LYS |
| 51 | n7 | 129 | TRP |
| 51 | n7 | 134 | LEU |
| 51 | n7 | 135 | ARG |
| 51 | N7 | 3 | LYS |
| 51 | N7 | 17 | ARG |
| 51 | N7 | 24 | VAL |
| 51 | N7 | 34 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 51 | N7 | 46 | ILE |
| 51 | N7 | 53 | VAL |
| 51 | N7 | 54 | THR |
| 51 | N7 | 64 | LYS |
| 51 | N7 | 81 | LEU |
| 51 | N7 | 83 | THR |
| 51 | N7 | 92 | PHE |
| 51 | N7 | 98 | THR |
| 51 | N7 | 102 | GLU |
| 51 | N7 | 103 | GLN |
| 51 | N7 | 109 | GLU |
| 51 | N7 | 120 | GLU |
| 51 | N7 | 121 | ARG |
| 51 | N7 | 127 | ASN |
| 51 | N7 | 134 | LEU |
| 52 | n8 | 4 | ARG |
| 52 | n8 | 8 | THR |
| 52 | n8 | 27 | LYS |
| 52 | n8 | 42 | ARG |
| 52 | n8 | 46 | ASP |
| 52 | n8 | 60 | TYR |
| 52 | n8 | 65 | GLN |
| 52 | n8 | 73 | LEU |
| 52 | n8 | 82 | ILE |
| 52 | n8 | 85 | ASP |
| 52 | n8 | 91 | LEU |
| 52 | n8 | 97 | GLU |
| 52 | n8 | 128 | ARG |
| 52 | n8 | 132 | LYS |
| 52 | n8 | 133 | LEU |
| 52 | n8 | 139 | ARG |
| 52 | N8 | 10 | LYS |
| 52 | N8 | 40 | HIS |
| 52 | N8 | 42 | ARG |
| 52 | N8 | 43 | ILE |
| 52 | N8 | 46 | ASP |
| 52 | N8 | 56 | VAL |
| 52 | N8 | 60 | TYR |
| 52 | N8 | 72 | VAL |
| 52 | N8 | 78 | LEU |
| 52 | N8 | 84 | GLU |
| 52 | N8 | 88 | ASP |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 52 | N8 | 91 | LEU |
| 52 | N8 | 96 | LYS |
| 52 | N8 | 120 | ASN |
| 52 | N8 | 133 | LEU |
| 52 | N8 | 139 | ARG |
| 53 | n9 | 8 | THR |
| 53 | n9 | 14 | ARG |
| 53 | n9 | 33 | LYS |
| 53 | n9 | 50 | THR |
| 53 | N9 | 7 | HIS |
| 53 | N9 | 8 | THR |
| 53 | N9 | 14 | ARG |
| 53 | N9 | 22 | LYS |
| 53 | N9 | 23 | LYS |
| 53 | N9 | 25 | LYS |
| 53 | N9 | 28 | LYS |
| 53 | N9 | 33 | LYS |
| 53 | N9 | 50 | THR |
| 53 | N9 | 58 | LYS |
| 54 | o0 | 6 | SER |
| 54 | o0 | 7 | GLN |
| 54 | o0 | 18 | ILE |
| 54 | o0 | 19 | LYS |
| 54 | o0 | 32 | LYS |
| 54 | o0 | 34 | LEU |
| 54 | o0 | 40 | LYS |
| 54 | o0 | 41 | LEU |
| 54 | o0 | 61 | MET |
| 54 | o0 | 86 | ARG |
| 54 | o0 | 87 | VAL |
| 54 | o0 | 100 | ILE |
| 54 | O0 | 16 | LEU |
| 54 | O0 | 32 | LYS |
| 54 | O0 | 34 | LEU |
| 54 | O0 | 36 | GLN |
| 54 | O0 | 40 | LYS |
| 54 | O0 | 43 | ILE |
| 54 | O0 | 48 | THR |
| 54 | O0 | 54 | SER |
| 54 | O0 | 61 | MET |
| 54 | O0 | 79 | THR |
| 54 | O0 | 83 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 54 | O0 | 93 | LEU |
| 54 | O0 | 100 | ILE |
| 55 | o1 | 6 | ASP |
| 55 | o1 | 8 | VAL |
| 55 | o1 | 13 | THR |
| 55 | o1 | 16 | LEU |
| 55 | o1 | 26 | LYS |
| 55 | o1 | 31 | ARG |
| 55 | o1 | 44 | MET |
| 55 | o1 | 55 | LEU |
| 55 | o1 | 64 | VAL |
| 55 | o1 | 76 | SER |
| 55 | o1 | 83 | GLU |
| 55 | o1 | 89 | LEU |
| 55 | o1 | 90 | PHE |
| 55 | o1 | 96 | VAL |
| 55 | o1 | 100 | SER |
| 55 | o1 | 102 | LYS |
| 55 | o1 | 106 | THR |
| 55 | o1 | 110 | GLU |
| 55 | O1 | 6 | ASP |
| 55 | O1 | 8 | VAL |
| 55 | O1 | 13 | THR |
| 55 | O1 | 16 | LEU |
| 55 | O1 | 26 | LYS |
| 55 | O1 | 31 | ARG |
| 55 | O1 | 46 | THR |
| 55 | O1 | 47 | ASP |
| 55 | O1 | 55 | LEU |
| 55 | O1 | 64 | VAL |
| 55 | O1 | 79 | ARG |
| 55 | O1 | 82 | GLU |
| 55 | O1 | 86 | LYS |
| 55 | O1 | 89 | LEU |
| 55 | O1 | 106 | THR |
| 56 | o2 | 19 | ARG |
| 56 | o2 | 24 | ARG |
| 56 | o2 | 25 | TYR |
| 56 | o2 | 33 | ARG |
| 56 | o2 | 40 | SER |
| 56 | o2 | 51 | SER |
| 56 | o2 | 63 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 56 | o2 | 73 | THR |
| 56 | o2 | 75 | LEU |
| 56 | o2 | 82 | LEU |
| 56 | o2 | 87 | MET |
| 56 | o2 | 89 | THR |
| 56 | o2 | 123 | LYS |
| 56 | o2 | 125 | ARG |
| 56 | o2 | 126 | LEU |
| 56 | o2 | 128 | LEU |
| 56 | O2 | 14 | THR |
| 56 | O2 | 19 | ARG |
| 56 | O2 | 27 | ARG |
| 56 | O2 | 33 | ARG |
| 56 | O2 | 51 | SER |
| 56 | O2 | 61 | LYS |
| 56 | O2 | 67 | SER |
| 56 | O2 | 73 | THR |
| 56 | O2 | 75 | LEU |
| 56 | O2 | 106 | VAL |
| 56 | O2 | 125 | ARG |
| 56 | O2 | 126 | LEU |
| 56 | O2 | 128 | LEU |
| 57 | o3 | 19 | SER |
| 57 | o3 | 28 | SER |
| 57 | o3 | 31 | LYS |
| 57 | o3 | 48 | ARG |
| 57 | o3 | 57 | LYS |
| 57 | o3 | 59 | VAL |
| 57 | o3 | 67 | MET |
| 57 | o3 | 70 | LYS |
| 57 | o3 | 80 | VAL |
| 57 | o3 | 81 | VAL |
| 57 | o3 | 86 | ARG |
| 57 | o3 | 98 | VAL |
| 57 | O3 | 3 | GLU |
| 57 | O3 | 4 | SER |
| 57 | O3 | 15 | SER |
| 57 | O3 | 19 | SER |
| 57 | O3 | 20 | LYS |
| 57 | O3 | 57 | LYS |
| 57 | O3 | 59 | VAL |
| 57 | O3 | 81 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 57 | O3 | 92 | LYS |
| 57 | O3 | 98 | VAL |
| 57 | O3 | 106 | ASN |
| 58 | o4 | 5 | VAL |
| 58 | o4 | 20 | ILE |
| 58 | o4 | 24 | LYS |
| 58 | o4 | 29 | ILE |
| 58 | o4 | 31 | ARG |
| 58 | o4 | 46 | ASP |
| 58 | o4 | 58 | ARG |
| 58 | o4 | 71 | THR |
| 58 | o4 | 79 | SER |
| 58 | o4 | 80 | ARG |
| 58 | o4 | 81 | CYS |
| 58 | o4 | 88 | ARG |
| 58 | O4 | 8 | ARG |
| 58 | O4 | 15 | THR |
| 58 | O4 | 16 | ARG |
| 58 | O4 | 20 | ILE |
| 58 | O4 | 24 | LYS |
| 58 | O4 | 29 | ILE |
| 58 | O4 | 33 | GLN |
| 58 | O4 | 44 | CYS |
| 58 | O4 | 58 | ARG |
| 58 | O4 | 65 | VAL |
| 58 | O4 | 71 | THR |
| 58 | O4 | 73 | SER |
| 58 | O4 | 79 | SER |
| 58 | O4 | 81 | CYS |
| 58 | O4 | 104 | VAL |
| 59 | o5 | 4 | VAL |
| 59 | o5 | 15 | GLU |
| 59 | o5 | 20 | GLN |
| 59 | o5 | 21 | LEU |
| 59 | o5 | 27 | GLU |
| 59 | o5 | 28 | LEU |
| 59 | o5 | 36 | LEU |
| 59 | o5 | 37 | SER |
| 59 | o5 | 40 | SER |
| 59 | o5 | 41 | LEU |
| 59 | o5 | 44 | ILE |
| 59 | o5 | 45 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 59 | o5 | 47 | VAL |
| 59 | o5 | 53 | CYS |
| 59 | o5 | 57 | VAL |
| 59 | o5 | 62 | GLN |
| 59 | o5 | 69 | LEU |
| 59 | o5 | 79 | ASP |
| 59 | o5 | 81 | ARG |
| 59 | o5 | 85 | THR |
| 59 | o5 | 89 | ARG |
| 59 | o5 | 90 | ARG |
| 59 | o5 | 94 | LYS |
| 59 | o5 | 98 | SER |
| 59 | o5 | 107 | LYS |
| 59 | o5 | 116 | TYR |
| 59 | O5 | 4 | VAL |
| 59 | O5 | 13 | SER |
| 59 | O5 | 15 | GLU |
| 59 | O5 | 20 | GLN |
| 59 | O5 | 21 | LEU |
| 59 | O5 | 27 | GLU |
| 59 | O5 | 31 | LEU |
| 59 | O5 | 44 | ILE |
| 59 | O5 | 46 | THR |
| 59 | O5 | 47 | VAL |
| 59 | O5 | 49 | LYS |
| 59 | O5 | 71 | LYS |
| 59 | O5 | 74 | LYS |
| 59 | O5 | 85 | THR |
| 59 | O5 | 89 | ARG |
| 59 | O5 | 96 | GLU |
| 59 | O5 | 100 | VAL |
| 59 | O5 | 101 | THR |
| 59 | O5 | 104 | GLN |
| 59 | O5 | 107 | LYS |
| 59 | O5 | 119 | LYS |
| 60 | o6 | 9 | ILE |
| 60 | o6 | 11 | LEU |
| 60 | o6 | 17 | VAL |
| 60 | o6 | 21 | THR |
| 60 | o6 | 26 | ILE |
| 60 | o6 | 29 | LYS |
| 60 | o6 | 36 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 60 | o6 | 43 | LEU |
| 60 | o6 | 45 | ARG |
| 60 | o6 | 57 | LEU |
| 60 | o6 | 58 | ILE |
| 60 | o6 | 60 | LEU |
| 60 | o6 | 61 | ILE |
| 60 | o6 | 68 | ARG |
| 60 | o6 | 75 | LYS |
| 60 | o6 | 76 | ARG |
| 60 | o6 | 81 | THR |
| 60 | o6 | 87 | VAL |
| 60 | o6 | 88 | GLU |
| 60 | o6 | 90 | MET |
| 60 | o6 | 94 | ILE |
| 60 | o6 | 98 | ARG |
| 60 | O6 | 11 | LEU |
| 60 | O6 | 13 | LYS |
| 60 | O6 | 17 | VAL |
| 60 | O6 | 20 | MET |
| 60 | O6 | 21 | THR |
| 60 | O6 | 26 | ILE |
| 60 | O6 | 29 | LYS |
| 60 | O6 | 36 | ARG |
| 60 | O6 | 45 | ARG |
| 60 | O6 | 57 | LEU |
| 60 | O6 | 58 | ILE |
| 60 | O6 | 60 | LEU |
| 60 | O6 | 62 | ARG |
| 60 | O6 | 63 | ASN |
| 60 | O6 | 68 | ARG |
| 60 | O6 | 76 | ARG |
| 60 | O6 | 79 | SER |
| 60 | O6 | 81 | THR |
| 60 | O6 | 99 | ARG |
| 61 | o7 | 17 | THR |
| 61 | o7 | 34 | CYS |
| 61 | o7 | 36 | SER |
| 61 | o7 | 55 | ARG |
| 61 | o7 | 59 | THR |
| 61 | o7 | 67 | LEU |
| 61 | o7 | 68 | LYS |
| 61 | o7 | 71 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 61 | o7 | 80 | THR |
| 61 | O7 | 5 | THR |
| 61 | O7 | 12 | HIS |
| 61 | O7 | 16 | HIS |
| 61 | O7 | 17 | THR |
| 61 | O7 | 19 | CYS |
| 61 | O7 | 24 | ARG |
| 61 | O7 | 25 | ARG |
| 61 | O7 | 33 | THR |
| 61 | O7 | 34 | CYS |
| 61 | O7 | 36 | SER |
| 61 | O7 | 43 | LYS |
| 61 | O7 | 58 | THR |
| 61 | O7 | 59 | THR |
| 61 | O7 | 67 | LEU |
| 61 | O7 | 75 | LYS |
| 61 | O7 | 87 | SER |
| 62 | o8 | 5 | ILE |
| 62 | o8 | 6 | THR |
| 62 | o8 | 24 | THR |
| 62 | o8 | 41 | THR |
| 62 | o8 | 50 | SER |
| 62 | o8 | 53 | THR |
| 62 | o8 | 61 | LYS |
| 62 | o8 | 63 | LYS |
| 62 | o8 | 64 | LYS |
| 62 | o8 | 65 | LEU |
| 62 | O8 | 5 | ILE |
| 62 | O8 | 6 | THR |
| 62 | O8 | 8 | ILE |
| 62 | O8 | 24 | THR |
| 62 | O8 | 31 | LEU |
| 62 | O8 | 41 | THR |
| 62 | O8 | 45 | VAL |
| 62 | O8 | 48 | SER |
| 62 | O8 | 51 | LEU |
| 62 | O8 | 52 | TYR |
| 62 | O8 | 53 | THR |
| 62 | O8 | 58 | ASP |
| 62 | O8 | 64 | LYS |
| 62 | O8 | 65 | LEU |
| 62 | O8 | 67 | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 62 | O8 | 77 | ARG |
| 63 | o9 | 15 | LYS |
| 63 | o9 | 21 | ARG |
| 63 | o9 | 23 | LEU |
| 63 | o9 | 29 | LEU |
| 63 | o9 | 45 | ARG |
| 63 | O9 | 4 | GLN |
| 63 | O9 | 5 | LYS |
| 63 | O9 | 21 | ARG |
| 63 | O9 | 23 | LEU |
| 63 | O9 | 36 | ARG |
| 63 | O9 | 45 | ARG |
| 63 | O9 | 49 | MET |
| 63 | O9 | 51 | ILE |
| 64 | q0 | 78 | ILE |
| 64 | q0 | 79 | GLU |
| 64 | q0 | 85 | LEU |
| 64 | q0 | 112 | LYS |
| 64 | q0 | 113 | ARG |
| 64 | q0 | 114 | LYS |
| 64 | q0 | 127 | LEU |
| 64 | Q0 | 85 | LEU |
| 64 | Q0 | 92 | ASP |
| 64 | Q0 | 94 | SER |
| 64 | Q0 | 97 | ARG |
| 64 | Q0 | 106 | ARG |
| 64 | Q0 | 113 | ARG |
| 64 | Q0 | 127 | LEU |
| 65 | q1 | 6 | ARG |
| 65 | q1 | 9 | ARG |
| 65 | q1 | 13 | LEU |
| 65 | q1 | 23 | ARG |
| 65 | Q1 | 2 | ARG |
| 65 | Q1 | 11 | ARG |
| 65 | Q1 | 19 | LYS |
| 65 | Q1 | 21 | ARG |
| 66 | q2 | 7 | THR |
| 66 | q2 | 8 | ARG |
| 66 | q2 | 34 | SER |
| 66 | q2 | 45 | ARG |
| 66 | q2 | 61 | LYS |
| 66 | q2 | 71 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 66 | q2 | 78 | LYS |
| 66 | q2 | 83 | LEU |
| 66 | q2 | 84 | THR |
| 66 | q2 | 85 | LEU |
| 66 | q2 | 89 | LYS |
| 66 | q2 | 93 | LEU |
| 66 | q2 | 104 | LEU |
| 66 | Q2 | 8 | ARG |
| 66 | Q2 | 9 | LYS |
| 66 | Q2 | 20 | HIS |
| 66 | Q2 | 29 | LYS |
| 66 | Q2 | 34 | SER |
| 66 | Q2 | 60 | LYS |
| 66 | Q2 | 61 | LYS |
| 66 | Q2 | 71 | ARG |
| 66 | Q2 | 72 | LEU |
| 66 | Q2 | 76 | LYS |
| 66 | Q2 | 78 | LYS |
| 66 | Q2 | 79 | THR |
| 66 | Q2 | 80 | ARG |
| 66 | Q2 | 83 | LEU |
| 66 | Q2 | 84 | THR |
| 66 | Q2 | 85 | LEU |
| 66 | Q2 | 93 | LEU |
| 66 | Q2 | 104 | LEU |
| 66 | Q2 | 105 | GLN |
| 67 | q3 | 3 | LYS |
| 67 | q3 | 24 | ARG |
| 67 | q3 | 36 | ARG |
| 67 | q3 | 42 | CYS |
| 67 | q3 | 45 | LYS |
| 67 | q3 | 46 | THR |
| 67 | q3 | 48 | LYS |
| 67 | q3 | 54 | ILE |
| 67 | q3 | 56 | THR |
| 67 | q3 | 57 | CYS |
| 67 | q3 | 59 | CYS |
| 67 | q3 | 60 | CYS |
| 67 | q3 | 80 | ARG |
| 67 | Q3 | 7 | LYS |
| 67 | Q3 | 11 | THR |
| 67 | Q3 | 24 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 67 | Q3 | 25 | GLN |
| 67 | Q3 | 45 | LYS |
| 67 | Q3 | 46 | THR |
| 67 | Q3 | 49 | ARG |
| 67 | Q3 | 60 | CYS |
| 67 | Q3 | 78 | THR |
| 67 | Q3 | 91 | GLU |
| 68 | S0 | 7 | PHE |
| 68 | S0 | 10 | THR |
| 68 | S0 | 27 | ARG |
| 68 | S0 | 45 | VAL |
| 68 | S0 | 50 | VAL |
| 68 | S0 | 57 | LEU |
| 68 | S0 | 62 | ARG |
| 68 | S0 | 76 | ILE |
| 68 | S0 | 84 | ARG |
| 68 | S0 | 87 | LEU |
| 68 | S0 | 88 | LYS |
| 68 | S0 | 101 | ARG |
| 68 | S0 | 103 | THR |
| 68 | S0 | 111 | ILE |
| 68 | S0 | 112 | THR |
| 68 | S0 | 117 | GLU |
| 68 | S0 | 119 | ARG |
| 68 | S0 | 123 | VAL |
| 68 | S0 | 131 | GLN |
| 68 | S0 | 135 | GLU |
| 68 | S0 | 139 | VAL |
| 68 | S0 | 154 | GLU |
| 68 | S0 | 157 | ASP |
| 68 | S0 | 165 | ARG |
| 68 | S0 | 170 | ILE |
| 68 | S0 | 172 | LEU |
| 68 | S0 | 177 | LEU |
| 68 | S0 | 184 | LEU |
| 68 | S0 | 185 | ARG |
| 68 | S0 | 200 | ASP |
| 68 | s0 | 6 | THR |
| 68 | s0 | 8 | ASP |
| 68 | s0 | 9 | LEU |
| 68 | s0 | 30 | GLN |
| 68 | s0 | 45 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 68 | s0 | 57 | LEU |
| 68 | s0 | 59 | LEU |
| 68 | s0 | 62 | ARG |
| 68 | s0 | 87 | LEU |
| 68 | s0 | 88 | LYS |
| 68 | s0 | 93 | THR |
| 68 | s0 | 101 | ARG |
| 68 | s0 | 103 | THR |
| 68 | s0 | 111 | ILE |
| 68 | s0 | 119 | ARG |
| 68 | s0 | 131 | GLN |
| 68 | s0 | 139 | VAL |
| 68 | s0 | 157 | ASP |
| 68 | s0 | 162 | CYS |
| 68 | s0 | 164 | ASN |
| 68 | s0 | 167 | LYS |
| 68 | s0 | 172 | LEU |
| 68 | s0 | 180 | GLU |
| 68 | s0 | 185 | ARG |
| 68 | s0 | 196 | SER |
| 68 | s0 | 202 | TYR |
| 68 | s0 | 203 | PHE |
| 69 | S1 | 21 | VAL |
| 69 | S1 | 22 | ASP |
| 69 | S1 | 24 | PHE |
| 69 | S1 | 25 | THR |
| 69 | S1 | 28 | GLU |
| 69 | S1 | 29 | TRP |
| 69 | S1 | 30 | PHE |
| 69 | S1 | 38 | PHE |
| 69 | S1 | 46 | THR |
| 69 | S1 | 47 | LEU |
| 69 | S1 | 55 | LYS |
| 69 | S1 | 58 | SER |
| 69 | S1 | 61 | LEU |
| 69 | S1 | 64 | ARG |
| 69 | S1 | 66 | VAL |
| 69 | S1 | 70 | LEU |
| 69 | S1 | 74 | GLN |
| 69 | S1 | 77 | GLU |
| 69 | S1 | 78 | ASP |
| 69 | S1 | 81 | PHE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 69 | S1 | 85 | LYS |
| 69 | S1 | 96 | LEU |
| 69 | S1 | 97 | LEU |
| 69 | S1 | 105 | PHE |
| 69 | S1 | 108 | ASP |
| 69 | S1 | 111 | ARG |
| 69 | S1 | 117 | TRP |
| 69 | S1 | 131 | ASP |
| 69 | S1 | 135 | LEU |
| 69 | S1 | 146 | GLN |
| 69 | S1 | 148 | ASN |
| 69 | S1 | 149 | GLN |
| 69 | S1 | 150 | VAL |
| 69 | S1 | 154 | SER |
| 69 | S1 | 177 | GLN |
| 69 | S1 | 180 | THR |
| 69 | S1 | 181 | LEU |
| 69 | S1 | 183 | GLN |
| 69 | S1 | 184 | LEU |
| 69 | S1 | 193 | ILE |
| 69 | S1 | 202 | LYS |
| 69 | S1 | 214 | LYS |
| 69 | S1 | 218 | LEU |
| 69 | S1 | 220 | GLN |
| 69 | S1 | 222 | LYS |
| 69 | S1 | 223 | PHE |
| 69 | S1 | 232 | HIS |
| 69 | s1 | 21 | VAL |
| 69 | s1 | 37 | THR |
| 69 | s1 | 40 | ASN |
| 69 | s1 | 47 | LEU |
| 69 | s1 | 61 | LEU |
| 69 | s1 | 62 | LYS |
| 69 | s1 | 70 | LEU |
| 69 | s1 | 81 | PHE |
| 69 | s1 | 82 | ARG |
| 69 | s1 | 83 | LYS |
| 69 | s1 | 85 | LYS |
| 69 | s1 | 88 | VAL |
| 69 | s1 | 89 | ASP |
| 69 | s1 | 90 | GLU |
| 69 | s1 | 91 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 69 | s1 | 96 | LEU |
| 69 | s1 | 105 | PHE |
| 69 | s1 | 108 | ASP |
| 69 | s1 | 110 | LEU |
| 69 | s1 | 125 | VAL |
| 69 | s1 | 150 | VAL |
| 69 | s1 | 153 | HIS |
| 69 | s1 | 159 | SER |
| 69 | s1 | 177 | GLN |
| 69 | s1 | 179 | SER |
| 69 | s1 | 180 | THR |
| 69 | s1 | 181 | LEU |
| 69 | s1 | 184 | LEU |
| 69 | s1 | 193 | ILE |
| 69 | s1 | 203 | ASP |
| 69 | s1 | 207 | LEU |
| 69 | s1 | 210 | ILE |
| 69 | s1 | 212 | VAL |
| 69 | s1 | 215 | VAL |
| 69 | s1 | 219 | LYS |
| 69 | s1 | 222 | LYS |
| 70 | S2 | 41 | LEU |
| 70 | S2 | 53 | ILE |
| 70 | S2 | 58 | LEU |
| 70 | S2 | 64 | LYS |
| 70 | S2 | 69 | ILE |
| 70 | S2 | 72 | LEU |
| 70 | S2 | 73 | LEU |
| 70 | S2 | 76 | LEU |
| 70 | S2 | 77 | GLN |
| 70 | S2 | 87 | GLN |
| 70 | S2 | 89 | GLN |
| 70 | S2 | 95 | ARG |
| 70 | S2 | 96 | THR |
| 70 | S2 | 97 | ARG |
| 70 | S2 | 108 | ASN |
| 70 | S2 | 111 | VAL |
| 70 | S2 | 117 | THR |
| 70 | S2 | 119 | LYS |
| 70 | S2 | 134 | LEU |
| 70 | S2 | 137 | ILE |
| 70 | S2 | 139 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 70 | S2 | 140 | ARG |
| 70 | S2 | 141 | ARG |
| 70 | S2 | 146 | THR |
| 70 | S2 | 148 | LEU |
| 70 | S2 | 159 | THR |
| 70 | S2 | 187 | LEU |
| 70 | S2 | 201 | ASN |
| 70 | S2 | 206 | THR |
| 70 | S2 | 208 | GLU |
| 70 | S2 | 218 | ILE |
| 70 | S2 | 221 | THR |
| 70 | S2 | 224 | PHE |
| 70 | S2 | 225 | LEU |
| 70 | S2 | 226 | THR |
| 70 | S2 | 237 | VAL |
| 70 | S2 | 240 | LEU |
| 70 | S2 | 246 | GLU |
| 70 | S2 | 250 | GLN |
| 70 | s2 | 53 | ILE |
| 70 | s2 | 55 | GLU |
| 70 | s2 | 69 | ILE |
| 70 | s2 | 72 | LEU |
| 70 | s2 | 76 | LEU |
| 70 | s2 | 77 | GLN |
| 70 | s2 | 80 | VAL |
| 70 | s2 | 81 | MET |
| 70 | s2 | 83 | ILE |
| 70 | s2 | 87 | GLN |
| 70 | s2 | 89 | GLN |
| 70 | s2 | 90 | THR |
| 70 | s2 | 97 | ARG |
| 70 | s2 | 106 | ASP |
| 70 | s2 | 111 | VAL |
| 70 | s2 | 117 | THR |
| 70 | s2 | 139 | ILE |
| 70 | s2 | 140 | ARG |
| 70 | s2 | 141 | ARG |
| 70 | s2 | 148 | LEU |
| 70 | s2 | 150 | GLN |
| 70 | s2 | 170 | ILE |
| 70 | s2 | 185 | LYS |
| 70 | s2 | 194 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 70 | s2 | 195 | ASP |
| 70 | s2 | 206 | THR |
| 70 | s2 | 207 | LEU |
| 70 | s2 | 218 | ILE |
| 70 | s2 | 225 | LEU |
| 70 | s2 | 229 | LEU |
| 70 | s2 | 233 | GLN |
| 70 | s2 | 237 | VAL |
| 70 | s2 | 250 | GLN |
| 71 | S3 | 4 | LEU |
| 71 | S3 | 7 | LYS |
| 71 | S3 | 9 | ARG |
| 71 | S3 | 10 | LYS |
| 71 | S3 | 23 | GLU |
| 71 | S3 | 57 | ASP |
| 71 | S3 | 65 | ARG |
| 71 | S3 | 66 | ILE |
| 71 | S3 | 84 | ILE |
| 71 | S3 | 92 | GLN |
| 71 | S3 | 93 | ASP |
| 71 | S3 | 94 | ARG |
| 71 | S3 | 103 | GLU |
| 71 | S3 | 105 | MET |
| 71 | S3 | 111 | ASN |
| 71 | S3 | 117 | ARG |
| 71 | S3 | 127 | MET |
| 71 | S3 | 134 | CYS |
| 71 | S3 | 141 | LYS |
| 71 | S3 | 142 | LEU |
| 71 | S3 | 151 | LYS |
| 71 | S3 | 158 | ILE |
| 71 | S3 | 170 | THR |
| 71 | S3 | 172 | THR |
| 71 | S3 | 175 | VAL |
| 71 | S3 | 176 | LEU |
| 71 | S3 | 187 | LYS |
| 71 | S3 | 190 | ARG |
| 71 | S3 | 195 | SER |
| 71 | S3 | 196 | ARG |
| 71 | S3 | 197 | THR |
| 71 | S3 | 215 | GLU |
| 71 | S3 | 218 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 71 | s3 | 4 | LEU |
| 71 | s3 | 10 | LYS |
| 71 | s3 | 21 | LEU |
| 71 | s3 | 26 | THR |
| 71 | s3 | 37 | VAL |
| 71 | s3 | 40 | ARG |
| 71 | s3 | 44 | THR |
| 71 | s3 | 55 | THR |
| 71 | s3 | 65 | ARG |
| 71 | s3 | 69 | LEU |
| 71 | s3 | 76 | ARG |
| 71 | s3 | 84 | ILE |
| 71 | s3 | 89 | GLU |
| 71 | s3 | 91 | VAL |
| 71 | s3 | 92 | GLN |
| 71 | s3 | 94 | ARG |
| 71 | s3 | 111 | ASN |
| 71 | s3 | 115 | ILE |
| 71 | s3 | 117 | ARG |
| 71 | s3 | 127 | MET |
| 71 | s3 | 148 | LYS |
| 71 | s3 | 150 | MET |
| 71 | s3 | 158 | ILE |
| 71 | s3 | 162 | GLN |
| 71 | s3 | 168 | ILE |
| 71 | s3 | 178 | ARG |
| 71 | s3 | 194 | LYS |
| 71 | s3 | 197 | THR |
| 71 | s3 | 202 | LEU |
| 71 | s3 | 212 | LYS |
| 71 | s3 | 213 | GLU |
| 71 | s3 | 215 | GLU |
| 71 | s3 | 223 | LYS |
| 71 | s3 | 225 | TYR |
| 72 | S4 | 6 | LYS |
| 72 | S4 | 7 | LYS |
| 72 | S4 | 9 | LEU |
| 72 | S4 | 23 | LEU |
| 72 | S4 | 38 | LEU |
| 72 | S4 | 39 | ARG |
| 72 | S4 | 40 | GLU |
| 72 | S4 | 67 | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 72 | S4 | 77 | ARG |
| 72 | S4 | 78 | THR |
| 72 | S4 | 92 | LEU |
| 72 | S4 | 116 | ASP |
| 72 | S4 | 126 | VAL |
| 72 | S4 | 129 | VAL |
| 72 | S4 | 133 | LYS |
| 72 | S4 | 139 | VAL |
| 72 | S4 | 146 | THR |
| 72 | S4 | 160 | VAL |
| 72 | S4 | 164 | LEU |
| 72 | S4 | 176 | ASP |
| 72 | S4 | 180 | LEU |
| 72 | S4 | 181 | VAL |
| 72 | S4 | 182 | TYR |
| 72 | S4 | 187 | ARG |
| 72 | S4 | 192 | ILE |
| 72 | S4 | 197 | HIS |
| 72 | S4 | 198 | LYS |
| 72 | S4 | 211 | LYS |
| 72 | S4 | 215 | ASP |
| 72 | S4 | 222 | LEU |
| 72 | S4 | 226 | PHE |
| 72 | S4 | 227 | VAL |
| 72 | S4 | 236 | ILE |
| 72 | S4 | 240 | LYS |
| 72 | S4 | 242 | LYS |
| 72 | S4 | 246 | LEU |
| 72 | S4 | 256 | ARG |
| 72 | S4 | 258 | GLN |
| 72 | s4 | 7 | LYS |
| 72 | s4 | 9 | LEU |
| 72 | s4 | 23 | LEU |
| 72 | s4 | 32 | SER |
| 72 | s4 | 38 | LEU |
| 72 | s4 | 39 | ARG |
| 72 | s4 | 42 | LEU |
| 72 | s4 | 49 | ARG |
| 72 | s4 | 51 | ARG |
| 72 | s4 | 67 | GLN |
| 72 | s4 | 78 | THR |
| 72 | s4 | 95 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 72 | s4 | 104 | ASP |
| 72 | s4 | 111 | VAL |
| 72 | s4 | 116 | ASP |
| 72 | s4 | 126 | VAL |
| 72 | s4 | 131 | LEU |
| 72 | s4 | 140 | VAL |
| 72 | s4 | 147 | ILE |
| 72 | s4 | 148 | ARG |
| 72 | s4 | 151 | ASP |
| 72 | s4 | 160 | VAL |
| 72 | s4 | 180 | LEU |
| 72 | s4 | 181 | VAL |
| 72 | s4 | 182 | TYR |
| 72 | s4 | 195 | ILE |
| 72 | s4 | 221 | ARG |
| 72 | s4 | 223 | ASN |
| 72 | s4 | 227 | VAL |
| 72 | s4 | 244 | ILE |
| 72 | s4 | 246 | LEU |
| 73 | S5 | 23 | VAL |
| 73 | S5 | 24 | VAL |
| 73 | S5 | 25 | LEU |
| 73 | S5 | 32 | GLU |
| 73 | S5 | 43 | PHE |
| 73 | S5 | 53 | VAL |
| 73 | S5 | 65 | ARG |
| 73 | S5 | 76 | ARG |
| 73 | S5 | 79 | ASN |
| 73 | S5 | 89 | ILE |
| 73 | S5 | 93 | LEU |
| 73 | S5 | 94 | THR |
| 73 | S5 | 99 | MET |
| 73 | S5 | 100 | ASN |
| 73 | S5 | 112 | ARG |
| 73 | S5 | 146 | THR |
| 73 | S5 | 147 | THR |
| 73 | S5 | 156 | ARG |
| 73 | S5 | 162 | VAL |
| 73 | S5 | 186 | ASN |
| 73 | S5 | 194 | LEU |
| 73 | S5 | 203 | LYS |
| 73 | S5 | 216 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 73 | S5 | 219 | ARG |
| 73 | S5 | 225 | ARG |
| 73 | s5 | 25 | LEU |
| 73 | s5 | 27 | THR |
| 73 | s5 | 31 | GLU |
| 73 | s5 | 32 | GLU |
| 73 | s5 | 39 | GLU |
| 73 | s5 | 43 | PHE |
| 73 | s5 | 51 | VAL |
| 73 | s5 | 59 | VAL |
| 73 | s5 | 63 | GLN |
| 73 | s5 | 64 | VAL |
| 73 | s5 | 68 | ILE |
| 73 | s5 | 76 | ARG |
| 73 | s5 | 84 | LYS |
| 73 | s5 | 89 | ILE |
| 73 | s5 | 93 | LEU |
| 73 | s5 | 94 | THR |
| 73 | s5 | 112 | ARG |
| 73 | s5 | 125 | THR |
| 73 | s5 | 128 | ASN |
| 73 | s5 | 130 | ILE |
| 73 | s5 | 132 | VAL |
| 73 | s5 | 133 | VAL |
| 73 | s5 | 148 | ARG |
| 73 | s5 | 156 | ARG |
| 73 | s5 | 157 | ARG |
| 73 | s5 | 161 | ASP |
| 73 | s5 | 162 | VAL |
| 73 | s5 | 170 | GLN |
| 73 | s5 | 187 | ILE |
| 73 | s5 | 188 | LYS |
| 73 | s5 | 194 | LEU |
| 73 | s5 | 203 | LYS |
| 73 | s5 | 208 | SER |
| 73 | s5 | 225 | ARG |
| 74 | S6 | 7 | TYR |
| 74 | S6 | 13 | GLN |
| 74 | S6 | 21 | GLU |
| 74 | S6 | 25 | ARG |
| 74 | S6 | 45 | PHE |
| 74 | S6 | 58 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 74 | S6 | 76 | LEU |
| 74 | S6 | 78 | THR |
| 74 | S6 | 79 | LYS |
| 74 | S6 | 82 | SER |
| 74 | S6 | 98 | ARG |
| 74 | S6 | 105 | ASP |
| 74 | S6 | 109 | LEU |
| 74 | S6 | 115 | LYS |
| 74 | S6 | 120 | GLU |
| 74 | S6 | 124 | LEU |
| 74 | S6 | 126 | ASP |
| 74 | S6 | 127 | THR |
| 74 | S6 | 129 | VAL |
| 74 | S6 | 132 | ARG |
| 74 | S6 | 133 | LEU |
| 74 | S6 | 137 | ARG |
| 74 | S6 | 143 | LYS |
| 74 | S6 | 151 | ASP |
| 74 | S6 | 154 | ARG |
| 74 | S6 | 155 | ASP |
| 74 | S6 | 163 | THR |
| 74 | S6 | 164 | LYS |
| 74 | S6 | 177 | ARG |
| 74 | S6 | 211 | LEU |
| 74 | S6 | 212 | LEU |
| 74 | S6 | 216 | LEU |
| 74 | s6 | 12 | SER |
| 74 | s6 | 15 | THR |
| 74 | s6 | 30 | LYS |
| 74 | s6 | 31 | ARG |
| 74 | s6 | 69 | LEU |
| 74 | s6 | 71 | THR |
| 74 | s6 | 78 | THR |
| 74 | s6 | 93 | LYS |
| 74 | s6 | 97 | VAL |
| 74 | s6 | 109 | LEU |
| 74 | s6 | 111 | LEU |
| 74 | s6 | 120 | GLU |
| 74 | s6 | 121 | LEU |
| 74 | s6 | 122 | GLU |
| 74 | s6 | 124 | LEU |
| 74 | s6 | 127 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 74 | s6 | 128 | THR |
| 74 | s6 | 129 | VAL |
| 74 | s6 | 143 | LYS |
| 74 | s6 | 150 | GLU |
| 74 | s6 | 151 | ASP |
| 74 | s6 | 154 | ARG |
| 74 | s6 | 155 | ASP |
| 74 | s6 | 169 | TYR |
| 74 | s6 | 170 | THR |
| 74 | s6 | 177 | ARG |
| 74 | s6 | 179 | VAL |
| 74 | s6 | 193 | LEU |
| 74 | s6 | 215 | ARG |
| 74 | s6 | 216 | LEU |
| 75 | s7 | 11 | GLN |
| 75 | s7 | 30 | SER |
| 75 | s7 | 35 | LYS |
| 75 | s7 | 41 | LEU |
| 75 | s7 | 42 | GLN |
| 75 | s7 | 49 | ILE |
| 75 | s7 | 50 | ASP |
| 75 | s7 | 67 | LEU |
| 75 | s7 | 77 | LEU |
| 75 | s7 | 86 | GLN |
| 75 | s7 | 88 | ARG |
| 75 | s7 | 97 | ARG |
| 75 | s7 | 105 | THR |
| 75 | s7 | 108 | GLN |
| 75 | s7 | 109 | VAL |
| 75 | s7 | 112 | ARG |
| 75 | s7 | 114 | ARG |
| 75 | s7 | 116 | ARG |
| 75 | s7 | 117 | THR |
| 75 | s7 | 126 | LEU |
| 75 | s7 | 134 | GLU |
| 75 | s7 | 143 | LEU |
| 75 | s7 | 144 | VAL |
| 75 | s7 | 159 | VAL |
| 75 | s7 | 162 | ILE |
| 75 | s7 | 185 | ILE |
| 75 | S7 | 9 | LEU |
| 75 | S7 | 14 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 75 | S7 | 28 | GLU |
| 75 | S7 | 29 | ASN |
| 75 | S7 | 37 | GLU |
| 75 | S7 | 38 | LEU |
| 75 | S7 | 42 | GLN |
| 75 | S7 | 46 | ILE |
| 75 | S7 | 50 | ASP |
| 75 | S7 | 60 | ILE |
| 75 | S7 | 64 | VAL |
| 75 | S7 | 70 | PHE |
| 75 | S7 | 71 | HIS |
| 75 | S7 | 75 | THR |
| 75 | S7 | 77 | LEU |
| 75 | S7 | 85 | PHE |
| 75 | S7 | 87 | ASP |
| 75 | S7 | 97 | ARG |
| 75 | S7 | 114 | ARG |
| 75 | S7 | 116 | ARG |
| 75 | S7 | 117 | THR |
| 75 | S7 | 126 | LEU |
| 75 | S7 | 131 | PHE |
| 75 | S7 | 136 | VAL |
| 75 | S7 | 139 | ARG |
| 75 | S7 | 144 | VAL |
| 75 | S7 | 163 | ASP |
| 75 | S7 | 168 | SER |
| 75 | S7 | 181 | ILE |
| 75 | S7 | 185 | ILE |
| 76 | s8 | 7 | SER |
| 76 | s8 | 8 | ARG |
| 76 | s8 | 25 | ARG |
| 76 | s8 | 28 | GLU |
| 76 | s8 | 29 | LEU |
| 76 | s8 | 36 | THR |
| 76 | s8 | 47 | ARG |
| 76 | s8 | 58 | LEU |
| 76 | s8 | 60 | ILE |
| 76 | s8 | 61 | GLU |
| 76 | s8 | 66 | SER |
| 76 | s8 | 74 | LYS |
| 76 | s8 | 76 | THR |
| 76 | s8 | 82 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 76 | s8 | 110 | ARG |
| 76 | s8 | 111 | GLN |
| 76 | s8 | 138 | ASN |
| 76 | s8 | 151 | LYS |
| 76 | s8 | 152 | ILE |
| 76 | s8 | 155 | SER |
| 76 | s8 | 168 | CYS |
| 76 | s8 | 176 | SER |
| 76 | s8 | 183 | ILE |
| 76 | s8 | 184 | LEU |
| 76 | S8 | 29 | LEU |
| 76 | S8 | 36 | THR |
| 76 | S8 | 47 | ARG |
| 76 | S8 | 49 | ARG |
| 76 | S8 | 56 | ARG |
| 76 | S8 | 58 | LEU |
| 76 | S8 | 66 | SER |
| 76 | S8 | 104 | ILE |
| 76 | S8 | 123 | LYS |
| 76 | S8 | 135 | LYS |
| 76 | S8 | 137 | LYS |
| 76 | S8 | 138 | ASN |
| 76 | S8 | 151 | LYS |
| 76 | S8 | 152 | ILE |
| 76 | S8 | 164 | ARG |
| 76 | S8 | 171 | SER |
| 76 | S8 | 184 | LEU |
| 76 | S8 | 187 | GLU |
| 76 | S8 | 193 | LEU |
| 76 | S8 | 196 | LEU |
| 77 | S9 | 3 | ARG |
| 77 | S9 | 6 | ARG |
| 77 | S9 | 7 | THR |
| 77 | S9 | 14 | THR |
| 77 | S9 | 28 | LEU |
| 77 | S9 | 39 | LYS |
| 77 | S9 | 49 | LEU |
| 77 | S9 | 60 | LEU |
| 77 | S9 | 78 | ARG |
| 77 | S9 | 79 | ARG |
| 77 | S9 | 89 | ASP |
| 77 | S9 | 92 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 77 | S9 | 93 | LEU |
| 77 | S9 | 96 | VAL |
| 77 | S9 | 97 | LEU |
| 77 | S9 | 99 | LEU |
| 77 | S9 | 105 | LEU |
| 77 | S9 | 109 | LEU |
| 77 | S9 | 110 | GLN |
| 77 | S9 | 118 | LEU |
| 77 | S9 | 126 | ARG |
| 77 | S9 | 130 | THR |
| 77 | S9 | 134 | ILE |
| 77 | S9 | 138 | LYS |
| 77 | S9 | 141 | VAL |
| 77 | S9 | 149 | ARG |
| 77 | S9 | 161 | THR |
| 77 | S9 | 171 | ARG |
| 77 | S9 | 180 | LYS |
| 77 | s9 | 3 | ARG |
| 77 | s9 | 7 | THR |
| 77 | s9 | 16 | LYS |
| 77 | s9 | 28 | LEU |
| 77 | s9 | 39 | LYS |
| 77 | s9 | 49 | LEU |
| 77 | s9 | 63 | ASP |
| 77 | s9 | 78 | ARG |
| 77 | s9 | 82 | ARG |
| 77 | s9 | 90 | LYS |
| 77 | s9 | 101 | VAL |
| 77 | s9 | 109 | LEU |
| 77 | s9 | 120 | LYS |
| 77 | s9 | 130 | THR |
| 77 | s9 | 133 | HIS |
| 77 | s9 | 134 | ILE |
| 77 | s9 | 151 | ASP |
| 77 | s9 | 152 | SER |
| 77 | s9 | 157 | ASP |
| 77 | s9 | 161 | THR |
| 77 | s9 | 180 | LYS |
| 77 | s9 | 184 | SER |
| 77 | s9 | 186 | GLU |
| 78 | sM | 30 | THR |
| 78 | sM | 37 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 78 | sM | 45 | SER |
| 78 | sM | 46 | LYS |
| 78 | sM | 48 | ARG |
| 78 | sM | 50 | ASN |
| 78 | sM | 51 | ARG |
| 78 | sM | 61 | ILE |
| 78 | sM | 68 | ARG |
| 78 | sM | 74 | LYS |
| 78 | sM | 77 | THR |
| 78 | sM | 78 | ASP |
| 78 | sM | 79 | SER |
| 78 | sM | 82 | THR |
| 78 | sM | 84 | LYS |
| 78 | sM | 88 | ARG |
| 78 | sM | 89 | ARG |
| 78 | sM | 91 | THR |
| 78 | sM | 96 | ARG |
| 78 | sM | 97 | THR |
| 78 | sM | 100 | THR |
| 78 | sM | 102 | THR |
| 78 | sM | 105 | LYS |
| 78 | sM | 112 | ASP |
| 78 | sM | 118 | SER |
| 78 | sM | 139 | GLU |
| 78 | SM | 23 | LYS |
| 78 | SM | 27 | LYS |
| 78 | SM | 30 | THR |
| 78 | SM | 34 | LYS |
| 78 | SM | 46 | LYS |
| 78 | SM | 51 | ARG |
| 78 | SM | 61 | ILE |
| 78 | SM | 63 | ASP |
| 78 | SM | 68 | ARG |
| 78 | SM | 70 | ASN |
| 78 | SM | 74 | LYS |
| 78 | SM | 75 | ASP |
| 78 | SM | 76 | VAL |
| 78 | SM | 77 | THR |
| 78 | SM | 84 | LYS |
| 78 | SM | 88 | ARG |
| 78 | SM | 89 | ARG |
| 78 | SM | 91 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 78 | SM | 97 | THR |
| 78 | SM | 100 | THR |
| 78 | SM | 102 | THR |
| 78 | SM | 105 | LYS |
| 78 | SM | 116 | GLU |
| 78 | SM | 139 | GLU |
| 79 | sR | 22 | SER |
| 79 | sR | 25 | THR |
| 79 | sR | 29 | GLN |
| 79 | sR | 42 | LEU |
| 79 | sR | 48 | THR |
| 79 | sR | 53 | LYS |
| 79 | sR | 58 | VAL |
| 79 | sR | 59 | ARG |
| 79 | sR | 64 | HIS |
| 79 | sR | 65 | SER |
| 79 | sR | 76 | ASP |
| 79 | sR | 96 | THR |
| 79 | sR | 106 | HIS |
| 79 | sR | 145 | LEU |
| 79 | sR | 163 | ASP |
| 79 | sR | 164 | ASP |
| 79 | sR | 167 | VAL |
| 79 | sR | 176 | LYS |
| 79 | sR | 184 | ASN |
| 79 | sR | 188 | ILE |
| 79 | sR | 202 | LEU |
| 79 | sR | 207 | ASP |
| 79 | sR | 232 | TYR |
| 79 | sR | 265 | LEU |
| 79 | sR | 274 | LEU |
| 79 | sR | 275 | ARG |
| 79 | sR | 297 | ASP |
| 79 | sR | 308 | ASN |
| 79 | sR | 309 | VAL |
| 79 | sR | 319 | ASN |
| 79 | SR | 4 | ASN |
| 79 | SR | 6 | VAL |
| 79 | SR | 14 | GLU |
| 79 | SR | 29 | GLN |
| 79 | SR | 44 | SER |
| 79 | SR | 46 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 79 | SR | 51 | ASP |
| 79 | SR | 52 | GLN |
| 79 | SR | 58 | VAL |
| 79 | SR | 59 | ARG |
| 79 | SR | 66 | HIS |
| 79 | SR | 76 | ASP |
| 79 | SR | 106 | HIS |
| 79 | SR | 117 | LYS |
| 79 | SR | 118 | LYS |
| 79 | SR | 123 | ILE |
| 79 | SR | 136 | ILE |
| 79 | SR | 137 | LYS |
| 79 | SR | 141 | LEU |
| 79 | SR | 153 | GLN |
| 79 | SR | 159 | ASN |
| 79 | SR | 165 | ASP |
| 79 | SR | 184 | ASN |
| 79 | SR | 195 | HIS |
| 79 | SR | 202 | LEU |
| 79 | SR | 207 | ASP |
| 79 | SR | 238 | ASP |
| 79 | SR | 250 | TYR |
| 79 | SR | 266 | ASP |
| 79 | SR | 268 | GLN |
| 79 | SR | 292 | LEU |
| 79 | SR | 308 | ASN |
| 79 | SR | 317 | THR |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 5 | c0 | 32 | HIS |
| 6 | c1 | 21 | ASN |
| 14 | c9 | 25 | GLN |
| 14 | c9 | 64 | HIS |
| 14 | c9 | 138 | GLN |
| 17 | d2 | 24 | GLN |
| 17 | d2 | 56 | HIS |
| 17 | D2 | 64 | GLN |
| 19 | d4 | 22 | GLN |
| 24 | D9 | 48 | ASN |
| 24 | D9 | 53 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | e0 | 17 | GLN |
| 27 | l2 | 83 | HIS |
| 27 | l2 | 86 | GLN |
| 27 | l2 | 194 | ASN |
| 30 | l5 | 40 | HIS |
| 31 | L6 | 97 | ASN |
| 33 | L8 | 145 | ASN |
| 33 | L8 | 240 | ASN |
| 34 | L9 | 5 | GLN |
| 35 | M0 | 14 | ASN |
| 36 | m1 | 109 | HIS |
| 37 | m3 | 114 | GLN |
| 39 | m5 | 138 | GLN |
| 39 | M5 | 87 | GLN |
| 39 | M5 | 138 | GLN |
| 42 | m8 | 58 | ASN |
| 45 | n1 | 146 | ASN |
| 47 | N3 | 98 | ASN |
| 51 | n7 | 57 | HIS |
| 52 | n8 | 14 | HIS |
| 52 | n8 | 28 | HIS |
| 52 | n8 | 64 | GLN |
| 52 | N8 | 41 | HIS |
| 53 | n9 | 43 | HIS |
| 53 | N9 | 45 | HIS |
| 56 | O2 | 35 | GLN |
| 59 | O5 | 16 | GLN |
| 61 | o7 | 12 | HIS |
| 63 | o9 | 4 | GLN |
| 66 | Q2 | 47 | GLN |
| 69 | S1 | 124 | ASN |
| 69 | S1 | 157 | GLN |
| 69 | s1 | 146 | GLN |
| 69 | s1 | 149 | GLN |
| 70 | s2 | 89 | GLN |
| 70 | s2 | 94 | GLN |
| 71 | s3 | 74 | GLN |
| 73 | s5 | 37 | GLN |
| 74 | s6 | 80 | ASN |
| 79 | sR | 106 | HIS |
| 79 | sR | 182 | ASN |
| 79 | sR | 184 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 79 | sR | 198 | ASN |
| 79 | SR | 195 | HIS |
| 79 | SR | 288 | HIS |

5.3.3 RNA [i](#)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------------|-------------------|-----------------|
| 1 | 1 | 3084/3396 (90%) | 644 (20%) | 99 (3%) |
| 1 | 5 | 3071/3396 (90%) | 615 (20%) | 70 (2%) |
| 2 | 2 | 1767/1800 (98%) | 481 (27%) | 62 (3%) |
| 2 | 6 | 1731/1800 (96%) | 411 (23%) | 55 (3%) |
| 3 | 3 | 120/121 (99%) | 17 (14%) | 1 (0%) |
| 3 | 7 | 120/121 (99%) | 15 (12%) | 1 (0%) |
| 4 | 4 | 157/158 (99%) | 32 (20%) | 4 (2%) |
| 4 | 8 | 157/158 (99%) | 33 (21%) | 4 (2%) |
| All | All | 10207/10950 (93%) | 2248 (22%) | 296 (2%) |

All (2248) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1 | 14 | U |
| 1 | 1 | 16 | A |
| 1 | 1 | 26 | A |
| 1 | 1 | 40 | A |
| 1 | 1 | 43 | A |
| 1 | 1 | 49 | A |
| 1 | 1 | 59 | G |
| 1 | 1 | 60 | A |
| 1 | 1 | 65 | A |
| 1 | 1 | 66 | A |
| 1 | 1 | 74 | G |
| 1 | 1 | 76 | G |
| 1 | 1 | 92 | G |
| 1 | 1 | 93 | C |
| 1 | 1 | 99 | A |
| 1 | 1 | 109 | A |
| 1 | 1 | 110 | G |
| 1 | 1 | 121 | A |
| 1 | 1 | 122 | A |
| 1 | 1 | 132 | C |
| 1 | 1 | 133 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 136 | G |
| 1 | 1 | 156 | G |
| 1 | 1 | 157 | A |
| 1 | 1 | 166 | C |
| 1 | 1 | 169 | U |
| 1 | 1 | 173 | G |
| 1 | 1 | 184 | U |
| 1 | 1 | 187 | A |
| 1 | 1 | 190 | U |
| 1 | 1 | 191 | U |
| 1 | 1 | 192 | C |
| 1 | 1 | 193 | C |
| 1 | 1 | 199 | A |
| 1 | 1 | 200 | C |
| 1 | 1 | 210 | U |
| 1 | 1 | 213 | A |
| 1 | 1 | 214 | G |
| 1 | 1 | 218 | G |
| 1 | 1 | 219 | A |
| 1 | 1 | 220 | G |
| 1 | 1 | 231 | G |
| 1 | 1 | 232 | G |
| 1 | 1 | 235 | A |
| 1 | 1 | 236 | G |
| 1 | 1 | 237 | G |
| 1 | 1 | 238 | A |
| 1 | 1 | 239 | G |
| 1 | 1 | 240 | U |
| 1 | 1 | 241 | G |
| 1 | 1 | 245 | U |
| 1 | 1 | 249 | U |
| 1 | 1 | 250 | U |
| 1 | 1 | 251 | G |
| 1 | 1 | 252 | U |
| 1 | 1 | 253 | A |
| 1 | 1 | 269 | G |
| 1 | 1 | 270 | U |
| 1 | 1 | 283 | G |
| 1 | 1 | 286 | U |
| 1 | 1 | 295 | A |
| 1 | 1 | 296 | A |
| 1 | 1 | 298 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 311 | C |
| 1 | 1 | 315 | C |
| 1 | 1 | 322 | U |
| 1 | 1 | 323 | A |
| 1 | 1 | 329 | U |
| 1 | 1 | 339 | C |
| 1 | 1 | 349 | A |
| 1 | 1 | 350 | C |
| 1 | 1 | 370 | U |
| 1 | 1 | 375 | A |
| 1 | 1 | 376 | G |
| 1 | 1 | 398 | A |
| 1 | 1 | 401 | U |
| 1 | 1 | 402 | A |
| 1 | 1 | 403 | C |
| 1 | 1 | 421 | G |
| 1 | 1 | 422 | A |
| 1 | 1 | 439 | C |
| 1 | 1 | 440 | A |
| 1 | 1 | 495 | G |
| 1 | 1 | 516 | A |
| 1 | 1 | 518 | G |
| 1 | 1 | 520 | U |
| 1 | 1 | 521 | A |
| 1 | 1 | 535 | G |
| 1 | 1 | 543 | C |
| 1 | 1 | 544 | C |
| 1 | 1 | 545 | U |
| 1 | 1 | 546 | C |
| 1 | 1 | 547 | G |
| 1 | 1 | 548 | G |
| 1 | 1 | 551 | A |
| 1 | 1 | 552 | G |
| 1 | 1 | 555 | U |
| 1 | 1 | 556 | U |
| 1 | 1 | 557 | A |
| 1 | 1 | 558 | U |
| 1 | 1 | 559 | A |
| 1 | 1 | 569 | A |
| 1 | 1 | 578 | A |
| 1 | 1 | 579 | G |
| 1 | 1 | 592 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 604 | G |
| 1 | 1 | 609 | G |
| 1 | 1 | 611 | A |
| 1 | 1 | 620 | U |
| 1 | 1 | 621 | A |
| 1 | 1 | 622 | A |
| 1 | 1 | 637 | C |
| 1 | 1 | 638 | C |
| 1 | 1 | 646 | A |
| 1 | 1 | 649 | A |
| 1 | 1 | 654 | C |
| 1 | 1 | 658 | G |
| 1 | 1 | 677 | A |
| 1 | 1 | 681 | U |
| 1 | 1 | 683 | U |
| 1 | 1 | 705 | A |
| 1 | 1 | 712 | G |
| 1 | 1 | 715 | A |
| 1 | 1 | 716 | A |
| 1 | 1 | 727 | G |
| 1 | 1 | 758 | C |
| 1 | 1 | 762 | U |
| 1 | 1 | 764 | U |
| 1 | 1 | 765 | C |
| 1 | 1 | 766 | U |
| 1 | 1 | 767 | U |
| 1 | 1 | 776 | U |
| 1 | 1 | 777 | U |
| 1 | 1 | 781 | G |
| 1 | 1 | 785 | G |
| 1 | 1 | 786 | A |
| 1 | 1 | 801 | A |
| 1 | 1 | 806 | A |
| 1 | 1 | 807 | A |
| 1 | 1 | 808 | 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 |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 896 | A |
| 1 | 1 | 907 | G |
| 1 | 1 | 908 | G |
| 1 | 1 | 913 | A |
| 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 | 937 | G |
| 1 | 1 | 943 | U |
| 1 | 1 | 944 | C |
| 1 | 1 | 953 | G |
| 1 | 1 | 959 | C |
| 1 | 1 | 960 | U |
| 1 | 1 | 974 | G |
| 1 | 1 | 978 | G |
| 1 | 1 | 979 | U |
| 1 | 1 | 980 | A |
| 1 | 1 | 981 | U |
| 1 | 1 | 982 | C |
| 1 | 1 | 993 | G |
| 1 | 1 | 994 | G |
| 1 | 1 | 1001 | G |
| 1 | 1 | 1002 | A |
| 1 | 1 | 1006 | A |
| 1 | 1 | 1010 | G |
| 1 | 1 | 1015 | U |
| 1 | 1 | 1016 | C |
| 1 | 1 | 1017 | C |
| 1 | 1 | 1018 | G |
| 1 | 1 | 1020 | G |
| 1 | 1 | 1021 | G |
| 1 | 1 | 1023 | C |
| 1 | 1 | 1024 | G |
| 1 | 1 | 1025 | A |
| 1 | 1 | 1027 | A |
| 1 | 1 | 1028 | U |
| 1 | 1 | 1029 | G |
| 1 | 1 | 1030 | A |
| 1 | 1 | 1033 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 1036 | A |
| 1 | 1 | 1037 | C |
| 1 | 1 | 1041 | U |
| 1 | 1 | 1047 | A |
| 1 | 1 | 1049 | C |
| 1 | 1 | 1052 | U |
| 1 | 1 | 1057 | A |
| 1 | 1 | 1064 | A |
| 1 | 1 | 1065 | A |
| 1 | 1 | 1071 | U |
| 1 | 1 | 1072 | G |
| 1 | 1 | 1081 | U |
| 1 | 1 | 1082 | U |
| 1 | 1 | 1087 | G |
| 1 | 1 | 1093 | A |
| 1 | 1 | 1094 | U |
| 1 | 1 | 1095 | U |
| 1 | 1 | 1096 | U |
| 1 | 1 | 1097 | G |
| 1 | 1 | 1098 | A |
| 1 | 1 | 1103 | A |
| 1 | 1 | 1104 | G |
| 1 | 1 | 1117 | G |
| 1 | 1 | 1128 | U |
| 1 | 1 | 1129 | A |
| 1 | 1 | 1131 | G |
| 1 | 1 | 1144 | U |
| 1 | 1 | 1153 | A |
| 1 | 1 | 1159 | A |
| 1 | 1 | 1160 | C |
| 1 | 1 | 1177 | G |
| 1 | 1 | 1180 | A |
| 1 | 1 | 1181 | U |
| 1 | 1 | 1182 | A |
| 1 | 1 | 1191 | U |
| 1 | 1 | 1192 | C |
| 1 | 1 | 1193 | A |
| 1 | 1 | 1201 | C |
| 1 | 1 | 1202 | A |
| 1 | 1 | 1206 | G |
| 1 | 1 | 1209 | G |
| 1 | 1 | 1218 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 1219 | C |
| 1 | 1 | 1221 | A |
| 1 | 1 | 1222 | G |
| 1 | 1 | 1225 | A |
| 1 | 1 | 1285 | G |
| 1 | 1 | 1292 | C |
| 1 | 1 | 1305 | U |
| 1 | 1 | 1307 | G |
| 1 | 1 | 1308 | A |
| 1 | 1 | 1309 | U |
| 1 | 1 | 1312 | C |
| 1 | 1 | 1313 | G |
| 1 | 1 | 1318 | A |
| 1 | 1 | 1325 | U |
| 1 | 1 | 1330 | A |
| 1 | 1 | 1348 | U |
| 1 | 1 | 1356 | U |
| 1 | 1 | 1357 | G |
| 1 | 1 | 1386 | A |
| 1 | 1 | 1392 | G |
| 1 | 1 | 1399 | A |
| 1 | 1 | 1400 | G |
| 1 | 1 | 1408 | G |
| 1 | 1 | 1416 | C |
| 1 | 1 | 1417 | G |
| 1 | 1 | 1419 | A |
| 1 | 1 | 1434 | G |
| 1 | 1 | 1437 | C |
| 1 | 1 | 1446 | A |
| 1 | 1 | 1450 | G |
| 1 | 1 | 1467 | A |
| 1 | 1 | 1481 | A |
| 1 | 1 | 1482 | A |
| 1 | 1 | 1485 | G |
| 1 | 1 | 1488 | G |
| 1 | 1 | 1503 | A |
| 1 | 1 | 1508 | C |
| 1 | 1 | 1533 | U |
| 1 | 1 | 1536 | G |
| 1 | 1 | 1539 | A |
| 1 | 1 | 1541 | G |
| 1 | 1 | 1547 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 1555 | U |
| 1 | 1 | 1556 | C |
| 1 | 1 | 1557 | A |
| 1 | 1 | 1560 | G |
| 1 | 1 | 1562 | C |
| 1 | 1 | 1563 | C |
| 1 | 1 | 1564 | U |
| 1 | 1 | 1565 | G |
| 1 | 1 | 1567 | U |
| 1 | 1 | 1568 | U |
| 1 | 1 | 1569 | U |
| 1 | 1 | 1570 | U |
| 1 | 1 | 1571 | A |
| 1 | 1 | 1572 | U |
| 1 | 1 | 1573 | G |
| 1 | 1 | 1574 | C |
| 1 | 1 | 1575 | A |
| 1 | 1 | 1576 | G |
| 1 | 1 | 1578 | C |
| 1 | 1 | 1580 | A |
| 1 | 1 | 1581 | C |
| 1 | 1 | 1582 | C |
| 1 | 1 | 1583 | A |
| 1 | 1 | 1587 | A |
| 1 | 1 | 1589 | A |
| 1 | 1 | 1593 | A |
| 1 | 1 | 1605 | A |
| 1 | 1 | 1607 | U |
| 1 | 1 | 1608 | C |
| 1 | 1 | 1620 | U |
| 1 | 1 | 1629 | U |
| 1 | 1 | 1632 | A |
| 1 | 1 | 1633 | C |
| 1 | 1 | 1639 | C |
| 1 | 1 | 1641 | U |
| 1 | 1 | 1643 | A |
| 1 | 1 | 1645 | U |
| 1 | 1 | 1657 | C |
| 1 | 1 | 1683 | A |
| 1 | 1 | 1687 | U |
| 1 | 1 | 1716 | U |
| 1 | 1 | 1717 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 1724 | U |
| 1 | 1 | 1725 | C |
| 1 | 1 | 1729 | A |
| 1 | 1 | 1736 | G |
| 1 | 1 | 1741 | A |
| 1 | 1 | 1750 | A |
| 1 | 1 | 1751 | G |
| 1 | 1 | 1759 | C |
| 1 | 1 | 1760 | A |
| 1 | 1 | 1761 | C |
| 1 | 1 | 1762 | C |
| 1 | 1 | 1763 | U |
| 1 | 1 | 1764 | U |
| 1 | 1 | 1765 | U |
| 1 | 1 | 1766 | G |
| 1 | 1 | 1767 | C |
| 1 | 1 | 1768 | U |
| 1 | 1 | 1770 | G |
| 1 | 1 | 1775 | G |
| 1 | 1 | 1780 | G |
| 1 | 1 | 1795 | U |
| 1 | 1 | 1797 | A |
| 1 | 1 | 1808 | G |
| 1 | 1 | 1810 | A |
| 1 | 1 | 1814 | A |
| 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 | 1841 | A |
| 1 | 1 | 1842 | A |
| 1 | 1 | 1845 | G |
| 1 | 1 | 1847 | A |
| 1 | 1 | 1849 | C |
| 1 | 1 | 1858 | A |
| 1 | 1 | 1867 | A |
| 1 | 1 | 1878 | G |
| 1 | 1 | 1879 | A |
| 1 | 1 | 1880 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 1886 | A |
| 1 | 1 | 1906 | G |
| 1 | 1 | 1915 | A |
| 1 | 1 | 1951 | C |
| 1 | 1 | 1952 | G |
| 1 | 1 | 2094 | C |
| 1 | 1 | 2101 | C |
| 1 | 1 | 2102 | U |
| 1 | 1 | 2107 | A |
| 1 | 1 | 2112 | U |
| 1 | 1 | 2113 | A |
| 1 | 1 | 2114 | C |
| 1 | 1 | 2121 | G |
| 1 | 1 | 2122 | G |
| 1 | 1 | 2125 | A |
| 1 | 1 | 2130 | G |
| 1 | 1 | 2131 | A |
| 1 | 1 | 2140 | U |
| 1 | 1 | 2158 | A |
| 1 | 1 | 2169 | G |
| 1 | 1 | 2170 | U |
| 1 | 1 | 2171 | G |
| 1 | 1 | 2201 | G |
| 1 | 1 | 2205 | U |
| 1 | 1 | 2206 | G |
| 1 | 1 | 2207 | A |
| 1 | 1 | 2208 | A |
| 1 | 1 | 2209 | U |
| 1 | 1 | 2210 | G |
| 1 | 1 | 2225 | U |
| 1 | 1 | 2228 | A |
| 1 | 1 | 2244 | A |
| 1 | 1 | 2249 | G |
| 1 | 1 | 2250 | G |
| 1 | 1 | 2252 | A |
| 1 | 1 | 2255 | A |
| 1 | 1 | 2256 | A |
| 1 | 1 | 2257 | C |
| 1 | 1 | 2272 | G |
| 1 | 1 | 2273 | G |
| 1 | 1 | 2280 | A |
| 1 | 1 | 2281 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 2282 | U |
| 1 | 1 | 2284 | C |
| 1 | 1 | 2288 | G |
| 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 | 2372 | A |
| 1 | 1 | 2373 | A |
| 1 | 1 | 2374 | C |
| 1 | 1 | 2375 | G |
| 1 | 1 | 2385 | G |
| 1 | 1 | 2393 | G |
| 1 | 1 | 2397 | A |
| 1 | 1 | 2401 | A |
| 1 | 1 | 2402 | A |
| 1 | 1 | 2403 | G |
| 1 | 1 | 2404 | A |
| 1 | 1 | 2411 | U |
| 1 | 1 | 2418 | G |
| 1 | 1 | 2419 | A |
| 1 | 1 | 2435 | G |
| 1 | 1 | 2437 | G |
| 1 | 1 | 2444 | C |
| 1 | 1 | 2505 | U |
| 1 | 1 | 2514 | U |
| 1 | 1 | 2515 | A |
| 1 | 1 | 2522 | G |
| 1 | 1 | 2523 | A |
| 1 | 1 | 2525 | G |
| 1 | 1 | 2526 | C |
| 1 | 1 | 2531 | C |
| 1 | 1 | 2532 | U |
| 1 | 1 | 2533 | G |
| 1 | 1 | 2537 | U |
| 1 | 1 | 2538 | U |
| 1 | 1 | 2539 | C |
| 1 | 1 | 2540 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 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 | 2553 | U |
| 1 | 1 | 2554 | A |
| 1 | 1 | 2555 | G |
| 1 | 1 | 2561 | A |
| 1 | 1 | 2567 | C |
| 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 | 2574 | G |
| 1 | 1 | 2577 | C |
| 1 | 1 | 2581 | U |
| 1 | 1 | 2585 | G |
| 1 | 1 | 2593 | A |
| 1 | 1 | 2594 | C |
| 1 | 1 | 2595 | A |
| 1 | 1 | 2606 | G |
| 1 | 1 | 2607 | G |
| 1 | 1 | 2614 | G |
| 1 | 1 | 2618 | G |
| 1 | 1 | 2619 | G |
| 1 | 1 | 2626 | A |
| 1 | 1 | 2634 | U |
| 1 | 1 | 2638 | C |
| 1 | 1 | 2652 | U |
| 1 | 1 | 2656 | A |
| 1 | 1 | 2657 | A |
| 1 | 1 | 2674 | A |
| 1 | 1 | 2676 | A |
| 1 | 1 | 2677 | G |
| 1 | 1 | 2681 | U |
| 1 | 1 | 2689 | A |
| 1 | 1 | 2690 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 2691 | A |
| 1 | 1 | 2694 | A |
| 1 | 1 | 2696 | A |
| 1 | 1 | 2705 | A |
| 1 | 1 | 2714 | G |
| 1 | 1 | 2719 | U |
| 1 | 1 | 2728 | G |
| 1 | 1 | 2729 | U |
| 1 | 1 | 2752 | U |
| 1 | 1 | 2753 | G |
| 1 | 1 | 2760 | C |
| 1 | 1 | 2762 | A |
| 1 | 1 | 2772 | C |
| 1 | 1 | 2777 | G |
| 1 | 1 | 2778 | G |
| 1 | 1 | 2779 | A |
| 1 | 1 | 2796 | G |
| 1 | 1 | 2799 | A |
| 1 | 1 | 2800 | G |
| 1 | 1 | 2801 | A |
| 1 | 1 | 2802 | A |
| 1 | 1 | 2810 | C |
| 1 | 1 | 2817 | A |
| 1 | 1 | 2818 | U |
| 1 | 1 | 2838 | A |
| 1 | 1 | 2842 | U |
| 1 | 1 | 2843 | U |
| 1 | 1 | 2845 | A |
| 1 | 1 | 2846 | U |
| 1 | 1 | 2853 | A |
| 1 | 1 | 2856 | G |
| 1 | 1 | 2860 | U |
| 1 | 1 | 2867 | C |
| 1 | 1 | 2871 | G |
| 1 | 1 | 2872 | A |
| 1 | 1 | 2873 | U |
| 1 | 1 | 2875 | U |
| 1 | 1 | 2887 | A |
| 1 | 1 | 2889 | C |
| 1 | 1 | 2896 | A |
| 1 | 1 | 2898 | G |
| 1 | 1 | 2899 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 2922 | G |
| 1 | 1 | 2923 | U |
| 1 | 1 | 2927 | C |
| 1 | 1 | 2935 | U |
| 1 | 1 | 2936 | A |
| 1 | 1 | 2938 | G |
| 1 | 1 | 2942 | C |
| 1 | 1 | 2945 | G |
| 1 | 1 | 2947 | G |
| 1 | 1 | 2951 | G |
| 1 | 1 | 2952 | G |
| 1 | 1 | 2957 | G |
| 1 | 1 | 2971 | A |
| 1 | 1 | 2974 | U |
| 1 | 1 | 2983 | C |
| 1 | 1 | 2990 | G |
| 1 | 1 | 2992 | U |
| 1 | 1 | 2997 | G |
| 1 | 1 | 3000 | A |
| 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 | 3116 | G |
| 1 | 1 | 3122 | A |
| 1 | 1 | 3123 | A |
| 1 | 1 | 3130 | A |
| 1 | 1 | 3131 | U |
| 1 | 1 | 3139 | A |
| 1 | 1 | 3142 | A |
| 1 | 1 | 3143 | C |
| 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 | 3158 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 3164 | C |
| 1 | 1 | 3165 | A |
| 1 | 1 | 3168 | A |
| 1 | 1 | 3169 | U |
| 1 | 1 | 3170 | A |
| 1 | 1 | 3171 | U |
| 1 | 1 | 3173 | G |
| 1 | 1 | 3174 | A |
| 1 | 1 | 3175 | U |
| 1 | 1 | 3176 | G |
| 1 | 1 | 3179 | U |
| 1 | 1 | 3180 | A |
| 1 | 1 | 3181 | C |
| 1 | 1 | 3187 | A |
| 1 | 1 | 3194 | C |
| 1 | 1 | 3199 | G |
| 1 | 1 | 3207 | U |
| 1 | 1 | 3210 | A |
| 1 | 1 | 3213 | A |
| 1 | 1 | 3217 | C |
| 1 | 1 | 3218 | A |
| 1 | 1 | 3219 | G |
| 1 | 1 | 3223 | A |
| 1 | 1 | 3224 | G |
| 1 | 1 | 3228 | C |
| 1 | 1 | 3229 | G |
| 1 | 1 | 3235 | C |
| 1 | 1 | 3239 | G |
| 1 | 1 | 3242 | G |
| 1 | 1 | 3245 | A |
| 1 | 1 | 3246 | G |
| 1 | 1 | 3247 | G |
| 1 | 1 | 3253 | G |
| 1 | 1 | 3259 | U |
| 1 | 1 | 3265 | C |
| 1 | 1 | 3270 | U |
| 1 | 1 | 3273 | A |
| 1 | 1 | 3276 | G |
| 1 | 1 | 3279 | A |
| 1 | 1 | 3281 | U |
| 1 | 1 | 3286 | G |
| 1 | 1 | 3287 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 3289 | G |
| 1 | 1 | 3294 | A |
| 1 | 1 | 3295 | A |
| 1 | 1 | 3303 | G |
| 1 | 1 | 3304 | U |
| 1 | 1 | 3307 | A |
| 1 | 1 | 3313 | U |
| 1 | 1 | 3316 | A |
| 1 | 1 | 3317 | U |
| 1 | 1 | 3318 | G |
| 1 | 1 | 3319 | U |
| 1 | 1 | 3320 | A |
| 1 | 1 | 3335 | A |
| 1 | 1 | 3342 | A |
| 1 | 1 | 3345 | G |
| 1 | 1 | 3347 | A |
| 1 | 1 | 3349 | C |
| 1 | 1 | 3350 | C |
| 1 | 1 | 3351 | U |
| 1 | 1 | 3352 | U |
| 1 | 1 | 3353 | G |
| 1 | 1 | 3354 | U |
| 1 | 1 | 3355 | U |
| 1 | 1 | 3356 | G |
| 1 | 1 | 3359 | A |
| 1 | 1 | 3360 | C |
| 1 | 1 | 3363 | 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 |
| 1 | 1 | 3383 | G |
| 1 | 1 | 3390 | G |
| 2 | 2 | 2 | A |
| 2 | 2 | 4 | C |
| 2 | 2 | 17 | C |
| 2 | 2 | 25 | C |
| 2 | 2 | 26 | A |
| 2 | 2 | 27 | U |
| 2 | 2 | 34 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 39 | A |
| 2 | 2 | 45 | U |
| 2 | 2 | 47 | A |
| 2 | 2 | 50 | C |
| 2 | 2 | 57 | G |
| 2 | 2 | 60 | U |
| 2 | 2 | 67 | A |
| 2 | 2 | 68 | A |
| 2 | 2 | 69 | G |
| 2 | 2 | 72 | A |
| 2 | 2 | 73 | U |
| 2 | 2 | 74 | U |
| 2 | 2 | 75 | U |
| 2 | 2 | 76 | A |
| 2 | 2 | 77 | U |
| 2 | 2 | 99 | C |
| 2 | 2 | 101 | U |
| 2 | 2 | 104 | A |
| 2 | 2 | 114 | C |
| 2 | 2 | 130 | C |
| 2 | 2 | 131 | C |
| 2 | 2 | 132 | U |
| 2 | 2 | 136 | C |
| 2 | 2 | 137 | U |
| 2 | 2 | 140 | A |
| 2 | 2 | 141 | U |
| 2 | 2 | 144 | U |
| 2 | 2 | 145 | A |
| 2 | 2 | 146 | U |
| 2 | 2 | 153 | G |
| 2 | 2 | 158 | U |
| 2 | 2 | 159 | U |
| 2 | 2 | 161 | U |
| 2 | 2 | 178 | U |
| 2 | 2 | 179 | A |
| 2 | 2 | 185 | U |
| 2 | 2 | 186 | C |
| 2 | 2 | 188 | A |
| 2 | 2 | 190 | C |
| 2 | 2 | 191 | C |
| 2 | 2 | 192 | U |
| 2 | 2 | 193 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 194 | U |
| 2 | 2 | 195 | G |
| 2 | 2 | 196 | G |
| 2 | 2 | 197 | A |
| 2 | 2 | 198 | A |
| 2 | 2 | 200 | A |
| 2 | 2 | 217 | A |
| 2 | 2 | 218 | A |
| 2 | 2 | 220 | A |
| 2 | 2 | 228 | G |
| 2 | 2 | 229 | U |
| 2 | 2 | 231 | U |
| 2 | 2 | 233 | C |
| 2 | 2 | 234 | G |
| 2 | 2 | 235 | G |
| 2 | 2 | 236 | A |
| 2 | 2 | 238 | U |
| 2 | 2 | 239 | C |
| 2 | 2 | 240 | U |
| 2 | 2 | 241 | U |
| 2 | 2 | 242 | U |
| 2 | 2 | 249 | U |
| 2 | 2 | 250 | C |
| 2 | 2 | 260 | U |
| 2 | 2 | 261 | U |
| 2 | 2 | 265 | A |
| 2 | 2 | 271 | A |
| 2 | 2 | 272 | U |
| 2 | 2 | 274 | G |
| 2 | 2 | 275 | C |
| 2 | 2 | 276 | C |
| 2 | 2 | 277 | U |
| 2 | 2 | 278 | U |
| 2 | 2 | 279 | G |
| 2 | 2 | 280 | U |
| 2 | 2 | 281 | G |
| 2 | 2 | 288 | A |
| 2 | 2 | 290 | G |
| 2 | 2 | 299 | A |
| 2 | 2 | 309 | C |
| 2 | 2 | 312 | A |
| 2 | 2 | 314 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 316 | A |
| 2 | 2 | 319 | U |
| 2 | 2 | 320 | U |
| 2 | 2 | 321 | C |
| 2 | 2 | 322 | G |
| 2 | 2 | 333 | A |
| 2 | 2 | 337 | G |
| 2 | 2 | 338 | C |
| 2 | 2 | 341 | A |
| 2 | 2 | 352 | A |
| 2 | 2 | 359 | A |
| 2 | 2 | 360 | A |
| 2 | 2 | 361 | C |
| 2 | 2 | 378 | A |
| 2 | 2 | 380 | U |
| 2 | 2 | 400 | A |
| 2 | 2 | 401 | A |
| 2 | 2 | 402 | C |
| 2 | 2 | 404 | G |
| 2 | 2 | 416 | A |
| 2 | 2 | 418 | G |
| 2 | 2 | 423 | G |
| 2 | 2 | 424 | C |
| 2 | 2 | 425 | A |
| 2 | 2 | 426 | G |
| 2 | 2 | 428 | A |
| 2 | 2 | 434 | G |
| 2 | 2 | 437 | A |
| 2 | 2 | 439 | U |
| 2 | 2 | 444 | C |
| 2 | 2 | 448 | C |
| 2 | 2 | 468 | A |
| 2 | 2 | 475 | A |
| 2 | 2 | 477 | A |
| 2 | 2 | 484 | C |
| 2 | 2 | 485 | A |
| 2 | 2 | 488 | G |
| 2 | 2 | 493 | U |
| 2 | 2 | 494 | U |
| 2 | 2 | 495 | C |
| 2 | 2 | 496 | G |
| 2 | 2 | 497 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 498 | G |
| 2 | 2 | 499 | U |
| 2 | 2 | 500 | C |
| 2 | 2 | 501 | U |
| 2 | 2 | 502 | U |
| 2 | 2 | 503 | G |
| 2 | 2 | 504 | U |
| 2 | 2 | 505 | A |
| 2 | 2 | 506 | A |
| 2 | 2 | 507 | U |
| 2 | 2 | 508 | U |
| 2 | 2 | 510 | G |
| 2 | 2 | 511 | A |
| 2 | 2 | 512 | A |
| 2 | 2 | 513 | U |
| 2 | 2 | 514 | G |
| 2 | 2 | 515 | A |
| 2 | 2 | 516 | G |
| 2 | 2 | 519 | C |
| 2 | 2 | 527 | A |
| 2 | 2 | 532 | U |
| 2 | 2 | 535 | A |
| 2 | 2 | 538 | A |
| 2 | 2 | 539 | G |
| 2 | 2 | 541 | A |
| 2 | 2 | 542 | A |
| 2 | 2 | 543 | C |
| 2 | 2 | 544 | A |
| 2 | 2 | 548 | G |
| 2 | 2 | 549 | G |
| 2 | 2 | 555 | A |
| 2 | 2 | 556 | A |
| 2 | 2 | 557 | G |
| 2 | 2 | 558 | U |
| 2 | 2 | 559 | C |
| 2 | 2 | 565 | C |
| 2 | 2 | 570 | A |
| 2 | 2 | 571 | G |
| 2 | 2 | 579 | A |
| 2 | 2 | 580 | A |
| 2 | 2 | 582 | U |
| 2 | 2 | 594 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 595 | G |
| 2 | 2 | 606 | A |
| 2 | 2 | 610 | G |
| 2 | 2 | 611 | U |
| 2 | 2 | 619 | A |
| 2 | 2 | 620 | A |
| 2 | 2 | 622 | A |
| 2 | 2 | 623 | A |
| 2 | 2 | 630 | A |
| 2 | 2 | 635 | A |
| 2 | 2 | 638 | U |
| 2 | 2 | 639 | U |
| 2 | 2 | 640 | U |
| 2 | 2 | 649 | U |
| 2 | 2 | 650 | U |
| 2 | 2 | 653 | C |
| 2 | 2 | 655 | G |
| 2 | 2 | 656 | G |
| 2 | 2 | 657 | U |
| 2 | 2 | 658 | C |
| 2 | 2 | 677 | G |
| 2 | 2 | 679 | U |
| 2 | 2 | 680 | U |
| 2 | 2 | 682 | C |
| 2 | 2 | 684 | A |
| 2 | 2 | 685 | A |
| 2 | 2 | 686 | C |
| 2 | 2 | 690 | G |
| 2 | 2 | 692 | C |
| 2 | 2 | 694 | U |
| 2 | 2 | 696 | C |
| 2 | 2 | 697 | C |
| 2 | 2 | 700 | C |
| 2 | 2 | 701 | U |
| 2 | 2 | 702 | G |
| 2 | 2 | 703 | G |
| 2 | 2 | 704 | C |
| 2 | 2 | 705 | U |
| 2 | 2 | 706 | A |
| 2 | 2 | 707 | A |
| 2 | 2 | 709 | C |
| 2 | 2 | 710 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 712 | G |
| 2 | 2 | 713 | A |
| 2 | 2 | 714 | G |
| 2 | 2 | 717 | C |
| 2 | 2 | 718 | U |
| 2 | 2 | 719 | U |
| 2 | 2 | 720 | G |
| 2 | 2 | 721 | U |
| 2 | 2 | 722 | G |
| 2 | 2 | 723 | G |
| 2 | 2 | 725 | U |
| 2 | 2 | 727 | U |
| 2 | 2 | 728 | U |
| 2 | 2 | 730 | G |
| 2 | 2 | 731 | C |
| 2 | 2 | 732 | G |
| 2 | 2 | 733 | A |
| 2 | 2 | 734 | A |
| 2 | 2 | 735 | C |
| 2 | 2 | 736 | C |
| 2 | 2 | 737 | A |
| 2 | 2 | 738 | G |
| 2 | 2 | 741 | C |
| 2 | 2 | 742 | U |
| 2 | 2 | 743 | U |
| 2 | 2 | 745 | U |
| 2 | 2 | 754 | A |
| 2 | 2 | 755 | A |
| 2 | 2 | 756 | A |
| 2 | 2 | 758 | U |
| 2 | 2 | 765 | G |
| 2 | 2 | 766 | U |
| 2 | 2 | 774 | A |
| 2 | 2 | 775 | G |
| 2 | 2 | 778 | G |
| 2 | 2 | 780 | A |
| 2 | 2 | 781 | U |
| 2 | 2 | 782 | U |
| 2 | 2 | 783 | G |
| 2 | 2 | 784 | C |
| 2 | 2 | 789 | A |
| 2 | 2 | 794 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 795 | U |
| 2 | 2 | 806 | A |
| 2 | 2 | 811 | A |
| 2 | 2 | 812 | A |
| 2 | 2 | 819 | G |
| 2 | 2 | 820 | U |
| 2 | 2 | 821 | U |
| 2 | 2 | 831 | U |
| 2 | 2 | 833 | U |
| 2 | 2 | 856 | A |
| 2 | 2 | 860 | U |
| 2 | 2 | 862 | A |
| 2 | 2 | 863 | A |
| 2 | 2 | 864 | U |
| 2 | 2 | 886 | U |
| 2 | 2 | 896 | U |
| 2 | 2 | 898 | A |
| 2 | 2 | 911 | U |
| 2 | 2 | 912 | U |
| 2 | 2 | 913 | G |
| 2 | 2 | 914 | G |
| 2 | 2 | 921 | U |
| 2 | 2 | 933 | A |
| 2 | 2 | 935 | U |
| 2 | 2 | 942 | G |
| 2 | 2 | 944 | A |
| 2 | 2 | 951 | A |
| 2 | 2 | 960 | U |
| 2 | 2 | 966 | A |
| 2 | 2 | 973 | A |
| 2 | 2 | 985 | G |
| 2 | 2 | 992 | A |
| 2 | 2 | 993 | A |
| 2 | 2 | 997 | G |
| 2 | 2 | 999 | U |
| 2 | 2 | 1004 | U |
| 2 | 2 | 1005 | A |
| 2 | 2 | 1020 | A |
| 2 | 2 | 1026 | A |
| 2 | 2 | 1028 | C |
| 2 | 2 | 1029 | U |
| 2 | 2 | 1032 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 1039 | A |
| 2 | 2 | 1040 | G |
| 2 | 2 | 1052 | U |
| 2 | 2 | 1053 | G |
| 2 | 2 | 1056 | U |
| 2 | 2 | 1057 | U |
| 2 | 2 | 1058 | U |
| 2 | 2 | 1059 | U |
| 2 | 2 | 1060 | U |
| 2 | 2 | 1061 | A |
| 2 | 2 | 1062 | A |
| 2 | 2 | 1064 | G |
| 2 | 2 | 1074 | G |
| 2 | 2 | 1076 | A |
| 2 | 2 | 1079 | U |
| 2 | 2 | 1082 | C |
| 2 | 2 | 1083 | G |
| 2 | 2 | 1091 | A |
| 2 | 2 | 1092 | A |
| 2 | 2 | 1096 | C |
| 2 | 2 | 1097 | U |
| 2 | 2 | 1098 | U |
| 2 | 2 | 1100 | G |
| 2 | 2 | 1109 | G |
| 2 | 2 | 1113 | A |
| 2 | 2 | 1138 | A |
| 2 | 2 | 1139 | A |
| 2 | 2 | 1146 | G |
| 2 | 2 | 1149 | G |
| 2 | 2 | 1150 | G |
| 2 | 2 | 1151 | A |
| 2 | 2 | 1155 | G |
| 2 | 2 | 1157 | A |
| 2 | 2 | 1158 | C |
| 2 | 2 | 1160 | A |
| 2 | 2 | 1162 | C |
| 2 | 2 | 1163 | A |
| 2 | 2 | 1167 | G |
| 2 | 2 | 1175 | U |
| 2 | 2 | 1185 | U |
| 2 | 2 | 1188 | G |
| 2 | 2 | 1194 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 1196 | A |
| 2 | 2 | 1197 | C |
| 2 | 2 | 1199 | G |
| 2 | 2 | 1200 | G |
| 2 | 2 | 1202 | A |
| 2 | 2 | 1207 | C |
| 2 | 2 | 1208 | A |
| 2 | 2 | 1217 | A |
| 2 | 2 | 1218 | G |
| 2 | 2 | 1227 | A |
| 2 | 2 | 1228 | G |
| 2 | 2 | 1229 | G |
| 2 | 2 | 1243 | G |
| 2 | 2 | 1244 | A |
| 2 | 2 | 1245 | G |
| 2 | 2 | 1250 | U |
| 2 | 2 | 1251 | U |
| 2 | 2 | 1257 | U |
| 2 | 2 | 1258 | U |
| 2 | 2 | 1284 | C |
| 2 | 2 | 1285 | U |
| 2 | 2 | 1286 | U |
| 2 | 2 | 1287 | A |
| 2 | 2 | 1301 | U |
| 2 | 2 | 1312 | A |
| 2 | 2 | 1314 | U |
| 2 | 2 | 1315 | U |
| 2 | 2 | 1321 | A |
| 2 | 2 | 1338 | C |
| 2 | 2 | 1339 | C |
| 2 | 2 | 1340 | U |
| 2 | 2 | 1341 | A |
| 2 | 2 | 1343 | U |
| 2 | 2 | 1344 | A |
| 2 | 2 | 1345 | A |
| 2 | 2 | 1349 | G |
| 2 | 2 | 1354 | G |
| 2 | 2 | 1360 | A |
| 2 | 2 | 1361 | U |
| 2 | 2 | 1363 | U |
| 2 | 2 | 1364 | G |
| 2 | 2 | 1370 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 1371 | A |
| 2 | 2 | 1372 | U |
| 2 | 2 | 1383 | G |
| 2 | 2 | 1388 | A |
| 2 | 2 | 1390 | U |
| 2 | 2 | 1398 | U |
| 2 | 2 | 1399 | C |
| 2 | 2 | 1410 | A |
| 2 | 2 | 1411 | A |
| 2 | 2 | 1412 | G |
| 2 | 2 | 1413 | U |
| 2 | 2 | 1414 | U |
| 2 | 2 | 1415 | U |
| 2 | 2 | 1427 | A |
| 2 | 2 | 1428 | G |
| 2 | 2 | 1432 | U |
| 2 | 2 | 1445 | G |
| 2 | 2 | 1446 | A |
| 2 | 2 | 1448 | G |
| 2 | 2 | 1457 | C |
| 2 | 2 | 1459 | C |
| 2 | 2 | 1460 | A |
| 2 | 2 | 1461 | C |
| 2 | 2 | 1471 | A |
| 2 | 2 | 1473 | U |
| 2 | 2 | 1474 | G |
| 2 | 2 | 1475 | A |
| 2 | 2 | 1481 | C |
| 2 | 2 | 1482 | C |
| 2 | 2 | 1486 | G |
| 2 | 2 | 1489 | U |
| 2 | 2 | 1490 | C |
| 2 | 2 | 1491 | U |
| 2 | 2 | 1492 | A |
| 2 | 2 | 1493 | A |
| 2 | 2 | 1499 | G |
| 2 | 2 | 1500 | C |
| 2 | 2 | 1506 | G |
| 2 | 2 | 1514 | U |
| 2 | 2 | 1515 | A |
| 2 | 2 | 1516 | A |
| 2 | 2 | 1517 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 1521 | G |
| 2 | 2 | 1523 | G |
| 2 | 2 | 1524 | A |
| 2 | 2 | 1530 | C |
| 2 | 2 | 1533 | C |
| 2 | 2 | 1535 | U |
| 2 | 2 | 1536 | G |
| 2 | 2 | 1537 | C |
| 2 | 2 | 1538 | U |
| 2 | 2 | 1539 | G |
| 2 | 2 | 1540 | G |
| 2 | 2 | 1542 | G |
| 2 | 2 | 1557 | U |
| 2 | 2 | 1559 | A |
| 2 | 2 | 1560 | U |
| 2 | 2 | 1569 | A |
| 2 | 2 | 1573 | A |
| 2 | 2 | 1574 | G |
| 2 | 2 | 1584 | G |
| 2 | 2 | 1590 | G |
| 2 | 2 | 1601 | G |
| 2 | 2 | 1614 | A |
| 2 | 2 | 1616 | G |
| 2 | 2 | 1618 | C |
| 2 | 2 | 1625 | C |
| 2 | 2 | 1626 | U |
| 2 | 2 | 1631 | A |
| 2 | 2 | 1639 | C |
| 2 | 2 | 1651 | A |
| 2 | 2 | 1657 | U |
| 2 | 2 | 1658 | G |
| 2 | 2 | 1680 | G |
| 2 | 2 | 1695 | G |
| 2 | 2 | 1731 | A |
| 2 | 2 | 1747 | G |
| 2 | 2 | 1750 | A |
| 2 | 2 | 1756 | A |
| 2 | 2 | 1757 | G |
| 2 | 2 | 1760 | G |
| 2 | 2 | 1762 | A |
| 2 | 2 | 1766 | A |
| 2 | 2 | 1769 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 1770 | U |
| 2 | 2 | 1780 | G |
| 2 | 2 | 1782 | A |
| 2 | 2 | 1783 | C |
| 2 | 2 | 1790 | A |
| 2 | 2 | 1791 | A |
| 2 | 2 | 1792 | G |
| 2 | 2 | 1793 | G |
| 2 | 2 | 1794 | A |
| 2 | 2 | 1795 | U |
| 2 | 2 | 1796 | C |
| 2 | 2 | 1798 | U |
| 3 | 3 | 7 | G |
| 3 | 3 | 13 | A |
| 3 | 3 | 17 | A |
| 3 | 3 | 22 | A |
| 3 | 3 | 41 | G |
| 3 | 3 | 51 | A |
| 3 | 3 | 53 | U |
| 3 | 3 | 54 | U |
| 3 | 3 | 65 | G |
| 3 | 3 | 74 | C |
| 3 | 3 | 76 | A |
| 3 | 3 | 91 | G |
| 3 | 3 | 93 | C |
| 3 | 3 | 95 | A |
| 3 | 3 | 102 | A |
| 3 | 3 | 112 | G |
| 3 | 3 | 121 | U |
| 4 | 4 | 21 | C |
| 4 | 4 | 34 | U |
| 4 | 4 | 35 | C |
| 4 | 4 | 51 | G |
| 4 | 4 | 59 | A |
| 4 | 4 | 62 | C |
| 4 | 4 | 63 | G |
| 4 | 4 | 71 | A |
| 4 | 4 | 79 | A |
| 4 | 4 | 80 | A |
| 4 | 4 | 81 | U |
| 4 | 4 | 82 | U |
| 4 | 4 | 83 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 4 | 4 | 84 | C |
| 4 | 4 | 86 | U |
| 4 | 4 | 87 | G |
| 4 | 4 | 90 | U |
| 4 | 4 | 95 | G |
| 4 | 4 | 104 | A |
| 4 | 4 | 106 | C |
| 4 | 4 | 111 | A |
| 4 | 4 | 112 | U |
| 4 | 4 | 113 | U |
| 4 | 4 | 125 | U |
| 4 | 4 | 126 | A |
| 4 | 4 | 128 | U |
| 4 | 4 | 138 | A |
| 4 | 4 | 151 | C |
| 4 | 4 | 152 | G |
| 4 | 4 | 155 | A |
| 4 | 4 | 157 | U |
| 4 | 4 | 158 | U |
| 1 | 5 | 6 | A |
| 1 | 5 | 15 | C |
| 1 | 5 | 26 | A |
| 1 | 5 | 40 | A |
| 1 | 5 | 43 | A |
| 1 | 5 | 49 | A |
| 1 | 5 | 60 | A |
| 1 | 5 | 65 | A |
| 1 | 5 | 66 | A |
| 1 | 5 | 68 | C |
| 1 | 5 | 76 | G |
| 1 | 5 | 85 | A |
| 1 | 5 | 89 | A |
| 1 | 5 | 92 | G |
| 1 | 5 | 93 | C |
| 1 | 5 | 96 | G |
| 1 | 5 | 99 | A |
| 1 | 5 | 109 | A |
| 1 | 5 | 110 | G |
| 1 | 5 | 111 | C |
| 1 | 5 | 112 | U |
| 1 | 5 | 113 | C |
| 1 | 5 | 116 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 5 | 121 | A |
| 1 | 5 | 122 | A |
| 1 | 5 | 133 | U |
| 1 | 5 | 134 | U |
| 1 | 5 | 135 | C |
| 1 | 5 | 136 | G |
| 1 | 5 | 147 | U |
| 1 | 5 | 150 | A |
| 1 | 5 | 152 | U |
| 1 | 5 | 156 | G |
| 1 | 5 | 157 | A |
| 1 | 5 | 166 | C |
| 1 | 5 | 170 | G |
| 1 | 5 | 175 | C |
| 1 | 5 | 182 | U |
| 1 | 5 | 187 | A |
| 1 | 5 | 190 | U |
| 1 | 5 | 191 | U |
| 1 | 5 | 200 | C |
| 1 | 5 | 212 | G |
| 1 | 5 | 219 | A |
| 1 | 5 | 220 | G |
| 1 | 5 | 240 | U |
| 1 | 5 | 242 | C |
| 1 | 5 | 244 | G |
| 1 | 5 | 248 | U |
| 1 | 5 | 249 | U |
| 1 | 5 | 250 | U |
| 1 | 5 | 251 | G |
| 1 | 5 | 252 | U |
| 1 | 5 | 254 | A |
| 1 | 5 | 269 | G |
| 1 | 5 | 282 | G |
| 1 | 5 | 283 | G |
| 1 | 5 | 284 | A |
| 1 | 5 | 286 | U |
| 1 | 5 | 295 | A |
| 1 | 5 | 305 | U |
| 1 | 5 | 315 | C |
| 1 | 5 | 323 | A |
| 1 | 5 | 329 | U |
| 1 | 5 | 334 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 5 | 339 | C |
| 1 | 5 | 349 | A |
| 1 | 5 | 350 | C |
| 1 | 5 | 370 | U |
| 1 | 5 | 376 | G |
| 1 | 5 | 390 | G |
| 1 | 5 | 398 | A |
| 1 | 5 | 399 | A |
| 1 | 5 | 401 | U |
| 1 | 5 | 402 | A |
| 1 | 5 | 403 | C |
| 1 | 5 | 404 | G |
| 1 | 5 | 421 | G |
| 1 | 5 | 422 | A |
| 1 | 5 | 425 | G |
| 1 | 5 | 439 | C |
| 1 | 5 | 440 | A |
| 1 | 5 | 520 | U |
| 1 | 5 | 521 | A |
| 1 | 5 | 542 | G |
| 1 | 5 | 546 | C |
| 1 | 5 | 547 | G |
| 1 | 5 | 548 | G |
| 1 | 5 | 555 | U |
| 1 | 5 | 556 | U |
| 1 | 5 | 557 | A |
| 1 | 5 | 559 | A |
| 1 | 5 | 561 | C |
| 1 | 5 | 569 | A |
| 1 | 5 | 578 | A |
| 1 | 5 | 579 | G |
| 1 | 5 | 581 | U |
| 1 | 5 | 588 | G |
| 1 | 5 | 592 | A |
| 1 | 5 | 594 | U |
| 1 | 5 | 604 | G |
| 1 | 5 | 609 | G |
| 1 | 5 | 611 | A |
| 1 | 5 | 620 | U |
| 1 | 5 | 621 | A |
| 1 | 5 | 622 | A |
| 1 | 5 | 636 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 5 | 649 | A |
| 1 | 5 | 654 | C |
| 1 | 5 | 660 | A |
| 1 | 5 | 675 | C |
| 1 | 5 | 677 | A |
| 1 | 5 | 681 | U |
| 1 | 5 | 705 | A |
| 1 | 5 | 712 | G |
| 1 | 5 | 715 | A |
| 1 | 5 | 716 | A |
| 1 | 5 | 719 | U |
| 1 | 5 | 720 | A |
| 1 | 5 | 726 | G |
| 1 | 5 | 727 | G |
| 1 | 5 | 735 | A |
| 1 | 5 | 736 | A |
| 1 | 5 | 758 | C |
| 1 | 5 | 766 | U |
| 1 | 5 | 767 | U |
| 1 | 5 | 776 | U |
| 1 | 5 | 777 | U |
| 1 | 5 | 780 | A |
| 1 | 5 | 781 | G |
| 1 | 5 | 785 | G |
| 1 | 5 | 786 | A |
| 1 | 5 | 806 | A |
| 1 | 5 | 816 | A |
| 1 | 5 | 817 | A |
| 1 | 5 | 824 | C |
| 1 | 5 | 829 | U |
| 1 | 5 | 830 | A |
| 1 | 5 | 846 | A |
| 1 | 5 | 851 | C |
| 1 | 5 | 852 | U |
| 1 | 5 | 856 | G |
| 1 | 5 | 857 | G |
| 1 | 5 | 861 | C |
| 1 | 5 | 869 | G |
| 1 | 5 | 874 | U |
| 1 | 5 | 879 | U |
| 1 | 5 | 883 | A |
| 1 | 5 | 890 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 5 | 896 | A |
| 1 | 5 | 907 | G |
| 1 | 5 | 908 | G |
| 1 | 5 | 914 | A |
| 1 | 5 | 916 | G |
| 1 | 5 | 917 | A |
| 1 | 5 | 921 | A |
| 1 | 5 | 923 | C |
| 1 | 5 | 924 | G |
| 1 | 5 | 937 | G |
| 1 | 5 | 943 | U |
| 1 | 5 | 944 | C |
| 1 | 5 | 959 | C |
| 1 | 5 | 960 | U |
| 1 | 5 | 961 | C |
| 1 | 5 | 979 | U |
| 1 | 5 | 980 | A |
| 1 | 5 | 981 | U |
| 1 | 5 | 982 | C |
| 1 | 5 | 994 | G |
| 1 | 5 | 1000 | C |
| 1 | 5 | 1001 | G |
| 1 | 5 | 1002 | A |
| 1 | 5 | 1003 | A |
| 1 | 5 | 1006 | A |
| 1 | 5 | 1010 | G |
| 1 | 5 | 1014 | U |
| 1 | 5 | 1015 | U |
| 1 | 5 | 1017 | C |
| 1 | 5 | 1021 | G |
| 1 | 5 | 1022 | U |
| 1 | 5 | 1023 | C |
| 1 | 5 | 1026 | A |
| 1 | 5 | 1027 | A |
| 1 | 5 | 1028 | U |
| 1 | 5 | 1029 | G |
| 1 | 5 | 1030 | A |
| 1 | 5 | 1047 | A |
| 1 | 5 | 1049 | C |
| 1 | 5 | 1064 | A |
| 1 | 5 | 1065 | A |
| 1 | 5 | 1071 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 5 | 1072 | G |
| 1 | 5 | 1079 | A |
| 1 | 5 | 1080 | A |
| 1 | 5 | 1081 | U |
| 1 | 5 | 1082 | U |
| 1 | 5 | 1085 | A |
| 1 | 5 | 1087 | G |
| 1 | 5 | 1093 | A |
| 1 | 5 | 1094 | U |
| 1 | 5 | 1095 | U |
| 1 | 5 | 1096 | U |
| 1 | 5 | 1097 | G |
| 1 | 5 | 1098 | A |
| 1 | 5 | 1102 | A |
| 1 | 5 | 1103 | A |
| 1 | 5 | 1104 | G |
| 1 | 5 | 1117 | G |
| 1 | 5 | 1129 | A |
| 1 | 5 | 1131 | G |
| 1 | 5 | 1152 | G |
| 1 | 5 | 1153 | A |
| 1 | 5 | 1159 | A |
| 1 | 5 | 1160 | C |
| 1 | 5 | 1177 | G |
| 1 | 5 | 1178 | G |
| 1 | 5 | 1180 | A |
| 1 | 5 | 1181 | U |
| 1 | 5 | 1182 | A |
| 1 | 5 | 1191 | U |
| 1 | 5 | 1192 | C |
| 1 | 5 | 1196 | C |
| 1 | 5 | 1200 | A |
| 1 | 5 | 1201 | C |
| 1 | 5 | 1202 | A |
| 1 | 5 | 1209 | G |
| 1 | 5 | 1212 | A |
| 1 | 5 | 1220 | U |
| 1 | 5 | 1221 | A |
| 1 | 5 | 1222 | G |
| 1 | 5 | 1225 | A |
| 1 | 5 | 1281 | G |
| 1 | 5 | 1284 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 5 | 1285 | G |
| 1 | 5 | 1286 | A |
| 1 | 5 | 1305 | U |
| 1 | 5 | 1307 | G |
| 1 | 5 | 1308 | A |
| 1 | 5 | 1309 | U |
| 1 | 5 | 1313 | G |
| 1 | 5 | 1329 | U |
| 1 | 5 | 1330 | A |
| 1 | 5 | 1347 | U |
| 1 | 5 | 1348 | U |
| 1 | 5 | 1355 | A |
| 1 | 5 | 1356 | U |
| 1 | 5 | 1357 | G |
| 1 | 5 | 1385 | C |
| 1 | 5 | 1386 | A |
| 1 | 5 | 1399 | A |
| 1 | 5 | 1400 | G |
| 1 | 5 | 1408 | G |
| 1 | 5 | 1416 | C |
| 1 | 5 | 1419 | A |
| 1 | 5 | 1431 | G |
| 1 | 5 | 1434 | G |
| 1 | 5 | 1437 | C |
| 1 | 5 | 1446 | A |
| 1 | 5 | 1450 | G |
| 1 | 5 | 1479 | U |
| 1 | 5 | 1481 | A |
| 1 | 5 | 1482 | A |
| 1 | 5 | 1484 | U |
| 1 | 5 | 1495 | U |
| 1 | 5 | 1503 | A |
| 1 | 5 | 1508 | C |
| 1 | 5 | 1533 | U |
| 1 | 5 | 1536 | G |
| 1 | 5 | 1549 | U |
| 1 | 5 | 1554 | U |
| 1 | 5 | 1555 | U |
| 1 | 5 | 1556 | C |
| 1 | 5 | 1557 | A |
| 1 | 5 | 1560 | G |
| 1 | 5 | 1562 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 5 | 1563 | C |
| 1 | 5 | 1564 | U |
| 1 | 5 | 1565 | G |
| 1 | 5 | 1571 | A |
| 1 | 5 | 1572 | U |
| 1 | 5 | 1574 | C |
| 1 | 5 | 1575 | A |
| 1 | 5 | 1578 | C |
| 1 | 5 | 1580 | A |
| 1 | 5 | 1581 | C |
| 1 | 5 | 1582 | C |
| 1 | 5 | 1583 | A |
| 1 | 5 | 1587 | A |
| 1 | 5 | 1589 | A |
| 1 | 5 | 1593 | A |
| 1 | 5 | 1607 | U |
| 1 | 5 | 1608 | C |
| 1 | 5 | 1620 | U |
| 1 | 5 | 1629 | U |
| 1 | 5 | 1639 | C |
| 1 | 5 | 1643 | A |
| 1 | 5 | 1644 | C |
| 1 | 5 | 1645 | U |
| 1 | 5 | 1655 | G |
| 1 | 5 | 1657 | C |
| 1 | 5 | 1658 | G |
| 1 | 5 | 1662 | G |
| 1 | 5 | 1683 | A |
| 1 | 5 | 1716 | U |
| 1 | 5 | 1717 | U |
| 1 | 5 | 1724 | U |
| 1 | 5 | 1725 | C |
| 1 | 5 | 1736 | G |
| 1 | 5 | 1750 | A |
| 1 | 5 | 1751 | G |
| 1 | 5 | 1756 | C |
| 1 | 5 | 1759 | C |
| 1 | 5 | 1760 | A |
| 1 | 5 | 1761 | C |
| 1 | 5 | 1769 | G |
| 1 | 5 | 1770 | G |
| 1 | 5 | 1780 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 5 | 1797 | A |
| 1 | 5 | 1813 | A |
| 1 | 5 | 1814 | A |
| 1 | 5 | 1816 | A |
| 1 | 5 | 1817 | G |
| 1 | 5 | 1818 | U |
| 1 | 5 | 1820 | U |
| 1 | 5 | 1821 | U |
| 1 | 5 | 1839 | A |
| 1 | 5 | 1841 | A |
| 1 | 5 | 1842 | A |
| 1 | 5 | 1846 | C |
| 1 | 5 | 1849 | C |
| 1 | 5 | 1850 | A |
| 1 | 5 | 1864 | A |
| 1 | 5 | 1879 | A |
| 1 | 5 | 1880 | U |
| 1 | 5 | 1885 | U |
| 1 | 5 | 1886 | A |
| 1 | 5 | 1894 | U |
| 1 | 5 | 1896 | A |
| 1 | 5 | 1906 | G |
| 1 | 5 | 1926 | C |
| 1 | 5 | 1952 | G |
| 1 | 5 | 1953 | G |
| 1 | 5 | 2100 | A |
| 1 | 5 | 2101 | C |
| 1 | 5 | 2102 | U |
| 1 | 5 | 2112 | U |
| 1 | 5 | 2113 | A |
| 1 | 5 | 2121 | G |
| 1 | 5 | 2122 | G |
| 1 | 5 | 2131 | A |
| 1 | 5 | 2140 | U |
| 1 | 5 | 2158 | A |
| 1 | 5 | 2159 | U |
| 1 | 5 | 2169 | G |
| 1 | 5 | 2176 | U |
| 1 | 5 | 2178 | A |
| 1 | 5 | 2179 | C |
| 1 | 5 | 2201 | G |
| 1 | 5 | 2204 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 5 | 2205 | U |
| 1 | 5 | 2206 | G |
| 1 | 5 | 2207 | A |
| 1 | 5 | 2208 | A |
| 1 | 5 | 2209 | U |
| 1 | 5 | 2210 | G |
| 1 | 5 | 2212 | C |
| 1 | 5 | 2223 | A |
| 1 | 5 | 2225 | U |
| 1 | 5 | 2228 | A |
| 1 | 5 | 2229 | A |
| 1 | 5 | 2244 | A |
| 1 | 5 | 2248 | C |
| 1 | 5 | 2249 | G |
| 1 | 5 | 2250 | G |
| 1 | 5 | 2252 | A |
| 1 | 5 | 2253 | G |
| 1 | 5 | 2255 | A |
| 1 | 5 | 2256 | A |
| 1 | 5 | 2257 | C |
| 1 | 5 | 2258 | U |
| 1 | 5 | 2260 | U |
| 1 | 5 | 2268 | U |
| 1 | 5 | 2269 | U |
| 1 | 5 | 2272 | G |
| 1 | 5 | 2273 | G |
| 1 | 5 | 2281 | A |
| 1 | 5 | 2282 | U |
| 1 | 5 | 2288 | G |
| 1 | 5 | 2306 | C |
| 1 | 5 | 2307 | G |
| 1 | 5 | 2308 | C |
| 1 | 5 | 2310 | U |
| 1 | 5 | 2313 | A |
| 1 | 5 | 2315 | G |
| 1 | 5 | 2318 | U |
| 1 | 5 | 2334 | U |
| 1 | 5 | 2336 | U |
| 1 | 5 | 2372 | A |
| 1 | 5 | 2373 | A |
| 1 | 5 | 2374 | C |
| 1 | 5 | 2375 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 5 | 2385 | G |
| 1 | 5 | 2393 | G |
| 1 | 5 | 2397 | A |
| 1 | 5 | 2398 | A |
| 1 | 5 | 2401 | A |
| 1 | 5 | 2402 | A |
| 1 | 5 | 2403 | G |
| 1 | 5 | 2404 | A |
| 1 | 5 | 2411 | U |
| 1 | 5 | 2414 | G |
| 1 | 5 | 2418 | G |
| 1 | 5 | 2419 | A |
| 1 | 5 | 2434 | U |
| 1 | 5 | 2435 | G |
| 1 | 5 | 2437 | G |
| 1 | 5 | 2439 | A |
| 1 | 5 | 2440 | G |
| 1 | 5 | 2441 | A |
| 1 | 5 | 2505 | U |
| 1 | 5 | 2508 | U |
| 1 | 5 | 2510 | U |
| 1 | 5 | 2511 | A |
| 1 | 5 | 2512 | C |
| 1 | 5 | 2513 | U |
| 1 | 5 | 2514 | U |
| 1 | 5 | 2515 | A |
| 1 | 5 | 2522 | G |
| 1 | 5 | 2523 | A |
| 1 | 5 | 2524 | A |
| 1 | 5 | 2526 | C |
| 1 | 5 | 2538 | U |
| 1 | 5 | 2539 | C |
| 1 | 5 | 2540 | A |
| 1 | 5 | 2541 | U |
| 1 | 5 | 2542 | U |
| 1 | 5 | 2543 | U |
| 1 | 5 | 2544 | U |
| 1 | 5 | 2545 | C |
| 1 | 5 | 2547 | A |
| 1 | 5 | 2549 | G |
| 1 | 5 | 2550 | U |
| 1 | 5 | 2552 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 5 | 2555 | G |
| 1 | 5 | 2566 | C |
| 1 | 5 | 2567 | C |
| 1 | 5 | 2568 | C |
| 1 | 5 | 2569 | A |
| 1 | 5 | 2570 | U |
| 1 | 5 | 2571 | U |
| 1 | 5 | 2572 | C |
| 1 | 5 | 2573 | G |
| 1 | 5 | 2574 | G |
| 1 | 5 | 2575 | G |
| 1 | 5 | 2584 | G |
| 1 | 5 | 2585 | G |
| 1 | 5 | 2589 | G |
| 1 | 5 | 2593 | A |
| 1 | 5 | 2594 | C |
| 1 | 5 | 2598 | G |
| 1 | 5 | 2600 | C |
| 1 | 5 | 2606 | G |
| 1 | 5 | 2607 | G |
| 1 | 5 | 2614 | G |
| 1 | 5 | 2640 | A |
| 1 | 5 | 2652 | U |
| 1 | 5 | 2656 | A |
| 1 | 5 | 2657 | A |
| 1 | 5 | 2662 | G |
| 1 | 5 | 2663 | G |
| 1 | 5 | 2667 | A |
| 1 | 5 | 2668 | U |
| 1 | 5 | 2674 | A |
| 1 | 5 | 2677 | G |
| 1 | 5 | 2683 | U |
| 1 | 5 | 2689 | A |
| 1 | 5 | 2690 | G |
| 1 | 5 | 2691 | A |
| 1 | 5 | 2694 | A |
| 1 | 5 | 2695 | A |
| 1 | 5 | 2696 | A |
| 1 | 5 | 2714 | G |
| 1 | 5 | 2728 | G |
| 1 | 5 | 2729 | U |
| 1 | 5 | 2737 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 5 | 2752 | U |
| 1 | 5 | 2753 | G |
| 1 | 5 | 2762 | A |
| 1 | 5 | 2771 | U |
| 1 | 5 | 2772 | C |
| 1 | 5 | 2773 | C |
| 1 | 5 | 2778 | G |
| 1 | 5 | 2779 | A |
| 1 | 5 | 2796 | G |
| 1 | 5 | 2799 | A |
| 1 | 5 | 2800 | G |
| 1 | 5 | 2801 | A |
| 1 | 5 | 2810 | C |
| 1 | 5 | 2814 | G |
| 1 | 5 | 2817 | A |
| 1 | 5 | 2818 | U |
| 1 | 5 | 2821 | C |
| 1 | 5 | 2845 | A |
| 1 | 5 | 2853 | A |
| 1 | 5 | 2856 | G |
| 1 | 5 | 2867 | C |
| 1 | 5 | 2871 | G |
| 1 | 5 | 2872 | A |
| 1 | 5 | 2873 | U |
| 1 | 5 | 2887 | A |
| 1 | 5 | 2889 | C |
| 1 | 5 | 2896 | A |
| 1 | 5 | 2899 | C |
| 1 | 5 | 2910 | A |
| 1 | 5 | 2923 | U |
| 1 | 5 | 2929 | C |
| 1 | 5 | 2935 | U |
| 1 | 5 | 2936 | A |
| 1 | 5 | 2942 | C |
| 1 | 5 | 2945 | G |
| 1 | 5 | 2947 | G |
| 1 | 5 | 2954 | U |
| 1 | 5 | 2957 | G |
| 1 | 5 | 2971 | A |
| 1 | 5 | 2979 | U |
| 1 | 5 | 2983 | C |
| 1 | 5 | 2990 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 5 | 2995 | A |
| 1 | 5 | 2996 | U |
| 1 | 5 | 2997 | G |
| 1 | 5 | 3049 | A |
| 1 | 5 | 3056 | U |
| 1 | 5 | 3059 | G |
| 1 | 5 | 3078 | U |
| 1 | 5 | 3079 | U |
| 1 | 5 | 3080 | G |
| 1 | 5 | 3086 | A |
| 1 | 5 | 3087 | A |
| 1 | 5 | 3092 | C |
| 1 | 5 | 3093 | C |
| 1 | 5 | 3122 | A |
| 1 | 5 | 3127 | A |
| 1 | 5 | 3129 | A |
| 1 | 5 | 3131 | U |
| 1 | 5 | 3142 | A |
| 1 | 5 | 3143 | C |
| 1 | 5 | 3150 | A |
| 1 | 5 | 3151 | U |
| 1 | 5 | 3153 | U |
| 1 | 5 | 3154 | C |
| 1 | 5 | 3155 | U |
| 1 | 5 | 3156 | U |
| 1 | 5 | 3157 | U |
| 1 | 5 | 3158 | G |
| 1 | 5 | 3170 | A |
| 1 | 5 | 3171 | U |
| 1 | 5 | 3172 | A |
| 1 | 5 | 3173 | G |
| 1 | 5 | 3174 | A |
| 1 | 5 | 3176 | G |
| 1 | 5 | 3179 | U |
| 1 | 5 | 3181 | C |
| 1 | 5 | 3187 | A |
| 1 | 5 | 3196 | U |
| 1 | 5 | 3198 | U |
| 1 | 5 | 3206 | C |
| 1 | 5 | 3207 | U |
| 1 | 5 | 3217 | C |
| 1 | 5 | 3218 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 5 | 3219 | G |
| 1 | 5 | 3224 | G |
| 1 | 5 | 3229 | G |
| 1 | 5 | 3235 | C |
| 1 | 5 | 3239 | G |
| 1 | 5 | 3244 | A |
| 1 | 5 | 3245 | A |
| 1 | 5 | 3246 | G |
| 1 | 5 | 3247 | G |
| 1 | 5 | 3249 | C |
| 1 | 5 | 3253 | G |
| 1 | 5 | 3259 | U |
| 1 | 5 | 3268 | A |
| 1 | 5 | 3269 | U |
| 1 | 5 | 3270 | U |
| 1 | 5 | 3271 | G |
| 1 | 5 | 3273 | A |
| 1 | 5 | 3276 | G |
| 1 | 5 | 3277 | U |
| 1 | 5 | 3279 | A |
| 1 | 5 | 3281 | U |
| 1 | 5 | 3285 | C |
| 1 | 5 | 3294 | A |
| 1 | 5 | 3304 | U |
| 1 | 5 | 3316 | A |
| 1 | 5 | 3317 | U |
| 1 | 5 | 3318 | G |
| 1 | 5 | 3319 | U |
| 1 | 5 | 3335 | A |
| 1 | 5 | 3341 | U |
| 1 | 5 | 3342 | A |
| 1 | 5 | 3345 | G |
| 1 | 5 | 3351 | U |
| 1 | 5 | 3352 | U |
| 1 | 5 | 3354 | U |
| 1 | 5 | 3355 | U |
| 1 | 5 | 3356 | G |
| 1 | 5 | 3363 | U |
| 1 | 5 | 3368 | U |
| 1 | 5 | 3369 | G |
| 1 | 5 | 3378 | C |
| 1 | 5 | 3383 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 5 | 3386 | G |
| 1 | 5 | 3389 | U |
| 1 | 5 | 3395 | G |
| 1 | 5 | 3396 | U |
| 2 | 6 | 2 | A |
| 2 | 6 | 4 | C |
| 2 | 6 | 17 | C |
| 2 | 6 | 25 | C |
| 2 | 6 | 26 | A |
| 2 | 6 | 27 | U |
| 2 | 6 | 34 | G |
| 2 | 6 | 45 | U |
| 2 | 6 | 46 | A |
| 2 | 6 | 47 | A |
| 2 | 6 | 57 | G |
| 2 | 6 | 60 | U |
| 2 | 6 | 67 | A |
| 2 | 6 | 68 | A |
| 2 | 6 | 69 | G |
| 2 | 6 | 73 | U |
| 2 | 6 | 74 | U |
| 2 | 6 | 75 | U |
| 2 | 6 | 76 | A |
| 2 | 6 | 77 | U |
| 2 | 6 | 78 | A |
| 2 | 6 | 79 | C |
| 2 | 6 | 104 | A |
| 2 | 6 | 114 | C |
| 2 | 6 | 115 | G |
| 2 | 6 | 126 | A |
| 2 | 6 | 129 | U |
| 2 | 6 | 130 | C |
| 2 | 6 | 131 | C |
| 2 | 6 | 132 | U |
| 2 | 6 | 137 | U |
| 2 | 6 | 138 | A |
| 2 | 6 | 140 | A |
| 2 | 6 | 141 | U |
| 2 | 6 | 144 | U |
| 2 | 6 | 145 | A |
| 2 | 6 | 158 | U |
| 2 | 6 | 159 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 6 | 166 | C |
| 2 | 6 | 177 | U |
| 2 | 6 | 178 | U |
| 2 | 6 | 179 | A |
| 2 | 6 | 185 | U |
| 2 | 6 | 188 | A |
| 2 | 6 | 189 | C |
| 2 | 6 | 190 | C |
| 2 | 6 | 192 | U |
| 2 | 6 | 193 | U |
| 2 | 6 | 194 | U |
| 2 | 6 | 195 | G |
| 2 | 6 | 197 | A |
| 2 | 6 | 198 | A |
| 2 | 6 | 199 | G |
| 2 | 6 | 200 | A |
| 2 | 6 | 215 | A |
| 2 | 6 | 216 | U |
| 2 | 6 | 217 | A |
| 2 | 6 | 218 | A |
| 2 | 6 | 219 | A |
| 2 | 6 | 223 | U |
| 2 | 6 | 230 | C |
| 2 | 6 | 231 | U |
| 2 | 6 | 232 | U |
| 2 | 6 | 233 | C |
| 2 | 6 | 234 | G |
| 2 | 6 | 235 | G |
| 2 | 6 | 237 | C |
| 2 | 6 | 238 | U |
| 2 | 6 | 239 | C |
| 2 | 6 | 240 | U |
| 2 | 6 | 241 | U |
| 2 | 6 | 242 | U |
| 2 | 6 | 250 | C |
| 2 | 6 | 257 | A |
| 2 | 6 | 260 | U |
| 2 | 6 | 261 | U |
| 2 | 6 | 265 | A |
| 2 | 6 | 271 | A |
| 2 | 6 | 272 | U |
| 2 | 6 | 273 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 6 | 276 | C |
| 2 | 6 | 277 | U |
| 2 | 6 | 278 | U |
| 2 | 6 | 280 | U |
| 2 | 6 | 281 | G |
| 2 | 6 | 299 | A |
| 2 | 6 | 314 | C |
| 2 | 6 | 316 | A |
| 2 | 6 | 320 | U |
| 2 | 6 | 321 | C |
| 2 | 6 | 331 | A |
| 2 | 6 | 333 | A |
| 2 | 6 | 337 | G |
| 2 | 6 | 338 | C |
| 2 | 6 | 341 | A |
| 2 | 6 | 352 | A |
| 2 | 6 | 359 | A |
| 2 | 6 | 360 | A |
| 2 | 6 | 361 | C |
| 2 | 6 | 400 | A |
| 2 | 6 | 401 | A |
| 2 | 6 | 402 | C |
| 2 | 6 | 404 | G |
| 2 | 6 | 416 | A |
| 2 | 6 | 417 | A |
| 2 | 6 | 418 | G |
| 2 | 6 | 423 | G |
| 2 | 6 | 424 | C |
| 2 | 6 | 425 | A |
| 2 | 6 | 426 | G |
| 2 | 6 | 434 | G |
| 2 | 6 | 437 | A |
| 2 | 6 | 439 | U |
| 2 | 6 | 444 | C |
| 2 | 6 | 448 | C |
| 2 | 6 | 468 | A |
| 2 | 6 | 475 | A |
| 2 | 6 | 485 | A |
| 2 | 6 | 486 | G |
| 2 | 6 | 487 | G |
| 2 | 6 | 488 | G |
| 2 | 6 | 489 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 6 | 490 | C |
| 2 | 6 | 491 | C |
| 2 | 6 | 492 | A |
| 2 | 6 | 493 | U |
| 2 | 6 | 494 | U |
| 2 | 6 | 495 | C |
| 2 | 6 | 496 | G |
| 2 | 6 | 497 | G |
| 2 | 6 | 498 | G |
| 2 | 6 | 500 | C |
| 2 | 6 | 501 | U |
| 2 | 6 | 502 | U |
| 2 | 6 | 504 | U |
| 2 | 6 | 505 | A |
| 2 | 6 | 506 | A |
| 2 | 6 | 507 | U |
| 2 | 6 | 508 | U |
| 2 | 6 | 510 | G |
| 2 | 6 | 511 | A |
| 2 | 6 | 512 | A |
| 2 | 6 | 513 | U |
| 2 | 6 | 514 | G |
| 2 | 6 | 515 | A |
| 2 | 6 | 519 | C |
| 2 | 6 | 527 | A |
| 2 | 6 | 535 | A |
| 2 | 6 | 539 | G |
| 2 | 6 | 540 | G |
| 2 | 6 | 541 | A |
| 2 | 6 | 542 | A |
| 2 | 6 | 543 | C |
| 2 | 6 | 544 | A |
| 2 | 6 | 548 | G |
| 2 | 6 | 549 | G |
| 2 | 6 | 555 | A |
| 2 | 6 | 556 | A |
| 2 | 6 | 557 | G |
| 2 | 6 | 558 | U |
| 2 | 6 | 559 | C |
| 2 | 6 | 565 | C |
| 2 | 6 | 568 | G |
| 2 | 6 | 570 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 6 | 574 | G |
| 2 | 6 | 578 | U |
| 2 | 6 | 579 | A |
| 2 | 6 | 580 | A |
| 2 | 6 | 582 | U |
| 2 | 6 | 594 | A |
| 2 | 6 | 595 | G |
| 2 | 6 | 609 | U |
| 2 | 6 | 610 | G |
| 2 | 6 | 611 | U |
| 2 | 6 | 619 | A |
| 2 | 6 | 620 | A |
| 2 | 6 | 621 | A |
| 2 | 6 | 622 | A |
| 2 | 6 | 623 | A |
| 2 | 6 | 624 | G |
| 2 | 6 | 639 | U |
| 2 | 6 | 640 | U |
| 2 | 6 | 652 | G |
| 2 | 6 | 653 | C |
| 2 | 6 | 679 | U |
| 2 | 6 | 680 | U |
| 2 | 6 | 681 | U |
| 2 | 6 | 682 | C |
| 2 | 6 | 684 | A |
| 2 | 6 | 685 | A |
| 2 | 6 | 691 | C |
| 2 | 6 | 694 | U |
| 2 | 6 | 695 | U |
| 2 | 6 | 696 | C |
| 2 | 6 | 733 | A |
| 2 | 6 | 741 | C |
| 2 | 6 | 742 | U |
| 2 | 6 | 754 | A |
| 2 | 6 | 755 | A |
| 2 | 6 | 756 | A |
| 2 | 6 | 765 | G |
| 2 | 6 | 774 | A |
| 2 | 6 | 775 | G |
| 2 | 6 | 779 | U |
| 2 | 6 | 780 | A |
| 2 | 6 | 781 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 6 | 782 | U |
| 2 | 6 | 783 | G |
| 2 | 6 | 789 | A |
| 2 | 6 | 793 | A |
| 2 | 6 | 794 | U |
| 2 | 6 | 795 | U |
| 2 | 6 | 806 | A |
| 2 | 6 | 811 | A |
| 2 | 6 | 812 | A |
| 2 | 6 | 819 | G |
| 2 | 6 | 828 | U |
| 2 | 6 | 829 | A |
| 2 | 6 | 833 | U |
| 2 | 6 | 856 | A |
| 2 | 6 | 861 | U |
| 2 | 6 | 862 | A |
| 2 | 6 | 863 | A |
| 2 | 6 | 873 | U |
| 2 | 6 | 876 | G |
| 2 | 6 | 898 | A |
| 2 | 6 | 912 | U |
| 2 | 6 | 913 | G |
| 2 | 6 | 914 | G |
| 2 | 6 | 926 | A |
| 2 | 6 | 933 | A |
| 2 | 6 | 935 | U |
| 2 | 6 | 942 | G |
| 2 | 6 | 951 | A |
| 2 | 6 | 959 | U |
| 2 | 6 | 960 | U |
| 2 | 6 | 966 | A |
| 2 | 6 | 969 | C |
| 2 | 6 | 970 | A |
| 2 | 6 | 971 | A |
| 2 | 6 | 992 | A |
| 2 | 6 | 993 | A |
| 2 | 6 | 995 | A |
| 2 | 6 | 997 | G |
| 2 | 6 | 1003 | A |
| 2 | 6 | 1004 | U |
| 2 | 6 | 1005 | A |
| 2 | 6 | 1021 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 6 | 1026 | A |
| 2 | 6 | 1028 | C |
| 2 | 6 | 1029 | U |
| 2 | 6 | 1039 | A |
| 2 | 6 | 1040 | G |
| 2 | 6 | 1052 | U |
| 2 | 6 | 1053 | G |
| 2 | 6 | 1054 | U |
| 2 | 6 | 1055 | U |
| 2 | 6 | 1056 | U |
| 2 | 6 | 1057 | U |
| 2 | 6 | 1058 | U |
| 2 | 6 | 1059 | U |
| 2 | 6 | 1060 | U |
| 2 | 6 | 1061 | A |
| 2 | 6 | 1062 | A |
| 2 | 6 | 1063 | U |
| 2 | 6 | 1064 | G |
| 2 | 6 | 1072 | C |
| 2 | 6 | 1074 | G |
| 2 | 6 | 1082 | C |
| 2 | 6 | 1092 | A |
| 2 | 6 | 1096 | C |
| 2 | 6 | 1097 | U |
| 2 | 6 | 1098 | U |
| 2 | 6 | 1100 | G |
| 2 | 6 | 1101 | G |
| 2 | 6 | 1109 | G |
| 2 | 6 | 1111 | G |
| 2 | 6 | 1138 | A |
| 2 | 6 | 1139 | A |
| 2 | 6 | 1150 | G |
| 2 | 6 | 1151 | A |
| 2 | 6 | 1155 | G |
| 2 | 6 | 1158 | C |
| 2 | 6 | 1159 | C |
| 2 | 6 | 1160 | A |
| 2 | 6 | 1162 | C |
| 2 | 6 | 1164 | G |
| 2 | 6 | 1167 | G |
| 2 | 6 | 1185 | U |
| 2 | 6 | 1191 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 6 | 1194 | A |
| 2 | 6 | 1196 | A |
| 2 | 6 | 1197 | C |
| 2 | 6 | 1199 | G |
| 2 | 6 | 1200 | G |
| 2 | 6 | 1202 | A |
| 2 | 6 | 1208 | A |
| 2 | 6 | 1217 | A |
| 2 | 6 | 1218 | G |
| 2 | 6 | 1219 | A |
| 2 | 6 | 1220 | C |
| 2 | 6 | 1228 | G |
| 2 | 6 | 1241 | G |
| 2 | 6 | 1243 | G |
| 2 | 6 | 1245 | G |
| 2 | 6 | 1262 | U |
| 2 | 6 | 1263 | G |
| 2 | 6 | 1276 | U |
| 2 | 6 | 1284 | C |
| 2 | 6 | 1285 | U |
| 2 | 6 | 1286 | U |
| 2 | 6 | 1288 | G |
| 2 | 6 | 1291 | G |
| 2 | 6 | 1314 | U |
| 2 | 6 | 1315 | U |
| 2 | 6 | 1316 | G |
| 2 | 6 | 1321 | A |
| 2 | 6 | 1337 | A |
| 2 | 6 | 1343 | U |
| 2 | 6 | 1344 | A |
| 2 | 6 | 1345 | A |
| 2 | 6 | 1346 | A |
| 2 | 6 | 1347 | U |
| 2 | 6 | 1354 | G |
| 2 | 6 | 1361 | U |
| 2 | 6 | 1362 | U |
| 2 | 6 | 1363 | U |
| 2 | 6 | 1364 | G |
| 2 | 6 | 1370 | U |
| 2 | 6 | 1371 | A |
| 2 | 6 | 1378 | U |
| 2 | 6 | 1383 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 6 | 1390 | U |
| 2 | 6 | 1396 | U |
| 2 | 6 | 1398 | U |
| 2 | 6 | 1399 | C |
| 2 | 6 | 1400 | A |
| 2 | 6 | 1402 | G |
| 2 | 6 | 1413 | U |
| 2 | 6 | 1414 | U |
| 2 | 6 | 1415 | U |
| 2 | 6 | 1424 | A |
| 2 | 6 | 1427 | A |
| 2 | 6 | 1428 | G |
| 2 | 6 | 1445 | G |
| 2 | 6 | 1446 | A |
| 2 | 6 | 1448 | G |
| 2 | 6 | 1459 | C |
| 2 | 6 | 1461 | C |
| 2 | 6 | 1471 | A |
| 2 | 6 | 1481 | C |
| 2 | 6 | 1482 | C |
| 2 | 6 | 1486 | G |
| 2 | 6 | 1489 | U |
| 2 | 6 | 1490 | C |
| 2 | 6 | 1491 | U |
| 2 | 6 | 1492 | A |
| 2 | 6 | 1493 | A |
| 2 | 6 | 1494 | C |
| 2 | 6 | 1506 | G |
| 2 | 6 | 1514 | U |
| 2 | 6 | 1515 | A |
| 2 | 6 | 1516 | A |
| 2 | 6 | 1521 | G |
| 2 | 6 | 1523 | G |
| 2 | 6 | 1524 | A |
| 2 | 6 | 1531 | G |
| 2 | 6 | 1535 | U |
| 2 | 6 | 1536 | G |
| 2 | 6 | 1537 | C |
| 2 | 6 | 1538 | U |
| 2 | 6 | 1540 | G |
| 2 | 6 | 1554 | U |
| 2 | 6 | 1557 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 6 | 1559 | A |
| 2 | 6 | 1569 | A |
| 2 | 6 | 1572 | G |
| 2 | 6 | 1573 | A |
| 2 | 6 | 1574 | G |
| 2 | 6 | 1575 | G |
| 2 | 6 | 1582 | U |
| 2 | 6 | 1584 | G |
| 2 | 6 | 1590 | G |
| 2 | 6 | 1601 | G |
| 2 | 6 | 1616 | G |
| 2 | 6 | 1621 | U |
| 2 | 6 | 1637 | C |
| 2 | 6 | 1638 | G |
| 2 | 6 | 1657 | U |
| 2 | 6 | 1658 | G |
| 2 | 6 | 1665 | U |
| 2 | 6 | 1681 | A |
| 2 | 6 | 1736 | G |
| 2 | 6 | 1756 | A |
| 2 | 6 | 1757 | G |
| 2 | 6 | 1760 | G |
| 2 | 6 | 1762 | A |
| 2 | 6 | 1766 | A |
| 2 | 6 | 1767 | G |
| 2 | 6 | 1769 | U |
| 2 | 6 | 1770 | U |
| 2 | 6 | 1780 | G |
| 2 | 6 | 1782 | A |
| 2 | 6 | 1783 | C |
| 2 | 6 | 1792 | G |
| 2 | 6 | 1793 | G |
| 2 | 6 | 1794 | A |
| 2 | 6 | 1795 | U |
| 2 | 6 | 1796 | C |
| 2 | 6 | 1799 | U |
| 2 | 6 | 1800 | A |
| 3 | 7 | 7 | G |
| 3 | 7 | 22 | A |
| 3 | 7 | 33 | U |
| 3 | 7 | 38 | U |
| 3 | 7 | 54 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 3 | 7 | 55 | A |
| 3 | 7 | 65 | G |
| 3 | 7 | 73 | C |
| 3 | 7 | 74 | C |
| 3 | 7 | 76 | A |
| 3 | 7 | 93 | C |
| 3 | 7 | 101 | G |
| 3 | 7 | 102 | A |
| 3 | 7 | 103 | A |
| 3 | 7 | 112 | G |
| 4 | 8 | 21 | C |
| 4 | 8 | 22 | U |
| 4 | 8 | 34 | U |
| 4 | 8 | 35 | C |
| 4 | 8 | 48 | A |
| 4 | 8 | 51 | G |
| 4 | 8 | 52 | A |
| 4 | 8 | 59 | A |
| 4 | 8 | 62 | C |
| 4 | 8 | 63 | G |
| 4 | 8 | 79 | A |
| 4 | 8 | 80 | A |
| 4 | 8 | 81 | U |
| 4 | 8 | 82 | U |
| 4 | 8 | 83 | C |
| 4 | 8 | 84 | C |
| 4 | 8 | 86 | U |
| 4 | 8 | 87 | G |
| 4 | 8 | 90 | U |
| 4 | 8 | 95 | G |
| 4 | 8 | 104 | A |
| 4 | 8 | 106 | C |
| 4 | 8 | 111 | A |
| 4 | 8 | 113 | U |
| 4 | 8 | 116 | G |
| 4 | 8 | 125 | U |
| 4 | 8 | 126 | A |
| 4 | 8 | 127 | U |
| 4 | 8 | 138 | A |
| 4 | 8 | 152 | G |
| 4 | 8 | 156 | U |
| 4 | 8 | 157 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 4 | 8 | 158 | U |

All (296) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 40 | A |
| 1 | 1 | 43 | A |
| 1 | 1 | 65 | A |
| 1 | 1 | 232 | G |
| 1 | 1 | 239 | G |
| 1 | 1 | 240 | U |
| 1 | 1 | 252 | U |
| 1 | 1 | 282 | G |
| 1 | 1 | 518 | G |
| 1 | 1 | 545 | U |
| 1 | 1 | 546 | C |
| 1 | 1 | 558 | U |
| 1 | 1 | 594 | U |
| 1 | 1 | 636 | C |
| 1 | 1 | 637 | C |
| 1 | 1 | 715 | A |
| 1 | 1 | 763 | G |
| 1 | 1 | 764 | U |
| 1 | 1 | 816 | A |
| 1 | 1 | 873 | C |
| 1 | 1 | 916 | G |
| 1 | 1 | 979 | U |
| 1 | 1 | 981 | U |
| 1 | 1 | 993 | G |
| 1 | 1 | 1000 | C |
| 1 | 1 | 1014 | U |
| 1 | 1 | 1015 | U |
| 1 | 1 | 1017 | C |
| 1 | 1 | 1024 | G |
| 1 | 1 | 1028 | U |
| 1 | 1 | 1029 | G |
| 1 | 1 | 1064 | A |
| 1 | 1 | 1081 | U |
| 1 | 1 | 1094 | U |
| 1 | 1 | 1097 | G |
| 1 | 1 | 1103 | A |
| 1 | 1 | 1201 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 1284 | C |
| 1 | 1 | 1307 | G |
| 1 | 1 | 1329 | U |
| 1 | 1 | 1355 | A |
| 1 | 1 | 1484 | U |
| 1 | 1 | 1514 | G |
| 1 | 1 | 1554 | U |
| 1 | 1 | 1556 | C |
| 1 | 1 | 1562 | C |
| 1 | 1 | 1568 | U |
| 1 | 1 | 1571 | A |
| 1 | 1 | 1572 | U |
| 1 | 1 | 1581 | C |
| 1 | 1 | 1582 | C |
| 1 | 1 | 1607 | U |
| 1 | 1 | 1716 | U |
| 1 | 1 | 1762 | C |
| 1 | 1 | 1815 | U |
| 1 | 1 | 1816 | A |
| 1 | 1 | 1820 | U |
| 1 | 1 | 2101 | C |
| 1 | 1 | 2112 | U |
| 1 | 1 | 2208 | A |
| 1 | 1 | 2209 | U |
| 1 | 1 | 2227 | C |
| 1 | 1 | 2249 | G |
| 1 | 1 | 2255 | A |
| 1 | 1 | 2256 | A |
| 1 | 1 | 2372 | A |
| 1 | 1 | 2400 | G |
| 1 | 1 | 2418 | G |
| 1 | 1 | 2513 | U |
| 1 | 1 | 2522 | G |
| 1 | 1 | 2525 | G |
| 1 | 1 | 2537 | U |
| 1 | 1 | 2538 | U |
| 1 | 1 | 2541 | U |
| 1 | 1 | 2554 | A |
| 1 | 1 | 2566 | C |
| 1 | 1 | 2570 | U |
| 1 | 1 | 2571 | U |
| 1 | 1 | 2585 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 1 | 2593 | A |
| 1 | 1 | 2689 | A |
| 1 | 1 | 2801 | A |
| 1 | 1 | 2818 | U |
| 1 | 1 | 3078 | U |
| 1 | 1 | 3121 | U |
| 1 | 1 | 3157 | U |
| 1 | 1 | 3169 | U |
| 1 | 1 | 3218 | A |
| 1 | 1 | 3228 | C |
| 1 | 1 | 3238 | G |
| 1 | 1 | 3259 | U |
| 1 | 1 | 3269 | U |
| 1 | 1 | 3316 | A |
| 1 | 1 | 3317 | U |
| 1 | 1 | 3350 | C |
| 1 | 1 | 3351 | U |
| 1 | 1 | 3353 | G |
| 1 | 1 | 3375 | A |
| 1 | 1 | 3389 | U |
| 2 | 2 | 1 | U |
| 2 | 2 | 25 | C |
| 2 | 2 | 68 | A |
| 2 | 2 | 72 | A |
| 2 | 2 | 73 | U |
| 2 | 2 | 74 | U |
| 2 | 2 | 76 | A |
| 2 | 2 | 103 | A |
| 2 | 2 | 114 | C |
| 2 | 2 | 139 | C |
| 2 | 2 | 144 | U |
| 2 | 2 | 158 | U |
| 2 | 2 | 187 | G |
| 2 | 2 | 232 | U |
| 2 | 2 | 240 | U |
| 2 | 2 | 278 | U |
| 2 | 2 | 280 | U |
| 2 | 2 | 319 | U |
| 2 | 2 | 321 | C |
| 2 | 2 | 417 | A |
| 2 | 2 | 484 | C |
| 2 | 2 | 497 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 499 | U |
| 2 | 2 | 501 | U |
| 2 | 2 | 503 | G |
| 2 | 2 | 512 | A |
| 2 | 2 | 555 | A |
| 2 | 2 | 558 | U |
| 2 | 2 | 622 | A |
| 2 | 2 | 685 | A |
| 2 | 2 | 704 | C |
| 2 | 2 | 720 | G |
| 2 | 2 | 721 | U |
| 2 | 2 | 734 | A |
| 2 | 2 | 755 | A |
| 2 | 2 | 781 | U |
| 2 | 2 | 782 | U |
| 2 | 2 | 794 | U |
| 2 | 2 | 913 | G |
| 2 | 2 | 1051 | G |
| 2 | 2 | 1081 | A |
| 2 | 2 | 1150 | G |
| 2 | 2 | 1157 | A |
| 2 | 2 | 1196 | A |
| 2 | 2 | 1207 | C |
| 2 | 2 | 1226 | A |
| 2 | 2 | 1244 | A |
| 2 | 2 | 1250 | U |
| 2 | 2 | 1285 | U |
| 2 | 2 | 1286 | U |
| 2 | 2 | 1339 | C |
| 2 | 2 | 1344 | A |
| 2 | 2 | 1370 | U |
| 2 | 2 | 1410 | A |
| 2 | 2 | 1481 | C |
| 2 | 2 | 1489 | U |
| 2 | 2 | 1490 | C |
| 2 | 2 | 1491 | U |
| 2 | 2 | 1568 | C |
| 2 | 2 | 1573 | A |
| 2 | 2 | 1615 | C |
| 2 | 2 | 1761 | U |
| 3 | 3 | 52 | G |
| 4 | 4 | 83 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 4 | 4 | 85 | G |
| 4 | 4 | 111 | A |
| 4 | 4 | 125 | U |
| 1 | 5 | 65 | A |
| 1 | 5 | 151 | A |
| 1 | 5 | 282 | G |
| 1 | 5 | 636 | C |
| 1 | 5 | 715 | A |
| 1 | 5 | 726 | G |
| 1 | 5 | 735 | A |
| 1 | 5 | 765 | C |
| 1 | 5 | 816 | A |
| 1 | 5 | 873 | C |
| 1 | 5 | 916 | G |
| 1 | 5 | 979 | U |
| 1 | 5 | 993 | G |
| 1 | 5 | 1064 | A |
| 1 | 5 | 1081 | U |
| 1 | 5 | 1152 | G |
| 1 | 5 | 1154 | A |
| 1 | 5 | 1284 | C |
| 1 | 5 | 1285 | G |
| 1 | 5 | 1307 | G |
| 1 | 5 | 1329 | U |
| 1 | 5 | 1355 | A |
| 1 | 5 | 1481 | A |
| 1 | 5 | 1581 | C |
| 1 | 5 | 1582 | C |
| 1 | 5 | 1607 | U |
| 1 | 5 | 1630 | U |
| 1 | 5 | 1716 | U |
| 1 | 5 | 1724 | U |
| 1 | 5 | 1816 | A |
| 1 | 5 | 1819 | U |
| 1 | 5 | 2101 | C |
| 1 | 5 | 2112 | U |
| 1 | 5 | 2204 | C |
| 1 | 5 | 2205 | U |
| 1 | 5 | 2206 | G |
| 1 | 5 | 2209 | U |
| 1 | 5 | 2249 | G |
| 1 | 5 | 2255 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 5 | 2257 | C |
| 1 | 5 | 2268 | U |
| 1 | 5 | 2272 | G |
| 1 | 5 | 2281 | A |
| 1 | 5 | 2373 | A |
| 1 | 5 | 2512 | C |
| 1 | 5 | 2513 | U |
| 1 | 5 | 2522 | G |
| 1 | 5 | 2537 | U |
| 1 | 5 | 2568 | C |
| 1 | 5 | 2569 | A |
| 1 | 5 | 2593 | A |
| 1 | 5 | 2662 | G |
| 1 | 5 | 2682 | C |
| 1 | 5 | 2772 | C |
| 1 | 5 | 2801 | A |
| 1 | 5 | 2817 | A |
| 1 | 5 | 2818 | U |
| 1 | 5 | 2872 | A |
| 1 | 5 | 3078 | U |
| 1 | 5 | 3121 | U |
| 1 | 5 | 3195 | U |
| 1 | 5 | 3218 | A |
| 1 | 5 | 3228 | C |
| 1 | 5 | 3269 | U |
| 1 | 5 | 3275 | U |
| 1 | 5 | 3317 | U |
| 1 | 5 | 3340 | G |
| 1 | 5 | 3341 | U |
| 1 | 5 | 3353 | G |
| 1 | 5 | 3395 | G |
| 2 | 6 | 66 | U |
| 2 | 6 | 75 | U |
| 2 | 6 | 76 | A |
| 2 | 6 | 77 | U |
| 2 | 6 | 78 | A |
| 2 | 6 | 103 | A |
| 2 | 6 | 114 | C |
| 2 | 6 | 130 | C |
| 2 | 6 | 137 | U |
| 2 | 6 | 139 | C |
| 2 | 6 | 158 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 6 | 187 | G |
| 2 | 6 | 192 | U |
| 2 | 6 | 217 | A |
| 2 | 6 | 238 | U |
| 2 | 6 | 240 | U |
| 2 | 6 | 272 | U |
| 2 | 6 | 277 | U |
| 2 | 6 | 319 | U |
| 2 | 6 | 417 | A |
| 2 | 6 | 488 | G |
| 2 | 6 | 490 | C |
| 2 | 6 | 512 | A |
| 2 | 6 | 542 | A |
| 2 | 6 | 555 | A |
| 2 | 6 | 557 | G |
| 2 | 6 | 558 | U |
| 2 | 6 | 652 | G |
| 2 | 6 | 694 | U |
| 2 | 6 | 695 | U |
| 2 | 6 | 741 | C |
| 2 | 6 | 755 | A |
| 2 | 6 | 781 | U |
| 2 | 6 | 827 | C |
| 2 | 6 | 856 | A |
| 2 | 6 | 1051 | G |
| 2 | 6 | 1058 | U |
| 2 | 6 | 1097 | U |
| 2 | 6 | 1196 | A |
| 2 | 6 | 1207 | C |
| 2 | 6 | 1227 | A |
| 2 | 6 | 1284 | C |
| 2 | 6 | 1344 | A |
| 2 | 6 | 1346 | A |
| 2 | 6 | 1413 | U |
| 2 | 6 | 1481 | C |
| 2 | 6 | 1489 | U |
| 2 | 6 | 1493 | A |
| 2 | 6 | 1535 | U |
| 2 | 6 | 1568 | C |
| 2 | 6 | 1573 | A |
| 2 | 6 | 1615 | C |
| 2 | 6 | 1620 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | 6 | 1637 | C |
| 2 | 6 | 1657 | U |
| 3 | 7 | 86 | U |
| 4 | 8 | 80 | A |
| 4 | 8 | 81 | U |
| 4 | 8 | 82 | U |
| 4 | 8 | 126 | A |

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1407 ligands modelled in this entry, 1382 are monoatomic - leaving 25 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 81 | 8UZ | 2 | 2031 | - | 35,35,35 | 0.37 | 0 | 49,52,52 | 1.02 | 3 (6%) |
| 81 | 8UZ | 1 | 3890 | - | 35,35,35 | 0.35 | 0 | 49,52,52 | 1.32 | 4 (8%) |
| 81 | 8UZ | 5 | 3855 | - | 35,35,35 | 0.35 | 0 | 49,52,52 | 1.28 | 8 (16%) |
| 81 | 8UZ | 1 | 3894 | - | 35,35,35 | 0.34 | 0 | 49,52,52 | 1.41 | 5 (10%) |
| 81 | 8UZ | 7 | 209 | - | 35,35,35 | 0.43 | 0 | 49,52,52 | 1.21 | 6 (12%) |
| 81 | 8UZ | 3 | 214 | - | 35,35,35 | 0.44 | 0 | 49,52,52 | 1.58 | 7 (14%) |
| 81 | 8UZ | 1 | 3895 | - | 35,35,35 | 0.34 | 0 | 49,52,52 | 1.27 | 7 (14%) |
| 81 | 8UZ | 1 | 3886 | - | 35,35,35 | 0.37 | 0 | 49,52,52 | 1.28 | 5 (10%) |
| 81 | 8UZ | 5 | 3857 | - | 35,35,35 | 0.36 | 0 | 49,52,52 | 0.96 | 3 (6%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 81 | 8UZ | 5 | 3852 | - | 35,35,35 | 0.36 | 0 | 49,52,52 | 1.23 | 3 (6%) |
| 81 | 8UZ | 6 | 2061 | - | 35,35,35 | 0.36 | 0 | 49,52,52 | 1.51 | 7 (14%) |
| 81 | 8UZ | 1 | 3891 | - | 35,35,35 | 0.36 | 0 | 49,52,52 | 1.37 | 7 (14%) |
| 81 | 8UZ | 1 | 3888 | - | 35,35,35 | 0.33 | 0 | 49,52,52 | 1.05 | 3 (6%) |
| 81 | 8UZ | 1 | 3889 | - | 35,35,35 | 0.19 | 0 | 49,52,52 | 0.80 | 2 (4%) |
| 81 | 8UZ | 2 | 2030 | - | 35,35,35 | 0.26 | 0 | 49,52,52 | 1.21 | 4 (8%) |
| 81 | 8UZ | 5 | 3854 | - | 35,35,35 | 0.34 | 0 | 49,52,52 | 1.79 | 6 (12%) |
| 81 | 8UZ | 5 | 3850 | - | 35,35,35 | 0.31 | 0 | 49,52,52 | 1.08 | 3 (6%) |
| 81 | 8UZ | 4 | 220 | - | 35,35,35 | 0.54 | 0 | 49,52,52 | 1.56 | 8 (16%) |
| 81 | 8UZ | 5 | 3856 | - | 35,35,35 | 0.28 | 0 | 49,52,52 | 1.45 | 7 (14%) |
| 81 | 8UZ | 5 | 3853 | - | 35,35,35 | 0.31 | 0 | 49,52,52 | 1.23 | 6 (12%) |
| 81 | 8UZ | 1 | 3892 | - | 35,35,35 | 0.44 | 0 | 49,52,52 | 1.35 | 4 (8%) |
| 81 | 8UZ | 5 | 3851 | - | 35,35,35 | 0.25 | 0 | 49,52,52 | 1.12 | 5 (10%) |
| 81 | 8UZ | 1 | 3887 | - | 35,35,35 | 0.42 | 0 | 49,52,52 | 1.30 | 3 (6%) |
| 81 | 8UZ | 2 | 2029 | - | 35,35,35 | 0.36 | 0 | 49,52,52 | 1.36 | 6 (12%) |
| 81 | 8UZ | 1 | 3893 | - | 35,35,35 | 0.54 | 0 | 49,52,52 | 0.96 | 3 (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. '2' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 81 | 8UZ | 2 | 2031 | - | - | 3/12/72/72 | 0/3/3/3 |
| 81 | 8UZ | 1 | 3890 | - | - | 6/12/72/72 | 0/3/3/3 |
| 81 | 8UZ | 5 | 3855 | - | - | 6/12/72/72 | 0/3/3/3 |
| 81 | 8UZ | 1 | 3894 | - | - | 3/12/72/72 | 0/3/3/3 |
| 81 | 8UZ | 7 | 209 | - | - | 7/12/72/72 | 0/3/3/3 |
| 81 | 8UZ | 3 | 214 | - | - | 4/12/72/72 | 0/3/3/3 |
| 81 | 8UZ | 1 | 3895 | - | - | 7/12/72/72 | 0/3/3/3 |
| 81 | 8UZ | 1 | 3886 | - | - | 4/12/72/72 | 0/3/3/3 |
| 81 | 8UZ | 5 | 3857 | - | - | 7/12/72/72 | 0/3/3/3 |
| 81 | 8UZ | 5 | 3852 | - | - | 3/12/72/72 | 0/3/3/3 |
| 81 | 8UZ | 6 | 2061 | - | - | 5/12/72/72 | 0/3/3/3 |
| 81 | 8UZ | 1 | 3891 | - | - | 8/12/72/72 | 0/3/3/3 |
| 81 | 8UZ | 1 | 3888 | - | - | 7/12/72/72 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-------------|---------|
| 81 | 8UZ | 1 | 3889 | - | - | 1/12/72/72 | 0/3/3/3 |
| 81 | 8UZ | 2 | 2030 | - | - | 5/12/72/72 | 0/3/3/3 |
| 81 | 8UZ | 5 | 3854 | - | - | 5/12/72/72 | 0/3/3/3 |
| 81 | 8UZ | 5 | 3850 | - | - | 3/12/72/72 | 0/3/3/3 |
| 81 | 8UZ | 4 | 220 | - | - | 6/12/72/72 | 0/3/3/3 |
| 81 | 8UZ | 5 | 3856 | - | - | 5/12/72/72 | 0/3/3/3 |
| 81 | 8UZ | 5 | 3853 | - | - | 6/12/72/72 | 0/3/3/3 |
| 81 | 8UZ | 1 | 3892 | - | - | 4/12/72/72 | 0/3/3/3 |
| 81 | 8UZ | 5 | 3851 | - | - | 4/12/72/72 | 0/3/3/3 |
| 81 | 8UZ | 1 | 3887 | - | - | 9/12/72/72 | 0/3/3/3 |
| 81 | 8UZ | 2 | 2029 | - | - | 10/12/72/72 | 0/3/3/3 |
| 81 | 8UZ | 1 | 3893 | - | - | 4/12/72/72 | 0/3/3/3 |

There are no bond length outliers.

All (125) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 81 | 5 | 3854 | 8UZ | C2-C15-N4 | 7.37 | 123.48 | 110.20 |
| 81 | 5 | 3854 | 8UZ | C14-C13-C12 | -6.83 | 96.24 | 111.06 |
| 81 | 6 | 2061 | 8UZ | C2-C15-N4 | 6.73 | 122.33 | 110.20 |
| 81 | 1 | 3894 | 8UZ | C2-C15-N4 | 5.79 | 120.64 | 110.20 |
| 81 | 3 | 214 | 8UZ | O1-C2-C15 | 5.52 | 117.72 | 108.22 |
| 81 | 1 | 3887 | 8UZ | C14-C13-C12 | -5.44 | 99.26 | 111.06 |
| 81 | 1 | 3892 | 8UZ | C2-C15-N4 | 5.34 | 119.82 | 110.20 |
| 81 | 5 | 3852 | 8UZ | O1-C2-C15 | -5.17 | 99.31 | 108.22 |
| 81 | 3 | 214 | 8UZ | C14-C13-C12 | -5.10 | 99.98 | 111.06 |
| 81 | 2 | 2030 | 8UZ | C2-C15-N4 | 5.03 | 119.26 | 110.20 |
| 81 | 5 | 3856 | 8UZ | C2-C15-N4 | 4.90 | 119.03 | 110.20 |
| 81 | 1 | 3887 | 8UZ | C2-C15-N4 | 4.79 | 118.84 | 110.20 |
| 81 | 5 | 3850 | 8UZ | O1-C2-C15 | 4.76 | 116.41 | 108.22 |
| 81 | 4 | 220 | 8UZ | C2-C15-N4 | 4.65 | 118.58 | 110.20 |
| 81 | 1 | 3891 | 8UZ | O1-C3-C4 | 4.60 | 120.15 | 109.18 |
| 81 | 1 | 3890 | 8UZ | C2-C15-N4 | 4.49 | 118.29 | 110.20 |
| 81 | 1 | 3886 | 8UZ | C2-C15-N4 | 4.48 | 118.27 | 110.20 |
| 81 | 1 | 3891 | 8UZ | C2-C15-N4 | 4.37 | 118.07 | 110.20 |
| 81 | 2 | 2029 | 8UZ | C2-C15-N4 | 4.11 | 117.62 | 110.20 |
| 81 | 4 | 220 | 8UZ | C9-C14-C13 | -4.00 | 105.03 | 110.40 |
| 81 | 1 | 3890 | 8UZ | O1-C2-C15 | 3.97 | 115.05 | 108.22 |
| 81 | 5 | 3856 | 8UZ | C6-C5-C4 | -3.89 | 103.20 | 111.18 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 81 | 1 | 3895 | 8UZ | C2-C15-N4 | 3.88 | 117.19 | 110.20 |
| 81 | 4 | 220 | 8UZ | C8-C3-C4 | 3.84 | 118.33 | 111.16 |
| 81 | 2 | 2029 | 8UZ | C9-C14-C13 | 3.78 | 115.47 | 110.40 |
| 81 | 5 | 3850 | 8UZ | C2-C15-N4 | 3.77 | 116.99 | 110.20 |
| 81 | 5 | 3851 | 8UZ | O1-C2-C15 | 3.74 | 114.65 | 108.22 |
| 81 | 7 | 209 | 8UZ | C2-C15-N4 | 3.72 | 116.91 | 110.20 |
| 81 | 5 | 3853 | 8UZ | C2-C15-N4 | 3.68 | 116.83 | 110.20 |
| 81 | 5 | 3856 | 8UZ | C14-C13-C12 | -3.59 | 103.26 | 111.06 |
| 81 | 1 | 3894 | 8UZ | O1-C3-C4 | 3.55 | 117.64 | 109.18 |
| 81 | 1 | 3886 | 8UZ | C14-C13-C12 | -3.48 | 103.51 | 111.06 |
| 81 | 1 | 3892 | 8UZ | O1-C3-C4 | 3.46 | 117.42 | 109.18 |
| 81 | 5 | 3854 | 8UZ | O1-C2-C15 | 3.41 | 114.09 | 108.22 |
| 81 | 1 | 3893 | 8UZ | C2-C15-N4 | 3.40 | 116.33 | 110.20 |
| 81 | 5 | 3852 | 8UZ | C2-C15-N4 | 3.35 | 116.23 | 110.20 |
| 81 | 1 | 3888 | 8UZ | C2-C15-N4 | 3.34 | 116.22 | 110.20 |
| 81 | 1 | 3890 | 8UZ | C14-C13-C12 | -3.32 | 103.86 | 111.06 |
| 81 | 6 | 2061 | 8UZ | C9-C14-C13 | 3.32 | 114.85 | 110.40 |
| 81 | 2 | 2029 | 8UZ | C14-C13-C12 | 3.31 | 118.24 | 111.06 |
| 81 | 1 | 3892 | 8UZ | O1-C2-C15 | 3.30 | 113.90 | 108.22 |
| 81 | 2 | 2031 | 8UZ | C8-C3-C4 | 3.26 | 117.24 | 111.16 |
| 81 | 1 | 3891 | 8UZ | O3-C8-C7 | 3.23 | 115.87 | 107.28 |
| 81 | 1 | 3892 | 8UZ | C14-C13-C12 | -3.19 | 104.13 | 111.06 |
| 81 | 3 | 214 | 8UZ | O-C2-C15 | 3.19 | 117.24 | 110.06 |
| 81 | 7 | 209 | 8UZ | O-C2-C15 | 3.19 | 117.22 | 110.06 |
| 81 | 5 | 3853 | 8UZ | C9-C14-C13 | -3.12 | 106.20 | 110.40 |
| 81 | 6 | 2061 | 8UZ | O1-C3-C4 | 3.11 | 116.60 | 109.18 |
| 81 | 5 | 3855 | 8UZ | C2-C15-N4 | 3.10 | 115.79 | 110.20 |
| 81 | 2 | 2029 | 8UZ | O3-C8-C7 | 3.10 | 115.53 | 107.28 |
| 81 | 3 | 214 | 8UZ | C2-C15-N4 | 3.08 | 115.75 | 110.20 |
| 81 | 5 | 3851 | 8UZ | C2-C15-N4 | 3.07 | 115.74 | 110.20 |
| 81 | 5 | 3856 | 8UZ | C8-C7-C6 | 3.06 | 117.10 | 109.63 |
| 81 | 5 | 3855 | 8UZ | C14-C13-C12 | -3.01 | 104.52 | 111.06 |
| 81 | 5 | 3853 | 8UZ | O3-C9-C14 | 2.99 | 115.85 | 108.10 |
| 81 | 3 | 214 | 8UZ | O1-C3-C4 | 2.97 | 116.25 | 109.18 |
| 81 | 5 | 3854 | 8UZ | C9-O4-C10 | 2.94 | 119.45 | 113.69 |
| 81 | 1 | 3894 | 8UZ | O1-C2-C15 | 2.88 | 113.17 | 108.22 |
| 81 | 4 | 220 | 8UZ | O3-C8-C7 | 2.87 | 114.92 | 107.28 |
| 81 | 5 | 3855 | 8UZ | C8-C7-C6 | -2.85 | 102.68 | 109.63 |
| 81 | 1 | 3895 | 8UZ | C9-O3-C8 | 2.76 | 124.80 | 117.96 |
| 81 | 6 | 2061 | 8UZ | O1-C2-C15 | 2.74 | 112.94 | 108.22 |
| 81 | 5 | 3856 | 8UZ | C7-C8-C3 | 2.74 | 117.92 | 111.66 |
| 81 | 1 | 3891 | 8UZ | O1-C2-C15 | 2.73 | 112.91 | 108.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 81 | 4 | 220 | 8UZ | O3-C9-O4 | 2.67 | 118.14 | 110.67 |
| 81 | 5 | 3855 | 8UZ | C5-C6-C7 | -2.67 | 106.01 | 110.04 |
| 81 | 5 | 3853 | 8UZ | C6-C5-C4 | -2.64 | 105.77 | 111.18 |
| 81 | 6 | 2061 | 8UZ | C9-O4-C10 | 2.63 | 118.85 | 113.69 |
| 81 | 5 | 3855 | 8UZ | O1-C2-C15 | 2.63 | 112.75 | 108.22 |
| 81 | 2 | 2031 | 8UZ | C2-C15-N4 | 2.63 | 114.94 | 110.20 |
| 81 | 1 | 3895 | 8UZ | O3-C9-C14 | 2.62 | 114.88 | 108.10 |
| 81 | 5 | 3855 | 8UZ | C6-C5-C4 | -2.61 | 105.82 | 111.18 |
| 81 | 1 | 3895 | 8UZ | O1-C2-C15 | 2.60 | 112.69 | 108.22 |
| 81 | 1 | 3894 | 8UZ | C9-C14-C13 | 2.59 | 113.87 | 110.40 |
| 81 | 5 | 3851 | 8UZ | O1-C3-C4 | 2.56 | 115.27 | 109.18 |
| 81 | 7 | 209 | 8UZ | C16-C17-C1 | -2.55 | 105.69 | 110.24 |
| 81 | 4 | 220 | 8UZ | O1-C2-C15 | 2.54 | 112.59 | 108.22 |
| 81 | 5 | 3857 | 8UZ | O1-C3-C4 | 2.53 | 115.22 | 109.18 |
| 81 | 2 | 2029 | 8UZ | C8-C7-C6 | -2.53 | 103.46 | 109.63 |
| 81 | 5 | 3855 | 8UZ | O2-C7-C8 | 2.49 | 116.53 | 109.94 |
| 81 | 6 | 2061 | 8UZ | C17-C16-C15 | -2.47 | 106.83 | 111.07 |
| 81 | 1 | 3893 | 8UZ | C14-C13-C12 | 2.46 | 116.39 | 111.06 |
| 81 | 1 | 3886 | 8UZ | C9-O3-C8 | 2.42 | 123.96 | 117.96 |
| 81 | 5 | 3856 | 8UZ | C8-C3-C4 | 2.41 | 115.67 | 111.16 |
| 81 | 5 | 3853 | 8UZ | C14-C13-C12 | -2.40 | 105.84 | 111.06 |
| 81 | 3 | 214 | 8UZ | C9-O4-C10 | 2.38 | 118.37 | 113.69 |
| 81 | 1 | 3894 | 8UZ | C16-C17-C1 | 2.37 | 114.47 | 110.24 |
| 81 | 5 | 3857 | 8UZ | C6-C5-C4 | 2.36 | 116.02 | 111.18 |
| 81 | 1 | 3889 | 8UZ | C14-C13-C12 | -2.34 | 105.97 | 111.06 |
| 81 | 5 | 3856 | 8UZ | C17-C16-C15 | -2.31 | 107.09 | 111.07 |
| 81 | 7 | 209 | 8UZ | C17-C16-C15 | -2.30 | 107.12 | 111.07 |
| 81 | 4 | 220 | 8UZ | O1-C3-C8 | -2.28 | 101.69 | 107.48 |
| 81 | 5 | 3851 | 8UZ | O-C2-C15 | 2.27 | 115.17 | 110.06 |
| 81 | 2 | 2030 | 8UZ | O1-C3-C8 | 2.26 | 113.23 | 107.48 |
| 81 | 5 | 3855 | 8UZ | O3-C8-C3 | 2.25 | 113.20 | 107.48 |
| 81 | 2 | 2030 | 8UZ | O3-C8-C7 | -2.24 | 101.31 | 107.28 |
| 81 | 1 | 3893 | 8UZ | C6-C5-C4 | 2.24 | 115.79 | 111.18 |
| 81 | 6 | 2061 | 8UZ | O4-C9-C14 | 2.24 | 115.09 | 110.35 |
| 81 | 5 | 3851 | 8UZ | C14-C13-C12 | -2.22 | 106.23 | 111.06 |
| 81 | 1 | 3895 | 8UZ | C6-C5-C4 | -2.21 | 106.64 | 111.18 |
| 81 | 5 | 3853 | 8UZ | C9-O3-C8 | 2.19 | 123.39 | 117.96 |
| 81 | 5 | 3850 | 8UZ | C14-C13-C12 | -2.18 | 106.32 | 111.06 |
| 81 | 1 | 3888 | 8UZ | C8-C7-C6 | 2.17 | 114.92 | 109.63 |
| 81 | 7 | 209 | 8UZ | O1-C2-C15 | 2.17 | 111.95 | 108.22 |
| 81 | 5 | 3852 | 8UZ | O-C1-C17 | 2.17 | 113.63 | 109.69 |
| 81 | 1 | 3891 | 8UZ | C9-C14-C13 | -2.17 | 107.49 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 81 | 3 | 214 | 8UZ | C2-O-C1 | 2.16 | 117.93 | 113.69 |
| 81 | 1 | 3886 | 8UZ | O3-C8-C3 | 2.16 | 112.96 | 107.48 |
| 81 | 2 | 2029 | 8UZ | O2-C7-C8 | 2.16 | 115.66 | 109.94 |
| 81 | 1 | 3887 | 8UZ | O1-C3-C4 | 2.12 | 114.23 | 109.18 |
| 81 | 1 | 3890 | 8UZ | O1-C3-C4 | 2.11 | 114.21 | 109.18 |
| 81 | 2 | 2030 | 8UZ | O3-C8-C3 | 2.08 | 112.75 | 107.48 |
| 81 | 1 | 3889 | 8UZ | O1-C2-C15 | -2.07 | 104.64 | 108.22 |
| 81 | 1 | 3891 | 8UZ | C7-C8-C3 | -2.07 | 106.94 | 111.66 |
| 81 | 5 | 3854 | 8UZ | C8-C3-C4 | 2.06 | 115.01 | 111.16 |
| 81 | 5 | 3857 | 8UZ | O-C2-C15 | 2.06 | 114.69 | 110.06 |
| 81 | 5 | 3854 | 8UZ | C9-C14-C13 | -2.06 | 107.63 | 110.40 |
| 81 | 2 | 2031 | 8UZ | O3-C8-C3 | 2.05 | 112.70 | 107.48 |
| 81 | 1 | 3888 | 8UZ | O1-C3-C4 | -2.05 | 104.28 | 109.18 |
| 81 | 7 | 209 | 8UZ | O9-C17-C1 | 2.05 | 114.39 | 109.30 |
| 81 | 1 | 3895 | 8UZ | O3-C8-C7 | -2.04 | 101.84 | 107.28 |
| 81 | 1 | 3895 | 8UZ | C8-C7-C6 | 2.04 | 114.62 | 109.63 |
| 81 | 4 | 220 | 8UZ | C14-C13-C12 | -2.04 | 106.62 | 111.06 |
| 81 | 1 | 3886 | 8UZ | O1-C2-C15 | 2.02 | 111.70 | 108.22 |
| 81 | 1 | 3891 | 8UZ | O3-C9-C14 | 2.01 | 113.32 | 108.10 |

There are no chirality outliers.

All (132) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|--------------|
| 81 | 1 | 3886 | 8UZ | C14-C9-O3-C8 |
| 81 | 1 | 3887 | 8UZ | N-C-C1-C17 |
| 81 | 1 | 3887 | 8UZ | N-C-C1-O |
| 81 | 1 | 3887 | 8UZ | C15-C2-O1-C3 |
| 81 | 1 | 3888 | 8UZ | N-C-C1-O |
| 81 | 1 | 3890 | 8UZ | C15-C2-O1-C3 |
| 81 | 1 | 3891 | 8UZ | C14-C9-O3-C8 |
| 81 | 1 | 3891 | 8UZ | N-C-C1-C17 |
| 81 | 1 | 3891 | 8UZ | N-C-C1-O |
| 81 | 1 | 3891 | 8UZ | C15-C2-O1-C3 |
| 81 | 1 | 3892 | 8UZ | C15-C2-O1-C3 |
| 81 | 1 | 3893 | 8UZ | N-C-C1-C17 |
| 81 | 1 | 3893 | 8UZ | N-C-C1-O |
| 81 | 1 | 3895 | 8UZ | C14-C9-O3-C8 |
| 81 | 1 | 3895 | 8UZ | N-C-C1-C17 |
| 81 | 1 | 3895 | 8UZ | N-C-C1-O |
| 81 | 2 | 2029 | 8UZ | N-C-C1-C17 |
| 81 | 2 | 2029 | 8UZ | N-C-C1-O |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|----------------|
| 81 | 2 | 2029 | 8UZ | C15-C2-O1-C3 |
| 81 | 2 | 2030 | 8UZ | C14-C9-O3-C8 |
| 81 | 3 | 214 | 8UZ | N-C-C1-O |
| 81 | 3 | 214 | 8UZ | C15-C2-O1-C3 |
| 81 | 4 | 220 | 8UZ | N-C-C1-C17 |
| 81 | 4 | 220 | 8UZ | N-C-C1-O |
| 81 | 4 | 220 | 8UZ | C15-C2-O1-C3 |
| 81 | 5 | 3852 | 8UZ | N-C-C1-C17 |
| 81 | 5 | 3853 | 8UZ | C14-C9-O3-C8 |
| 81 | 5 | 3853 | 8UZ | N-C-C1-O |
| 81 | 5 | 3854 | 8UZ | N-C-C1-O |
| 81 | 5 | 3854 | 8UZ | C15-C2-O1-C3 |
| 81 | 5 | 3855 | 8UZ | N-C-C1-C17 |
| 81 | 5 | 3855 | 8UZ | N-C-C1-O |
| 81 | 5 | 3856 | 8UZ | N-C-C1-C17 |
| 81 | 5 | 3856 | 8UZ | N-C-C1-O |
| 81 | 5 | 3856 | 8UZ | C15-C2-O1-C3 |
| 81 | 5 | 3857 | 8UZ | N-C-C1-C17 |
| 81 | 5 | 3857 | 8UZ | N-C-C1-O |
| 81 | 5 | 3857 | 8UZ | C4-C3-O1-C2 |
| 81 | 6 | 2061 | 8UZ | C15-C2-O1-C3 |
| 81 | 7 | 209 | 8UZ | N-C-C1-O |
| 81 | 7 | 209 | 8UZ | C15-C2-O1-C3 |
| 81 | 2 | 2029 | 8UZ | O4-C9-O3-C8 |
| 81 | 2 | 2031 | 8UZ | O4-C9-O3-C8 |
| 81 | 5 | 3854 | 8UZ | O-C2-O1-C3 |
| 81 | 6 | 2061 | 8UZ | O-C2-O1-C3 |
| 81 | 1 | 3886 | 8UZ | O4-C9-O3-C8 |
| 81 | 2 | 2030 | 8UZ | O4-C9-O3-C8 |
| 81 | 2 | 2029 | 8UZ | C14-C9-O3-C8 |
| 81 | 5 | 3857 | 8UZ | O4-C9-O3-C8 |
| 81 | 5 | 3857 | 8UZ | C14-C9-O3-C8 |
| 81 | 5 | 3850 | 8UZ | C12-C10-C11-O5 |
| 81 | 6 | 2061 | 8UZ | C14-C9-O3-C8 |
| 81 | 1 | 3887 | 8UZ | C12-C10-C11-O5 |
| 81 | 5 | 3850 | 8UZ | O4-C10-C11-O5 |
| 81 | 1 | 3887 | 8UZ | O4-C9-O3-C8 |
| 81 | 1 | 3887 | 8UZ | O-C2-O1-C3 |
| 81 | 1 | 3894 | 8UZ | O4-C9-O3-C8 |
| 81 | 1 | 3888 | 8UZ | O4-C9-O3-C8 |
| 81 | 6 | 2061 | 8UZ | O4-C9-O3-C8 |
| 81 | 1 | 3894 | 8UZ | C14-C9-O3-C8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|----------------|
| 81 | 7 | 209 | 8UZ | C12-C10-C11-O5 |
| 81 | 1 | 3888 | 8UZ | C14-C9-O3-C8 |
| 81 | 5 | 3853 | 8UZ | O4-C10-C11-O5 |
| 81 | 5 | 3855 | 8UZ | O4-C10-C11-O5 |
| 81 | 1 | 3888 | 8UZ | O-C2-O1-C3 |
| 81 | 1 | 3890 | 8UZ | O4-C10-C11-O5 |
| 81 | 7 | 209 | 8UZ | O4-C10-C11-O5 |
| 81 | 1 | 3887 | 8UZ | O4-C10-C11-O5 |
| 81 | 4 | 220 | 8UZ | O4-C10-C11-O5 |
| 81 | 5 | 3854 | 8UZ | O4-C10-C11-O5 |
| 81 | 1 | 3887 | 8UZ | C14-C9-O3-C8 |
| 81 | 2 | 2030 | 8UZ | O4-C10-C11-O5 |
| 81 | 5 | 3853 | 8UZ | C12-C10-C11-O5 |
| 81 | 1 | 3892 | 8UZ | C14-C9-O3-C8 |
| 81 | 2 | 2030 | 8UZ | C12-C10-C11-O5 |
| 81 | 4 | 220 | 8UZ | C12-C10-C11-O5 |
| 81 | 1 | 3890 | 8UZ | C12-C10-C11-O5 |
| 81 | 5 | 3854 | 8UZ | C12-C10-C11-O5 |
| 81 | 1 | 3892 | 8UZ | O4-C9-O3-C8 |
| 81 | 1 | 3891 | 8UZ | O4-C10-C11-O5 |
| 81 | 2 | 2031 | 8UZ | C3-C8-O3-C9 |
| 81 | 5 | 3853 | 8UZ | O-C2-O1-C3 |
| 81 | 5 | 3855 | 8UZ | C12-C10-C11-O5 |
| 81 | 1 | 3895 | 8UZ | O4-C10-C11-O5 |
| 81 | 5 | 3856 | 8UZ | O-C2-O1-C3 |
| 81 | 1 | 3891 | 8UZ | C8-C3-O1-C2 |
| 81 | 1 | 3888 | 8UZ | O4-C10-C11-O5 |
| 81 | 1 | 3893 | 8UZ | O4-C10-C11-O5 |
| 81 | 5 | 3851 | 8UZ | C12-C10-C11-O5 |
| 81 | 2 | 2029 | 8UZ | C8-C3-O1-C2 |
| 81 | 1 | 3891 | 8UZ | C12-C10-C11-O5 |
| 81 | 2 | 2029 | 8UZ | O4-C10-C11-O5 |
| 81 | 1 | 3889 | 8UZ | O4-C10-C11-O5 |
| 81 | 5 | 3852 | 8UZ | O4-C10-C11-O5 |
| 81 | 5 | 3851 | 8UZ | O4-C10-C11-O5 |
| 81 | 5 | 3853 | 8UZ | C8-C3-O1-C2 |
| 81 | 1 | 3894 | 8UZ | O4-C10-C11-O5 |
| 81 | 5 | 3850 | 8UZ | O-C2-O1-C3 |
| 81 | 2 | 2031 | 8UZ | C7-C8-O3-C9 |
| 81 | 7 | 209 | 8UZ | N-C-C1-C17 |
| 81 | 2 | 2029 | 8UZ | C3-C8-O3-C9 |
| 81 | 5 | 3857 | 8UZ | C8-C3-O1-C2 |

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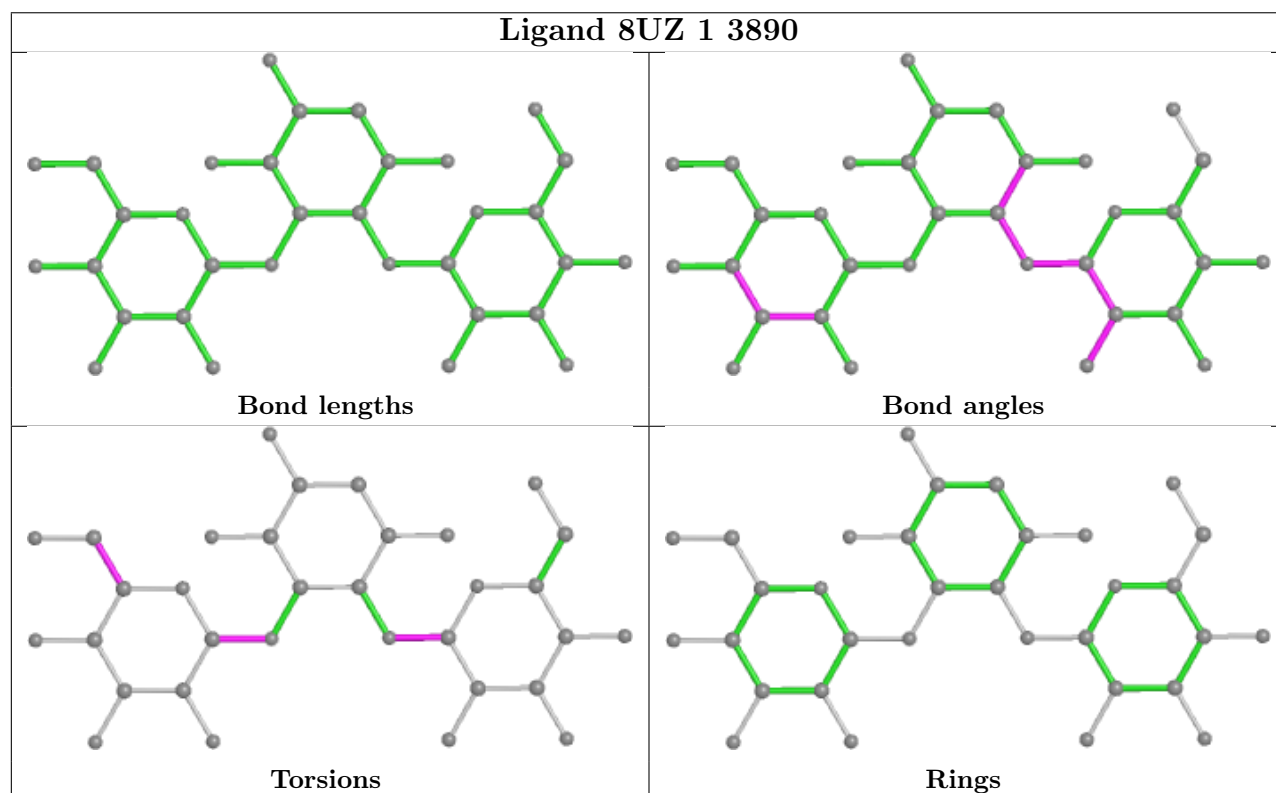
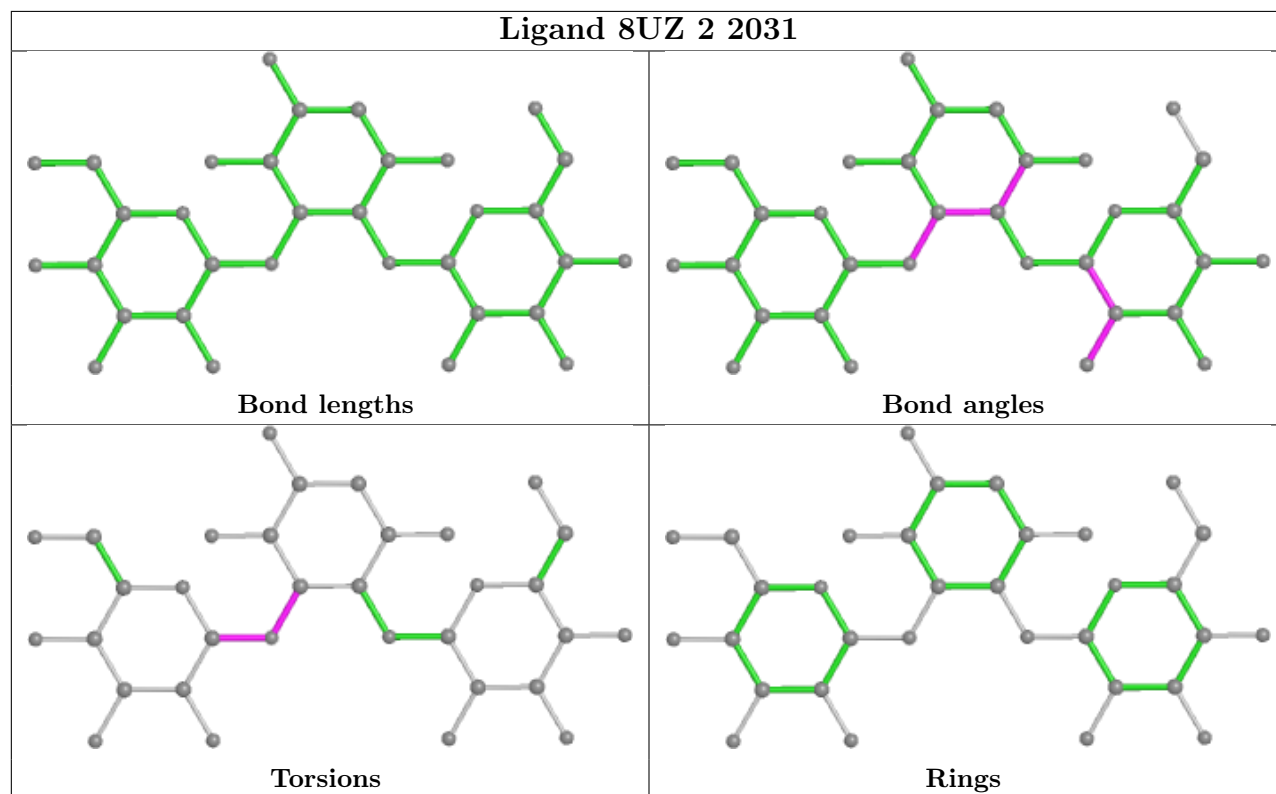
| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|----------------|
| 81 | 3 | 214 | 8UZ | C3-C8-O3-C9 |
| 81 | 1 | 3887 | 8UZ | C8-C3-O1-C2 |
| 81 | 3 | 214 | 8UZ | C7-C8-O3-C9 |
| 81 | 5 | 3857 | 8UZ | C12-C10-C11-O5 |
| 81 | 2 | 2029 | 8UZ | C7-C8-O3-C9 |
| 81 | 1 | 3895 | 8UZ | O4-C9-O3-C8 |
| 81 | 4 | 220 | 8UZ | C8-C3-O1-C2 |
| 81 | 5 | 3852 | 8UZ | C8-C3-O1-C2 |
| 81 | 1 | 3892 | 8UZ | N-C-C1-O |
| 81 | 1 | 3886 | 8UZ | C12-C10-C11-O5 |
| 81 | 2 | 2030 | 8UZ | N-C-C1-C17 |
| 81 | 1 | 3895 | 8UZ | C15-C2-O1-C3 |
| 81 | 1 | 3888 | 8UZ | C7-C8-O3-C9 |
| 81 | 7 | 209 | 8UZ | C3-C8-O3-C9 |
| 81 | 5 | 3856 | 8UZ | C7-C8-O3-C9 |
| 81 | 5 | 3851 | 8UZ | O-C2-O1-C3 |
| 81 | 1 | 3888 | 8UZ | C3-C8-O3-C9 |
| 81 | 1 | 3890 | 8UZ | C14-C9-O3-C8 |
| 81 | 5 | 3855 | 8UZ | C7-C8-O3-C9 |
| 81 | 5 | 3855 | 8UZ | C3-C8-O3-C9 |
| 81 | 1 | 3890 | 8UZ | O-C2-O1-C3 |
| 81 | 6 | 2061 | 8UZ | C8-C3-O1-C2 |
| 81 | 7 | 209 | 8UZ | C7-C8-O3-C9 |
| 81 | 1 | 3891 | 8UZ | C4-C3-O1-C2 |
| 81 | 2 | 2029 | 8UZ | C4-C3-O1-C2 |
| 81 | 5 | 3851 | 8UZ | C3-C8-O3-C9 |
| 81 | 1 | 3886 | 8UZ | N-C-C1-C17 |
| 81 | 1 | 3890 | 8UZ | O4-C9-O3-C8 |
| 81 | 1 | 3893 | 8UZ | C15-C2-O1-C3 |
| 81 | 1 | 3895 | 8UZ | C12-C10-C11-O5 |

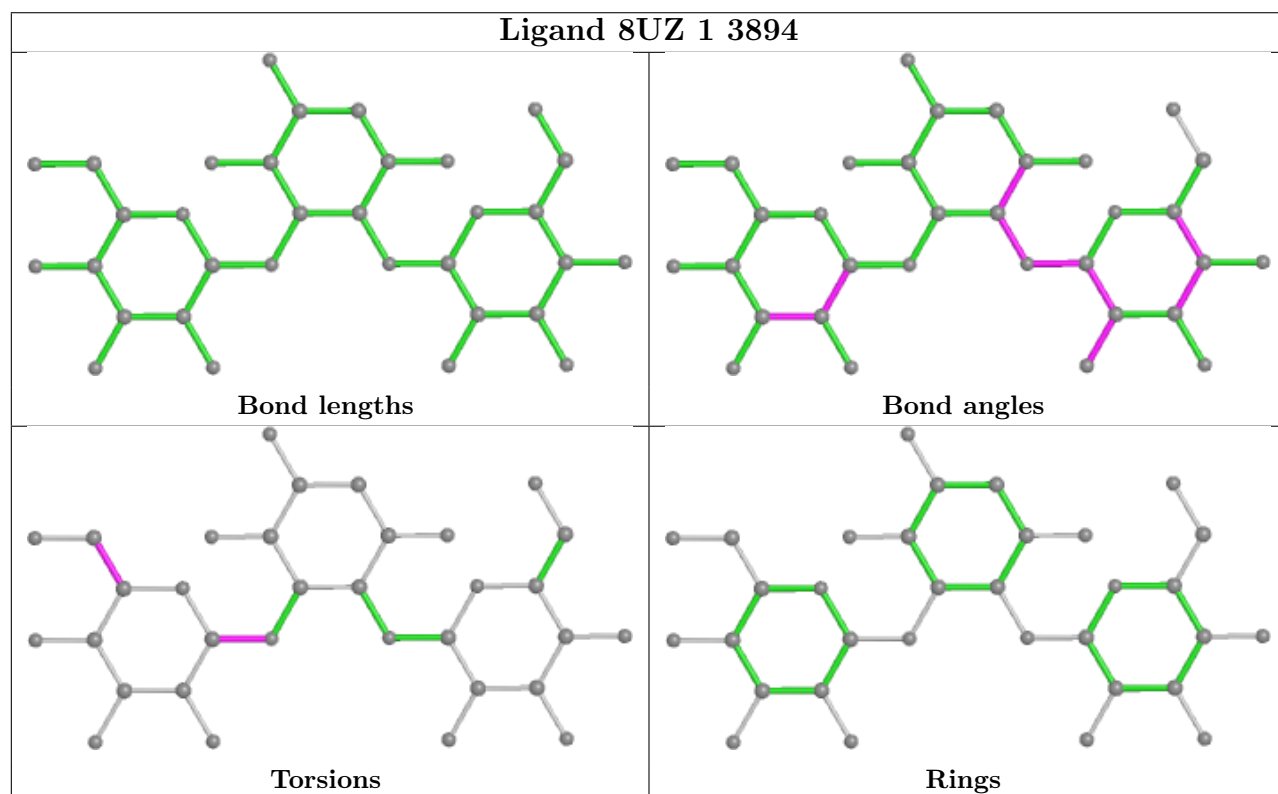
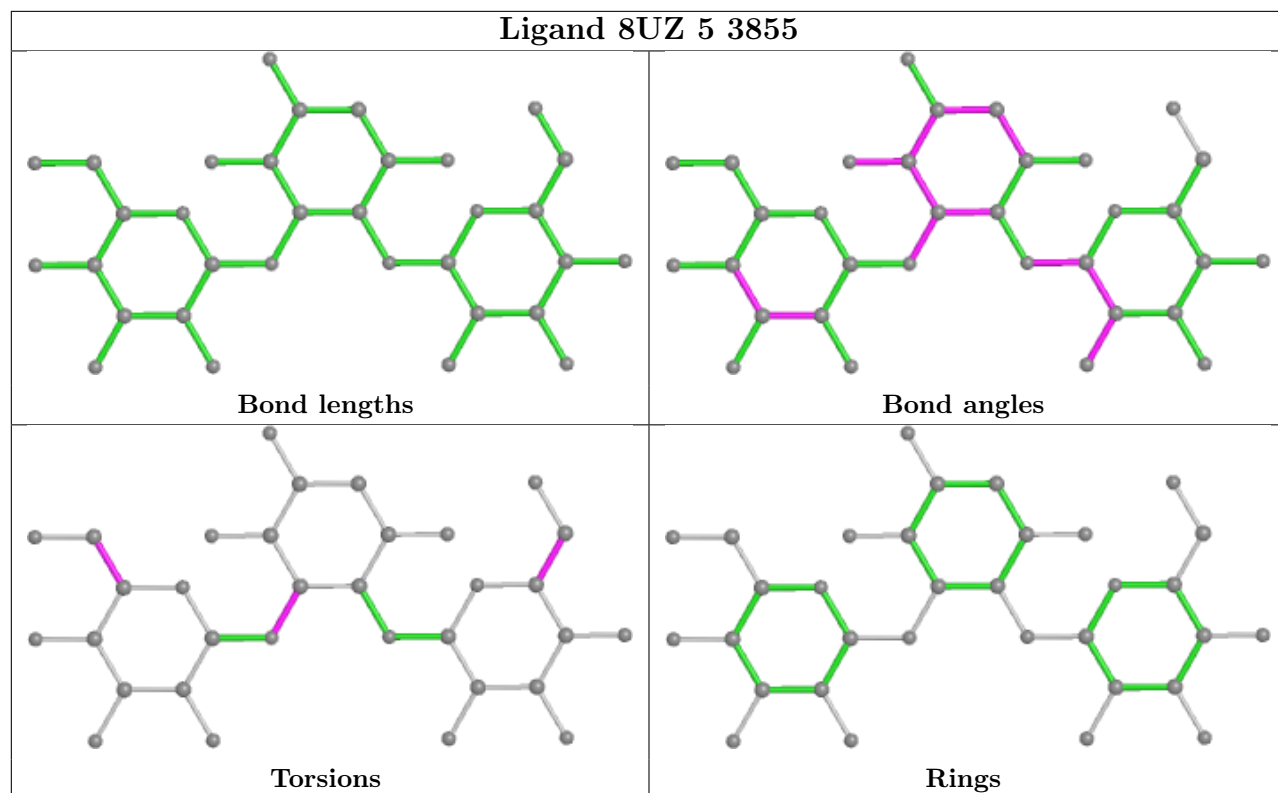
There are no ring outliers.

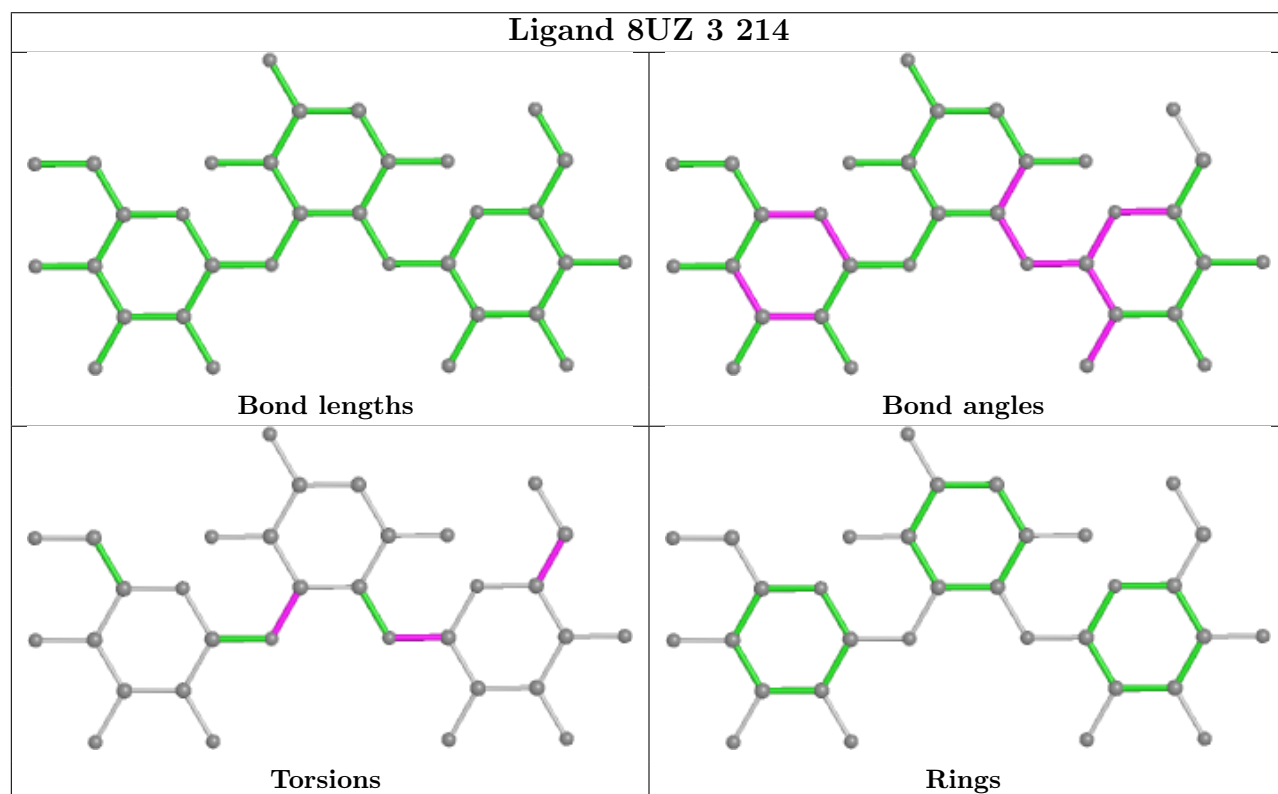
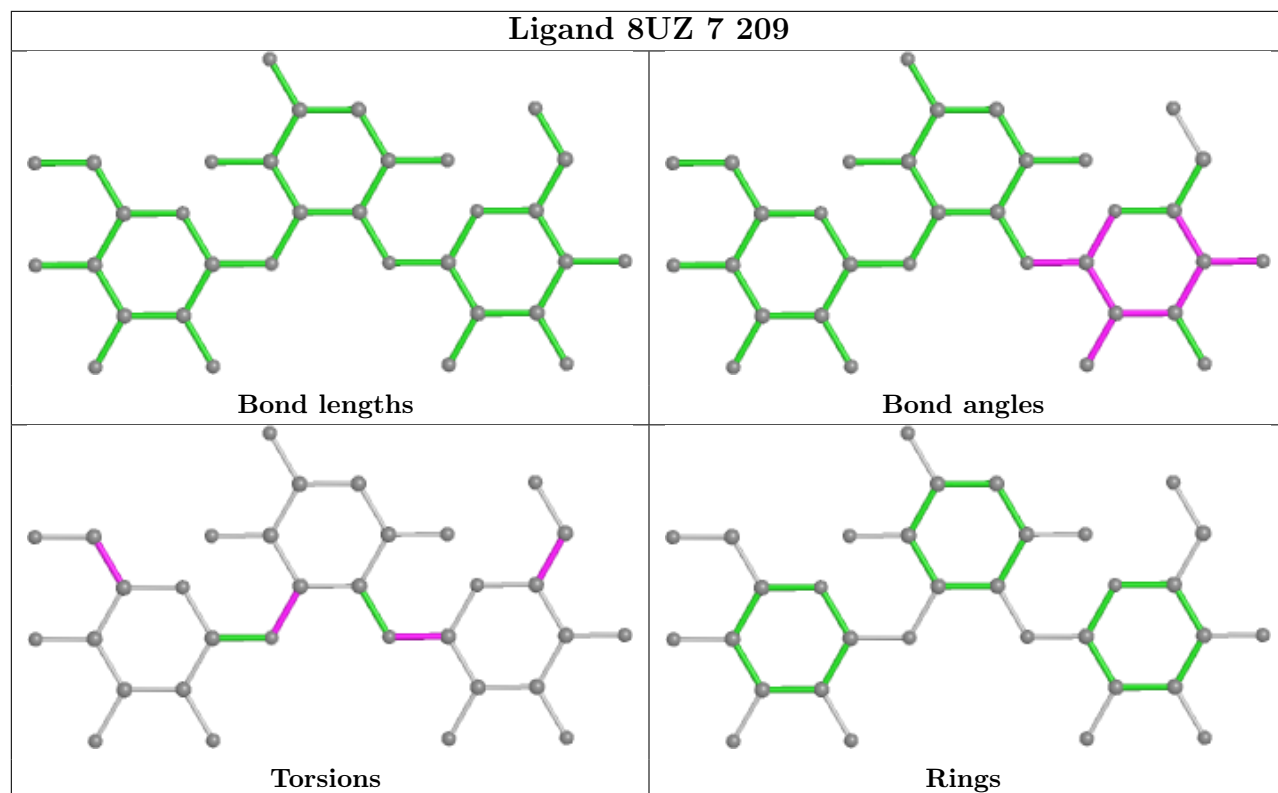
No monomer is involved in short contacts.

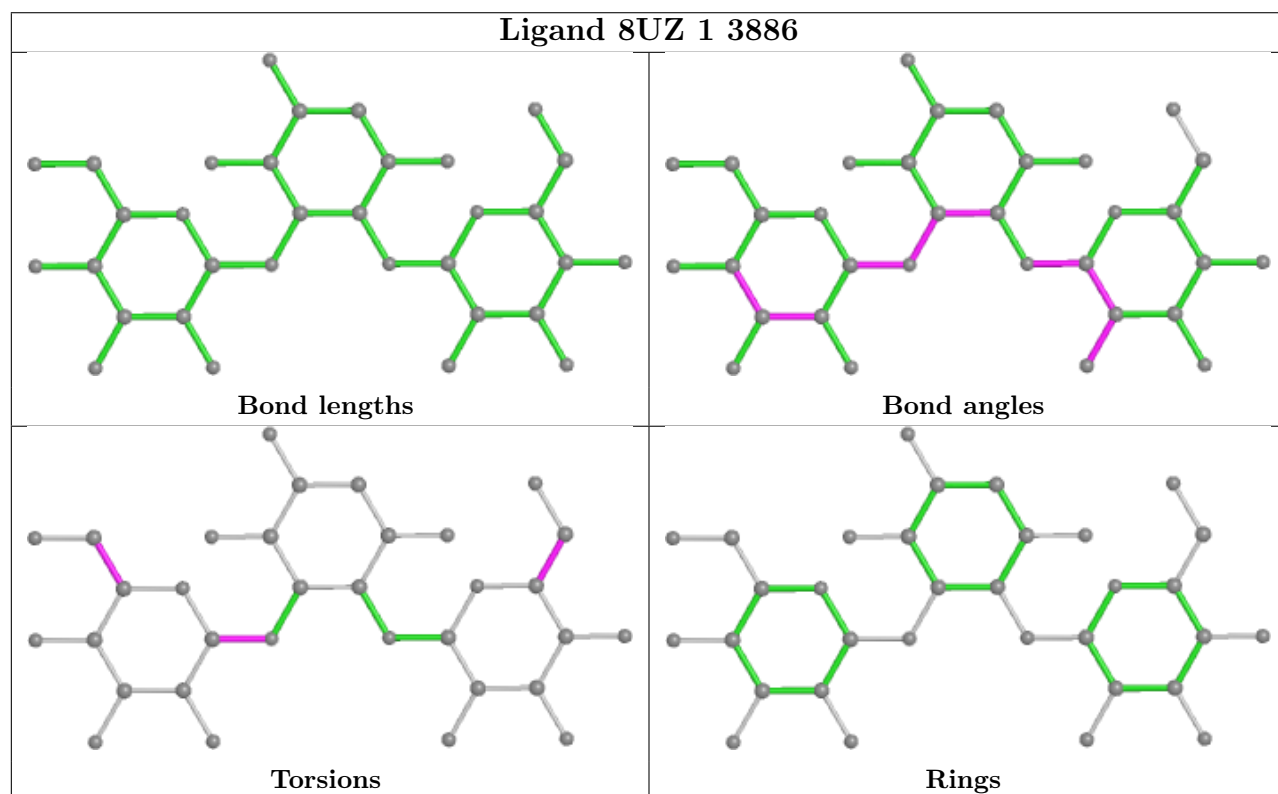
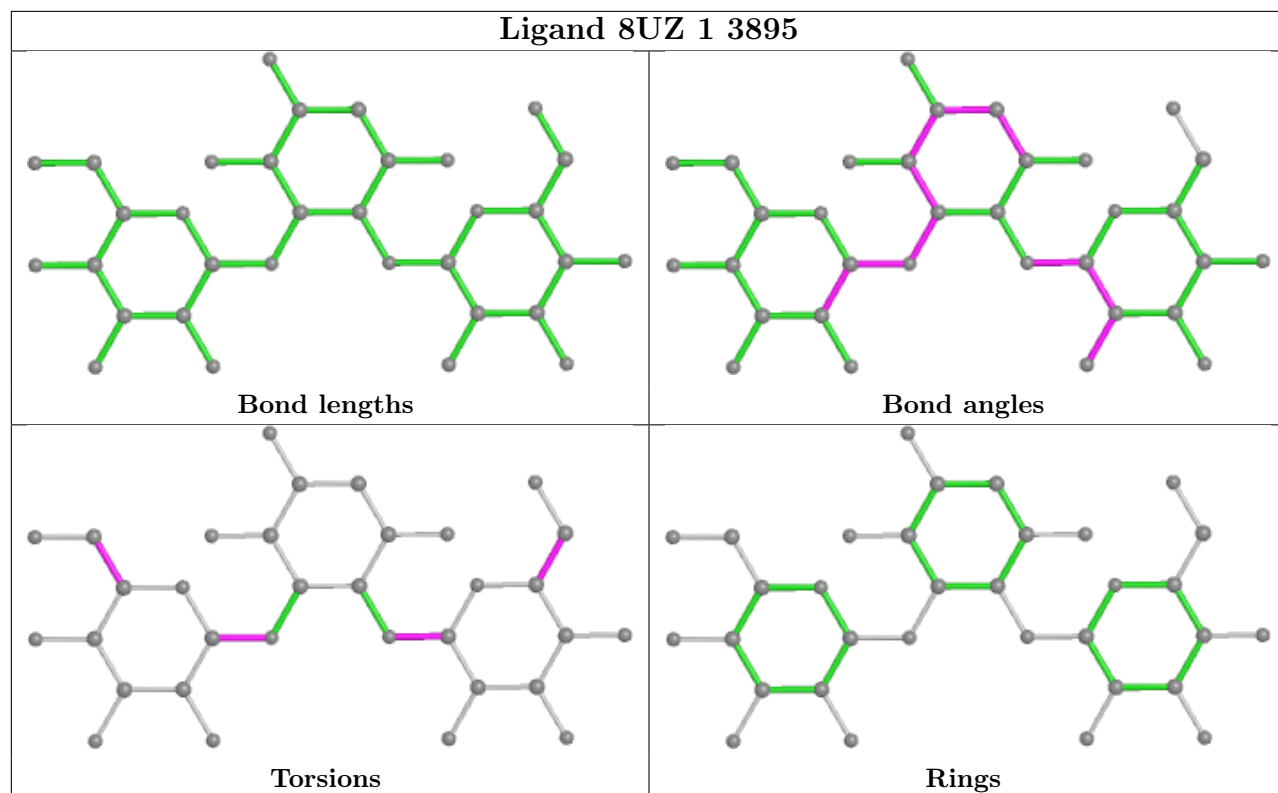
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

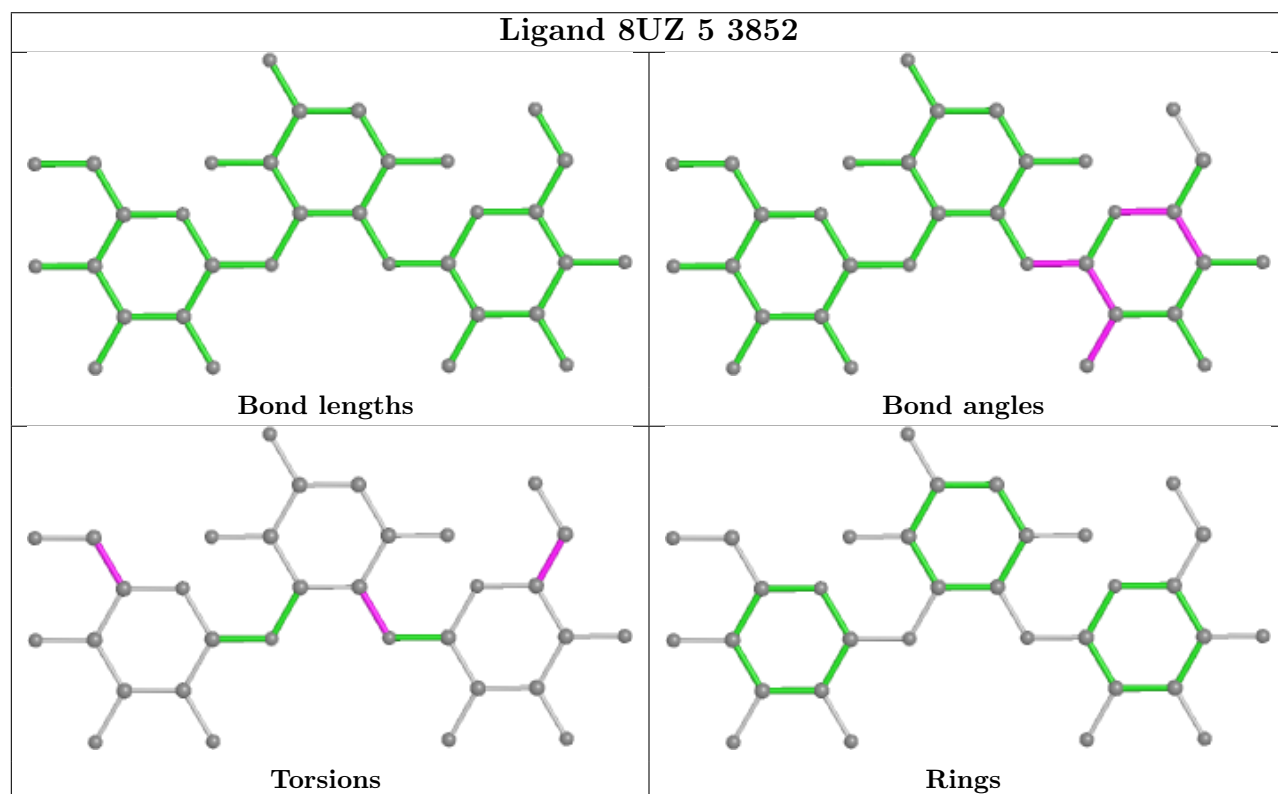
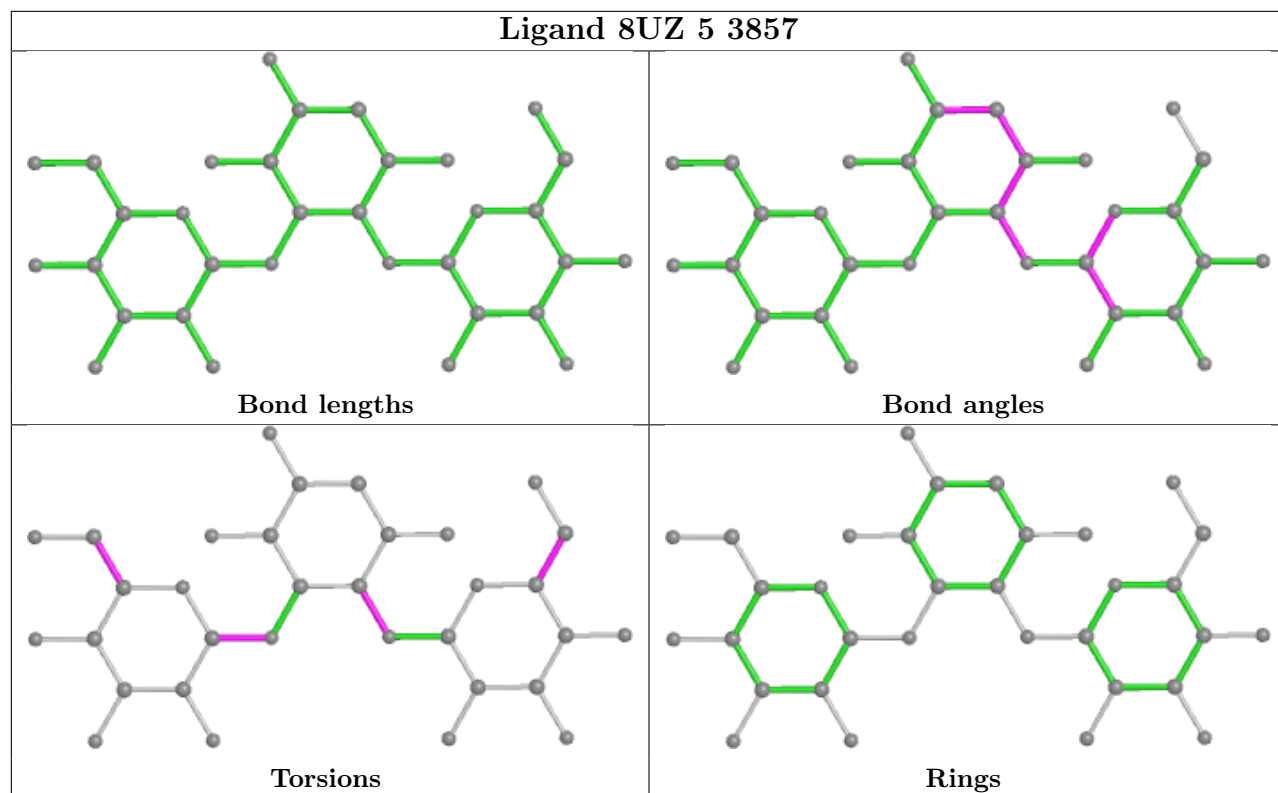
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

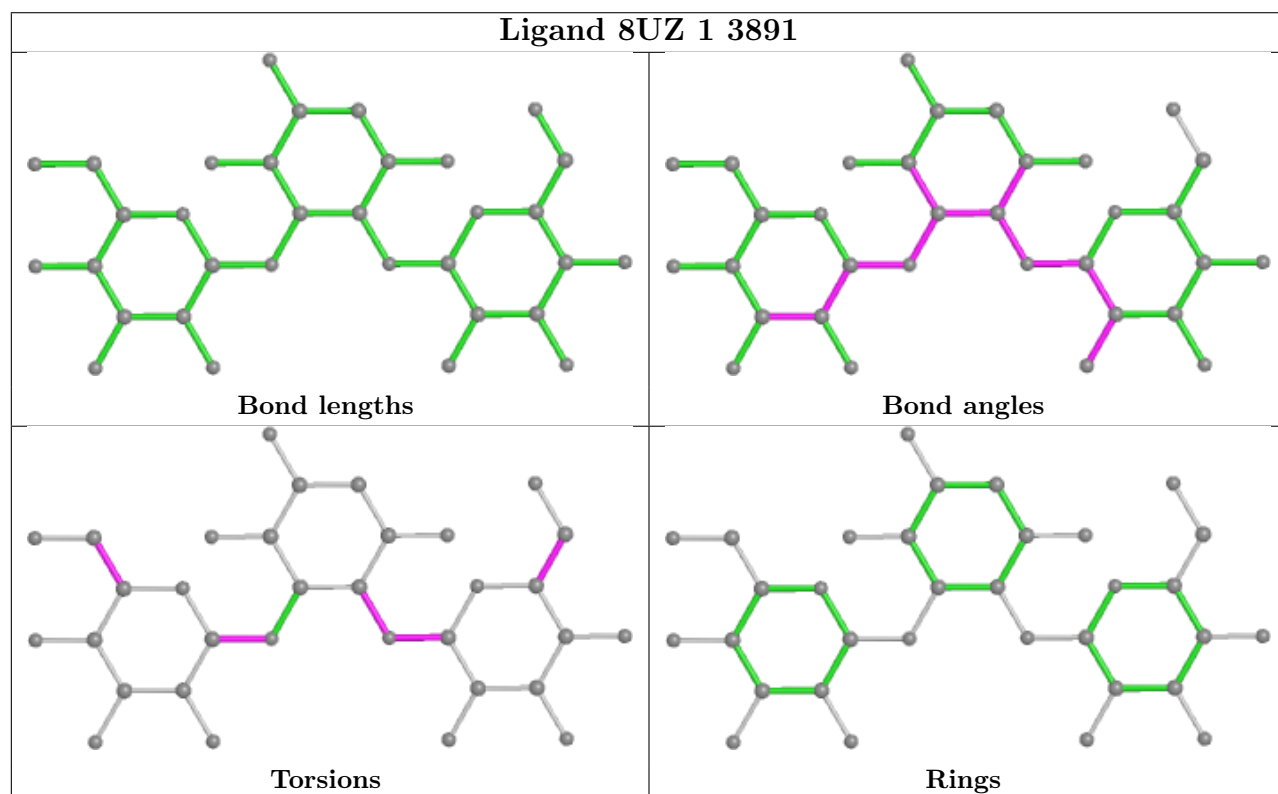
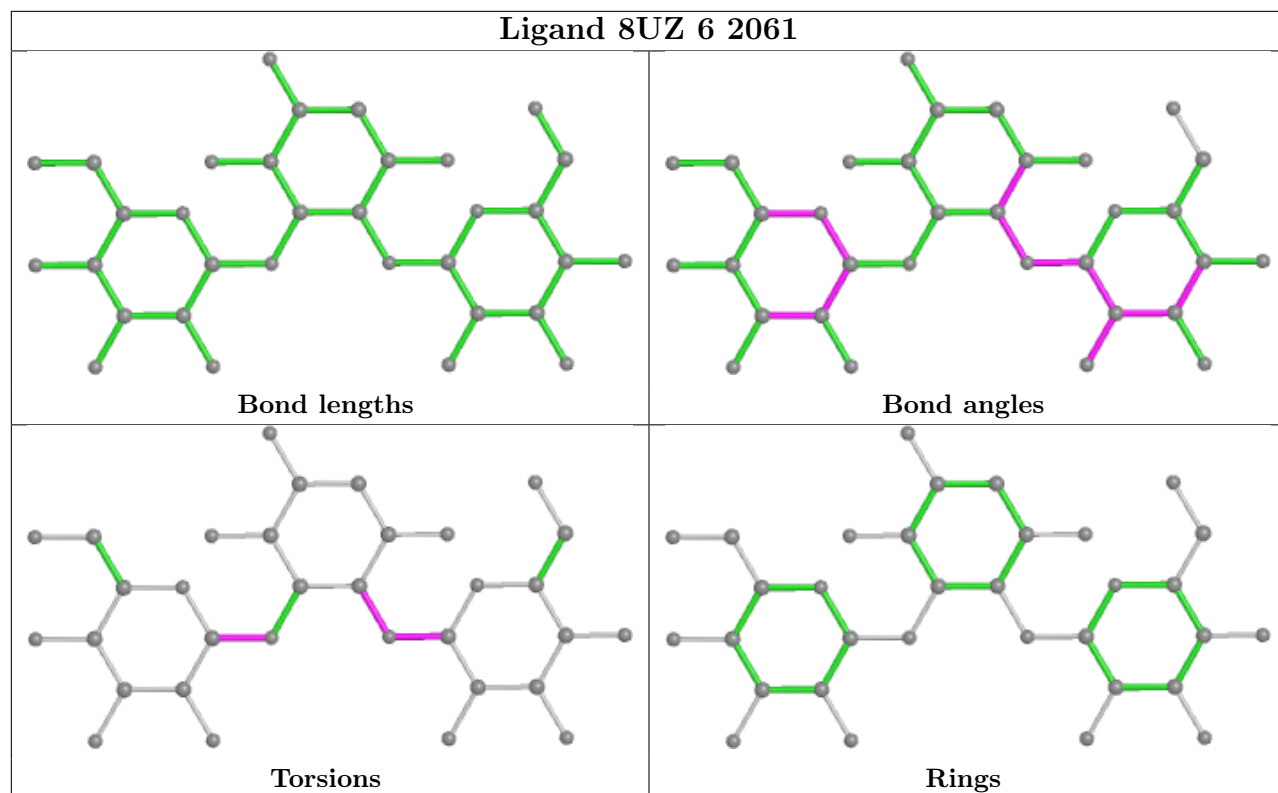


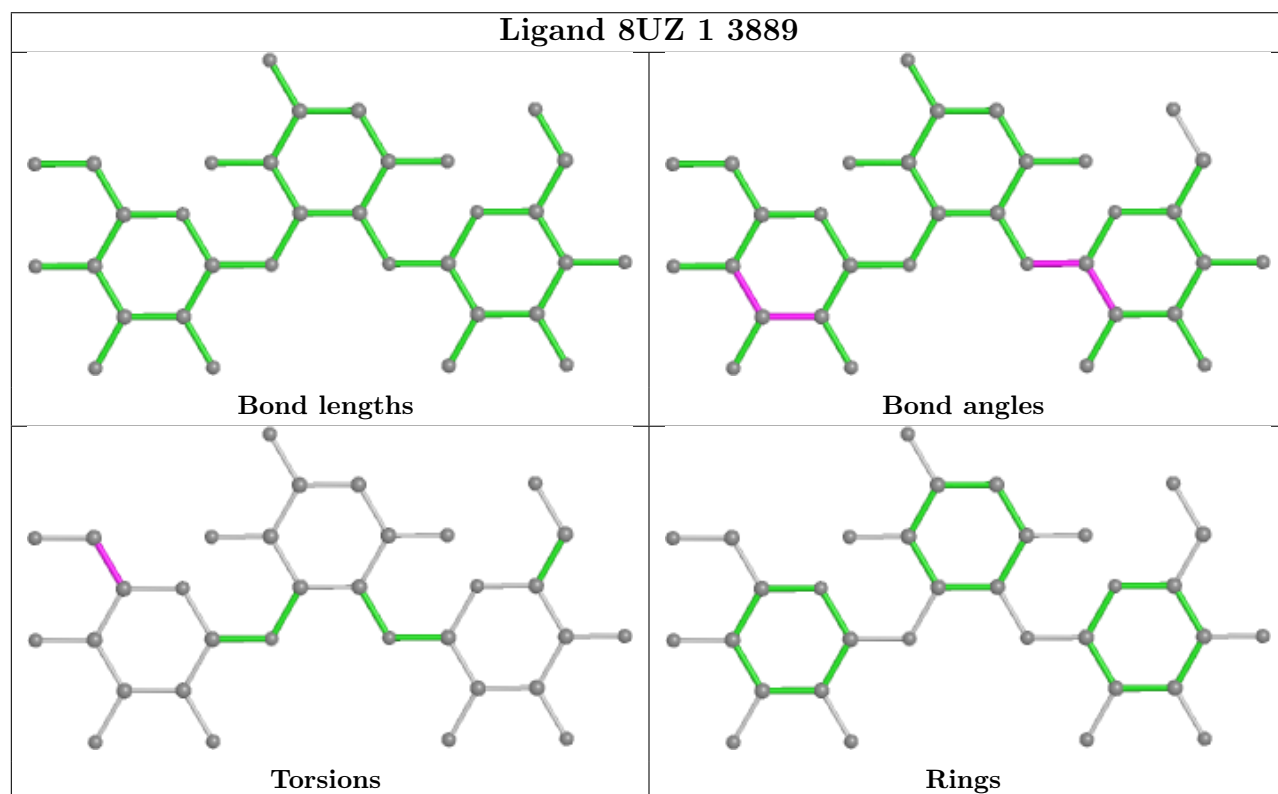
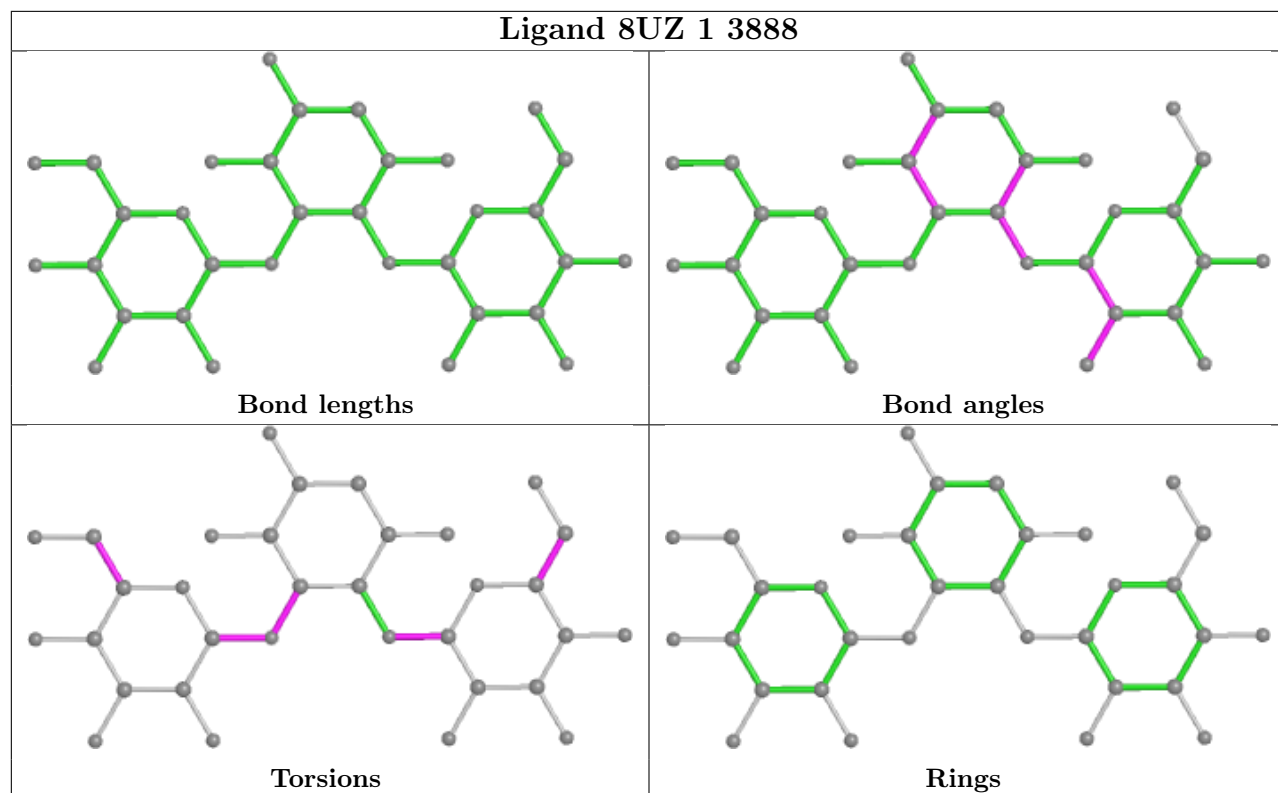


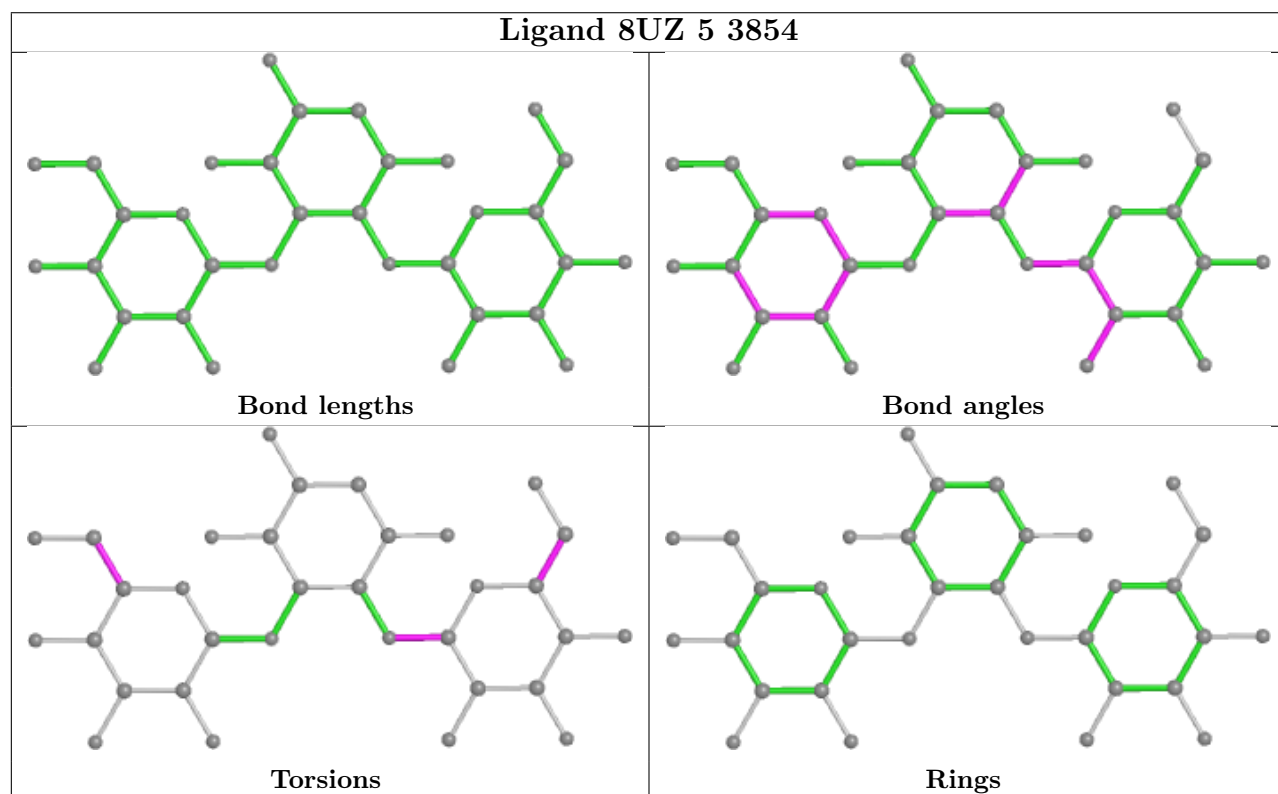
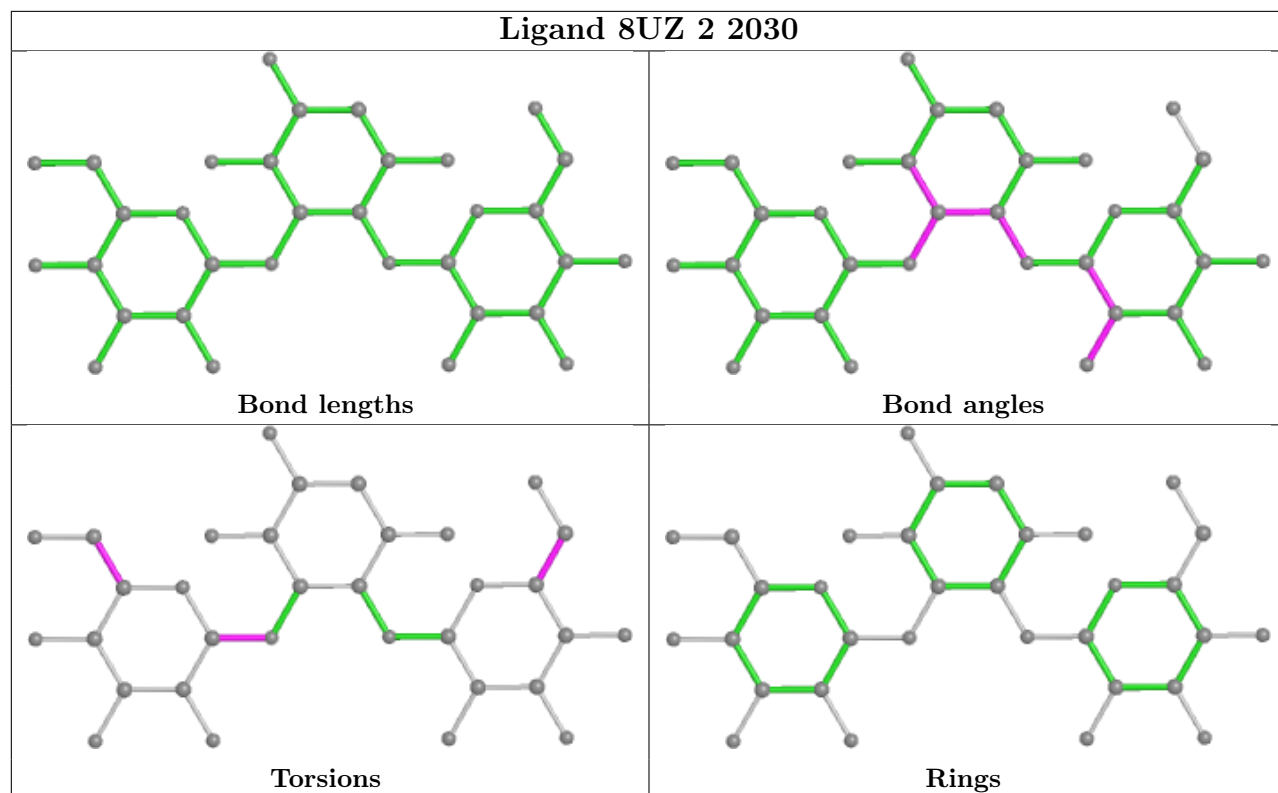


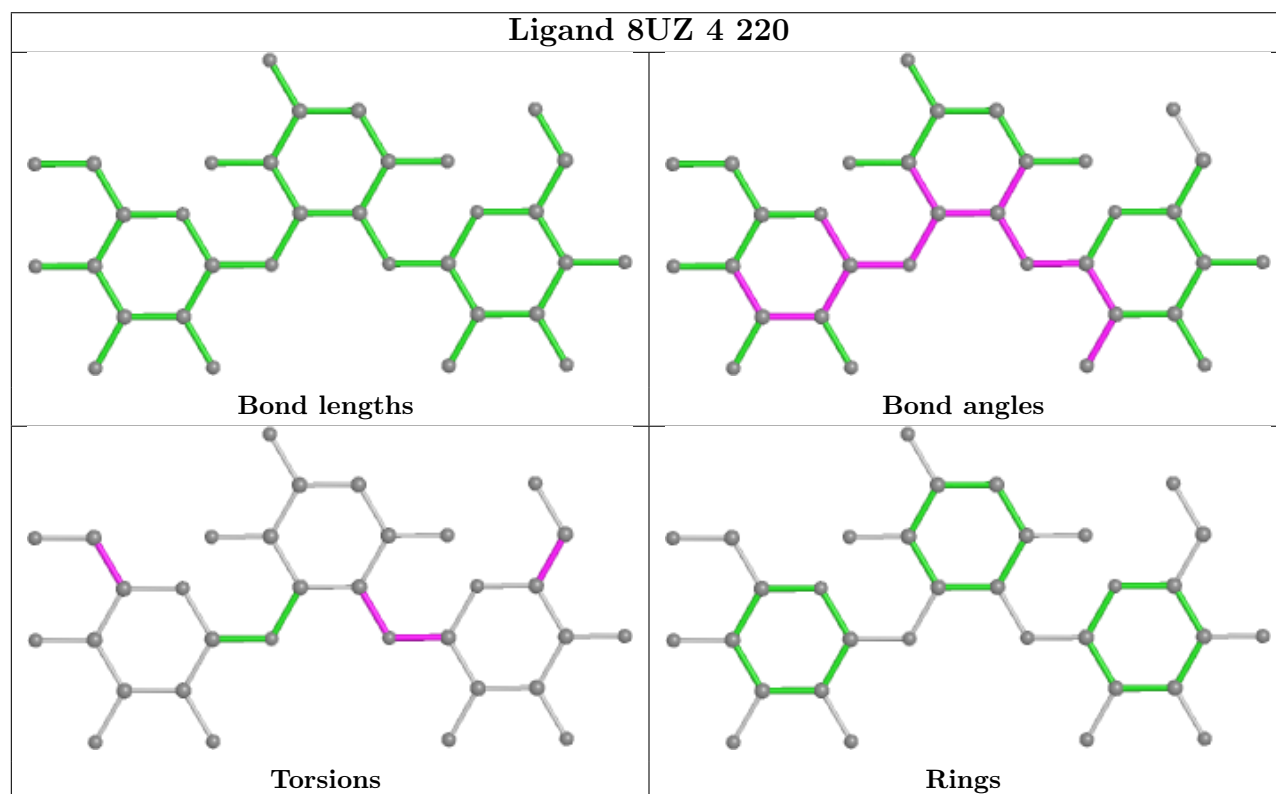
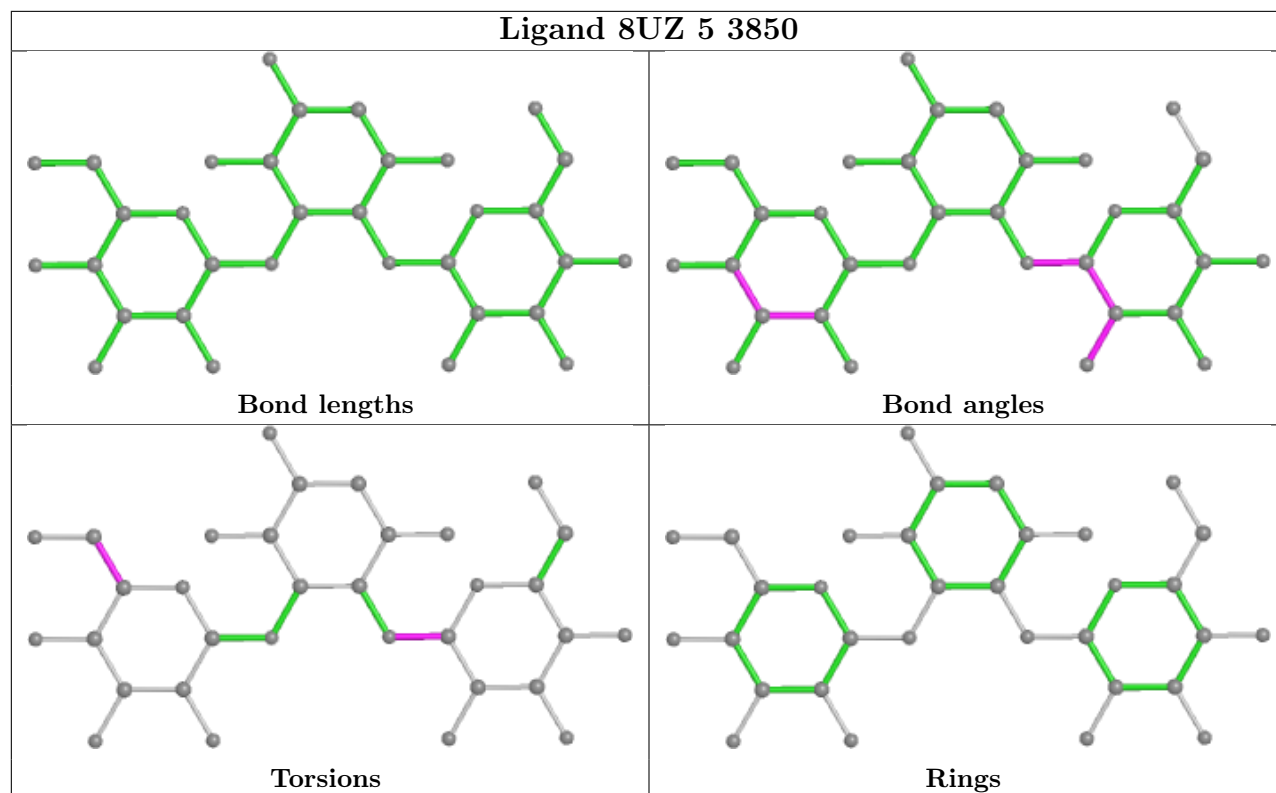


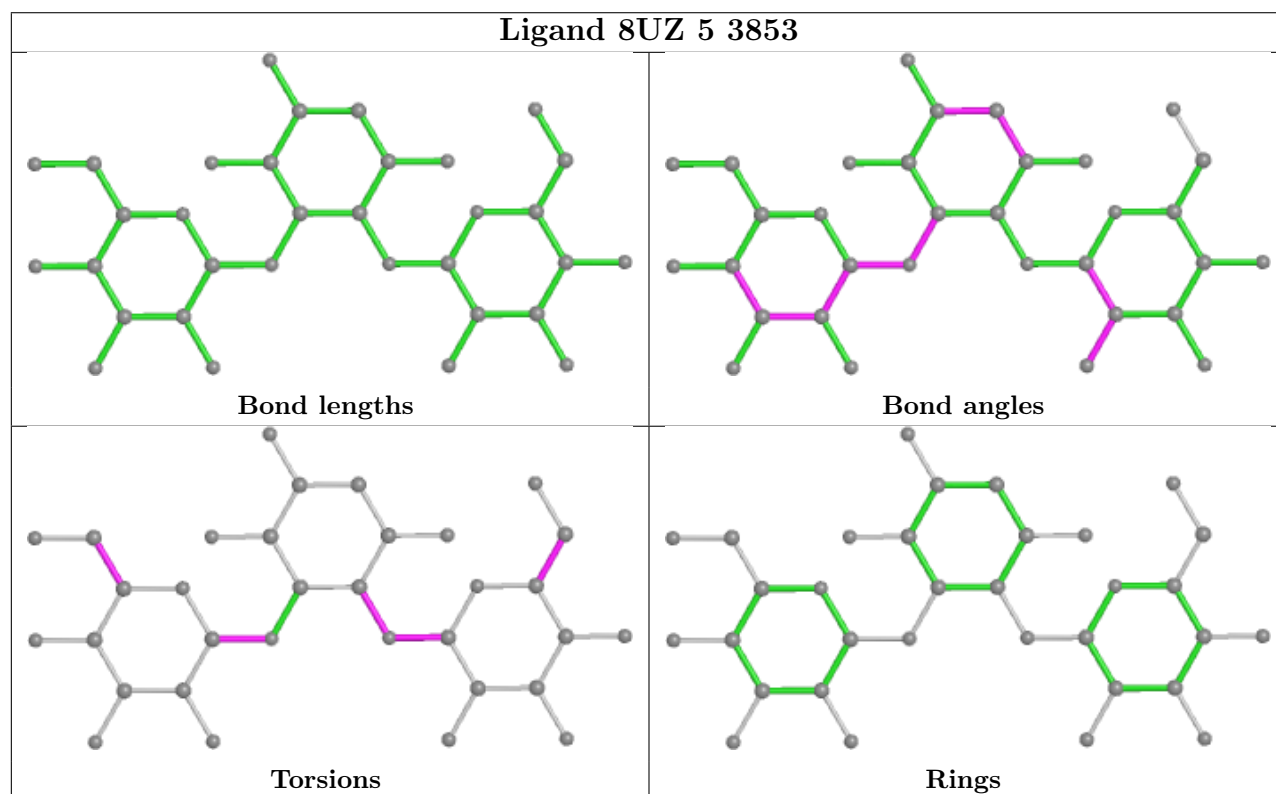
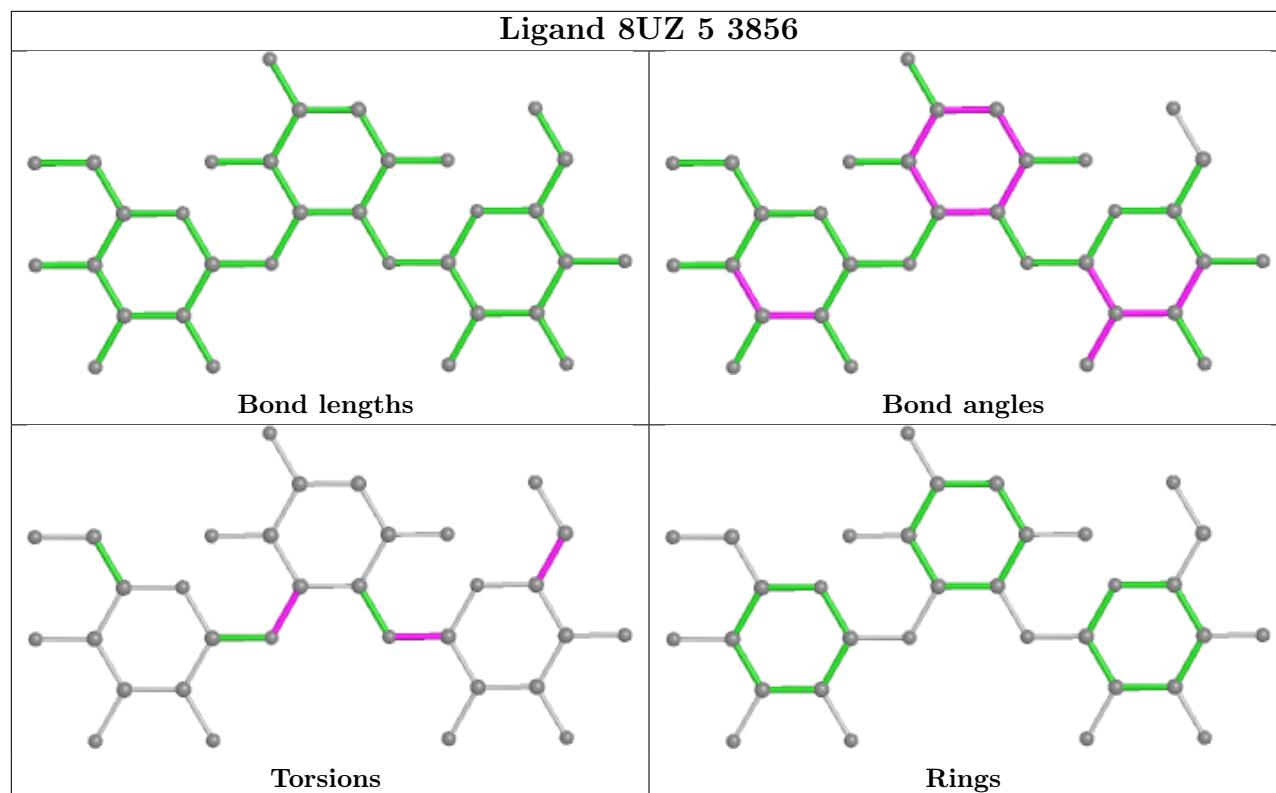


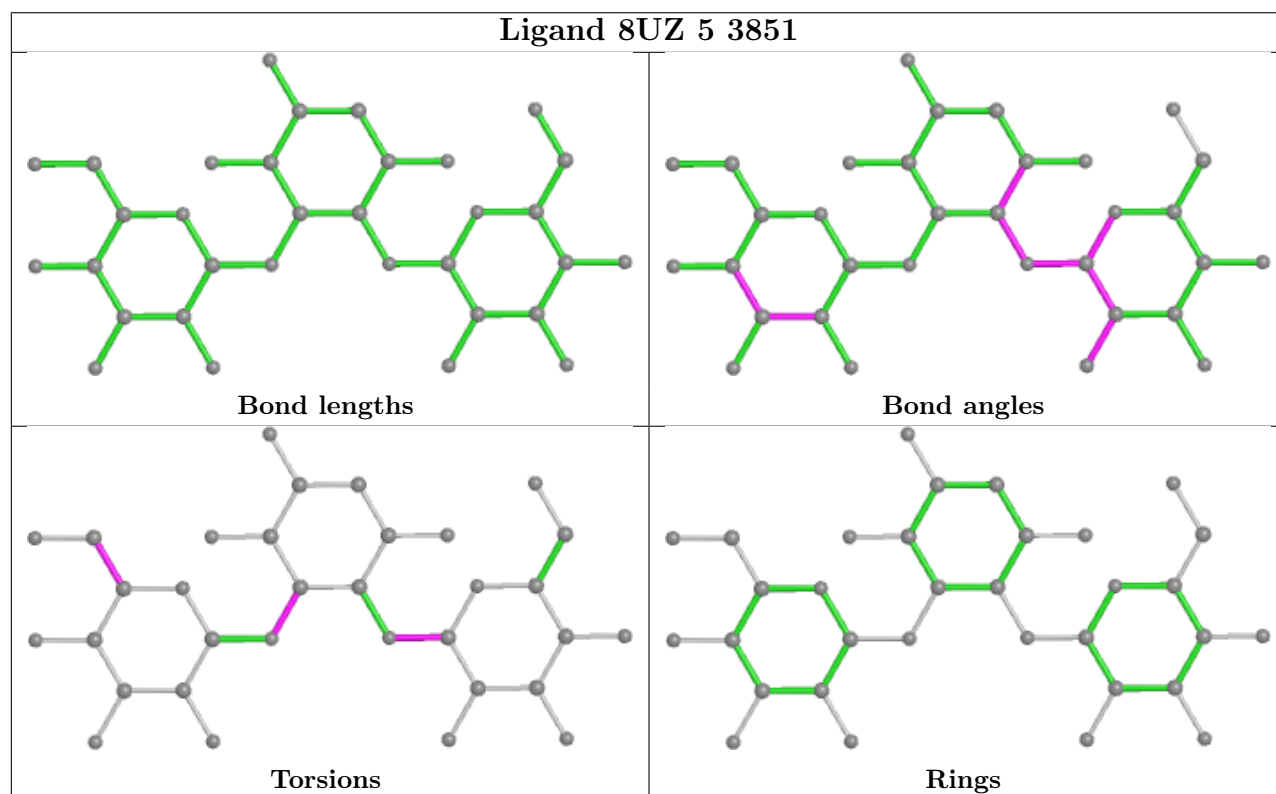
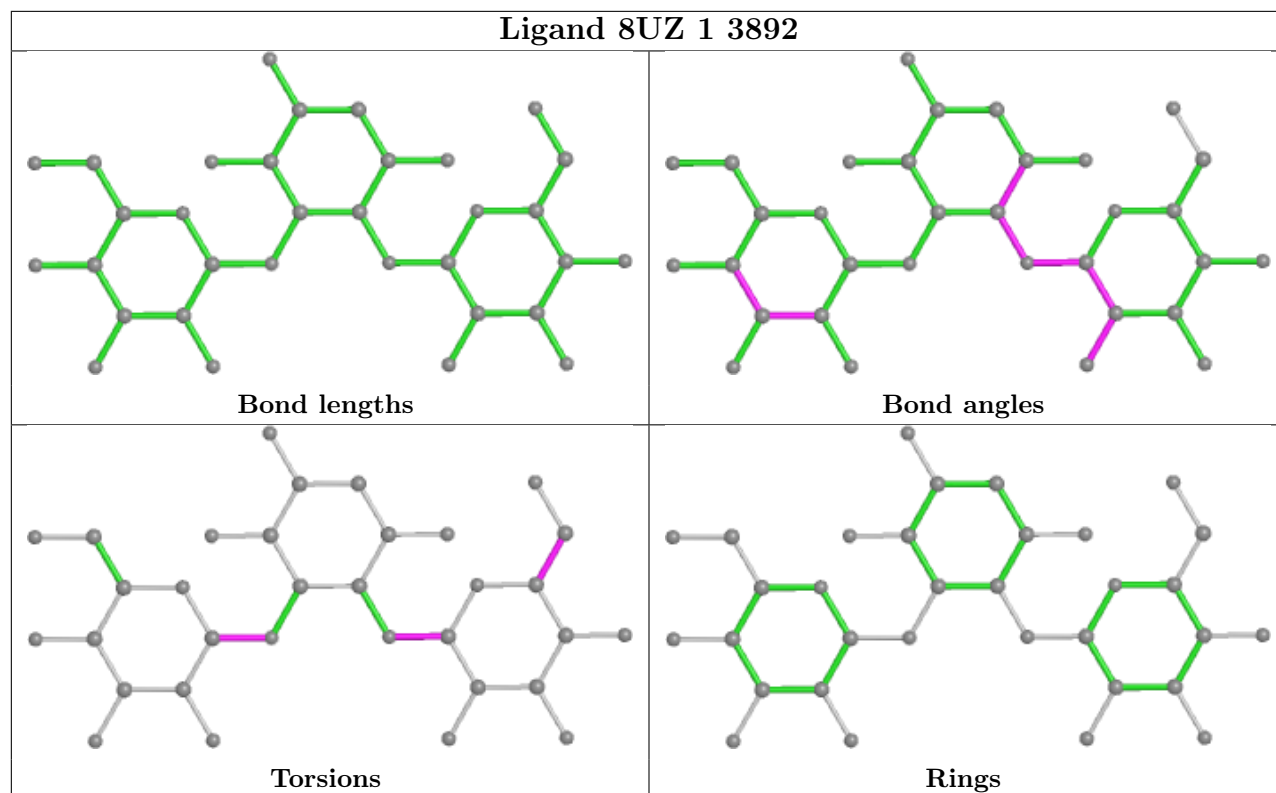


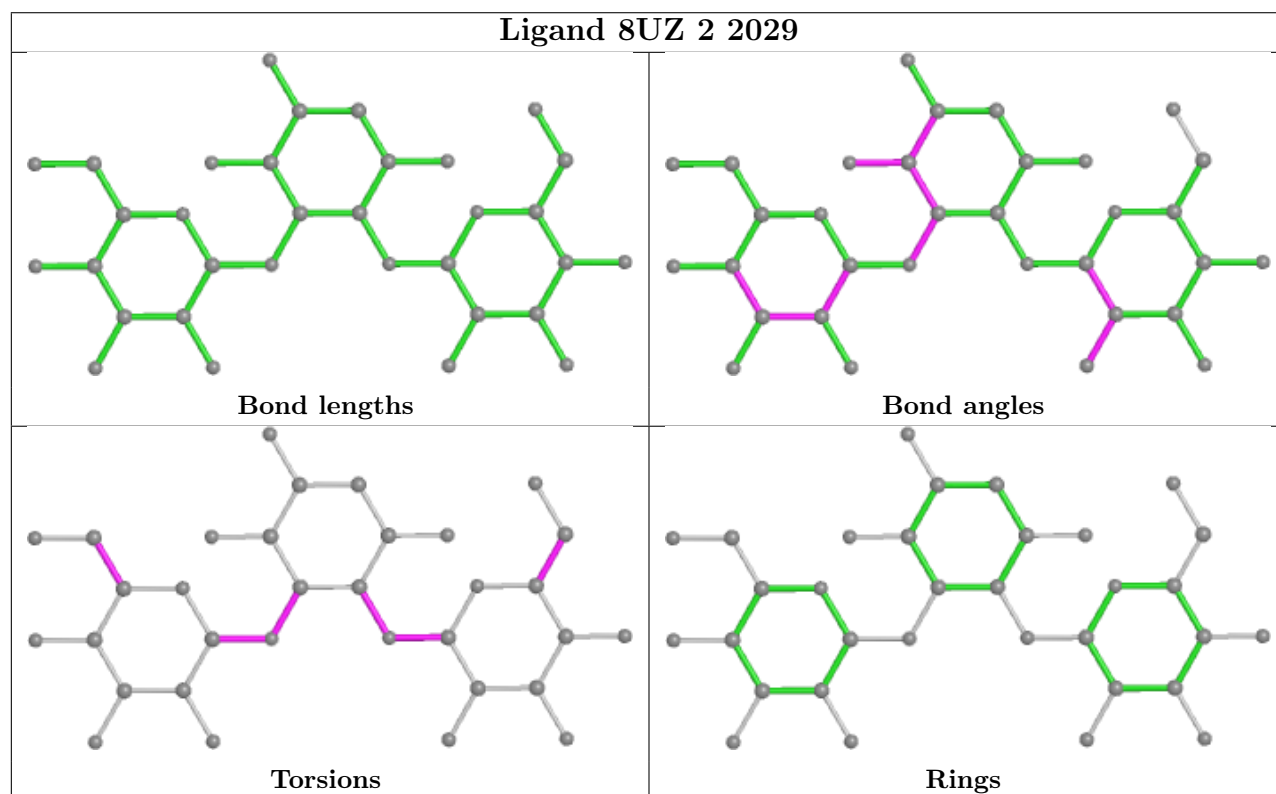
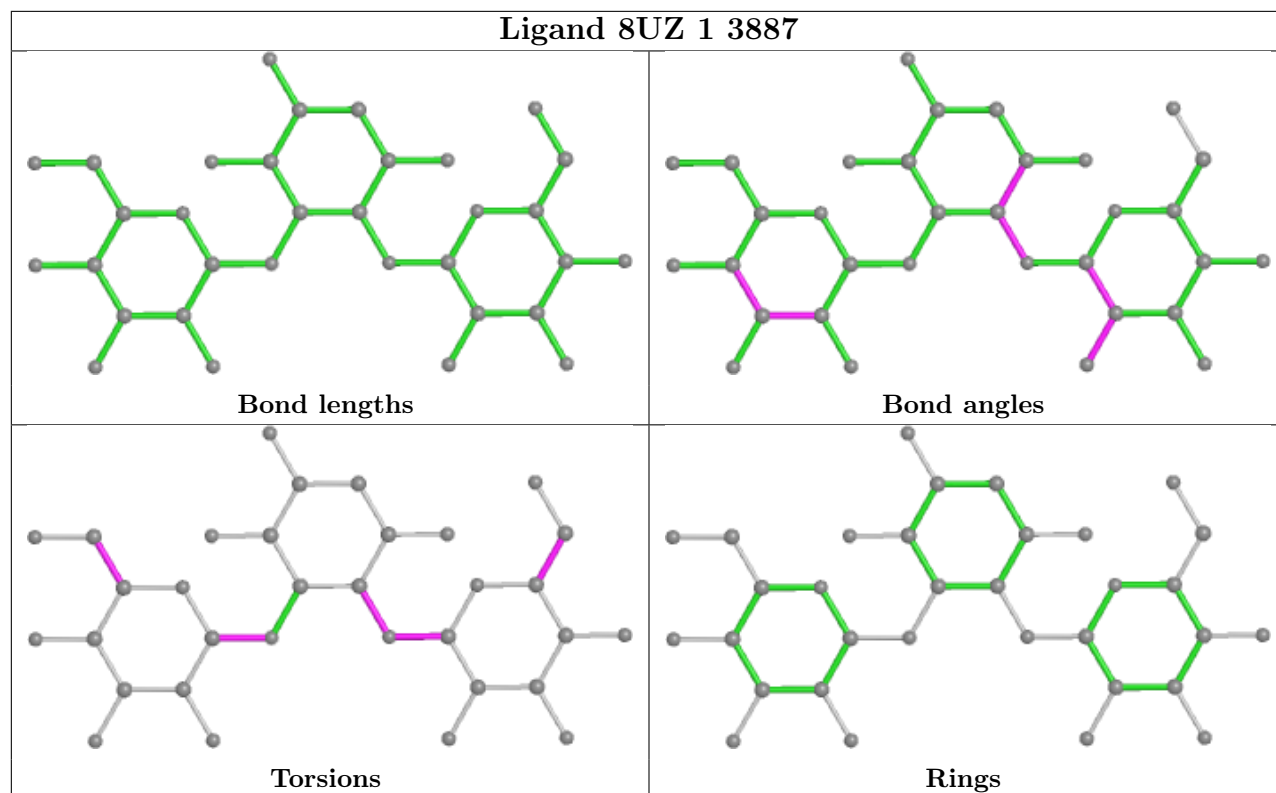


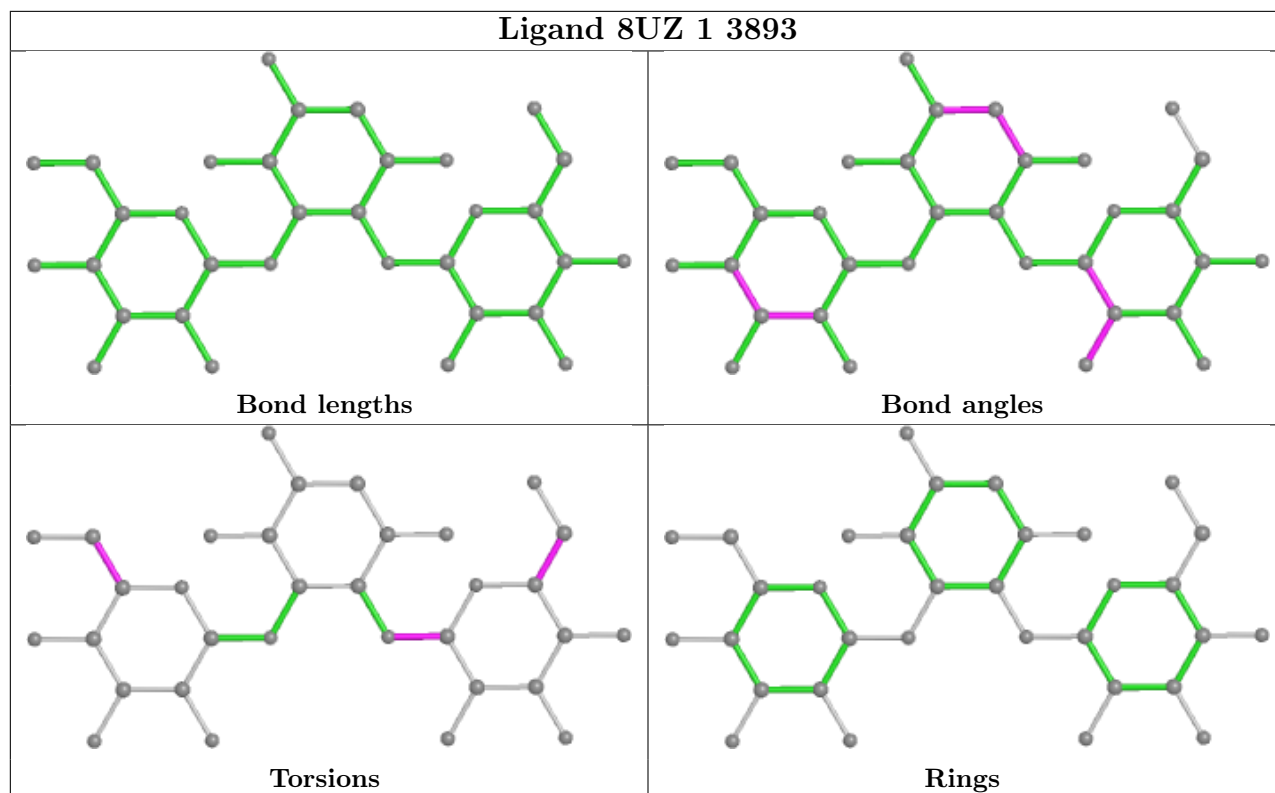












5.7 Other polymers [i](#)

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 |
|-----|-------|------------------|
| 1 | 5 | 1 |
| 78 | sM | 1 |
| 51 | n7 | 1 |
| 37 | M3 | 1 |
| 50 | n6 | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | 5 | 1017:C | O3' | 1018:G | P | 6.05 |
| 1 | sM | 50:ASN | C | 51:ARG | N | 3.56 |
| 1 | n7 | 36:HIS | C | 37:PRO | N | 1.73 |
| 1 | M3 | 125:VAL | C | 126:PHE | N | 1.18 |
| 1 | n6 | 99:LEU | C | 100:HIS | N | 1.17 |

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 | 3090/3396 (90%) | -0.01 | 15 (0%) 91 85 | 73, 114, 221, 384 | 0 |
| 1 | 5 | 3080/3396 (90%) | -0.04 | 16 (0%) 91 85 | 75, 122, 223, 357 | 0 |
| 2 | 2 | 1770/1800 (98%) | -0.13 | 46 (2%) 56 43 | 91, 158, 320, 453 | 0 |
| 2 | 6 | 1736/1800 (96%) | -0.26 | 13 (0%) 87 81 | 95, 154, 275, 374 | 0 |
| 3 | 3 | 121/121 (100%) | -0.51 | 0 100 100 | 88, 150, 179, 215 | 0 |
| 3 | 7 | 121/121 (100%) | -0.54 | 0 100 100 | 90, 171, 210, 226 | 0 |
| 4 | 4 | 158/158 (100%) | -0.11 | 1 (0%) 89 83 | 82, 126, 196, 327 | 0 |
| 4 | 8 | 158/158 (100%) | -0.06 | 3 (1%) 66 55 | 88, 138, 203, 271 | 0 |
| 5 | C0 | 96/105 (91%) | 1.54 | 34 (35%) 0 0 | 138, 198, 247, 261 | 0 |
| 5 | c0 | 93/105 (88%) | 0.80 | 20 (21%) 0 0 | 161, 209, 265, 317 | 0 |
| 6 | C1 | 154/156 (98%) | 1.47 | 47 (30%) 0 0 | 114, 150, 268, 325 | 0 |
| 6 | c1 | 146/156 (93%) | 0.91 | 20 (13%) 3 3 | 103, 137, 199, 244 | 0 |
| 7 | C2 | 119/143 (83%) | 2.08 | 56 (47%) 0 0 | 207, 274, 323, 343 | 0 |
| 7 | c2 | 124/143 (86%) | 1.98 | 55 (44%) 0 0 | 215, 274, 321, 343 | 0 |
| 8 | C3 | 150/150 (100%) | 0.39 | 7 (4%) 31 23 | 120, 171, 208, 232 | 0 |
| 8 | c3 | 150/150 (100%) | 0.74 | 13 (8%) 10 7 | 117, 157, 195, 229 | 0 |
| 9 | C4 | 127/128 (99%) | 0.12 | 6 (4%) 31 23 | 111, 171, 218, 250 | 0 |
| 9 | c4 | 128/128 (100%) | 1.01 | 27 (21%) 1 0 | 126, 185, 232, 278 | 0 |
| 10 | C5 | 124/141 (87%) | 0.76 | 14 (11%) 5 4 | 139, 185, 244, 296 | 0 |
| 10 | c5 | 125/141 (88%) | 0.55 | 19 (15%) 2 2 | 132, 180, 239, 260 | 0 |
| 11 | C6 | 141/141 (100%) | 1.39 | 46 (32%) 0 0 | 113, 175, 232, 275 | 0 |
| 11 | c6 | 141/141 (100%) | 1.20 | 43 (30%) 0 0 | 124, 171, 219, 243 | 0 |
| 12 | C7 | 120/136 (88%) | 0.74 | 21 (17%) 1 1 | 127, 192, 251, 284 | 0 |
| 12 | c7 | 121/136 (88%) | 0.24 | 7 (5%) 23 16 | 135, 186, 246, 340 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 13 | C8 | 145/145 (100%) | 0.65 | 16 (11%) 5 4 | 127, 194, 255, 283 | 0 |
| 13 | c8 | 145/145 (100%) | 0.48 | 15 (10%) 6 5 | 133, 175, 221, 248 | 0 |
| 14 | C9 | 143/143 (100%) | 0.51 | 14 (9%) 7 6 | 128, 175, 216, 241 | 0 |
| 14 | c9 | 143/143 (100%) | 0.53 | 12 (8%) 11 8 | 137, 175, 210, 252 | 0 |
| 15 | D0 | 105/107 (98%) | 1.46 | 40 (38%) 0 0 | 117, 174, 261, 277 | 0 |
| 15 | d0 | 104/107 (97%) | 0.51 | 10 (9%) 8 6 | 133, 188, 257, 300 | 0 |
| 16 | D1 | 87/87 (100%) | 0.66 | 9 (10%) 6 5 | 137, 174, 221, 251 | 0 |
| 16 | d1 | 87/87 (100%) | 0.67 | 9 (10%) 6 5 | 132, 168, 212, 238 | 0 |
| 17 | D2 | 129/129 (100%) | 1.09 | 20 (15%) 2 1 | 114, 154, 185, 229 | 0 |
| 17 | d2 | 129/129 (100%) | 0.77 | 17 (13%) 3 3 | 112, 145, 171, 199 | 0 |
| 18 | D3 | 144/144 (100%) | 0.49 | 10 (6%) 16 11 | 101, 132, 166, 191 | 0 |
| 18 | d3 | 144/144 (100%) | 0.50 | 5 (3%) 44 33 | 96, 127, 154, 192 | 0 |
| 19 | D4 | 134/134 (100%) | 0.50 | 15 (11%) 5 4 | 144, 199, 233, 275 | 0 |
| 19 | d4 | 134/134 (100%) | 0.25 | 8 (5%) 21 15 | 122, 174, 224, 254 | 0 |
| 20 | D5 | 70/70 (100%) | 1.36 | 22 (31%) 0 0 | 146, 212, 265, 290 | 0 |
| 20 | d5 | 69/70 (98%) | 0.68 | 12 (17%) 1 1 | 159, 205, 240, 250 | 0 |
| 21 | D6 | 97/97 (100%) | 0.77 | 12 (12%) 4 4 | 108, 149, 225, 242 | 0 |
| 21 | d6 | 97/97 (100%) | 1.32 | 30 (30%) 0 0 | 108, 151, 241, 257 | 0 |
| 22 | D7 | 81/81 (100%) | 0.32 | 5 (6%) 20 14 | 119, 192, 254, 273 | 0 |
| 22 | d7 | 81/81 (100%) | 1.01 | 17 (20%) 1 0 | 130, 170, 251, 277 | 0 |
| 23 | D8 | 63/63 (100%) | 0.99 | 14 (22%) 0 0 | 137, 199, 263, 293 | 0 |
| 23 | d8 | 63/63 (100%) | 0.55 | 5 (7%) 12 9 | 144, 195, 229, 255 | 0 |
| 24 | D9 | 52/53 (98%) | 1.32 | 17 (32%) 0 0 | 121, 148, 181, 242 | 0 |
| 24 | d9 | 53/53 (100%) | 0.67 | 8 (15%) 2 2 | 131, 155, 201, 270 | 0 |
| 25 | E0 | 60/61 (98%) | 0.80 | 10 (16%) 1 1 | 127, 175, 237, 256 | 0 |
| 25 | e0 | 61/61 (100%) | 0.57 | 8 (13%) 3 3 | 118, 172, 231, 265 | 0 |
| 26 | E1 | 71/73 (97%) | 1.71 | 24 (33%) 0 0 | 184, 254, 297, 331 | 0 |
| 26 | e1 | 73/73 (100%) | 1.50 | 21 (28%) 0 0 | 194, 252, 323, 356 | 0 |
| 27 | L2 | 252/252 (100%) | 0.29 | 4 (1%) 72 61 | 70, 117, 155, 210 | 0 |
| 27 | l2 | 252/252 (100%) | 0.29 | 8 (3%) 47 35 | 85, 129, 167, 268 | 0 |
| 28 | L3 | 386/386 (100%) | 0.47 | 28 (7%) 15 11 | 71, 106, 143, 204 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 28 | l3 | 386/386 (100%) | 0.14 | 4 (1%) 82 73 | 71, 103, 141, 238 | 0 |
| 29 | L4 | 361/361 (100%) | 0.18 | 3 (0%) 86 78 | 77, 120, 160, 215 | 0 |
| 29 | l4 | 361/361 (100%) | 0.10 | 4 (1%) 80 71 | 83, 129, 171, 207 | 0 |
| 30 | L5 | 296/296 (100%) | 0.73 | 42 (14%) 2 2 | 101, 165, 219, 253 | 0 |
| 30 | l5 | 294/296 (99%) | 0.99 | 62 (21%) 1 0 | 130, 193, 248, 273 | 0 |
| 31 | L6 | 157/176 (89%) | -0.09 | 1 (0%) 89 83 | 87, 119, 160, 180 | 0 |
| 31 | l6 | 157/176 (89%) | 0.04 | 2 (1%) 77 67 | 82, 112, 171, 222 | 0 |
| 32 | L7 | 222/223 (99%) | 0.47 | 19 (8%) 10 8 | 83, 113, 169, 245 | 0 |
| 32 | l7 | 223/223 (100%) | 0.22 | 4 (1%) 68 57 | 77, 113, 161, 269 | 0 |
| 33 | L8 | 233/233 (100%) | 0.54 | 18 (7%) 13 10 | 124, 171, 236, 295 | 0 |
| 33 | l8 | 231/233 (99%) | 0.51 | 23 (9%) 7 5 | 134, 182, 244, 323 | 0 |
| 34 | L9 | 191/191 (100%) | 0.46 | 17 (8%) 9 7 | 85, 123, 158, 208 | 0 |
| 34 | l9 | 191/191 (100%) | 0.53 | 8 (4%) 36 27 | 82, 116, 147, 226 | 0 |
| 35 | M0 | 211/221 (95%) | 0.05 | 3 (1%) 75 64 | 82, 111, 181, 250 | 0 |
| 35 | m0 | 209/221 (94%) | 0.27 | 7 (3%) 46 35 | 89, 118, 180, 278 | 0 |
| 36 | M1 | 169/169 (100%) | 0.36 | 10 (5%) 22 15 | 123, 155, 188, 203 | 0 |
| 36 | m1 | 169/169 (100%) | 0.61 | 14 (8%) 11 9 | 136, 183, 219, 250 | 0 |
| 37 | M3 | 193/194 (99%) | -0.04 | 4 (2%) 63 52 | 79, 144, 187, 263 | 0 |
| 37 | m3 | 194/194 (100%) | 0.28 | 10 (5%) 27 20 | 106, 162, 211, 286 | 0 |
| 38 | M4 | 136/137 (99%) | 0.24 | 4 (2%) 51 39 | 96, 123, 157, 191 | 0 |
| 38 | m4 | 137/137 (100%) | 0.05 | 1 (0%) 87 81 | 87, 111, 137, 182 | 0 |
| 39 | M5 | 203/203 (100%) | 1.06 | 28 (13%) 2 3 | 88, 124, 150, 166 | 0 |
| 39 | m5 | 203/203 (100%) | 1.11 | 36 (17%) 1 1 | 96, 140, 170, 183 | 0 |
| 40 | M6 | 197/197 (100%) | 0.17 | 2 (1%) 82 73 | 67, 97, 140, 196 | 0 |
| 40 | m6 | 197/197 (100%) | 0.09 | 0 100 100 | 67, 94, 138, 166 | 0 |
| 41 | M7 | 183/184 (99%) | 0.13 | 4 (2%) 62 50 | 75, 99, 184, 250 | 0 |
| 41 | m7 | 183/184 (99%) | 0.45 | 4 (2%) 62 50 | 76, 105, 176, 253 | 0 |
| 42 | M8 | 185/185 (100%) | 0.75 | 24 (12%) 3 3 | 89, 121, 149, 183 | 0 |
| 42 | m8 | 185/185 (100%) | 0.67 | 27 (14%) 2 2 | 93, 138, 166, 194 | 0 |
| 43 | M9 | 188/188 (100%) | 0.16 | 10 (5%) 26 20 | 92, 134, 244, 336 | 0 |
| 43 | m9 | 184/188 (97%) | 0.32 | 12 (6%) 18 12 | 101, 137, 218, 301 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 44 | N0 | 172/172 (100%) | 0.88 | 19 (11%) 5 4 | 88, 115, 150, 188 | 0 |
| 44 | n0 | 171/172 (99%) | 0.43 | 7 (4%) 37 27 | 80, 108, 139, 189 | 0 |
| 45 | N1 | 159/159 (100%) | 1.13 | 32 (20%) 1 0 | 94, 126, 187, 212 | 0 |
| 45 | n1 | 159/159 (100%) | 1.18 | 47 (29%) 0 0 | 100, 136, 187, 244 | 0 |
| 46 | N2 | 100/100 (100%) | 0.60 | 12 (12%) 4 4 | 126, 172, 211, 237 | 0 |
| 46 | n2 | 98/100 (98%) | 0.38 | 13 (13%) 3 3 | 139, 180, 223, 247 | 0 |
| 47 | N3 | 136/136 (100%) | 0.52 | 6 (4%) 34 25 | 69, 105, 149, 254 | 0 |
| 47 | n3 | 135/136 (99%) | 0.37 | 3 (2%) 62 50 | 72, 100, 135, 178 | 0 |
| 48 | N4 | 130/155 (83%) | 1.18 | 25 (19%) 1 1 | 88, 171, 291, 313 | 0 |
| 48 | n4 | 130/155 (83%) | 0.70 | 19 (14%) 2 2 | 93, 180, 259, 294 | 0 |
| 49 | N5 | 121/121 (100%) | 0.50 | 8 (6%) 18 12 | 105, 138, 175, 245 | 0 |
| 49 | n5 | 120/121 (99%) | 1.37 | 35 (29%) 0 0 | 113, 150, 191, 229 | 0 |
| 50 | N6 | 126/126 (100%) | 0.55 | 4 (3%) 47 35 | 96, 127, 164, 209 | 0 |
| 50 | n6 | 122/126 (96%) | 0.68 | 10 (8%) 11 9 | 104, 144, 177, 183 | 0 |
| 51 | N7 | 135/135 (100%) | 0.96 | 26 (19%) 1 1 | 143, 184, 224, 242 | 0 |
| 51 | n7 | 135/135 (100%) | 0.77 | 15 (11%) 5 4 | 137, 187, 227, 253 | 0 |
| 52 | N8 | 148/148 (100%) | 0.77 | 10 (6%) 17 12 | 79, 123, 170, 199 | 0 |
| 52 | n8 | 148/148 (100%) | 0.65 | 18 (12%) 4 4 | 90, 144, 188, 213 | 0 |
| 53 | N9 | 58/58 (100%) | 1.33 | 14 (24%) 0 0 | 82, 135, 196, 215 | 0 |
| 53 | n9 | 56/58 (96%) | 1.65 | 21 (37%) 0 0 | 91, 158, 203, 245 | 0 |
| 54 | O0 | 97/100 (97%) | 0.52 | 8 (8%) 11 9 | 138, 162, 212, 221 | 0 |
| 54 | o0 | 100/100 (100%) | 0.37 | 7 (7%) 16 11 | 128, 165, 222, 241 | 0 |
| 55 | O1 | 109/109 (100%) | 0.61 | 8 (7%) 15 11 | 81, 119, 186, 224 | 0 |
| 55 | o1 | 109/109 (100%) | 0.59 | 8 (7%) 15 11 | 89, 124, 204, 257 | 0 |
| 56 | O2 | 127/127 (100%) | 0.17 | 0 100 100 | 77, 100, 133, 192 | 0 |
| 56 | o2 | 127/127 (100%) | 0.35 | 2 (1%) 72 61 | 75, 108, 139, 200 | 0 |
| 57 | O3 | 106/106 (100%) | 0.16 | 1 (0%) 84 76 | 74, 97, 130, 145 | 0 |
| 57 | o3 | 106/106 (100%) | 0.30 | 0 100 100 | 76, 95, 123, 162 | 0 |
| 58 | O4 | 112/112 (100%) | 1.21 | 25 (22%) 0 0 | 102, 143, 228, 286 | 0 |
| 58 | o4 | 112/112 (100%) | 0.50 | 11 (9%) 7 6 | 109, 150, 203, 243 | 0 |
| 59 | O5 | 119/119 (100%) | 0.30 | 3 (2%) 57 45 | 109, 146, 190, 230 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 59 | o5 | 119/119 (100%) | 0.73 | 12 (10%) 7 5 | 126, 157, 193, 207 | 0 |
| 60 | O6 | 99/99 (100%) | 0.38 | 5 (5%) 28 21 | 126, 151, 195, 302 | 0 |
| 60 | o6 | 99/99 (100%) | 0.35 | 8 (8%) 12 9 | 128, 169, 209, 289 | 0 |
| 61 | O7 | 87/87 (100%) | 0.06 | 0 100 100 | 80, 104, 186, 209 | 0 |
| 61 | o7 | 83/87 (95%) | 0.23 | 3 (3%) 42 32 | 91, 119, 150, 202 | 0 |
| 62 | O8 | 77/77 (100%) | 0.83 | 13 (16%) 1 1 | 132, 168, 205, 227 | 0 |
| 62 | o8 | 77/77 (100%) | 1.24 | 16 (20%) 1 0 | 150, 180, 220, 227 | 0 |
| 63 | O9 | 50/50 (100%) | 0.61 | 2 (4%) 38 28 | 94, 117, 133, 144 | 0 |
| 63 | o9 | 50/50 (100%) | 1.44 | 10 (20%) 1 0 | 108, 125, 145, 152 | 0 |
| 64 | Q0 | 52/52 (100%) | 0.07 | 1 (1%) 66 55 | 92, 110, 155, 190 | 0 |
| 64 | q0 | 52/52 (100%) | 0.30 | 2 (3%) 40 30 | 83, 106, 135, 148 | 0 |
| 65 | Q1 | 25/25 (100%) | 0.45 | 0 100 100 | 96, 115, 136, 144 | 0 |
| 65 | q1 | 25/25 (100%) | 0.30 | 1 (4%) 38 28 | 102, 117, 148, 156 | 0 |
| 66 | Q2 | 105/105 (100%) | 0.88 | 18 (17%) 1 1 | 86, 132, 166, 258 | 0 |
| 66 | q2 | 104/105 (99%) | 1.14 | 28 (26%) 0 0 | 111, 156, 199, 215 | 0 |
| 67 | Q3 | 91/91 (100%) | 0.01 | 0 100 100 | 88, 127, 175, 217 | 0 |
| 67 | q3 | 91/91 (100%) | 0.18 | 1 (1%) 80 71 | 79, 131, 176, 210 | 0 |
| 68 | S0 | 206/206 (100%) | 0.56 | 20 (9%) 7 6 | 128, 178, 224, 271 | 0 |
| 68 | s0 | 206/206 (100%) | 0.39 | 22 (10%) 6 5 | 133, 174, 214, 262 | 0 |
| 69 | S1 | 214/216 (99%) | 0.75 | 33 (15%) 2 1 | 138, 201, 253, 279 | 0 |
| 69 | s1 | 216/216 (100%) | 1.30 | 69 (31%) 0 0 | 139, 202, 254, 312 | 0 |
| 70 | S2 | 217/217 (100%) | 0.79 | 29 (13%) 3 3 | 120, 161, 202, 244 | 0 |
| 70 | s2 | 217/217 (100%) | 0.57 | 22 (10%) 7 5 | 114, 155, 195, 226 | 0 |
| 71 | S3 | 223/223 (100%) | 1.13 | 47 (21%) 1 0 | 113, 166, 236, 306 | 0 |
| 71 | s3 | 223/223 (100%) | 0.53 | 24 (10%) 5 4 | 137, 174, 236, 267 | 0 |
| 72 | S4 | 260/260 (100%) | 1.02 | 55 (21%) 0 0 | 131, 181, 213, 254 | 0 |
| 72 | s4 | 260/260 (100%) | 0.45 | 15 (5%) 23 16 | 109, 159, 203, 253 | 0 |
| 73 | S5 | 206/206 (100%) | 1.16 | 42 (20%) 1 0 | 125, 189, 236, 278 | 0 |
| 73 | s5 | 206/206 (100%) | 0.98 | 35 (16%) 1 1 | 145, 185, 230, 264 | 0 |
| 74 | S6 | 226/236 (95%) | 0.84 | 45 (19%) 1 0 | 125, 186, 246, 272 | 0 |
| 74 | s6 | 218/236 (92%) | 0.63 | 32 (14%) 2 2 | 111, 162, 216, 258 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | OWAB(Å ²) | Q<0.9 | |
|-----|-------|-------------------|--------|-----------|----|-----------------------|--------------------|---|
| 75 | S7 | 184/184 (100%) | 0.83 | 33 (17%) | 1 | 1 | 154, 208, 268, 305 | 0 |
| 75 | s7 | 184/184 (100%) | 0.46 | 19 (10%) | 6 | 5 | 133, 195, 250, 297 | 0 |
| 76 | S8 | 188/200 (94%) | 1.01 | 35 (18%) | 1 | 1 | 113, 154, 219, 291 | 0 |
| 76 | s8 | 185/200 (92%) | 0.87 | 29 (15%) | 2 | 1 | 101, 142, 204, 250 | 0 |
| 77 | S9 | 185/185 (100%) | 0.98 | 36 (19%) | 1 | 1 | 129, 186, 240, 279 | 0 |
| 77 | s9 | 185/185 (100%) | 0.87 | 29 (15%) | 2 | 1 | 119, 169, 223, 263 | 0 |
| 78 | SM | 159/272 (58%) | 0.51 | 22 (13%) | 2 | 3 | 117, 185, 279, 371 | 0 |
| 78 | sM | 131/272 (48%) | 0.38 | 15 (11%) | 4 | 4 | 129, 182, 270, 311 | 0 |
| 79 | SR | 318/318 (100%) | 1.13 | 77 (24%) | 0 | 0 | 164, 221, 281, 318 | 0 |
| 79 | sR | 316/318 (99%) | 0.58 | 40 (12%) | 3 | 4 | 143, 199, 251, 293 | 0 |
| All | All | 32778/34100 (96%) | 0.41 | 2743 (8%) | 11 | 8 | 67, 147, 242, 453 | 0 |

All (2743) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 78 | SM | 19 | VAL | 12.3 |
| 34 | l9 | 191 | LEU | 12.0 |
| 1 | 5 | 1565 | G | 11.1 |
| 54 | o0 | 6 | SER | 10.7 |
| 78 | SM | 18 | VAL | 9.3 |
| 26 | e1 | 106 | TYR | 9.3 |
| 7 | c2 | 62 | LEU | 8.2 |
| 7 | c2 | 97 | LEU | 8.1 |
| 79 | SR | 212 | ALA | 8.0 |
| 79 | SR | 213 | SER | 7.8 |
| 78 | sM | 53 | ARG | 7.7 |
| 44 | N0 | 1 | MET | 7.5 |
| 7 | C2 | 62 | LEU | 7.4 |
| 48 | N4 | 65 | GLU | 7.3 |
| 6 | C1 | 36 | LYS | 7.0 |
| 2 | 2 | 709 | C | 7.0 |
| 69 | s1 | 100 | PHE | 6.9 |
| 79 | SR | 156 | VAL | 6.9 |
| 73 | S5 | 152 | GLY | 6.8 |
| 79 | SR | 211 | ILE | 6.7 |
| 73 | s5 | 152 | GLY | 6.7 |
| 7 | c2 | 111 | ASN | 6.7 |
| 26 | E1 | 152 | ALA | 6.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 7 | c2 | 63 | VAL | 6.6 |
| 33 | l8 | 198 | ALA | 6.6 |
| 7 | C2 | 119 | SER | 6.6 |
| 5 | C0 | 22 | VAL | 6.6 |
| 79 | SR | 32 | LEU | 6.6 |
| 39 | M5 | 2 | GLY | 6.6 |
| 45 | N1 | 34 | TYR | 6.5 |
| 26 | E1 | 145 | HIS | 6.4 |
| 7 | c2 | 104 | GLY | 6.3 |
| 75 | S7 | 93 | LEU | 6.3 |
| 5 | C0 | 23 | ALA | 6.3 |
| 17 | D2 | 122 | SER | 6.2 |
| 75 | s7 | 92 | PHE | 6.2 |
| 13 | C8 | 2 | SER | 6.2 |
| 39 | M5 | 3 | ALA | 6.1 |
| 7 | C2 | 25 | GLU | 6.0 |
| 5 | C0 | 21 | VAL | 6.0 |
| 7 | C2 | 61 | VAL | 6.0 |
| 44 | N0 | 2 | ALA | 5.9 |
| 7 | c2 | 121 | VAL | 5.9 |
| 26 | E1 | 93 | HIS | 5.8 |
| 74 | S6 | 96 | SER | 5.8 |
| 39 | m5 | 3 | ALA | 5.8 |
| 75 | s7 | 93 | LEU | 5.8 |
| 79 | SR | 178 | VAL | 5.8 |
| 2 | 2 | 135 | A | 5.8 |
| 45 | n1 | 66 | ASN | 5.8 |
| 73 | s5 | 153 | GLY | 5.7 |
| 7 | c2 | 90 | LYS | 5.7 |
| 69 | s1 | 212 | VAL | 5.7 |
| 5 | c0 | 23 | ALA | 5.7 |
| 48 | N4 | 99 | GLU | 5.6 |
| 79 | SR | 204 | ALA | 5.6 |
| 78 | SM | 170 | VAL | 5.6 |
| 79 | SR | 25 | THR | 5.6 |
| 48 | N4 | 86 | SER | 5.6 |
| 5 | C0 | 25 | LYS | 5.6 |
| 73 | s5 | 129 | PRO | 5.6 |
| 74 | s6 | 89 | ASP | 5.6 |
| 7 | C2 | 71 | ILE | 5.6 |
| 33 | L8 | 198 | ALA | 5.5 |
| 48 | n4 | 67 | VAL | 5.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 75 | s7 | 134 | GLU | 5.5 |
| 79 | SR | 263 | PHE | 5.5 |
| 45 | n1 | 34 | TYR | 5.5 |
| 7 | C2 | 69 | ALA | 5.5 |
| 70 | S2 | 90 | THR | 5.5 |
| 79 | SR | 210 | LEU | 5.4 |
| 6 | c1 | 4 | GLU | 5.4 |
| 7 | c2 | 102 | GLY | 5.4 |
| 33 | l8 | 199 | ALA | 5.4 |
| 6 | C1 | 150 | ASN | 5.4 |
| 62 | o8 | 5 | ILE | 5.4 |
| 69 | s1 | 89 | ASP | 5.4 |
| 11 | C6 | 132 | LYS | 5.4 |
| 39 | m5 | 58 | GLY | 5.4 |
| 51 | N7 | 11 | ALA | 5.3 |
| 1 | 1 | 2539 | C | 5.3 |
| 48 | N4 | 97 | LYS | 5.3 |
| 30 | l5 | 69 | ILE | 5.3 |
| 79 | sR | 211 | ILE | 5.3 |
| 25 | E0 | 45 | VAL | 5.3 |
| 73 | S5 | 154 | ALA | 5.3 |
| 75 | S7 | 94 | ALA | 5.2 |
| 15 | D0 | 107 | THR | 5.2 |
| 7 | c2 | 28 | LEU | 5.2 |
| 6 | C1 | 152 | GLN | 5.2 |
| 30 | l5 | 127 | GLY | 5.2 |
| 79 | SR | 252 | LEU | 5.2 |
| 26 | e1 | 107 | LYS | 5.1 |
| 75 | S7 | 47 | ARG | 5.1 |
| 45 | n1 | 77 | ASN | 5.1 |
| 69 | S1 | 156 | ALA | 5.1 |
| 45 | n1 | 65 | TYR | 5.1 |
| 9 | c4 | 135 | ARG | 5.1 |
| 79 | SR | 192 | PHE | 5.1 |
| 69 | s1 | 140 | ILE | 5.1 |
| 7 | c2 | 119 | SER | 5.1 |
| 24 | D9 | 56 | ARG | 5.1 |
| 7 | c2 | 70 | ASN | 5.1 |
| 7 | C2 | 63 | VAL | 5.1 |
| 9 | c4 | 98 | GLY | 5.1 |
| 74 | s6 | 153 | VAL | 5.1 |
| 79 | sR | 121 | MET | 5.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 69 | s1 | 101 | HIS | 5.0 |
| 26 | e1 | 100 | LEU | 5.0 |
| 11 | c6 | 114 | ARG | 5.0 |
| 62 | o8 | 43 | PHE | 5.0 |
| 22 | d7 | 51 | GLN | 5.0 |
| 43 | m9 | 185 | LEU | 5.0 |
| 2 | 2 | 721 | U | 5.0 |
| 7 | C2 | 28 | LEU | 5.0 |
| 72 | S4 | 149 | TYR | 5.0 |
| 26 | e1 | 116 | LYS | 5.0 |
| 69 | s1 | 122 | GLU | 5.0 |
| 45 | n1 | 67 | VAL | 4.9 |
| 2 | 2 | 729 | G | 4.9 |
| 60 | o6 | 66 | GLU | 4.9 |
| 9 | C4 | 14 | PHE | 4.9 |
| 21 | d6 | 45 | VAL | 4.9 |
| 48 | n4 | 68 | ALA | 4.9 |
| 15 | D0 | 65 | ILE | 4.8 |
| 15 | D0 | 84 | MET | 4.8 |
| 66 | q2 | 72 | LEU | 4.8 |
| 74 | s6 | 88 | ARG | 4.8 |
| 7 | C2 | 29 | LYS | 4.8 |
| 7 | C2 | 33 | ARG | 4.8 |
| 79 | SR | 115 | ILE | 4.8 |
| 2 | 2 | 1709 | C | 4.8 |
| 30 | l5 | 55 | PHE | 4.8 |
| 6 | C1 | 146 | ALA | 4.8 |
| 78 | SM | 21 | PRO | 4.8 |
| 70 | S2 | 91 | ARG | 4.8 |
| 33 | l8 | 150 | LEU | 4.8 |
| 1 | 5 | 2539 | C | 4.8 |
| 48 | N4 | 66 | GLU | 4.8 |
| 58 | O4 | 33 | GLN | 4.8 |
| 69 | s1 | 99 | ASN | 4.8 |
| 7 | c2 | 103 | LEU | 4.8 |
| 23 | D8 | 67 | ARG | 4.8 |
| 48 | N4 | 95 | SER | 4.8 |
| 6 | C1 | 3 | THR | 4.8 |
| 16 | d1 | 55 | LEU | 4.8 |
| 79 | sR | 33 | LEU | 4.8 |
| 75 | S7 | 48 | GLU | 4.8 |
| 45 | n1 | 78 | LYS | 4.8 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 74 | S6 | 156 | PHE | 4.8 |
| 53 | n9 | 43 | HIS | 4.7 |
| 7 | c2 | 115 | VAL | 4.7 |
| 30 | L5 | 62 | CYS | 4.7 |
| 73 | s5 | 37 | GLN | 4.7 |
| 73 | S5 | 71 | ALA | 4.7 |
| 66 | q2 | 81 | ALA | 4.7 |
| 60 | O6 | 100 | HIS | 4.7 |
| 54 | o0 | 105 | ALA | 4.7 |
| 74 | S6 | 88 | ARG | 4.7 |
| 70 | S2 | 97 | ARG | 4.7 |
| 71 | s3 | 148 | LYS | 4.7 |
| 79 | SR | 203 | THR | 4.7 |
| 72 | S4 | 45 | ILE | 4.7 |
| 73 | S5 | 151 | GLY | 4.7 |
| 35 | M0 | 220 | GLN | 4.7 |
| 46 | N2 | 95 | PHE | 4.6 |
| 23 | D8 | 66 | LEU | 4.6 |
| 39 | m5 | 143 | ARG | 4.6 |
| 48 | N4 | 108 | LYS | 4.6 |
| 5 | C0 | 64 | TYR | 4.6 |
| 15 | d0 | 64 | LYS | 4.6 |
| 24 | D9 | 5 | ASN | 4.6 |
| 7 | c2 | 122 | VAL | 4.6 |
| 39 | m5 | 148 | TYR | 4.6 |
| 77 | s9 | 134 | ILE | 4.6 |
| 26 | E1 | 87 | THR | 4.6 |
| 62 | O8 | 43 | PHE | 4.6 |
| 66 | Q2 | 106 | PHE | 4.6 |
| 13 | C8 | 48 | LYS | 4.6 |
| 11 | C6 | 55 | VAL | 4.6 |
| 73 | s5 | 71 | ALA | 4.6 |
| 77 | S9 | 141 | VAL | 4.6 |
| 11 | c6 | 47 | LYS | 4.6 |
| 17 | D2 | 121 | VAL | 4.6 |
| 15 | D0 | 82 | TYR | 4.6 |
| 45 | N1 | 72 | VAL | 4.6 |
| 7 | C2 | 32 | LEU | 4.6 |
| 54 | o0 | 7 | GLN | 4.5 |
| 15 | D0 | 111 | GLY | 4.5 |
| 7 | c2 | 91 | VAL | 4.5 |
| 7 | c2 | 93 | ASP | 4.5 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 77 | s9 | 86 | LEU | 4.5 |
| 7 | c2 | 100 | TRP | 4.5 |
| 79 | SR | 181 | TRP | 4.5 |
| 26 | E1 | 90 | LYS | 4.5 |
| 30 | l5 | 163 | LEU | 4.5 |
| 53 | n9 | 47 | LEU | 4.5 |
| 79 | SR | 171 | SER | 4.5 |
| 26 | E1 | 89 | LYS | 4.5 |
| 33 | l8 | 197 | VAL | 4.5 |
| 73 | S5 | 158 | GLN | 4.5 |
| 71 | S3 | 206 | VAL | 4.5 |
| 20 | D5 | 36 | ALA | 4.5 |
| 25 | e0 | 60 | PRO | 4.5 |
| 43 | M9 | 184 | LEU | 4.4 |
| 72 | S4 | 12 | LEU | 4.4 |
| 69 | s1 | 213 | ARG | 4.4 |
| 45 | n1 | 32 | LYS | 4.4 |
| 69 | s1 | 235 | GLY | 4.4 |
| 25 | e0 | 53 | LYS | 4.4 |
| 50 | n6 | 109 | LEU | 4.4 |
| 69 | s1 | 97 | LEU | 4.4 |
| 7 | C2 | 60 | VAL | 4.4 |
| 30 | L5 | 4 | GLN | 4.4 |
| 22 | d7 | 46 | VAL | 4.4 |
| 78 | sM | 54 | PRO | 4.4 |
| 7 | c2 | 110 | GLY | 4.4 |
| 77 | s9 | 118 | LEU | 4.4 |
| 75 | S7 | 5 | GLN | 4.4 |
| 77 | S9 | 6 | ARG | 4.4 |
| 79 | SR | 231 | MET | 4.4 |
| 11 | c6 | 44 | LEU | 4.4 |
| 30 | L5 | 38 | THR | 4.4 |
| 7 | c2 | 49 | THR | 4.4 |
| 17 | D2 | 46 | TYR | 4.4 |
| 51 | N7 | 14 | VAL | 4.3 |
| 59 | O5 | 75 | TYR | 4.3 |
| 14 | C9 | 27 | LYS | 4.3 |
| 6 | C1 | 137 | PHE | 4.3 |
| 7 | C2 | 70 | ASN | 4.3 |
| 39 | M5 | 6 | TYR | 4.3 |
| 60 | O6 | 2 | THR | 4.3 |
| 7 | C2 | 89 | ILE | 4.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 77 | S9 | 2 | PRO | 4.3 |
| 7 | c2 | 92 | ALA | 4.3 |
| 73 | s5 | 80 | LYS | 4.3 |
| 78 | SM | 176 | LYS | 4.3 |
| 15 | d0 | 65 | ILE | 4.3 |
| 21 | d6 | 73 | TYR | 4.3 |
| 6 | C1 | 151 | LYS | 4.3 |
| 7 | c2 | 109 | GLU | 4.3 |
| 48 | n4 | 66 | GLU | 4.3 |
| 68 | S0 | 107 | PHE | 4.3 |
| 79 | sR | 79 | TYR | 4.3 |
| 48 | n4 | 90 | ILE | 4.3 |
| 62 | o8 | 40 | GLN | 4.3 |
| 30 | l5 | 61 | ILE | 4.3 |
| 79 | SR | 193 | ILE | 4.3 |
| 11 | C6 | 54 | LEU | 4.3 |
| 79 | SR | 7 | LEU | 4.3 |
| 39 | M5 | 123 | GLN | 4.3 |
| 5 | C0 | 41 | TYR | 4.3 |
| 9 | c4 | 102 | LEU | 4.3 |
| 45 | N1 | 67 | VAL | 4.2 |
| 70 | S2 | 96 | THR | 4.2 |
| 74 | S6 | 157 | VAL | 4.2 |
| 66 | q2 | 79 | THR | 4.2 |
| 26 | E1 | 119 | ARG | 4.2 |
| 2 | 2 | 493 | U | 4.2 |
| 11 | C6 | 51 | PRO | 4.2 |
| 2 | 6 | 239 | C | 4.2 |
| 63 | o9 | 38 | ASN | 4.2 |
| 33 | L8 | 199 | ALA | 4.2 |
| 69 | S1 | 140 | ILE | 4.2 |
| 11 | C6 | 21 | HIS | 4.2 |
| 11 | c6 | 51 | PRO | 4.2 |
| 78 | SM | 171 | PRO | 4.2 |
| 17 | D2 | 61 | ILE | 4.2 |
| 79 | sR | 204 | ALA | 4.2 |
| 69 | s1 | 141 | ALA | 4.2 |
| 77 | s9 | 2 | PRO | 4.2 |
| 78 | SM | 22 | PRO | 4.2 |
| 7 | C2 | 64 | SER | 4.2 |
| 26 | e1 | 108 | VAL | 4.2 |
| 74 | S6 | 179 | VAL | 4.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | 2 | 719 | U | 4.2 |
| 16 | D1 | 33 | GLN | 4.2 |
| 26 | e1 | 99 | LYS | 4.2 |
| 50 | n6 | 108 | LYS | 4.2 |
| 19 | D4 | 119 | PHE | 4.2 |
| 26 | e1 | 134 | ASN | 4.2 |
| 45 | N1 | 92 | ARG | 4.2 |
| 32 | L7 | 135 | ALA | 4.1 |
| 46 | n2 | 95 | PHE | 4.1 |
| 53 | n9 | 39 | PHE | 4.1 |
| 26 | E1 | 109 | ASP | 4.1 |
| 51 | n7 | 41 | ALA | 4.1 |
| 7 | C2 | 36 | LEU | 4.1 |
| 79 | SR | 33 | LEU | 4.1 |
| 79 | SR | 190 | ALA | 4.1 |
| 30 | l5 | 49 | TYR | 4.1 |
| 5 | C0 | 45 | ALA | 4.1 |
| 6 | C1 | 149 | ALA | 4.1 |
| 52 | N8 | 149 | ALA | 4.1 |
| 27 | l2 | 252 | THR | 4.1 |
| 20 | D5 | 50 | ILE | 4.1 |
| 43 | M9 | 183 | ALA | 4.1 |
| 58 | O4 | 79 | SER | 4.1 |
| 66 | q2 | 8 | ARG | 4.1 |
| 77 | S9 | 134 | ILE | 4.1 |
| 5 | C0 | 20 | VAL | 4.1 |
| 51 | N7 | 15 | ARG | 4.1 |
| 53 | N9 | 43 | HIS | 4.1 |
| 18 | D3 | 4 | GLY | 4.1 |
| 26 | e1 | 132 | LEU | 4.1 |
| 23 | d8 | 65 | ARG | 4.1 |
| 74 | s6 | 80 | ASN | 4.1 |
| 48 | n4 | 87 | LEU | 4.1 |
| 2 | 2 | 697 | C | 4.1 |
| 7 | c2 | 98 | GLY | 4.1 |
| 22 | d7 | 32 | PHE | 4.1 |
| 5 | C0 | 68 | LEU | 4.1 |
| 26 | E1 | 104 | SER | 4.1 |
| 21 | d6 | 83 | ILE | 4.1 |
| 24 | D9 | 27 | HIS | 4.1 |
| 33 | l8 | 132 | VAL | 4.1 |
| 58 | o4 | 3 | GLN | 4.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 79 | sR | 32 | LEU | 4.1 |
| 26 | e1 | 118 | ARG | 4.1 |
| 70 | s2 | 90 | THR | 4.1 |
| 39 | M5 | 58 | GLY | 4.0 |
| 71 | S3 | 134 | CYS | 4.0 |
| 72 | S4 | 157 | ASN | 4.0 |
| 7 | C2 | 100 | TRP | 4.0 |
| 79 | SR | 169 | ILE | 4.0 |
| 22 | D7 | 24 | LEU | 4.0 |
| 34 | L9 | 191 | LEU | 4.0 |
| 45 | n1 | 64 | VAL | 4.0 |
| 76 | S8 | 8 | ARG | 4.0 |
| 58 | O4 | 78 | GLY | 4.0 |
| 58 | O4 | 77 | GLY | 4.0 |
| 60 | o6 | 69 | ALA | 4.0 |
| 48 | N4 | 1 | MET | 4.0 |
| 10 | C5 | 101 | ALA | 4.0 |
| 11 | c6 | 48 | VAL | 4.0 |
| 42 | M8 | 140 | LEU | 4.0 |
| 69 | S1 | 122 | GLU | 4.0 |
| 9 | C4 | 114 | ARG | 4.0 |
| 25 | E0 | 55 | ARG | 4.0 |
| 48 | N4 | 96 | LEU | 4.0 |
| 23 | D8 | 33 | LEU | 4.0 |
| 25 | e0 | 62 | VAL | 4.0 |
| 55 | O1 | 71 | LEU | 4.0 |
| 76 | S8 | 148 | ALA | 4.0 |
| 48 | n4 | 130 | SER | 4.0 |
| 70 | s2 | 224 | PHE | 4.0 |
| 66 | q2 | 25 | VAL | 4.0 |
| 7 | c2 | 42 | ALA | 4.0 |
| 11 | c6 | 138 | PHE | 4.0 |
| 21 | d6 | 44 | ILE | 4.0 |
| 46 | N2 | 69 | ALA | 4.0 |
| 63 | o9 | 2 | ALA | 4.0 |
| 73 | s5 | 44 | ASN | 4.0 |
| 2 | 2 | 718 | U | 4.0 |
| 11 | c6 | 57 | LEU | 4.0 |
| 10 | C5 | 125 | PRO | 4.0 |
| 42 | m8 | 169 | GLY | 4.0 |
| 6 | c1 | 147 | GLY | 4.0 |
| 36 | m1 | 91 | LEU | 4.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 33 | l8 | 131 | ALA | 4.0 |
| 68 | S0 | 120 | LEU | 3.9 |
| 79 | SR | 222 | LEU | 3.9 |
| 79 | SR | 234 | LEU | 3.9 |
| 21 | d6 | 38 | ARG | 3.9 |
| 77 | S9 | 13 | SER | 3.9 |
| 71 | S3 | 137 | VAL | 3.9 |
| 2 | 2 | 724 | C | 3.9 |
| 70 | S2 | 92 | ALA | 3.9 |
| 69 | S1 | 45 | LYS | 3.9 |
| 2 | 2 | 711 | U | 3.9 |
| 70 | s2 | 91 | ARG | 3.9 |
| 7 | C2 | 41 | LEU | 3.9 |
| 73 | s5 | 43 | PHE | 3.9 |
| 79 | SR | 232 | TYR | 3.9 |
| 14 | c9 | 28 | LEU | 3.9 |
| 39 | m5 | 135 | VAL | 3.9 |
| 58 | o4 | 2 | ALA | 3.9 |
| 72 | S4 | 44 | LEU | 3.9 |
| 78 | SM | 175 | VAL | 3.9 |
| 53 | N9 | 33 | LYS | 3.9 |
| 69 | S1 | 138 | PHE | 3.9 |
| 42 | m8 | 167 | SER | 3.9 |
| 7 | C2 | 95 | LYS | 3.9 |
| 46 | N2 | 71 | PHE | 3.9 |
| 8 | c3 | 69 | ASN | 3.9 |
| 69 | s1 | 218 | LEU | 3.9 |
| 45 | n1 | 39 | ILE | 3.9 |
| 24 | D9 | 55 | PHE | 3.9 |
| 69 | s1 | 84 | ILE | 3.9 |
| 5 | c0 | 21 | VAL | 3.9 |
| 30 | l5 | 146 | LEU | 3.9 |
| 46 | n2 | 56 | VAL | 3.9 |
| 20 | D5 | 102 | THR | 3.9 |
| 21 | d6 | 17 | HIS | 3.9 |
| 45 | n1 | 90 | ASN | 3.9 |
| 75 | S7 | 91 | ILE | 3.9 |
| 26 | E1 | 132 | LEU | 3.9 |
| 72 | S4 | 154 | ILE | 3.9 |
| 71 | s3 | 150 | MET | 3.9 |
| 69 | s1 | 90 | GLU | 3.8 |
| 79 | sR | 313 | TRP | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 11 | C6 | 121 | SER | 3.8 |
| 69 | S1 | 84 | ILE | 3.8 |
| 74 | S6 | 95 | LYS | 3.8 |
| 30 | l5 | 75 | LEU | 3.8 |
| 39 | m5 | 134 | LEU | 3.8 |
| 45 | n1 | 98 | HIS | 3.8 |
| 7 | c2 | 45 | LEU | 3.8 |
| 31 | l6 | 109 | GLU | 3.8 |
| 7 | c2 | 59 | LEU | 3.8 |
| 26 | e1 | 104 | SER | 3.8 |
| 26 | E1 | 86 | THR | 3.8 |
| 73 | S5 | 198 | LEU | 3.8 |
| 5 | C0 | 16 | PHE | 3.8 |
| 46 | N2 | 70 | LYS | 3.8 |
| 69 | s1 | 216 | LYS | 3.8 |
| 77 | S9 | 118 | LEU | 3.8 |
| 79 | SR | 73 | LEU | 3.8 |
| 13 | c8 | 61 | LEU | 3.8 |
| 15 | D0 | 64 | LYS | 3.8 |
| 20 | D5 | 91 | PRO | 3.8 |
| 63 | o9 | 51 | ILE | 3.8 |
| 76 | S8 | 167 | ALA | 3.8 |
| 7 | c2 | 101 | ALA | 3.8 |
| 52 | N8 | 144 | VAL | 3.8 |
| 21 | d6 | 68 | TYR | 3.8 |
| 50 | n6 | 45 | ILE | 3.8 |
| 79 | SR | 265 | LEU | 3.8 |
| 11 | c6 | 82 | ARG | 3.8 |
| 73 | S5 | 153 | GLY | 3.8 |
| 7 | c2 | 71 | ILE | 3.8 |
| 16 | d1 | 33 | GLN | 3.8 |
| 72 | S4 | 175 | PHE | 3.8 |
| 78 | sM | 55 | SER | 3.8 |
| 78 | sM | 66 | ALA | 3.8 |
| 21 | D6 | 62 | TYR | 3.8 |
| 1 | 1 | 2540 | A | 3.8 |
| 7 | c2 | 61 | VAL | 3.8 |
| 51 | n7 | 75 | VAL | 3.8 |
| 39 | m5 | 185 | ALA | 3.8 |
| 51 | N7 | 2 | ALA | 3.8 |
| 79 | SR | 191 | ASP | 3.7 |
| 51 | n7 | 82 | PRO | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 59 | o5 | 78 | LYS | 3.7 |
| 11 | C6 | 92 | TYR | 3.7 |
| 10 | c5 | 89 | MET | 3.7 |
| 20 | d5 | 42 | LEU | 3.7 |
| 49 | n5 | 121 | LYS | 3.7 |
| 70 | S2 | 95 | ARG | 3.7 |
| 53 | n9 | 40 | ARG | 3.7 |
| 69 | s1 | 211 | HIS | 3.7 |
| 35 | M0 | 221 | ALA | 3.7 |
| 67 | q3 | 92 | ALA | 3.7 |
| 74 | s6 | 161 | GLU | 3.7 |
| 30 | L5 | 127 | GLY | 3.7 |
| 7 | C2 | 143 | GLN | 3.7 |
| 30 | l5 | 41 | LYS | 3.7 |
| 70 | S2 | 113 | LEU | 3.7 |
| 30 | L5 | 78 | ALA | 3.7 |
| 60 | O6 | 8 | ALA | 3.7 |
| 6 | C1 | 155 | LYS | 3.7 |
| 44 | N0 | 30 | PHE | 3.7 |
| 15 | D0 | 110 | PRO | 3.7 |
| 71 | s3 | 134 | CYS | 3.7 |
| 16 | d1 | 87 | ARG | 3.7 |
| 30 | l5 | 216 | GLU | 3.7 |
| 12 | C7 | 71 | PHE | 3.7 |
| 15 | d0 | 66 | SER | 3.7 |
| 62 | O8 | 40 | GLN | 3.7 |
| 77 | s9 | 156 | ILE | 3.7 |
| 7 | C2 | 128 | ALA | 3.7 |
| 7 | C2 | 68 | GLU | 3.7 |
| 79 | sR | 7 | LEU | 3.7 |
| 55 | O1 | 14 | ILE | 3.7 |
| 69 | s1 | 121 | ILE | 3.7 |
| 79 | sR | 314 | GLN | 3.7 |
| 45 | N1 | 91 | LEU | 3.7 |
| 75 | s7 | 129 | LEU | 3.7 |
| 79 | SR | 241 | PHE | 3.7 |
| 25 | e0 | 2 | ALA | 3.7 |
| 30 | l5 | 137 | ASP | 3.7 |
| 73 | S5 | 155 | ALA | 3.7 |
| 71 | s3 | 152 | PHE | 3.7 |
| 77 | s9 | 105 | LEU | 3.7 |
| 2 | 2 | 696 | C | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 75 | S7 | 98 | ILE | 3.7 |
| 27 | L2 | 71 | LEU | 3.7 |
| 79 | SR | 254 | ALA | 3.7 |
| 77 | s9 | 37 | LYS | 3.6 |
| 71 | S3 | 16 | VAL | 3.6 |
| 24 | D9 | 50 | ILE | 3.6 |
| 52 | N8 | 109 | TYR | 3.6 |
| 71 | S3 | 184 | ILE | 3.6 |
| 75 | s7 | 91 | ILE | 3.6 |
| 72 | S4 | 48 | LEU | 3.6 |
| 30 | l5 | 38 | THR | 3.6 |
| 73 | s5 | 151 | GLY | 3.6 |
| 1 | 5 | 1815 | U | 3.6 |
| 5 | c0 | 25 | LYS | 3.6 |
| 59 | O5 | 2 | ALA | 3.6 |
| 74 | s6 | 133 | LEU | 3.6 |
| 79 | sR | 263 | PHE | 3.6 |
| 5 | c0 | 64 | TYR | 3.6 |
| 7 | C2 | 90 | LYS | 3.6 |
| 16 | d1 | 54 | ALA | 3.6 |
| 30 | L5 | 31 | TYR | 3.6 |
| 48 | n4 | 82 | ILE | 3.6 |
| 2 | 6 | 731 | C | 3.6 |
| 6 | C1 | 43 | LYS | 3.6 |
| 30 | l5 | 181 | PRO | 3.6 |
| 5 | C0 | 28 | ASN | 3.6 |
| 5 | C0 | 54 | TYR | 3.6 |
| 48 | n4 | 65 | GLU | 3.6 |
| 79 | SR | 208 | GLY | 3.6 |
| 50 | n6 | 73 | VAL | 3.6 |
| 48 | n4 | 85 | ALA | 3.6 |
| 10 | C5 | 109 | PRO | 3.6 |
| 16 | D1 | 22 | ARG | 3.6 |
| 71 | S3 | 50 | ILE | 3.6 |
| 19 | D4 | 17 | LEU | 3.6 |
| 24 | D9 | 36 | LEU | 3.6 |
| 30 | l5 | 48 | LYS | 3.6 |
| 47 | N3 | 100 | GLY | 3.6 |
| 49 | n5 | 62 | VAL | 3.6 |
| 12 | C7 | 125 | SER | 3.6 |
| 26 | E1 | 131 | PHE | 3.6 |
| 12 | C7 | 74 | GLN | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 49 | n5 | 60 | TYR | 3.6 |
| 14 | c9 | 31 | PRO | 3.6 |
| 72 | S4 | 47 | PHE | 3.6 |
| 42 | m8 | 176 | ARG | 3.6 |
| 77 | S9 | 3 | ARG | 3.6 |
| 53 | n9 | 29 | TYR | 3.6 |
| 77 | s9 | 97 | LEU | 3.6 |
| 11 | C6 | 59 | LYS | 3.6 |
| 39 | m5 | 6 | TYR | 3.6 |
| 73 | S5 | 133 | VAL | 3.6 |
| 30 | l5 | 67 | SER | 3.6 |
| 41 | m7 | 160 | ALA | 3.6 |
| 30 | l5 | 37 | VAL | 3.6 |
| 69 | s1 | 215 | VAL | 3.6 |
| 74 | S6 | 158 | ILE | 3.6 |
| 75 | S7 | 49 | ILE | 3.6 |
| 69 | s1 | 120 | LEU | 3.6 |
| 71 | S3 | 8 | LYS | 3.5 |
| 5 | C0 | 66 | TYR | 3.5 |
| 7 | C2 | 121 | VAL | 3.5 |
| 34 | l9 | 25 | VAL | 3.5 |
| 53 | n9 | 51 | ALA | 3.5 |
| 58 | o4 | 32 | ALA | 3.5 |
| 15 | D0 | 90 | TYR | 3.5 |
| 45 | N1 | 31 | LEU | 3.5 |
| 39 | m5 | 144 | ARG | 3.5 |
| 10 | c5 | 103 | ASN | 3.5 |
| 7 | C2 | 72 | ILE | 3.5 |
| 58 | O4 | 7 | PHE | 3.5 |
| 24 | D9 | 13 | ARG | 3.5 |
| 48 | N4 | 110 | LYS | 3.5 |
| 7 | C2 | 59 | LEU | 3.5 |
| 33 | l8 | 94 | PHE | 3.5 |
| 79 | sR | 34 | LEU | 3.5 |
| 20 | D5 | 101 | TYR | 3.5 |
| 42 | m8 | 174 | ARG | 3.5 |
| 72 | s4 | 25 | GLY | 3.5 |
| 25 | E0 | 48 | THR | 3.5 |
| 19 | d4 | 119 | PHE | 3.5 |
| 69 | s1 | 139 | ALA | 3.5 |
| 78 | SM | 20 | LEU | 3.5 |
| 72 | S4 | 138 | TYR | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 11 | C6 | 39 | VAL | 3.5 |
| 1 | 1 | 1581 | C | 3.5 |
| 30 | l5 | 223 | PHE | 3.5 |
| 2 | 2 | 277 | U | 3.5 |
| 71 | S3 | 39 | VAL | 3.5 |
| 7 | c2 | 117 | GLY | 3.5 |
| 72 | S4 | 139 | VAL | 3.5 |
| 75 | s7 | 90 | VAL | 3.5 |
| 22 | d7 | 73 | LEU | 3.5 |
| 32 | L7 | 88 | ARG | 3.5 |
| 51 | n7 | 11 | ALA | 3.5 |
| 12 | c7 | 2 | GLY | 3.5 |
| 35 | m0 | 56 | GLU | 3.5 |
| 71 | S3 | 138 | VAL | 3.5 |
| 74 | S6 | 97 | VAL | 3.5 |
| 7 | c2 | 32 | LEU | 3.5 |
| 62 | O8 | 29 | LYS | 3.5 |
| 69 | s1 | 136 | ARG | 3.5 |
| 30 | l5 | 70 | THR | 3.5 |
| 74 | S6 | 166 | GLU | 3.5 |
| 30 | L5 | 34 | LYS | 3.5 |
| 52 | N8 | 79 | TRP | 3.5 |
| 68 | s0 | 174 | TRP | 3.5 |
| 76 | s8 | 38 | ILE | 3.5 |
| 22 | d7 | 49 | HIS | 3.5 |
| 2 | 2 | 234 | G | 3.5 |
| 20 | D5 | 54 | VAL | 3.5 |
| 51 | N7 | 65 | ARG | 3.5 |
| 5 | c0 | 66 | TYR | 3.5 |
| 17 | D2 | 69 | LEU | 3.5 |
| 77 | S9 | 86 | LEU | 3.5 |
| 72 | s4 | 69 | HIS | 3.5 |
| 30 | L5 | 60 | ILE | 3.5 |
| 76 | S8 | 67 | TRP | 3.5 |
| 30 | l5 | 42 | ALA | 3.5 |
| 15 | D0 | 66 | SER | 3.5 |
| 30 | L5 | 69 | ILE | 3.5 |
| 66 | q2 | 70 | LEU | 3.5 |
| 74 | s6 | 156 | PHE | 3.5 |
| 7 | C2 | 111 | ASN | 3.4 |
| 51 | n7 | 42 | LEU | 3.4 |
| 2 | 2 | 1370 | U | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 9 | c4 | 14 | PHE | 3.4 |
| 32 | L7 | 134 | VAL | 3.4 |
| 71 | s3 | 136 | VAL | 3.4 |
| 76 | S8 | 156 | VAL | 3.4 |
| 28 | L3 | 47 | LEU | 3.4 |
| 46 | N2 | 105 | LEU | 3.4 |
| 30 | l5 | 34 | LYS | 3.4 |
| 42 | m8 | 186 | VAL | 3.4 |
| 44 | N0 | 136 | LYS | 3.4 |
| 77 | S9 | 85 | VAL | 3.4 |
| 79 | SR | 233 | THR | 3.4 |
| 15 | D0 | 63 | LEU | 3.4 |
| 16 | d1 | 34 | ILE | 3.4 |
| 34 | L9 | 91 | ARG | 3.4 |
| 46 | n2 | 15 | PHE | 3.4 |
| 53 | N9 | 34 | GLY | 3.4 |
| 73 | S5 | 197 | GLU | 3.4 |
| 12 | C7 | 62 | GLN | 3.4 |
| 16 | D1 | 34 | ILE | 3.4 |
| 73 | S5 | 194 | LEU | 3.4 |
| 74 | S6 | 93 | LYS | 3.4 |
| 77 | S9 | 92 | LYS | 3.4 |
| 24 | D9 | 52 | PHE | 3.4 |
| 45 | n1 | 30 | TYR | 3.4 |
| 30 | l5 | 68 | THR | 3.4 |
| 45 | N1 | 151 | LEU | 3.4 |
| 54 | O0 | 89 | VAL | 3.4 |
| 70 | s2 | 196 | VAL | 3.4 |
| 11 | c6 | 92 | TYR | 3.4 |
| 12 | c7 | 74 | GLN | 3.4 |
| 69 | S1 | 151 | LYS | 3.4 |
| 73 | S5 | 76 | ARG | 3.4 |
| 79 | SR | 236 | ALA | 3.4 |
| 79 | SR | 302 | PHE | 3.4 |
| 2 | 2 | 1707 | A | 3.4 |
| 73 | S5 | 178 | GLY | 3.4 |
| 77 | s9 | 36 | LEU | 3.4 |
| 79 | SR | 179 | LYS | 3.4 |
| 16 | D1 | 39 | VAL | 3.4 |
| 32 | L7 | 244 | ASN | 3.4 |
| 54 | O0 | 59 | TYR | 3.4 |
| 17 | D2 | 37 | PHE | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 45 | n1 | 33 | VAL | 3.4 |
| 72 | S4 | 77 | ARG | 3.4 |
| 45 | N1 | 44 | ALA | 3.4 |
| 71 | s3 | 149 | ALA | 3.4 |
| 73 | s5 | 198 | LEU | 3.4 |
| 74 | S6 | 75 | LEU | 3.4 |
| 77 | s9 | 99 | LEU | 3.4 |
| 66 | Q2 | 24 | LYS | 3.4 |
| 5 | c0 | 62 | GLN | 3.4 |
| 33 | l8 | 34 | PHE | 3.4 |
| 53 | n9 | 32 | LEU | 3.4 |
| 58 | O4 | 30 | LEU | 3.4 |
| 21 | d6 | 67 | THR | 3.4 |
| 76 | S8 | 192 | TYR | 3.4 |
| 69 | s1 | 91 | VAL | 3.4 |
| 77 | S9 | 104 | PHE | 3.4 |
| 10 | C5 | 112 | LEU | 3.4 |
| 44 | n0 | 57 | GLU | 3.4 |
| 69 | s1 | 217 | LEU | 3.4 |
| 6 | C1 | 35 | TYR | 3.4 |
| 73 | s5 | 41 | LYS | 3.4 |
| 9 | c4 | 26 | THR | 3.4 |
| 15 | D0 | 27 | THR | 3.4 |
| 27 | L2 | 72 | ARG | 3.4 |
| 35 | m0 | 55 | ASN | 3.4 |
| 60 | o6 | 68 | ARG | 3.4 |
| 62 | o8 | 2 | ALA | 3.4 |
| 68 | s0 | 75 | ALA | 3.4 |
| 75 | S7 | 105 | THR | 3.4 |
| 26 | E1 | 82 | LYS | 3.4 |
| 30 | l5 | 222 | LEU | 3.4 |
| 37 | m3 | 190 | LYS | 3.4 |
| 53 | n9 | 24 | PRO | 3.4 |
| 79 | sR | 73 | LEU | 3.4 |
| 1 | 1 | 1221 | A | 3.4 |
| 49 | n5 | 123 | TYR | 3.4 |
| 52 | N8 | 124 | ILE | 3.4 |
| 79 | SR | 253 | ALA | 3.4 |
| 69 | s1 | 138 | PHE | 3.3 |
| 74 | s6 | 162 | VAL | 3.3 |
| 46 | N2 | 93 | ILE | 3.3 |
| 69 | s1 | 113 | MET | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 46 | N2 | 15 | PHE | 3.3 |
| 72 | S4 | 99 | PHE | 3.3 |
| 66 | q2 | 83 | LEU | 3.3 |
| 9 | C4 | 112 | ILE | 3.3 |
| 30 | l5 | 62 | CYS | 3.3 |
| 20 | d5 | 91 | PRO | 3.3 |
| 15 | D0 | 93 | LEU | 3.3 |
| 63 | o9 | 23 | LEU | 3.3 |
| 2 | 2 | 716 | C | 3.3 |
| 11 | C6 | 16 | ALA | 3.3 |
| 25 | e0 | 54 | ARG | 3.3 |
| 53 | n9 | 31 | SER | 3.3 |
| 64 | Q0 | 128 | LYS | 3.3 |
| 77 | S9 | 96 | VAL | 3.3 |
| 14 | c9 | 22 | LEU | 3.3 |
| 45 | n1 | 89 | LEU | 3.3 |
| 7 | c2 | 27 | ALA | 3.3 |
| 17 | d2 | 61 | ILE | 3.3 |
| 7 | C2 | 110 | GLY | 3.3 |
| 11 | C6 | 106 | LYS | 3.3 |
| 15 | D0 | 112 | VAL | 3.3 |
| 45 | n1 | 31 | LEU | 3.3 |
| 12 | C7 | 69 | ILE | 3.3 |
| 9 | c4 | 23 | PHE | 3.3 |
| 74 | S6 | 86 | PRO | 3.3 |
| 74 | S6 | 178 | LEU | 3.3 |
| 7 | c2 | 64 | SER | 3.3 |
| 16 | D1 | 23 | ILE | 3.3 |
| 69 | S1 | 137 | ILE | 3.3 |
| 69 | S1 | 141 | ALA | 3.3 |
| 71 | S3 | 52 | ALA | 3.3 |
| 30 | L5 | 163 | LEU | 3.3 |
| 6 | C1 | 136 | ARG | 3.3 |
| 7 | C2 | 120 | VAL | 3.3 |
| 39 | M5 | 148 | TYR | 3.3 |
| 21 | D6 | 82 | ARG | 3.3 |
| 69 | S1 | 143 | THR | 3.3 |
| 59 | o5 | 120 | ALA | 3.3 |
| 9 | c4 | 92 | LYS | 3.3 |
| 45 | n1 | 35 | LYS | 3.3 |
| 49 | n5 | 66 | PRO | 3.3 |
| 20 | D5 | 71 | ILE | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 42 | m8 | 96 | PHE | 3.3 |
| 71 | s3 | 188 | ILE | 3.3 |
| 39 | M5 | 141 | ALA | 3.3 |
| 6 | C1 | 73 | GLY | 3.3 |
| 69 | s1 | 70 | LEU | 3.3 |
| 23 | d8 | 67 | ARG | 3.3 |
| 73 | S5 | 157 | ARG | 3.3 |
| 36 | M1 | 122 | ILE | 3.3 |
| 72 | S4 | 137 | PRO | 3.3 |
| 16 | d1 | 1 | MET | 3.3 |
| 70 | S2 | 119 | LYS | 3.3 |
| 73 | s5 | 83 | ARG | 3.3 |
| 53 | n9 | 37 | PRO | 3.3 |
| 69 | S1 | 104 | ASP | 3.3 |
| 11 | c6 | 112 | TYR | 3.3 |
| 74 | S6 | 83 | CYS | 3.3 |
| 28 | L3 | 369 | ARG | 3.3 |
| 48 | N4 | 64 | THR | 3.3 |
| 17 | d2 | 27 | ILE | 3.3 |
| 72 | S4 | 173 | ILE | 3.3 |
| 17 | d2 | 3 | ARG | 3.3 |
| 73 | S5 | 193 | THR | 3.3 |
| 44 | N0 | 135 | VAL | 3.3 |
| 46 | N2 | 28 | PHE | 3.3 |
| 68 | S0 | 122 | ILE | 3.3 |
| 71 | s3 | 25 | PHE | 3.3 |
| 7 | c2 | 52 | LEU | 3.3 |
| 11 | c6 | 20 | ALA | 3.3 |
| 26 | e1 | 105 | TYR | 3.3 |
| 47 | n3 | 81 | GLN | 3.3 |
| 79 | sR | 252 | LEU | 3.3 |
| 1 | 1 | 1565 | G | 3.3 |
| 69 | s1 | 152 | ARG | 3.3 |
| 11 | c6 | 22 | VAL | 3.3 |
| 39 | m5 | 61 | ILE | 3.3 |
| 42 | M8 | 101 | VAL | 3.3 |
| 76 | S8 | 102 | VAL | 3.3 |
| 79 | sR | 203 | THR | 3.3 |
| 2 | 6 | 493 | U | 3.2 |
| 48 | N4 | 71 | ARG | 3.2 |
| 58 | o4 | 33 | GLN | 3.2 |
| 66 | q2 | 82 | GLN | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 23 | D8 | 45 | LYS | 3.2 |
| 7 | c2 | 22 | VAL | 3.2 |
| 53 | n9 | 35 | VAL | 3.2 |
| 1 | 1 | 494 | G | 3.2 |
| 9 | c4 | 60 | ALA | 3.2 |
| 13 | c8 | 3 | LEU | 3.2 |
| 70 | S2 | 86 | VAL | 3.2 |
| 70 | S2 | 98 | PHE | 3.2 |
| 1 | 1 | 1569 | U | 3.2 |
| 11 | C6 | 44 | LEU | 3.2 |
| 68 | S0 | 146 | LEU | 3.2 |
| 26 | E1 | 106 | TYR | 3.2 |
| 51 | N7 | 75 | VAL | 3.2 |
| 71 | S3 | 213 | GLU | 3.2 |
| 74 | S6 | 91 | GLU | 3.2 |
| 12 | C7 | 25 | THR | 3.2 |
| 2 | 6 | 75 | U | 3.2 |
| 11 | C6 | 48 | VAL | 3.2 |
| 69 | s1 | 231 | LEU | 3.2 |
| 75 | S7 | 138 | LYS | 3.2 |
| 11 | c6 | 55 | VAL | 3.2 |
| 72 | S4 | 70 | VAL | 3.2 |
| 75 | S7 | 108 | GLN | 3.2 |
| 2 | 2 | 710 | U | 3.2 |
| 12 | C7 | 70 | SER | 3.2 |
| 72 | S4 | 13 | ALA | 3.2 |
| 16 | d1 | 82 | VAL | 3.2 |
| 30 | l5 | 297 | GLN | 3.2 |
| 73 | S5 | 37 | GLN | 3.2 |
| 23 | d8 | 66 | LEU | 3.2 |
| 76 | S8 | 165 | LEU | 3.2 |
| 11 | C6 | 60 | PHE | 3.2 |
| 45 | n1 | 44 | ALA | 3.2 |
| 11 | C6 | 133 | GLY | 3.2 |
| 8 | c3 | 16 | ILE | 3.2 |
| 20 | D5 | 51 | LEU | 3.2 |
| 22 | d7 | 22 | LYS | 3.2 |
| 25 | E0 | 53 | LYS | 3.2 |
| 28 | L3 | 50 | LYS | 3.2 |
| 2 | 2 | 730 | G | 3.2 |
| 7 | C2 | 93 | ASP | 3.2 |
| 30 | L5 | 41 | LYS | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 76 | s8 | 56 | ARG | 3.2 |
| 58 | O4 | 72 | VAL | 3.2 |
| 76 | s8 | 192 | TYR | 3.2 |
| 45 | N1 | 43 | LYS | 3.2 |
| 7 | c2 | 96 | GLN | 3.2 |
| 9 | c4 | 91 | THR | 3.2 |
| 6 | C1 | 144 | ALA | 3.2 |
| 76 | S8 | 15 | GLY | 3.2 |
| 10 | c5 | 112 | LEU | 3.2 |
| 20 | d5 | 51 | LEU | 3.2 |
| 30 | l5 | 150 | LEU | 3.2 |
| 45 | n1 | 96 | ILE | 3.2 |
| 66 | q2 | 22 | GLN | 3.2 |
| 12 | C7 | 9 | VAL | 3.2 |
| 7 | c2 | 21 | GLU | 3.2 |
| 2 | 6 | 492 | A | 3.2 |
| 78 | SM | 113 | ASP | 3.2 |
| 13 | C8 | 72 | ILE | 3.2 |
| 21 | d6 | 65 | PRO | 3.2 |
| 48 | N4 | 70 | LYS | 3.2 |
| 49 | n5 | 47 | ALA | 3.2 |
| 70 | S2 | 115 | ILE | 3.2 |
| 11 | c6 | 12 | LYS | 3.2 |
| 24 | d9 | 46 | LYS | 3.2 |
| 71 | S3 | 152 | PHE | 3.2 |
| 45 | n1 | 42 | ILE | 3.2 |
| 69 | s1 | 103 | MET | 3.2 |
| 79 | SR | 225 | LEU | 3.2 |
| 69 | S1 | 153 | HIS | 3.2 |
| 71 | S3 | 170 | THR | 3.2 |
| 32 | L7 | 87 | VAL | 3.2 |
| 53 | n9 | 33 | LYS | 3.2 |
| 53 | N9 | 44 | LYS | 3.2 |
| 79 | SR | 290 | VAL | 3.2 |
| 22 | d7 | 5 | GLN | 3.1 |
| 63 | o9 | 24 | PRO | 3.1 |
| 6 | C1 | 138 | ASN | 3.1 |
| 72 | S4 | 26 | CYS | 3.1 |
| 18 | D3 | 3 | LYS | 3.1 |
| 54 | O0 | 90 | VAL | 3.1 |
| 58 | O4 | 80 | ARG | 3.1 |
| 6 | C1 | 147 | GLY | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | 2 | 1708 | U | 3.1 |
| 77 | S9 | 93 | LEU | 3.1 |
| 79 | SR | 226 | ALA | 3.1 |
| 51 | N7 | 131 | PHE | 3.1 |
| 66 | q2 | 91 | PHE | 3.1 |
| 74 | s6 | 131 | LYS | 3.1 |
| 5 | c0 | 22 | VAL | 3.1 |
| 17 | d2 | 68 | ARG | 3.1 |
| 43 | m9 | 49 | THR | 3.1 |
| 5 | C0 | 3 | MET | 3.1 |
| 15 | D0 | 52 | LYS | 3.1 |
| 2 | 2 | 723 | G | 3.1 |
| 28 | L3 | 321 | PHE | 3.1 |
| 25 | e0 | 61 | SER | 3.1 |
| 7 | C2 | 107 | ASP | 3.1 |
| 13 | C8 | 146 | ALA | 3.1 |
| 16 | D1 | 54 | ALA | 3.1 |
| 20 | d5 | 41 | ILE | 3.1 |
| 30 | l5 | 60 | ILE | 3.1 |
| 71 | S3 | 171 | ALA | 3.1 |
| 73 | S5 | 121 | ILE | 3.1 |
| 76 | s8 | 44 | HIS | 3.1 |
| 76 | S8 | 200 | LYS | 3.1 |
| 69 | S1 | 100 | PHE | 3.1 |
| 79 | SR | 251 | TRP | 3.1 |
| 7 | C2 | 52 | LEU | 3.1 |
| 76 | S8 | 166 | TYR | 3.1 |
| 79 | SR | 34 | LEU | 3.1 |
| 2 | 2 | 722 | G | 3.1 |
| 7 | c2 | 66 | VAL | 3.1 |
| 71 | S3 | 25 | PHE | 3.1 |
| 79 | sR | 251 | TRP | 3.1 |
| 17 | D2 | 85 | ASP | 3.1 |
| 74 | s6 | 93 | LYS | 3.1 |
| 17 | D2 | 128 | PHE | 3.1 |
| 8 | c3 | 151 | ASN | 3.1 |
| 11 | C6 | 123 | ARG | 3.1 |
| 45 | N1 | 24 | ALA | 3.1 |
| 73 | s5 | 130 | ILE | 3.1 |
| 33 | L8 | 165 | PHE | 3.1 |
| 45 | n1 | 74 | VAL | 3.1 |
| 73 | S5 | 148 | ARG | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 9 | c4 | 126 | THR | 3.1 |
| 11 | C6 | 77 | GLN | 3.1 |
| 59 | o5 | 83 | LYS | 3.1 |
| 7 | C2 | 65 | SER | 3.1 |
| 79 | sR | 315 | VAL | 3.1 |
| 66 | q2 | 24 | LYS | 3.1 |
| 9 | c4 | 132 | ARG | 3.1 |
| 76 | s8 | 195 | ARG | 3.1 |
| 75 | s7 | 48 | GLU | 3.1 |
| 22 | d7 | 7 | LEU | 3.1 |
| 24 | D9 | 46 | LYS | 3.1 |
| 76 | S8 | 199 | LYS | 3.1 |
| 1 | 5 | 1570 | U | 3.1 |
| 10 | c5 | 85 | ILE | 3.1 |
| 7 | c2 | 67 | THR | 3.1 |
| 19 | D4 | 27 | VAL | 3.1 |
| 51 | N7 | 53 | VAL | 3.1 |
| 58 | O4 | 32 | ALA | 3.1 |
| 69 | S1 | 139 | ALA | 3.1 |
| 72 | S4 | 208 | VAL | 3.1 |
| 9 | c4 | 47 | LYS | 3.1 |
| 6 | C1 | 126 | GLY | 3.1 |
| 7 | C2 | 31 | VAL | 3.1 |
| 7 | c2 | 94 | ALA | 3.1 |
| 55 | O1 | 12 | TYR | 3.1 |
| 55 | O1 | 73 | LEU | 3.1 |
| 20 | D5 | 88 | ILE | 3.1 |
| 45 | n1 | 84 | TYR | 3.1 |
| 70 | S2 | 215 | PHE | 3.1 |
| 38 | M4 | 138 | ALA | 3.1 |
| 73 | S5 | 62 | VAL | 3.1 |
| 73 | S5 | 77 | TYR | 3.1 |
| 69 | s1 | 137 | ILE | 3.1 |
| 32 | L7 | 86 | VAL | 3.0 |
| 5 | C0 | 52 | LYS | 3.0 |
| 39 | m5 | 2 | GLY | 3.0 |
| 22 | d7 | 33 | LEU | 3.0 |
| 71 | S3 | 150 | MET | 3.0 |
| 77 | S9 | 20 | GLU | 3.0 |
| 48 | N4 | 12 | LYS | 3.0 |
| 71 | s3 | 135 | GLU | 3.0 |
| 79 | sR | 202 | LEU | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 69 | s1 | 46 | THR | 3.0 |
| 71 | S3 | 221 | SER | 3.0 |
| 33 | l8 | 130 | TYR | 3.0 |
| 52 | N8 | 55 | LYS | 3.0 |
| 5 | C0 | 40 | LEU | 3.0 |
| 30 | L5 | 55 | PHE | 3.0 |
| 45 | n1 | 72 | VAL | 3.0 |
| 70 | S2 | 178 | ILE | 3.0 |
| 6 | C1 | 148 | LYS | 3.0 |
| 39 | M5 | 128 | LYS | 3.0 |
| 62 | O8 | 44 | LYS | 3.0 |
| 15 | D0 | 18 | GLN | 3.0 |
| 30 | l5 | 142 | PHE | 3.0 |
| 79 | sR | 158 | PRO | 3.0 |
| 5 | C0 | 24 | LYS | 3.0 |
| 7 | c2 | 120 | VAL | 3.0 |
| 74 | S6 | 71 | THR | 3.0 |
| 76 | S8 | 117 | TYR | 3.0 |
| 78 | SM | 85 | SER | 3.0 |
| 11 | C6 | 68 | ARG | 3.0 |
| 77 | S9 | 164 | PHE | 3.0 |
| 11 | C6 | 17 | THR | 3.0 |
| 49 | n5 | 126 | LEU | 3.0 |
| 69 | s1 | 135 | LEU | 3.0 |
| 45 | n1 | 82 | ASN | 3.0 |
| 39 | m5 | 131 | GLU | 3.0 |
| 19 | D4 | 117 | LYS | 3.0 |
| 43 | M9 | 188 | ASP | 3.0 |
| 79 | SR | 266 | ASP | 3.0 |
| 30 | l5 | 92 | LEU | 3.0 |
| 51 | N7 | 134 | LEU | 3.0 |
| 10 | c5 | 127 | ARG | 3.0 |
| 30 | l5 | 109 | THR | 3.0 |
| 76 | s8 | 97 | THR | 3.0 |
| 15 | D0 | 22 | ILE | 3.0 |
| 77 | S9 | 101 | VAL | 3.0 |
| 11 | c6 | 89 | LEU | 3.0 |
| 68 | S0 | 23 | HIS | 3.0 |
| 68 | s0 | 110 | TYR | 3.0 |
| 76 | s8 | 96 | LEU | 3.0 |
| 11 | C6 | 70 | THR | 3.0 |
| 12 | c7 | 71 | PHE | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 73 | s5 | 156 | ARG | 3.0 |
| 14 | C9 | 71 | VAL | 3.0 |
| 70 | s2 | 184 | VAL | 3.0 |
| 72 | s4 | 45 | ILE | 3.0 |
| 19 | d4 | 122 | GLY | 3.0 |
| 49 | n5 | 32 | PHE | 3.0 |
| 66 | Q2 | 15 | LYS | 3.0 |
| 69 | S1 | 103 | MET | 3.0 |
| 12 | C7 | 26 | LEU | 3.0 |
| 45 | N1 | 30 | TYR | 3.0 |
| 18 | D3 | 2 | GLY | 3.0 |
| 50 | n6 | 77 | LYS | 3.0 |
| 5 | c0 | 20 | VAL | 3.0 |
| 17 | D2 | 129 | VAL | 3.0 |
| 44 | N0 | 93 | GLU | 3.0 |
| 74 | s6 | 18 | ILE | 3.0 |
| 74 | S6 | 82 | SER | 3.0 |
| 30 | l5 | 171 | LEU | 3.0 |
| 32 | L7 | 112 | ASN | 3.0 |
| 52 | N8 | 110 | GLY | 3.0 |
| 66 | q2 | 51 | GLY | 3.0 |
| 76 | S8 | 22 | ARG | 3.0 |
| 10 | C5 | 85 | ILE | 3.0 |
| 11 | c6 | 21 | HIS | 3.0 |
| 34 | l9 | 99 | ILE | 3.0 |
| 45 | n1 | 80 | VAL | 3.0 |
| 7 | c2 | 88 | LEU | 3.0 |
| 30 | l5 | 143 | LYS | 3.0 |
| 39 | m5 | 62 | TYR | 3.0 |
| 53 | N9 | 41 | ARG | 3.0 |
| 7 | C2 | 123 | VAL | 3.0 |
| 51 | N7 | 23 | VAL | 3.0 |
| 39 | m5 | 57 | GLN | 3.0 |
| 39 | m5 | 63 | ARG | 3.0 |
| 49 | n5 | 141 | TYR | 3.0 |
| 68 | S0 | 174 | TRP | 3.0 |
| 69 | S1 | 213 | ARG | 3.0 |
| 46 | N2 | 27 | VAL | 3.0 |
| 79 | SR | 136 | ILE | 3.0 |
| 13 | c8 | 12 | GLN | 3.0 |
| 51 | N7 | 22 | LYS | 3.0 |
| 51 | N7 | 4 | PHE | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 52 | n8 | 53 | PHE | 3.0 |
| 33 | L8 | 99 | PRO | 3.0 |
| 42 | M8 | 99 | THR | 3.0 |
| 69 | s1 | 114 | VAL | 3.0 |
| 11 | c6 | 85 | ILE | 3.0 |
| 7 | C2 | 88 | LEU | 3.0 |
| 11 | c6 | 117 | LEU | 3.0 |
| 36 | m1 | 60 | ARG | 3.0 |
| 43 | M9 | 173 | ARG | 3.0 |
| 71 | S3 | 151 | LYS | 3.0 |
| 71 | S3 | 149 | ALA | 2.9 |
| 71 | S3 | 220 | PRO | 2.9 |
| 79 | SR | 177 | MET | 2.9 |
| 72 | s4 | 26 | CYS | 2.9 |
| 28 | L3 | 46 | PHE | 2.9 |
| 11 | C6 | 134 | ALA | 2.9 |
| 21 | d6 | 72 | HIS | 2.9 |
| 30 | L5 | 77 | ALA | 2.9 |
| 42 | M8 | 84 | VAL | 2.9 |
| 17 | d2 | 125 | ILE | 2.9 |
| 15 | D0 | 109 | GLU | 2.9 |
| 48 | N4 | 98 | PRO | 2.9 |
| 74 | S6 | 78 | THR | 2.9 |
| 69 | s1 | 43 | VAL | 2.9 |
| 73 | s5 | 68 | ILE | 2.9 |
| 76 | S8 | 152 | ILE | 2.9 |
| 2 | 2 | 676 | G | 2.9 |
| 6 | c1 | 5 | LEU | 2.9 |
| 30 | l5 | 128 | GLU | 2.9 |
| 38 | M4 | 37 | GLU | 2.9 |
| 45 | n1 | 91 | LEU | 2.9 |
| 49 | N5 | 40 | LEU | 2.9 |
| 74 | S6 | 76 | LEU | 2.9 |
| 74 | s6 | 149 | LYS | 2.9 |
| 73 | S5 | 69 | PHE | 2.9 |
| 11 | C6 | 36 | ILE | 2.9 |
| 45 | N1 | 95 | HIS | 2.9 |
| 66 | Q2 | 27 | GLN | 2.9 |
| 69 | s1 | 124 | ASN | 2.9 |
| 21 | d6 | 19 | LYS | 2.9 |
| 60 | O6 | 50 | LEU | 2.9 |
| 77 | S9 | 5 | PRO | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 79 | sR | 210 | LEU | 2.9 |
| 30 | L5 | 53 | VAL | 2.9 |
| 79 | sR | 6 | VAL | 2.9 |
| 21 | d6 | 36 | ILE | 2.9 |
| 76 | S8 | 183 | ILE | 2.9 |
| 33 | L8 | 150 | LEU | 2.9 |
| 30 | L5 | 180 | PHE | 2.9 |
| 33 | l8 | 42 | PRO | 2.9 |
| 39 | M5 | 145 | ASP | 2.9 |
| 70 | s2 | 95 | ARG | 2.9 |
| 72 | s4 | 56 | LEU | 2.9 |
| 77 | S9 | 97 | LEU | 2.9 |
| 48 | N4 | 75 | THR | 2.9 |
| 62 | o8 | 6 | THR | 2.9 |
| 71 | S3 | 186 | VAL | 2.9 |
| 73 | s5 | 133 | VAL | 2.9 |
| 79 | SR | 262 | VAL | 2.9 |
| 11 | C6 | 143 | ARG | 2.9 |
| 17 | D2 | 51 | GLU | 2.9 |
| 69 | S1 | 228 | LEU | 2.9 |
| 5 | c0 | 26 | ASP | 2.9 |
| 79 | sR | 302 | PHE | 2.9 |
| 11 | C6 | 41 | PRO | 2.9 |
| 6 | C1 | 38 | ALA | 2.9 |
| 71 | S3 | 88 | ALA | 2.9 |
| 51 | N7 | 5 | LEU | 2.9 |
| 59 | o5 | 86 | ARG | 2.9 |
| 74 | s6 | 91 | GLU | 2.9 |
| 21 | D6 | 73 | TYR | 2.9 |
| 45 | N1 | 42 | ILE | 2.9 |
| 14 | c9 | 54 | PHE | 2.9 |
| 2 | 6 | 742 | U | 2.9 |
| 11 | c6 | 79 | TYR | 2.9 |
| 46 | N2 | 106 | ALA | 2.9 |
| 68 | s0 | 98 | ILE | 2.9 |
| 69 | S1 | 96 | LEU | 2.9 |
| 79 | SR | 194 | GLY | 2.9 |
| 15 | D0 | 104 | THR | 2.9 |
| 21 | d6 | 39 | MET | 2.9 |
| 76 | s8 | 95 | THR | 2.9 |
| 30 | l5 | 144 | VAL | 2.9 |
| 16 | d1 | 53 | TYR | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 66 | q2 | 9 | LYS | 2.9 |
| 22 | d7 | 24 | LEU | 2.9 |
| 26 | e1 | 139 | LEU | 2.9 |
| 41 | m7 | 81 | ALA | 2.9 |
| 69 | s1 | 82 | ARG | 2.9 |
| 39 | m5 | 132 | VAL | 2.9 |
| 45 | N1 | 126 | VAL | 2.9 |
| 77 | s9 | 96 | VAL | 2.9 |
| 30 | l5 | 226 | TYR | 2.9 |
| 37 | M3 | 21 | ARG | 2.9 |
| 49 | n5 | 142 | ILE | 2.9 |
| 78 | sM | 62 | ARG | 2.9 |
| 11 | c6 | 116 | LEU | 2.9 |
| 33 | L8 | 197 | VAL | 2.9 |
| 46 | n2 | 70 | LYS | 2.9 |
| 48 | n4 | 100 | VAL | 2.9 |
| 74 | s6 | 79 | LYS | 2.9 |
| 1 | 1 | 2538 | U | 2.9 |
| 13 | c8 | 125 | ILE | 2.9 |
| 19 | d4 | 7 | ILE | 2.9 |
| 26 | E1 | 91 | ILE | 2.9 |
| 42 | M8 | 76 | ALA | 2.9 |
| 42 | M8 | 124 | LEU | 2.9 |
| 19 | d4 | 123 | LYS | 2.9 |
| 46 | n2 | 13 | LYS | 2.9 |
| 53 | N9 | 42 | ASN | 2.9 |
| 79 | sR | 294 | TRP | 2.9 |
| 5 | C0 | 65 | TYR | 2.9 |
| 42 | m8 | 170 | ARG | 2.9 |
| 53 | N9 | 47 | LEU | 2.9 |
| 77 | S9 | 119 | ALA | 2.9 |
| 79 | SR | 220 | ILE | 2.9 |
| 24 | D9 | 33 | LYS | 2.9 |
| 58 | O4 | 5 | VAL | 2.9 |
| 5 | C0 | 35 | ILE | 2.9 |
| 11 | C6 | 81 | ILE | 2.9 |
| 74 | s6 | 109 | LEU | 2.9 |
| 45 | N1 | 32 | LYS | 2.9 |
| 52 | n8 | 56 | VAL | 2.9 |
| 2 | 2 | 720 | G | 2.9 |
| 14 | C9 | 28 | LEU | 2.9 |
| 16 | d1 | 8 | LEU | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 44 | N0 | 29 | ILE | 2.9 |
| 78 | SM | 16 | ASP | 2.9 |
| 11 | c6 | 7 | VAL | 2.8 |
| 39 | m5 | 43 | THR | 2.8 |
| 69 | S1 | 233 | GLY | 2.8 |
| 72 | S4 | 14 | ALA | 2.9 |
| 72 | S4 | 22 | LYS | 2.8 |
| 41 | M7 | 161 | ALA | 2.8 |
| 78 | SM | 15 | ALA | 2.8 |
| 48 | n4 | 81 | PRO | 2.8 |
| 69 | S1 | 82 | ARG | 2.8 |
| 2 | 2 | 136 | C | 2.8 |
| 2 | 2 | 1695 | G | 2.8 |
| 15 | D0 | 86 | ILE | 2.8 |
| 69 | S1 | 207 | LEU | 2.8 |
| 42 | m8 | 87 | VAL | 2.8 |
| 73 | s5 | 134 | VAL | 2.8 |
| 18 | d3 | 141 | GLU | 2.8 |
| 45 | n1 | 83 | ARG | 2.8 |
| 12 | c7 | 53 | TYR | 2.8 |
| 30 | l5 | 51 | LEU | 2.8 |
| 53 | n9 | 23 | LYS | 2.8 |
| 77 | S9 | 10 | LYS | 2.8 |
| 20 | D5 | 60 | VAL | 2.8 |
| 50 | N6 | 79 | ALA | 2.8 |
| 52 | n8 | 64 | GLN | 2.8 |
| 70 | S2 | 112 | GLY | 2.8 |
| 1 | 1 | 1563 | C | 2.8 |
| 2 | 2 | 731 | C | 2.8 |
| 42 | M8 | 92 | ARG | 2.8 |
| 20 | d5 | 50 | ILE | 2.8 |
| 68 | s0 | 122 | ILE | 2.8 |
| 76 | S8 | 143 | TRP | 2.8 |
| 30 | L5 | 49 | TYR | 2.8 |
| 31 | l6 | 2 | SER | 2.8 |
| 42 | M8 | 85 | GLY | 2.8 |
| 42 | M8 | 102 | ALA | 2.8 |
| 71 | S3 | 9 | ARG | 2.8 |
| 34 | L9 | 189 | GLU | 2.8 |
| 28 | L3 | 359 | ILE | 2.8 |
| 73 | s5 | 42 | LEU | 2.8 |
| 75 | S7 | 154 | LEU | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 76 | s8 | 83 | TYR | 2.8 |
| 7 | c2 | 116 | VAL | 2.8 |
| 15 | D0 | 116 | VAL | 2.8 |
| 37 | m3 | 2 | ALA | 2.8 |
| 68 | S0 | 73 | VAL | 2.8 |
| 71 | S3 | 51 | ARG | 2.8 |
| 5 | c0 | 24 | LYS | 2.8 |
| 72 | S4 | 101 | LEU | 2.8 |
| 75 | S7 | 153 | LEU | 2.8 |
| 7 | c2 | 23 | THR | 2.8 |
| 47 | N3 | 137 | VAL | 2.8 |
| 52 | n8 | 48 | TYR | 2.8 |
| 66 | Q2 | 25 | VAL | 2.8 |
| 13 | C8 | 123 | ARG | 2.8 |
| 10 | c5 | 56 | PHE | 2.8 |
| 17 | D2 | 27 | ILE | 2.8 |
| 28 | l3 | 140 | ASP | 2.8 |
| 30 | l5 | 64 | ILE | 2.8 |
| 30 | L5 | 61 | ILE | 2.8 |
| 42 | m8 | 153 | PHE | 2.8 |
| 42 | M8 | 96 | PHE | 2.8 |
| 51 | n7 | 134 | LEU | 2.8 |
| 75 | S7 | 60 | ILE | 2.8 |
| 5 | c0 | 37 | THR | 2.8 |
| 5 | C0 | 12 | HIS | 2.8 |
| 30 | L5 | 131 | LEU | 2.8 |
| 36 | m1 | 64 | LYS | 2.8 |
| 7 | C2 | 136 | ILE | 2.8 |
| 43 | M9 | 187 | GLU | 2.8 |
| 48 | N4 | 106 | GLU | 2.8 |
| 53 | n9 | 36 | ASP | 2.8 |
| 62 | o8 | 3 | ARG | 2.8 |
| 69 | S1 | 123 | ALA | 2.8 |
| 70 | S2 | 93 | GLY | 2.8 |
| 49 | n5 | 49 | LYS | 2.8 |
| 53 | n9 | 25 | LYS | 2.8 |
| 62 | O8 | 26 | LYS | 2.8 |
| 69 | s1 | 98 | THR | 2.8 |
| 6 | C1 | 42 | PHE | 2.8 |
| 31 | L6 | 109 | GLU | 2.8 |
| 39 | M5 | 142 | ILE | 2.8 |
| 77 | S9 | 99 | LEU | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 45 | N1 | 149 | GLN | 2.8 |
| 45 | n1 | 28 | SER | 2.8 |
| 76 | S8 | 83 | TYR | 2.8 |
| 78 | SM | 17 | VAL | 2.8 |
| 19 | d4 | 128 | LYS | 2.8 |
| 66 | Q2 | 36 | PHE | 2.8 |
| 71 | s3 | 21 | LEU | 2.8 |
| 13 | c8 | 21 | ASN | 2.8 |
| 72 | S4 | 219 | VAL | 2.8 |
| 11 | c6 | 56 | GLY | 2.8 |
| 33 | L8 | 196 | ALA | 2.8 |
| 41 | m7 | 161 | ALA | 2.8 |
| 78 | sM | 83 | LYS | 2.8 |
| 50 | n6 | 48 | LEU | 2.8 |
| 55 | o1 | 71 | LEU | 2.8 |
| 20 | D5 | 100 | ILE | 2.8 |
| 30 | l5 | 126 | GLU | 2.8 |
| 74 | S6 | 162 | VAL | 2.8 |
| 78 | SM | 69 | ARG | 2.8 |
| 70 | S2 | 186 | LYS | 2.8 |
| 43 | M9 | 169 | ALA | 2.8 |
| 69 | s1 | 102 | GLY | 2.8 |
| 72 | s4 | 207 | LEU | 2.8 |
| 44 | N0 | 96 | ASP | 2.8 |
| 71 | S3 | 136 | VAL | 2.8 |
| 71 | s3 | 186 | VAL | 2.8 |
| 8 | c3 | 61 | THR | 2.8 |
| 7 | C2 | 104 | GLY | 2.8 |
| 33 | L8 | 169 | LEU | 2.8 |
| 45 | N1 | 125 | ALA | 2.8 |
| 24 | d9 | 56 | ARG | 2.8 |
| 44 | N0 | 121 | ILE | 2.8 |
| 55 | O1 | 75 | ILE | 2.8 |
| 77 | S9 | 148 | VAL | 2.8 |
| 8 | C3 | 141 | TYR | 2.8 |
| 17 | d2 | 37 | PHE | 2.8 |
| 20 | D5 | 62 | VAL | 2.7 |
| 39 | M5 | 135 | VAL | 2.7 |
| 45 | N1 | 25 | VAL | 2.7 |
| 6 | C1 | 127 | GLN | 2.7 |
| 39 | M5 | 57 | GLN | 2.7 |
| 79 | SR | 79 | TYR | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 69 | S1 | 46 | THR | 2.7 |
| 75 | S7 | 59 | ALA | 2.7 |
| 75 | S7 | 126 | LEU | 2.7 |
| 23 | d8 | 45 | LYS | 2.7 |
| 43 | M9 | 181 | ARG | 2.7 |
| 77 | s9 | 141 | VAL | 2.7 |
| 76 | s8 | 188 | GLU | 2.7 |
| 11 | C6 | 79 | TYR | 2.7 |
| 7 | c2 | 78 | LEU | 2.7 |
| 9 | c4 | 99 | GLN | 2.7 |
| 12 | C7 | 16 | LEU | 2.7 |
| 42 | M8 | 2 | GLY | 2.7 |
| 49 | n5 | 50 | ALA | 2.7 |
| 73 | S5 | 93 | LEU | 2.7 |
| 13 | c8 | 126 | ARG | 2.7 |
| 14 | c9 | 92 | LYS | 2.7 |
| 15 | D0 | 61 | LYS | 2.7 |
| 48 | n4 | 69 | LYS | 2.7 |
| 68 | S0 | 119 | ARG | 2.7 |
| 53 | N9 | 31 | SER | 2.7 |
| 69 | s1 | 210 | ILE | 2.7 |
| 11 | c6 | 49 | TYR | 2.7 |
| 77 | S9 | 12 | TYR | 2.7 |
| 30 | l5 | 113 | LEU | 2.7 |
| 76 | s8 | 67 | TRP | 2.7 |
| 77 | s9 | 93 | LEU | 2.7 |
| 2 | 2 | 717 | C | 2.7 |
| 19 | D4 | 118 | ILE | 2.7 |
| 30 | l5 | 65 | ILE | 2.7 |
| 45 | N1 | 93 | VAL | 2.7 |
| 73 | S5 | 162 | VAL | 2.7 |
| 13 | C8 | 25 | ASN | 2.7 |
| 33 | L8 | 202 | GLU | 2.7 |
| 6 | C1 | 60 | PHE | 2.7 |
| 5 | C0 | 19 | GLY | 2.7 |
| 50 | n6 | 79 | ALA | 2.7 |
| 15 | D0 | 83 | GLU | 2.7 |
| 42 | m8 | 168 | THR | 2.7 |
| 68 | s0 | 97 | PRO | 2.7 |
| 69 | s1 | 228 | LEU | 2.7 |
| 28 | L3 | 48 | GLY | 2.7 |
| 34 | L9 | 134 | ILE | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 68 | s0 | 54 | TRP | 2.7 |
| 8 | c3 | 141 | TYR | 2.7 |
| 27 | l2 | 76 | PHE | 2.7 |
| 71 | s3 | 24 | PHE | 2.7 |
| 76 | S8 | 182 | TYR | 2.7 |
| 48 | N4 | 109 | LEU | 2.7 |
| 6 | C1 | 33 | ARG | 2.7 |
| 6 | c1 | 2 | SER | 2.7 |
| 8 | C3 | 42 | ARG | 2.7 |
| 19 | d4 | 127 | LYS | 2.7 |
| 49 | n5 | 28 | THR | 2.7 |
| 53 | N9 | 40 | ARG | 2.7 |
| 61 | o7 | 65 | ARG | 2.7 |
| 9 | c4 | 28 | VAL | 2.7 |
| 22 | d7 | 2 | VAL | 2.7 |
| 30 | l5 | 175 | HIS | 2.7 |
| 38 | m4 | 44 | VAL | 2.7 |
| 39 | m5 | 133 | ILE | 2.7 |
| 69 | s1 | 123 | ALA | 2.7 |
| 15 | D0 | 15 | GLN | 2.7 |
| 63 | o9 | 36 | ARG | 2.7 |
| 7 | c2 | 60 | VAL | 2.7 |
| 34 | l9 | 93 | VAL | 2.7 |
| 51 | n7 | 96 | VAL | 2.7 |
| 68 | s0 | 144 | ILE | 2.7 |
| 11 | C6 | 13 | LYS | 2.7 |
| 71 | S3 | 17 | PHE | 2.7 |
| 77 | S9 | 34 | PHE | 2.7 |
| 18 | D3 | 42 | PRO | 2.7 |
| 73 | S5 | 130 | ILE | 2.7 |
| 11 | c6 | 60 | PHE | 2.7 |
| 19 | d4 | 85 | PHE | 2.7 |
| 20 | D5 | 58 | ARG | 2.7 |
| 30 | L5 | 146 | LEU | 2.7 |
| 45 | N1 | 35 | LYS | 2.7 |
| 45 | N1 | 50 | LYS | 2.7 |
| 58 | O4 | 37 | LYS | 2.7 |
| 58 | O4 | 58 | ARG | 2.7 |
| 69 | S1 | 83 | LYS | 2.7 |
| 69 | s1 | 151 | LYS | 2.7 |
| 76 | S8 | 109 | PHE | 2.7 |
| 79 | SR | 145 | LEU | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 74 | s6 | 81 | VAL | 2.7 |
| 10 | c5 | 84 | ILE | 2.7 |
| 44 | N0 | 76 | GLY | 2.7 |
| 1 | 5 | 3155 | U | 2.7 |
| 6 | C1 | 26 | LYS | 2.7 |
| 10 | C5 | 110 | GLU | 2.7 |
| 62 | o8 | 11 | PHE | 2.7 |
| 70 | s2 | 225 | LEU | 2.7 |
| 72 | s4 | 47 | PHE | 2.7 |
| 58 | O4 | 16 | ARG | 2.7 |
| 58 | O4 | 74 | ARG | 2.7 |
| 12 | C7 | 24 | LEU | 2.7 |
| 16 | D1 | 55 | LEU | 2.7 |
| 17 | d2 | 26 | LEU | 2.7 |
| 27 | l2 | 111 | THR | 2.7 |
| 59 | o5 | 84 | LYS | 2.7 |
| 66 | q2 | 80 | ARG | 2.7 |
| 71 | S3 | 69 | LEU | 2.7 |
| 61 | o7 | 66 | TYR | 2.7 |
| 72 | S4 | 27 | TYR | 2.7 |
| 32 | l7 | 231 | ASN | 2.7 |
| 10 | c5 | 133 | ALA | 2.7 |
| 71 | s3 | 171 | ALA | 2.7 |
| 30 | l5 | 115 | LEU | 2.7 |
| 59 | O5 | 78 | LYS | 2.7 |
| 77 | S9 | 76 | LEU | 2.7 |
| 15 | d0 | 88 | LYS | 2.7 |
| 17 | D2 | 99 | PHE | 2.7 |
| 62 | O8 | 30 | LYS | 2.7 |
| 78 | SM | 84 | LYS | 2.7 |
| 37 | m3 | 186 | ARG | 2.7 |
| 30 | l5 | 53 | VAL | 2.7 |
| 61 | o7 | 84 | SER | 2.7 |
| 12 | C7 | 8 | THR | 2.7 |
| 23 | D8 | 19 | THR | 2.7 |
| 71 | s3 | 120 | TYR | 2.7 |
| 54 | o0 | 100 | ILE | 2.7 |
| 2 | 2 | 714 | G | 2.7 |
| 6 | C1 | 69 | LYS | 2.7 |
| 11 | C6 | 57 | LEU | 2.6 |
| 13 | C8 | 128 | PHE | 2.7 |
| 51 | N7 | 21 | LYS | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 68 | s0 | 146 | LEU | 2.6 |
| 30 | l5 | 52 | VAL | 2.6 |
| 66 | Q2 | 73 | GLU | 2.6 |
| 2 | 6 | 232 | U | 2.6 |
| 8 | C3 | 45 | LEU | 2.6 |
| 17 | d2 | 128 | PHE | 2.6 |
| 25 | E0 | 44 | PHE | 2.6 |
| 35 | M0 | 219 | ALA | 2.6 |
| 41 | M7 | 160 | ALA | 2.6 |
| 46 | n2 | 14 | THR | 2.6 |
| 51 | n7 | 131 | PHE | 2.6 |
| 76 | S8 | 63 | GLY | 2.6 |
| 24 | d9 | 4 | GLU | 2.6 |
| 68 | s0 | 181 | VAL | 2.6 |
| 73 | S5 | 142 | PRO | 2.6 |
| 5 | c0 | 44 | LYS | 2.6 |
| 6 | c1 | 38 | ALA | 2.6 |
| 11 | c6 | 11 | GLY | 2.6 |
| 69 | S1 | 121 | ILE | 2.6 |
| 71 | S3 | 187 | LYS | 2.6 |
| 49 | n5 | 82 | LEU | 2.6 |
| 72 | S4 | 220 | THR | 2.6 |
| 45 | N1 | 94 | GLU | 2.6 |
| 53 | N9 | 24 | PRO | 2.6 |
| 75 | S7 | 95 | GLU | 2.6 |
| 20 | d5 | 46 | LYS | 2.6 |
| 77 | S9 | 156 | ILE | 2.6 |
| 15 | D0 | 23 | ARG | 2.6 |
| 25 | E0 | 54 | ARG | 2.6 |
| 44 | N0 | 4 | PHE | 2.6 |
| 76 | s8 | 113 | PHE | 2.6 |
| 79 | sR | 246 | SER | 2.6 |
| 36 | M1 | 109 | HIS | 2.6 |
| 69 | s1 | 119 | THR | 2.6 |
| 74 | s6 | 76 | LEU | 2.6 |
| 6 | C1 | 37 | ASN | 2.6 |
| 27 | l2 | 75 | ILE | 2.6 |
| 28 | L3 | 49 | TYR | 2.6 |
| 60 | o6 | 9 | ILE | 2.6 |
| 74 | S6 | 84 | TYR | 2.6 |
| 12 | C7 | 2 | GLY | 2.6 |
| 21 | d6 | 29 | SER | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 24 | d9 | 12 | ARG | 2.6 |
| 48 | n4 | 95 | SER | 2.6 |
| 42 | M8 | 100 | THR | 2.6 |
| 59 | o5 | 85 | THR | 2.6 |
| 1 | 5 | 1582 | C | 2.6 |
| 10 | c5 | 111 | MET | 2.6 |
| 8 | C3 | 78 | ASN | 2.6 |
| 9 | c4 | 27 | PHE | 2.6 |
| 21 | d6 | 85 | ARG | 2.6 |
| 60 | O6 | 78 | GLY | 2.6 |
| 62 | O8 | 28 | ASN | 2.6 |
| 72 | S4 | 200 | ARG | 2.6 |
| 70 | s2 | 154 | LEU | 2.6 |
| 5 | C0 | 56 | LYS | 2.6 |
| 6 | C1 | 105 | LYS | 2.6 |
| 7 | C2 | 126 | TRP | 2.6 |
| 34 | L9 | 86 | TYR | 2.6 |
| 53 | n9 | 27 | TYR | 2.6 |
| 45 | n1 | 88 | ARG | 2.6 |
| 68 | s0 | 76 | ILE | 2.6 |
| 24 | D9 | 23 | VAL | 2.6 |
| 36 | m1 | 62 | ASN | 2.6 |
| 58 | O4 | 18 | ASN | 2.6 |
| 58 | O4 | 39 | ALA | 2.6 |
| 66 | q2 | 27 | GLN | 2.6 |
| 45 | n1 | 97 | LYS | 2.6 |
| 46 | n2 | 67 | SER | 2.6 |
| 79 | SR | 157 | VAL | 2.6 |
| 79 | SR | 261 | LYS | 2.6 |
| 30 | L5 | 126 | GLU | 2.6 |
| 6 | c1 | 11 | ARG | 2.6 |
| 69 | S1 | 47 | LEU | 2.6 |
| 21 | d6 | 37 | LYS | 2.6 |
| 53 | n9 | 22 | LYS | 2.6 |
| 62 | O8 | 45 | VAL | 2.6 |
| 1 | 5 | 1573 | G | 2.6 |
| 1 | 5 | 1953 | G | 2.6 |
| 32 | L7 | 89 | ILE | 2.6 |
| 59 | o5 | 89 | ARG | 2.6 |
| 73 | S5 | 209 | TYR | 2.6 |
| 42 | M8 | 138 | LEU | 2.6 |
| 76 | s8 | 165 | LEU | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 6 | c1 | 29 | LYS | 2.6 |
| 12 | C7 | 63 | LYS | 2.6 |
| 14 | C9 | 92 | LYS | 2.6 |
| 43 | m9 | 177 | VAL | 2.6 |
| 62 | o8 | 30 | LYS | 2.6 |
| 79 | sR | 156 | VAL | 2.6 |
| 43 | m9 | 7 | GLN | 2.6 |
| 15 | d0 | 91 | ILE | 2.6 |
| 45 | N1 | 96 | ILE | 2.6 |
| 51 | n7 | 92 | PHE | 2.6 |
| 7 | C2 | 58 | LEU | 2.6 |
| 22 | D7 | 33 | LEU | 2.6 |
| 36 | M1 | 172 | LEU | 2.6 |
| 52 | N8 | 78 | LEU | 2.6 |
| 45 | n1 | 93 | VAL | 2.6 |
| 53 | n9 | 34 | GLY | 2.6 |
| 69 | s1 | 160 | HIS | 2.6 |
| 11 | C6 | 47 | LYS | 2.6 |
| 42 | M8 | 81 | VAL | 2.6 |
| 66 | q2 | 13 | LYS | 2.6 |
| 79 | SR | 130 | THR | 2.6 |
| 2 | 6 | 655 | G | 2.6 |
| 11 | C6 | 52 | LEU | 2.6 |
| 25 | E0 | 46 | ASN | 2.6 |
| 63 | o9 | 7 | PHE | 2.6 |
| 9 | C4 | 15 | GLY | 2.6 |
| 69 | S1 | 212 | VAL | 2.6 |
| 74 | s6 | 90 | GLY | 2.6 |
| 18 | D3 | 117 | ILE | 2.6 |
| 17 | D2 | 41 | MET | 2.6 |
| 33 | l8 | 52 | TRP | 2.6 |
| 75 | s7 | 154 | LEU | 2.6 |
| 30 | l5 | 125 | VAL | 2.6 |
| 45 | n1 | 36 | VAL | 2.6 |
| 71 | S3 | 185 | LYS | 2.6 |
| 77 | S9 | 4 | ALA | 2.6 |
| 11 | C6 | 46 | PHE | 2.6 |
| 14 | C9 | 113 | ILE | 2.6 |
| 15 | D0 | 20 | ILE | 2.6 |
| 30 | l5 | 105 | ILE | 2.6 |
| 36 | m1 | 125 | MET | 2.6 |
| 42 | M8 | 71 | LEU | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 45 | n1 | 76 | ILE | 2.6 |
| 68 | s0 | 120 | LEU | 2.6 |
| 73 | s5 | 58 | LEU | 2.6 |
| 72 | S4 | 33 | ALA | 2.6 |
| 14 | C9 | 134 | ARG | 2.6 |
| 13 | c8 | 73 | MET | 2.6 |
| 24 | d9 | 34 | TYR | 2.6 |
| 33 | l8 | 152 | LEU | 2.6 |
| 33 | l8 | 162 | LEU | 2.6 |
| 70 | S2 | 87 | GLN | 2.6 |
| 79 | SR | 170 | ILE | 2.6 |
| 34 | L9 | 90 | MET | 2.6 |
| 51 | N7 | 13 | VAL | 2.6 |
| 11 | C6 | 20 | ALA | 2.6 |
| 13 | c8 | 44 | ASN | 2.6 |
| 2 | 2 | 192 | U | 2.6 |
| 13 | c8 | 131 | LEU | 2.6 |
| 21 | D6 | 17 | HIS | 2.6 |
| 75 | S7 | 61 | PHE | 2.6 |
| 12 | C7 | 42 | GLN | 2.6 |
| 42 | m8 | 171 | LYS | 2.6 |
| 49 | n5 | 95 | ILE | 2.6 |
| 63 | o9 | 40 | LYS | 2.6 |
| 13 | C8 | 133 | VAL | 2.6 |
| 68 | S0 | 32 | HIS | 2.5 |
| 73 | S5 | 190 | ILE | 2.5 |
| 2 | 6 | 494 | U | 2.5 |
| 13 | c8 | 58 | ALA | 2.5 |
| 36 | M1 | 102 | PHE | 2.5 |
| 22 | D7 | 8 | LEU | 2.5 |
| 23 | D8 | 9 | LEU | 2.5 |
| 49 | n5 | 120 | LYS | 2.5 |
| 75 | S7 | 149 | ILE | 2.5 |
| 5 | C0 | 58 | GLN | 2.5 |
| 26 | e1 | 109 | ASP | 2.5 |
| 72 | S4 | 225 | VAL | 2.5 |
| 72 | S4 | 100 | ARG | 2.5 |
| 62 | o8 | 29 | LYS | 2.5 |
| 20 | D5 | 40 | VAL | 2.5 |
| 6 | C1 | 88 | ARG | 2.5 |
| 52 | n8 | 79 | TRP | 2.5 |
| 28 | L3 | 337 | THR | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 69 | s1 | 156 | ALA | 2.5 |
| 20 | d5 | 92 | ILE | 2.5 |
| 32 | L7 | 228 | SER | 2.5 |
| 71 | S3 | 12 | VAL | 2.5 |
| 6 | C1 | 34 | TRP | 2.5 |
| 66 | Q2 | 18 | ARG | 2.5 |
| 6 | C1 | 145 | ALA | 2.5 |
| 9 | c4 | 106 | ALA | 2.5 |
| 17 | d2 | 60 | LYS | 2.5 |
| 43 | m9 | 174 | ALA | 2.5 |
| 49 | n5 | 45 | LYS | 2.5 |
| 69 | s1 | 105 | PHE | 2.5 |
| 71 | S3 | 204 | ASP | 2.5 |
| 6 | c1 | 30 | ARG | 2.5 |
| 25 | E0 | 2 | ALA | 2.5 |
| 26 | e1 | 128 | ALA | 2.5 |
| 72 | S4 | 109 | PHE | 2.5 |
| 70 | S2 | 211 | LEU | 2.5 |
| 33 | l8 | 202 | GLU | 2.5 |
| 77 | S9 | 147 | MET | 2.5 |
| 6 | c1 | 141 | LYS | 2.5 |
| 71 | S3 | 200 | LYS | 2.5 |
| 74 | S6 | 64 | LYS | 2.5 |
| 79 | SR | 223 | TRP | 2.5 |
| 6 | c1 | 140 | VAL | 2.5 |
| 7 | c2 | 89 | ILE | 2.5 |
| 49 | N5 | 24 | LEU | 2.5 |
| 79 | sR | 193 | ILE | 2.5 |
| 66 | q2 | 11 | TYR | 2.5 |
| 66 | q2 | 21 | THR | 2.5 |
| 68 | s0 | 180 | GLU | 2.5 |
| 71 | S3 | 40 | ARG | 2.5 |
| 6 | c1 | 34 | TRP | 2.5 |
| 7 | C2 | 94 | ALA | 2.5 |
| 10 | c5 | 101 | ALA | 2.5 |
| 29 | l4 | 187 | LEU | 2.5 |
| 34 | l9 | 95 | ALA | 2.5 |
| 51 | N7 | 50 | PRO | 2.5 |
| 2 | 2 | 249 | U | 2.5 |
| 46 | n2 | 93 | ILE | 2.5 |
| 62 | o8 | 54 | LEU | 2.5 |
| 6 | c1 | 33 | ARG | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 13 | C8 | 127 | HIS | 2.5 |
| 49 | n5 | 26 | VAL | 2.5 |
| 51 | N7 | 12 | VAL | 2.5 |
| 26 | e1 | 80 | ARG | 2.5 |
| 26 | e1 | 85 | TYR | 2.5 |
| 45 | n1 | 45 | ASN | 2.5 |
| 62 | o8 | 52 | TYR | 2.5 |
| 73 | S5 | 181 | GLU | 2.5 |
| 5 | C0 | 37 | THR | 2.5 |
| 5 | C0 | 57 | THR | 2.5 |
| 15 | d0 | 67 | THR | 2.5 |
| 19 | D4 | 128 | LYS | 2.5 |
| 24 | d9 | 33 | LYS | 2.5 |
| 1 | 5 | 1571 | A | 2.5 |
| 73 | s5 | 69 | PHE | 2.5 |
| 48 | N4 | 125 | ALA | 2.5 |
| 51 | n7 | 81 | LEU | 2.5 |
| 70 | s2 | 92 | ALA | 2.5 |
| 79 | SR | 180 | ALA | 2.5 |
| 12 | C7 | 41 | ILE | 2.5 |
| 45 | n1 | 63 | VAL | 2.5 |
| 62 | o8 | 25 | VAL | 2.5 |
| 75 | s7 | 62 | VAL | 2.5 |
| 30 | L5 | 198 | TYR | 2.5 |
| 42 | m8 | 164 | ARG | 2.5 |
| 44 | N0 | 122 | HIS | 2.5 |
| 28 | L3 | 365 | PHE | 2.5 |
| 39 | M5 | 181 | ASN | 2.5 |
| 66 | Q2 | 32 | LYS | 2.5 |
| 75 | s7 | 133 | THR | 2.5 |
| 8 | c3 | 57 | ALA | 2.5 |
| 12 | C7 | 13 | SER | 2.5 |
| 18 | d3 | 120 | VAL | 2.5 |
| 43 | m9 | 32 | ILE | 2.5 |
| 70 | S2 | 104 | VAL | 2.5 |
| 5 | C0 | 13 | GLN | 2.5 |
| 1 | 1 | 1566 | A | 2.5 |
| 33 | L8 | 177 | TYR | 2.5 |
| 43 | m9 | 53 | LYS | 2.5 |
| 48 | n4 | 91 | LYS | 2.5 |
| 51 | N7 | 31 | GLU | 2.5 |
| 55 | o1 | 110 | GLU | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 69 | s1 | 153 | HIS | 2.5 |
| 45 | n1 | 46 | GLY | 2.5 |
| 64 | q0 | 92 | ASP | 2.5 |
| 45 | N1 | 29 | THR | 2.5 |
| 75 | S7 | 137 | GLY | 2.5 |
| 11 | c6 | 81 | ILE | 2.5 |
| 11 | c6 | 90 | VAL | 2.5 |
| 17 | D2 | 102 | VAL | 2.5 |
| 71 | s3 | 208 | ILE | 2.5 |
| 76 | s8 | 100 | ALA | 2.5 |
| 55 | o1 | 74 | ARG | 2.5 |
| 71 | s3 | 116 | ARG | 2.5 |
| 45 | n1 | 57 | TYR | 2.5 |
| 50 | N6 | 3 | LYS | 2.5 |
| 52 | n8 | 38 | GLN | 2.5 |
| 74 | S6 | 135 | PRO | 2.5 |
| 33 | l8 | 230 | LYS | 2.5 |
| 6 | C1 | 156 | PHE | 2.5 |
| 69 | s1 | 38 | PHE | 2.5 |
| 45 | N1 | 98 | HIS | 2.5 |
| 9 | c4 | 33 | LEU | 2.5 |
| 34 | l9 | 144 | ILE | 2.5 |
| 39 | m5 | 114 | ARG | 2.5 |
| 49 | N5 | 25 | LYS | 2.5 |
| 74 | s6 | 177 | ARG | 2.5 |
| 79 | sR | 35 | SER | 2.5 |
| 46 | n2 | 71 | PHE | 2.5 |
| 69 | s1 | 142 | PHE | 2.5 |
| 73 | S5 | 75 | GLY | 2.5 |
| 73 | s5 | 70 | VAL | 2.5 |
| 75 | s7 | 52 | ALA | 2.5 |
| 77 | S9 | 113 | VAL | 2.5 |
| 77 | s9 | 135 | ALA | 2.5 |
| 26 | E1 | 83 | LYS | 2.5 |
| 53 | N9 | 58 | LYS | 2.5 |
| 71 | s3 | 151 | LYS | 2.5 |
| 78 | SM | 53 | ARG | 2.5 |
| 79 | sR | 74 | THR | 2.5 |
| 5 | C0 | 62 | GLN | 2.5 |
| 6 | c1 | 97 | TYR | 2.5 |
| 20 | d5 | 101 | TYR | 2.5 |
| 39 | m5 | 59 | PHE | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 70 | s2 | 215 | PHE | 2.5 |
| 6 | C1 | 66 | ILE | 2.5 |
| 38 | M4 | 15 | VAL | 2.5 |
| 45 | N1 | 88 | ARG | 2.5 |
| 70 | s2 | 115 | ILE | 2.5 |
| 73 | s5 | 62 | VAL | 2.5 |
| 49 | N5 | 121 | LYS | 2.5 |
| 5 | C0 | 75 | TYR | 2.5 |
| 11 | c6 | 10 | PHE | 2.5 |
| 15 | D0 | 92 | ASP | 2.5 |
| 68 | s0 | 107 | PHE | 2.5 |
| 15 | d0 | 24 | ILE | 2.5 |
| 24 | d9 | 54 | LYS | 2.5 |
| 58 | O4 | 9 | ARG | 2.5 |
| 11 | C6 | 120 | ASP | 2.4 |
| 77 | s9 | 34 | PHE | 2.5 |
| 20 | D5 | 47 | TYR | 2.4 |
| 32 | l7 | 149 | TYR | 2.4 |
| 36 | m1 | 167 | TYR | 2.4 |
| 8 | c3 | 14 | SER | 2.4 |
| 25 | e0 | 56 | MET | 2.4 |
| 32 | L7 | 108 | LEU | 2.4 |
| 68 | S0 | 18 | LEU | 2.4 |
| 72 | S4 | 52 | LEU | 2.4 |
| 13 | C8 | 5 | VAL | 2.4 |
| 15 | D0 | 85 | ARG | 2.4 |
| 34 | L9 | 144 | ILE | 2.4 |
| 51 | N7 | 74 | VAL | 2.4 |
| 76 | S8 | 101 | ILE | 2.4 |
| 10 | C5 | 102 | PHE | 2.4 |
| 13 | c8 | 129 | TRP | 2.4 |
| 32 | l7 | 214 | TRP | 2.4 |
| 47 | N3 | 85 | TRP | 2.4 |
| 49 | N5 | 84 | PHE | 2.4 |
| 51 | N7 | 129 | TRP | 2.4 |
| 76 | s8 | 191 | PHE | 2.4 |
| 20 | D5 | 67 | ASP | 2.4 |
| 77 | S9 | 36 | LEU | 2.4 |
| 6 | C1 | 140 | VAL | 2.4 |
| 26 | E1 | 92 | LYS | 2.4 |
| 68 | S0 | 76 | ILE | 2.4 |
| 70 | s2 | 97 | ARG | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 73 | s5 | 102 | ARG | 2.4 |
| 74 | S6 | 92 | ARG | 2.4 |
| 76 | s8 | 22 | ARG | 2.4 |
| 28 | L3 | 51 | ALA | 2.4 |
| 35 | m0 | 221 | ALA | 2.4 |
| 42 | m8 | 102 | ALA | 2.4 |
| 76 | s8 | 86 | SER | 2.4 |
| 36 | m1 | 163 | PHE | 2.4 |
| 30 | L5 | 30 | TYR | 2.4 |
| 48 | N4 | 107 | GLU | 2.4 |
| 68 | S0 | 36 | TYR | 2.4 |
| 20 | D5 | 98 | GLN | 2.4 |
| 26 | E1 | 94 | LYS | 2.4 |
| 30 | L5 | 143 | LYS | 2.4 |
| 68 | s0 | 74 | VAL | 2.4 |
| 69 | S1 | 152 | ARG | 2.4 |
| 76 | S8 | 123 | LYS | 2.4 |
| 9 | c4 | 15 | GLY | 2.4 |
| 14 | c9 | 62 | ALA | 2.4 |
| 21 | d6 | 43 | ASN | 2.4 |
| 37 | m3 | 3 | ILE | 2.4 |
| 39 | m5 | 183 | THR | 2.4 |
| 45 | n1 | 62 | GLY | 2.4 |
| 49 | n5 | 48 | SER | 2.4 |
| 76 | S8 | 30 | GLY | 2.4 |
| 33 | l8 | 91 | PHE | 2.4 |
| 17 | d2 | 46 | TYR | 2.4 |
| 26 | e1 | 103 | LEU | 2.4 |
| 77 | s9 | 30 | LEU | 2.4 |
| 79 | sR | 81 | LEU | 2.4 |
| 68 | S0 | 86 | VAL | 2.4 |
| 9 | C4 | 12 | GLN | 2.4 |
| 21 | d6 | 33 | ASP | 2.4 |
| 23 | D8 | 40 | ILE | 2.4 |
| 2 | 2 | 733 | A | 2.4 |
| 2 | 2 | 1710 | U | 2.4 |
| 4 | 8 | 38 | U | 2.4 |
| 28 | L3 | 44 | THR | 2.4 |
| 39 | M5 | 185 | ALA | 2.4 |
| 78 | sM | 42 | ALA | 2.4 |
| 62 | O8 | 57 | ASN | 2.4 |
| 9 | c4 | 127 | ARG | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 23 | D8 | 56 | LEU | 2.4 |
| 24 | D9 | 16 | LYS | 2.4 |
| 51 | n7 | 87 | LEU | 2.4 |
| 30 | L5 | 52 | VAL | 2.4 |
| 63 | o9 | 37 | TYR | 2.4 |
| 66 | q2 | 73 | GLU | 2.4 |
| 71 | S3 | 132 | LYS | 2.4 |
| 30 | L5 | 174 | PRO | 2.4 |
| 36 | m1 | 59 | ILE | 2.4 |
| 52 | n8 | 34 | MET | 2.4 |
| 6 | C1 | 118 | GLN | 2.4 |
| 77 | s9 | 158 | PHE | 2.4 |
| 25 | e0 | 22 | GLU | 2.4 |
| 30 | l5 | 44 | TYR | 2.4 |
| 30 | L5 | 173 | VAL | 2.4 |
| 68 | s0 | 119 | ARG | 2.4 |
| 74 | S6 | 109 | LEU | 2.4 |
| 2 | 2 | 754 | A | 2.4 |
| 6 | c1 | 66 | ILE | 2.4 |
| 68 | s0 | 170 | ILE | 2.4 |
| 79 | SR | 221 | MET | 2.4 |
| 76 | s8 | 103 | GLN | 2.4 |
| 5 | c0 | 40 | LEU | 2.4 |
| 11 | C6 | 15 | SER | 2.4 |
| 12 | C7 | 113 | LEU | 2.4 |
| 46 | N2 | 94 | ARG | 2.4 |
| 52 | n8 | 63 | LYS | 2.4 |
| 68 | S0 | 123 | VAL | 2.4 |
| 70 | S2 | 225 | LEU | 2.4 |
| 29 | L4 | 18 | ASN | 2.4 |
| 69 | s1 | 193 | ILE | 2.4 |
| 12 | c7 | 24 | LEU | 2.4 |
| 79 | sR | 62 | LYS | 2.4 |
| 2 | 2 | 726 | C | 2.4 |
| 7 | C2 | 26 | ASP | 2.4 |
| 48 | n4 | 99 | GLU | 2.4 |
| 58 | O4 | 6 | THR | 2.4 |
| 66 | Q2 | 28 | TYR | 2.4 |
| 72 | s4 | 220 | THR | 2.4 |
| 79 | SR | 209 | THR | 2.4 |
| 10 | C5 | 56 | PHE | 2.4 |
| 13 | C8 | 73 | MET | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 58 | O4 | 11 | ASN | 2.4 |
| 66 | q2 | 101 | GLY | 2.4 |
| 56 | o2 | 77 | ALA | 2.4 |
| 69 | S1 | 142 | PHE | 2.4 |
| 71 | S3 | 205 | ALA | 2.4 |
| 9 | c4 | 42 | VAL | 2.4 |
| 30 | l5 | 50 | ARG | 2.4 |
| 55 | o1 | 93 | VAL | 2.4 |
| 56 | o2 | 76 | VAL | 2.4 |
| 58 | O4 | 23 | VAL | 2.4 |
| 66 | q2 | 69 | VAL | 2.4 |
| 77 | s9 | 136 | VAL | 2.4 |
| 77 | s9 | 148 | VAL | 2.4 |
| 79 | sR | 225 | LEU | 2.4 |
| 35 | m0 | 134 | ILE | 2.4 |
| 42 | M8 | 86 | THR | 2.4 |
| 74 | S6 | 180 | THR | 2.4 |
| 40 | M6 | 182 | ASN | 2.4 |
| 52 | N8 | 116 | GLY | 2.4 |
| 77 | S9 | 91 | LYS | 2.4 |
| 35 | m0 | 51 | HIS | 2.4 |
| 39 | m5 | 116 | LEU | 2.4 |
| 7 | c2 | 99 | GLU | 2.4 |
| 39 | m5 | 119 | TYR | 2.4 |
| 15 | D0 | 91 | ILE | 2.4 |
| 58 | o4 | 29 | ILE | 2.4 |
| 78 | sM | 61 | ILE | 2.4 |
| 2 | 2 | 712 | G | 2.4 |
| 21 | d6 | 8 | ASN | 2.4 |
| 30 | L5 | 233 | ALA | 2.4 |
| 39 | M5 | 5 | LYS | 2.4 |
| 39 | M5 | 176 | LYS | 2.4 |
| 76 | s8 | 54 | LYS | 2.4 |
| 76 | S8 | 135 | LYS | 2.4 |
| 2 | 2 | 725 | U | 2.4 |
| 7 | C2 | 75 | VAL | 2.4 |
| 11 | c6 | 52 | LEU | 2.4 |
| 53 | n9 | 11 | ASN | 2.4 |
| 66 | q2 | 18 | ARG | 2.4 |
| 13 | C8 | 4 | VAL | 2.4 |
| 17 | d2 | 121 | VAL | 2.4 |
| 43 | m9 | 51 | VAL | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 6 | C1 | 4 | GLU | 2.4 |
| 30 | l5 | 129 | TYR | 2.4 |
| 76 | s8 | 32 | GLN | 2.4 |
| 11 | c6 | 36 | ILE | 2.4 |
| 68 | S0 | 38 | PHE | 2.4 |
| 75 | S7 | 181 | ILE | 2.4 |
| 76 | S8 | 78 | ILE | 2.4 |
| 2 | 2 | 541 | A | 2.4 |
| 28 | L3 | 45 | SER | 2.4 |
| 32 | l7 | 90 | LYS | 2.4 |
| 33 | l8 | 120 | LYS | 2.4 |
| 71 | s3 | 187 | LYS | 2.4 |
| 11 | c6 | 86 | ALA | 2.4 |
| 62 | O8 | 39 | ARG | 2.4 |
| 9 | C4 | 13 | VAL | 2.4 |
| 17 | d2 | 25 | VAL | 2.4 |
| 21 | d6 | 69 | ASN | 2.4 |
| 14 | C9 | 55 | TYR | 2.4 |
| 45 | n1 | 87 | LYS | 2.4 |
| 58 | o4 | 24 | LYS | 2.4 |
| 15 | D0 | 102 | ARG | 2.4 |
| 21 | D6 | 63 | ALA | 2.4 |
| 24 | D9 | 12 | ARG | 2.4 |
| 34 | l9 | 91 | ARG | 2.4 |
| 26 | E1 | 108 | VAL | 2.4 |
| 37 | m3 | 54 | LEU | 2.4 |
| 48 | n4 | 64 | THR | 2.4 |
| 14 | C9 | 18 | TYR | 2.4 |
| 15 | D0 | 24 | ILE | 2.4 |
| 15 | D0 | 87 | HIS | 2.4 |
| 18 | D3 | 107 | PHE | 2.4 |
| 18 | D3 | 118 | PRO | 2.4 |
| 32 | L7 | 90 | LYS | 2.4 |
| 43 | m9 | 52 | LYS | 2.4 |
| 44 | N0 | 129 | ILE | 2.4 |
| 73 | s5 | 72 | HIS | 2.4 |
| 74 | s6 | 16 | PHE | 2.4 |
| 76 | s8 | 43 | ILE | 2.4 |
| 76 | s8 | 65 | PHE | 2.4 |
| 11 | c6 | 133 | GLY | 2.4 |
| 24 | D9 | 22 | ARG | 2.4 |
| 39 | m5 | 186 | GLY | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 70 | S2 | 163 | GLY | 2.4 |
| 11 | C6 | 105 | LEU | 2.4 |
| 19 | D4 | 25 | VAL | 2.4 |
| 42 | m8 | 175 | ALA | 2.4 |
| 49 | n5 | 57 | LEU | 2.4 |
| 70 | S2 | 103 | VAL | 2.4 |
| 74 | S6 | 77 | LEU | 2.4 |
| 79 | SR | 230 | ALA | 2.4 |
| 1 | 5 | 250 | U | 2.4 |
| 66 | q2 | 7 | THR | 2.4 |
| 28 | L3 | 314 | TYR | 2.4 |
| 21 | d6 | 16 | GLY | 2.4 |
| 39 | m5 | 162 | ARG | 2.4 |
| 39 | M5 | 37 | HIS | 2.4 |
| 72 | s4 | 57 | ASN | 2.4 |
| 6 | C1 | 154 | ALA | 2.4 |
| 60 | o6 | 8 | ALA | 2.4 |
| 73 | S5 | 70 | VAL | 2.4 |
| 15 | d0 | 27 | THR | 2.4 |
| 30 | l5 | 43 | LYS | 2.4 |
| 34 | L9 | 99 | ILE | 2.3 |
| 47 | N3 | 95 | PHE | 2.4 |
| 52 | n8 | 55 | LYS | 2.4 |
| 11 | c6 | 124 | PRO | 2.3 |
| 10 | C5 | 83 | MET | 2.3 |
| 30 | l5 | 182 | GLY | 2.3 |
| 33 | L8 | 152 | LEU | 2.3 |
| 45 | N1 | 77 | ASN | 2.3 |
| 75 | S7 | 53 | GLY | 2.3 |
| 18 | D3 | 122 | PHE | 2.3 |
| 76 | S8 | 86 | SER | 2.3 |
| 11 | C6 | 40 | GLU | 2.3 |
| 28 | l3 | 106 | TRP | 2.3 |
| 77 | s9 | 6 | ARG | 2.3 |
| 26 | e1 | 98 | VAL | 2.3 |
| 35 | m0 | 52 | LEU | 2.3 |
| 5 | C0 | 30 | ALA | 2.3 |
| 39 | m5 | 64 | VAL | 2.3 |
| 53 | n9 | 57 | ALA | 2.3 |
| 39 | m5 | 152 | CYS | 2.3 |
| 1 | 5 | 2571 | U | 2.3 |
| 5 | C0 | 27 | PHE | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 18 | d3 | 11 | SER | 2.3 |
| 54 | o0 | 35 | ARG | 2.3 |
| 7 | C2 | 49 | THR | 2.3 |
| 10 | c5 | 83 | MET | 2.3 |
| 15 | D0 | 50 | LEU | 2.3 |
| 33 | L8 | 162 | LEU | 2.3 |
| 42 | m8 | 166 | LEU | 2.3 |
| 69 | s1 | 37 | THR | 2.3 |
| 74 | S6 | 102 | VAL | 2.3 |
| 77 | s9 | 5 | PRO | 2.3 |
| 12 | C7 | 14 | LYS | 2.3 |
| 9 | c4 | 115 | ILE | 2.3 |
| 12 | c7 | 17 | ILE | 2.3 |
| 2 | 6 | 930 | A | 2.3 |
| 17 | d2 | 30 | SER | 2.3 |
| 26 | e1 | 119 | ARG | 2.3 |
| 30 | l5 | 133 | GLU | 2.3 |
| 39 | m5 | 201 | ARG | 2.3 |
| 57 | O3 | 51 | TYR | 2.3 |
| 73 | s5 | 90 | ILE | 2.3 |
| 44 | n0 | 93 | GLU | 2.3 |
| 69 | s1 | 154 | SER | 2.3 |
| 1 | 5 | 2306 | C | 2.3 |
| 7 | c2 | 26 | ASP | 2.3 |
| 7 | c2 | 126 | TRP | 2.3 |
| 34 | L9 | 34 | LEU | 2.3 |
| 11 | C6 | 128 | LYS | 2.3 |
| 39 | M5 | 102 | ALA | 2.3 |
| 58 | O4 | 12 | PRO | 2.3 |
| 74 | S6 | 79 | LYS | 2.3 |
| 78 | sM | 34 | LYS | 2.3 |
| 17 | d2 | 53 | ILE | 2.3 |
| 37 | m3 | 89 | TYR | 2.3 |
| 39 | m5 | 142 | ILE | 2.3 |
| 39 | M5 | 143 | ARG | 2.3 |
| 46 | n2 | 108 | TYR | 2.3 |
| 53 | n9 | 41 | ARG | 2.3 |
| 72 | S4 | 39 | ARG | 2.3 |
| 74 | S6 | 94 | ARG | 2.3 |
| 74 | S6 | 208 | TYR | 2.3 |
| 19 | D4 | 74 | LEU | 2.3 |
| 30 | L5 | 37 | VAL | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 42 | m8 | 124 | LEU | 2.3 |
| 43 | m9 | 127 | SER | 2.3 |
| 72 | S4 | 207 | LEU | 2.3 |
| 76 | S8 | 70 | GLU | 2.3 |
| 47 | N3 | 16 | GLY | 2.3 |
| 78 | sM | 110 | TRP | 2.3 |
| 7 | C2 | 73 | LYS | 2.3 |
| 77 | s9 | 94 | ASP | 2.3 |
| 30 | L5 | 223 | PHE | 2.3 |
| 6 | C1 | 30 | ARG | 2.3 |
| 30 | L5 | 244 | HIS | 2.3 |
| 33 | L8 | 130 | TYR | 2.3 |
| 48 | N4 | 47 | ARG | 2.3 |
| 54 | o0 | 44 | ILE | 2.3 |
| 64 | q0 | 77 | ILE | 2.3 |
| 1 | 1 | 1762 | C | 2.3 |
| 13 | C8 | 124 | GLY | 2.3 |
| 18 | d3 | 24 | TRP | 2.3 |
| 21 | d6 | 34 | LYS | 2.3 |
| 21 | d6 | 66 | LYS | 2.3 |
| 44 | N0 | 27 | MET | 2.3 |
| 74 | S6 | 54 | GLY | 2.3 |
| 8 | c3 | 26 | PHE | 2.3 |
| 75 | S7 | 150 | GLN | 2.3 |
| 78 | sM | 52 | PRO | 2.3 |
| 79 | sR | 253 | ALA | 2.3 |
| 5 | C0 | 79 | TYR | 2.3 |
| 7 | c2 | 24 | ILE | 2.3 |
| 10 | c5 | 121 | ILE | 2.3 |
| 11 | C6 | 82 | ARG | 2.3 |
| 11 | c6 | 68 | ARG | 2.3 |
| 27 | L2 | 70 | ARG | 2.3 |
| 28 | L3 | 80 | ASP | 2.3 |
| 14 | c9 | 66 | TYR | 2.3 |
| 21 | D6 | 18 | VAL | 2.3 |
| 50 | n6 | 111 | LEU | 2.3 |
| 66 | Q2 | 70 | LEU | 2.3 |
| 71 | S3 | 135 | GLU | 2.3 |
| 54 | O0 | 11 | ASN | 2.3 |
| 78 | sM | 84 | LYS | 2.3 |
| 21 | d6 | 35 | ALA | 2.3 |
| 44 | n0 | 4 | PHE | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 45 | n1 | 49 | GLN | 2.3 |
| 69 | s1 | 60 | ALA | 2.3 |
| 49 | n5 | 67 | ILE | 2.3 |
| 68 | s0 | 141 | ILE | 2.3 |
| 78 | SM | 54 | PRO | 2.3 |
| 6 | c1 | 31 | THR | 2.3 |
| 10 | c5 | 9 | LYS | 2.3 |
| 33 | L8 | 211 | LEU | 2.3 |
| 42 | M8 | 83 | VAL | 2.3 |
| 49 | n5 | 124 | VAL | 2.3 |
| 59 | o5 | 80 | LEU | 2.3 |
| 59 | o5 | 96 | GLU | 2.3 |
| 69 | s1 | 207 | LEU | 2.3 |
| 18 | D3 | 71 | CYS | 2.3 |
| 16 | D1 | 87 | ARG | 2.3 |
| 21 | d6 | 15 | ARG | 2.3 |
| 47 | N3 | 81 | GLN | 2.3 |
| 48 | N4 | 90 | ILE | 2.3 |
| 69 | s1 | 165 | ARG | 2.3 |
| 70 | s2 | 183 | ALA | 2.3 |
| 74 | S6 | 85 | ARG | 2.3 |
| 6 | c1 | 139 | VAL | 2.3 |
| 10 | C5 | 124 | THR | 2.3 |
| 10 | c5 | 76 | VAL | 2.3 |
| 15 | d0 | 63 | LEU | 2.3 |
| 51 | n7 | 12 | VAL | 2.3 |
| 71 | S3 | 48 | VAL | 2.3 |
| 65 | q1 | 5 | TRP | 2.3 |
| 79 | sR | 61 | PHE | 2.3 |
| 79 | SR | 195 | HIS | 2.3 |
| 14 | c9 | 94 | ILE | 2.3 |
| 76 | s8 | 72 | ILE | 2.3 |
| 24 | D9 | 34 | TYR | 2.3 |
| 53 | N9 | 35 | VAL | 2.3 |
| 71 | s3 | 138 | VAL | 2.3 |
| 72 | S4 | 76 | VAL | 2.3 |
| 75 | S7 | 67 | LEU | 2.3 |
| 76 | S8 | 82 | VAL | 2.3 |
| 76 | S8 | 184 | LEU | 2.3 |
| 79 | SR | 270 | LEU | 2.3 |
| 6 | C1 | 121 | ASP | 2.3 |
| 32 | L7 | 109 | THR | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 33 | l8 | 196 | ALA | 2.3 |
| 1 | 1 | 1800 | A | 2.3 |
| 38 | M4 | 32 | LEU | 2.3 |
| 39 | M5 | 62 | TYR | 2.3 |
| 43 | M9 | 185 | LEU | 2.3 |
| 51 | n7 | 74 | VAL | 2.3 |
| 74 | s6 | 135 | PRO | 2.3 |
| 77 | s9 | 144 | PRO | 2.3 |
| 77 | s9 | 145 | SER | 2.3 |
| 30 | l5 | 180 | PHE | 2.3 |
| 27 | l2 | 77 | ILE | 2.3 |
| 30 | l5 | 8 | LYS | 2.3 |
| 46 | n2 | 105 | LEU | 2.3 |
| 53 | N9 | 32 | LEU | 2.3 |
| 66 | Q2 | 78 | LYS | 2.3 |
| 70 | s2 | 211 | LEU | 2.3 |
| 71 | s3 | 142 | LEU | 2.3 |
| 68 | S0 | 109 | ASN | 2.3 |
| 77 | S9 | 145 | SER | 2.3 |
| 21 | D6 | 89 | ARG | 2.3 |
| 34 | L9 | 190 | ASP | 2.3 |
| 42 | m8 | 178 | ARG | 2.3 |
| 45 | n1 | 79 | MET | 2.3 |
| 58 | O4 | 10 | ARG | 2.3 |
| 74 | s6 | 145 | PHE | 2.3 |
| 79 | sR | 72 | THR | 2.3 |
| 27 | l2 | 251 | LYS | 2.3 |
| 49 | n5 | 113 | LEU | 2.3 |
| 73 | S5 | 72 | HIS | 2.3 |
| 30 | L5 | 63 | GLN | 2.3 |
| 7 | C2 | 99 | GLU | 2.3 |
| 2 | 6 | 234 | G | 2.3 |
| 23 | D8 | 42 | ARG | 2.3 |
| 30 | l5 | 36 | LEU | 2.3 |
| 34 | L9 | 112 | ILE | 2.3 |
| 39 | m5 | 176 | LYS | 2.3 |
| 44 | N0 | 31 | ALA | 2.3 |
| 51 | N7 | 68 | ILE | 2.3 |
| 62 | O8 | 2 | ALA | 2.3 |
| 71 | S3 | 7 | LYS | 2.3 |
| 73 | S5 | 125 | THR | 2.3 |
| 49 | n5 | 107 | VAL | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5 | c0 | 29 | GLN | 2.3 |
| 60 | o6 | 80 | PHE | 2.3 |
| 66 | Q2 | 8 | ARG | 2.3 |
| 73 | s5 | 76 | ARG | 2.3 |
| 74 | S6 | 72 | ARG | 2.3 |
| 74 | S6 | 145 | PHE | 2.3 |
| 11 | c6 | 106 | LYS | 2.3 |
| 46 | n2 | 69 | ALA | 2.3 |
| 51 | n7 | 126 | LYS | 2.3 |
| 75 | S7 | 46 | ILE | 2.3 |
| 20 | d5 | 43 | ASP | 2.3 |
| 36 | M1 | 171 | VAL | 2.3 |
| 50 | N6 | 73 | VAL | 2.3 |
| 14 | c9 | 18 | TYR | 2.3 |
| 66 | Q2 | 54 | THR | 2.3 |
| 33 | L8 | 228 | GLU | 2.2 |
| 44 | N0 | 95 | ARG | 2.2 |
| 66 | Q2 | 80 | ARG | 2.2 |
| 28 | L3 | 309 | GLY | 2.2 |
| 78 | SM | 52 | PRO | 2.2 |
| 55 | O1 | 93 | VAL | 2.2 |
| 59 | o5 | 88 | LEU | 2.2 |
| 73 | s5 | 97 | LEU | 2.2 |
| 79 | sR | 301 | LEU | 2.2 |
| 79 | SR | 244 | ALA | 2.2 |
| 68 | S0 | 121 | VAL | 2.2 |
| 17 | D2 | 101 | TYR | 2.2 |
| 68 | s0 | 157 | ASP | 2.2 |
| 70 | s2 | 140 | ARG | 2.2 |
| 11 | C6 | 124 | PRO | 2.2 |
| 39 | m5 | 184 | LYS | 2.2 |
| 45 | n1 | 103 | GLN | 2.2 |
| 73 | S5 | 204 | GLY | 2.2 |
| 79 | SR | 206 | PRO | 2.2 |
| 10 | c5 | 86 | VAL | 2.2 |
| 19 | D4 | 7 | ILE | 2.2 |
| 48 | N4 | 20 | LEU | 2.2 |
| 62 | O8 | 27 | ILE | 2.2 |
| 71 | s3 | 206 | VAL | 2.2 |
| 72 | S4 | 147 | ILE | 2.2 |
| 79 | sR | 223 | TRP | 2.2 |
| 30 | L5 | 44 | TYR | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 74 | S6 | 98 | ARG | 2.2 |
| 1 | 5 | 781 | G | 2.2 |
| 10 | C5 | 71 | GLU | 2.2 |
| 6 | C1 | 59 | PRO | 2.2 |
| 10 | c5 | 132 | GLY | 2.2 |
| 14 | C9 | 65 | ILE | 2.2 |
| 50 | n6 | 70 | ILE | 2.2 |
| 55 | o1 | 75 | ILE | 2.2 |
| 72 | S4 | 31 | PRO | 2.2 |
| 72 | S4 | 56 | LEU | 2.2 |
| 74 | s6 | 83 | CYS | 2.2 |
| 79 | sR | 157 | VAL | 2.2 |
| 6 | C1 | 11 | ARG | 2.2 |
| 11 | C6 | 66 | ARG | 2.2 |
| 49 | n5 | 46 | TYR | 2.2 |
| 74 | s6 | 92 | ARG | 2.2 |
| 76 | s8 | 21 | PHE | 2.2 |
| 2 | 2 | 708 | C | 2.2 |
| 9 | c4 | 128 | LYS | 2.2 |
| 22 | d7 | 70 | LYS | 2.2 |
| 41 | m7 | 80 | LYS | 2.2 |
| 78 | SM | 174 | LYS | 2.2 |
| 2 | 2 | 820 | U | 2.2 |
| 6 | C1 | 63 | LEU | 2.2 |
| 7 | c2 | 75 | VAL | 2.2 |
| 14 | C9 | 124 | ILE | 2.2 |
| 22 | d7 | 26 | GLN | 2.2 |
| 71 | s3 | 140 | GLY | 2.2 |
| 15 | D0 | 118 | VAL | 2.2 |
| 30 | l5 | 134 | ALA | 2.2 |
| 30 | L5 | 150 | LEU | 2.2 |
| 35 | m0 | 152 | LEU | 2.2 |
| 79 | sR | 180 | ALA | 2.2 |
| 49 | n5 | 56 | ARG | 2.2 |
| 58 | o4 | 10 | ARG | 2.2 |
| 20 | D5 | 85 | LYS | 2.2 |
| 30 | L5 | 27 | LYS | 2.2 |
| 40 | M6 | 42 | ASN | 2.2 |
| 32 | L7 | 114 | GLY | 2.2 |
| 52 | n8 | 37 | GLY | 2.2 |
| 15 | D0 | 56 | VAL | 2.2 |
| 16 | D1 | 47 | PRO | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 26 | e1 | 102 | VAL | 2.2 |
| 52 | n8 | 78 | LEU | 2.2 |
| 54 | O0 | 42 | ILE | 2.2 |
| 74 | s6 | 75 | LEU | 2.2 |
| 74 | s6 | 97 | VAL | 2.2 |
| 75 | s7 | 126 | LEU | 2.2 |
| 44 | n0 | 88 | HIS | 2.2 |
| 75 | s7 | 63 | PRO | 2.2 |
| 20 | D5 | 97 | LYS | 2.2 |
| 48 | N4 | 102 | LYS | 2.2 |
| 37 | m3 | 95 | ILE | 2.2 |
| 75 | S7 | 99 | LEU | 2.2 |
| 73 | S5 | 117 | THR | 2.2 |
| 79 | SR | 168 | THR | 2.2 |
| 79 | SR | 227 | ALA | 2.2 |
| 11 | c6 | 135 | ARG | 2.2 |
| 13 | c8 | 128 | PHE | 2.2 |
| 63 | o9 | 30 | ARG | 2.2 |
| 34 | L9 | 87 | LYS | 2.2 |
| 74 | S6 | 164 | LYS | 2.2 |
| 74 | S6 | 171 | LYS | 2.2 |
| 76 | S8 | 65 | PHE | 2.2 |
| 2 | 2 | 657 | U | 2.2 |
| 7 | C2 | 122 | VAL | 2.2 |
| 15 | D0 | 58 | LEU | 2.2 |
| 42 | m8 | 140 | LEU | 2.2 |
| 75 | S7 | 62 | VAL | 2.2 |
| 20 | d5 | 39 | ALA | 2.2 |
| 9 | c4 | 94 | PRO | 2.2 |
| 21 | D6 | 70 | LYS | 2.2 |
| 36 | m1 | 159 | THR | 2.2 |
| 43 | m9 | 182 | ASP | 2.2 |
| 45 | N1 | 69 | LYS | 2.2 |
| 60 | o6 | 2 | THR | 2.2 |
| 70 | s2 | 64 | LYS | 2.2 |
| 76 | S8 | 95 | THR | 2.2 |
| 7 | C2 | 66 | VAL | 2.2 |
| 24 | D9 | 17 | GLY | 2.2 |
| 26 | E1 | 84 | VAL | 2.2 |
| 43 | M9 | 17 | VAL | 2.2 |
| 68 | S0 | 144 | ILE | 2.2 |
| 69 | s1 | 53 | GLY | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 70 | S2 | 139 | ILE | 2.2 |
| 44 | N0 | 8 | GLN | 2.2 |
| 45 | N1 | 55 | LYS | 2.2 |
| 49 | n5 | 65 | GLN | 2.2 |
| 73 | s5 | 154 | ALA | 2.2 |
| 75 | s7 | 42 | GLN | 2.2 |
| 77 | S9 | 100 | LYS | 2.2 |
| 47 | n3 | 85 | TRP | 2.2 |
| 13 | c8 | 15 | LEU | 2.2 |
| 20 | D5 | 65 | LEU | 2.2 |
| 28 | L3 | 74 | GLU | 2.2 |
| 36 | M1 | 19 | LEU | 2.2 |
| 54 | O0 | 43 | ILE | 2.2 |
| 71 | S3 | 208 | ILE | 2.2 |
| 73 | S5 | 96 | SER | 2.2 |
| 5 | c0 | 38 | LYS | 2.2 |
| 13 | c8 | 48 | LYS | 2.2 |
| 28 | L3 | 308 | MET | 2.2 |
| 23 | d8 | 54 | LEU | 2.2 |
| 28 | L3 | 77 | THR | 2.2 |
| 74 | S6 | 80 | ASN | 2.2 |
| 52 | n8 | 41 | HIS | 2.2 |
| 69 | s1 | 188 | LEU | 2.2 |
| 76 | S8 | 97 | THR | 2.2 |
| 9 | c4 | 22 | SER | 2.2 |
| 24 | D9 | 31 | ILE | 2.2 |
| 30 | l5 | 173 | VAL | 2.2 |
| 30 | L5 | 65 | ILE | 2.2 |
| 39 | M5 | 60 | VAL | 2.2 |
| 42 | M8 | 82 | VAL | 2.2 |
| 72 | S4 | 49 | ARG | 2.2 |
| 7 | C2 | 112 | ALA | 2.2 |
| 17 | D2 | 108 | ALA | 2.2 |
| 14 | c9 | 55 | TYR | 2.2 |
| 74 | S6 | 65 | GLN | 2.2 |
| 30 | L5 | 95 | TRP | 2.2 |
| 7 | c2 | 31 | VAL | 2.2 |
| 19 | D4 | 98 | GLU | 2.2 |
| 30 | L5 | 236 | LEU | 2.2 |
| 42 | M8 | 97 | PRO | 2.2 |
| 37 | m3 | 189 | GLU | 2.2 |
| 49 | n5 | 119 | THR | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 69 | s1 | 96 | LEU | 2.2 |
| 5 | c0 | 27 | PHE | 2.2 |
| 21 | d6 | 32 | LYS | 2.2 |
| 27 | l2 | 110 | GLY | 2.2 |
| 44 | N0 | 149 | LYS | 2.2 |
| 69 | s1 | 111 | ARG | 2.2 |
| 72 | s4 | 80 | THR | 2.2 |
| 32 | L7 | 219 | LYS | 2.2 |
| 70 | s2 | 116 | LYS | 2.2 |
| 71 | S3 | 156 | PHE | 2.2 |
| 79 | SR | 235 | SER | 2.2 |
| 8 | c3 | 62 | GLN | 2.2 |
| 36 | M1 | 108 | GLU | 2.2 |
| 43 | m9 | 123 | LEU | 2.2 |
| 70 | S2 | 184 | VAL | 2.2 |
| 70 | S2 | 196 | VAL | 2.2 |
| 71 | S3 | 21 | LEU | 2.2 |
| 7 | C2 | 105 | LYS | 2.2 |
| 42 | m8 | 151 | ARG | 2.2 |
| 62 | o8 | 66 | ILE | 2.2 |
| 36 | m1 | 109 | HIS | 2.2 |
| 42 | m8 | 152 | HIS | 2.2 |
| 71 | S3 | 53 | THR | 2.2 |
| 79 | SR | 245 | PHE | 2.2 |
| 8 | c3 | 60 | VAL | 2.2 |
| 23 | D8 | 54 | LEU | 2.2 |
| 45 | n1 | 43 | LYS | 2.2 |
| 45 | n1 | 85 | LEU | 2.2 |
| 49 | n5 | 24 | LEU | 2.2 |
| 62 | o8 | 14 | LEU | 2.2 |
| 21 | D6 | 83 | ILE | 2.2 |
| 42 | m8 | 173 | GLU | 2.2 |
| 47 | n3 | 3 | GLY | 2.2 |
| 48 | N4 | 63 | ILE | 2.2 |
| 66 | q2 | 6 | LYS | 2.2 |
| 74 | S6 | 73 | ILE | 2.2 |
| 29 | L4 | 89 | ALA | 2.2 |
| 30 | l5 | 78 | ALA | 2.2 |
| 73 | S5 | 94 | THR | 2.2 |
| 15 | d0 | 82 | TYR | 2.2 |
| 34 | L9 | 146 | LEU | 2.2 |
| 42 | M8 | 62 | VAL | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 51 | N7 | 51 | LEU | 2.2 |
| 72 | S4 | 130 | GLN | 2.2 |
| 13 | C8 | 69 | ILE | 2.2 |
| 28 | L3 | 209 | PHE | 2.2 |
| 34 | l9 | 41 | ILE | 2.2 |
| 71 | s3 | 184 | ILE | 2.2 |
| 73 | s5 | 79 | ASN | 2.2 |
| 6 | c1 | 88 | ARG | 2.2 |
| 46 | n2 | 65 | VAL | 2.2 |
| 54 | O0 | 25 | LEU | 2.2 |
| 58 | o4 | 23 | VAL | 2.2 |
| 45 | N1 | 58 | GLN | 2.2 |
| 58 | O4 | 31 | ARG | 2.2 |
| 7 | C2 | 102 | GLY | 2.1 |
| 51 | N7 | 118 | PHE | 2.2 |
| 60 | o6 | 65 | GLY | 2.1 |
| 77 | s9 | 104 | PHE | 2.2 |
| 72 | s4 | 31 | PRO | 2.1 |
| 21 | D6 | 35 | ALA | 2.1 |
| 11 | C6 | 127 | LYS | 2.1 |
| 15 | D0 | 26 | LEU | 2.1 |
| 23 | D8 | 11 | LYS | 2.1 |
| 25 | E0 | 49 | LEU | 2.1 |
| 28 | L3 | 336 | VAL | 2.1 |
| 36 | m1 | 49 | LYS | 2.1 |
| 49 | N5 | 38 | LEU | 2.1 |
| 52 | N8 | 63 | LYS | 2.1 |
| 62 | O8 | 25 | VAL | 2.1 |
| 68 | s0 | 158 | VAL | 2.1 |
| 69 | s1 | 64 | ARG | 2.1 |
| 69 | s1 | 143 | THR | 2.1 |
| 76 | s8 | 90 | LEU | 2.1 |
| 19 | D4 | 22 | GLN | 2.1 |
| 69 | s1 | 67 | GLU | 2.1 |
| 72 | S4 | 90 | ILE | 2.1 |
| 2 | 2 | 913 | G | 2.1 |
| 11 | C6 | 80 | ALA | 2.1 |
| 72 | S4 | 84 | ALA | 2.1 |
| 74 | S6 | 62 | PRO | 2.1 |
| 76 | s8 | 85 | PRO | 2.1 |
| 5 | c0 | 75 | TYR | 2.1 |
| 11 | c6 | 13 | LYS | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 20 | D5 | 57 | TYR | 2.1 |
| 27 | l2 | 156 | LYS | 2.1 |
| 48 | n4 | 93 | ARG | 2.1 |
| 70 | S2 | 61 | LEU | 2.1 |
| 28 | L3 | 358 | TRP | 2.1 |
| 29 | L4 | 114 | ASN | 2.1 |
| 37 | m3 | 12 | ASN | 2.1 |
| 69 | S1 | 124 | ASN | 2.1 |
| 77 | S9 | 52 | ILE | 2.1 |
| 10 | C5 | 113 | GLY | 2.1 |
| 4 | 8 | 52 | A | 2.1 |
| 33 | l8 | 129 | PRO | 2.1 |
| 6 | C1 | 139 | VAL | 2.1 |
| 22 | d7 | 82 | LYS | 2.1 |
| 49 | n5 | 122 | ALA | 2.1 |
| 70 | S2 | 190 | LEU | 2.1 |
| 72 | s4 | 128 | LYS | 2.1 |
| 73 | S5 | 159 | ALA | 2.1 |
| 23 | D8 | 49 | ARG | 2.1 |
| 26 | E1 | 130 | VAL | 2.1 |
| 30 | l5 | 218 | ARG | 2.1 |
| 55 | o1 | 92 | TYR | 2.1 |
| 66 | Q2 | 72 | LEU | 2.1 |
| 8 | C3 | 16 | ILE | 2.1 |
| 30 | l5 | 56 | THR | 2.1 |
| 34 | L9 | 45 | PHE | 2.1 |
| 69 | s1 | 24 | PHE | 2.1 |
| 2 | 6 | 1228 | G | 2.1 |
| 7 | c2 | 25 | GLU | 2.1 |
| 8 | C3 | 62 | GLN | 2.1 |
| 34 | L9 | 59 | ASN | 2.1 |
| 45 | N1 | 70 | SER | 2.1 |
| 52 | n8 | 46 | ASP | 2.1 |
| 77 | s9 | 133 | HIS | 2.1 |
| 52 | n8 | 54 | GLY | 2.1 |
| 5 | c0 | 45 | ALA | 2.1 |
| 12 | c7 | 9 | VAL | 2.1 |
| 17 | d2 | 124 | LYS | 2.1 |
| 41 | M7 | 158 | ALA | 2.1 |
| 42 | M8 | 91 | ALA | 2.1 |
| 20 | d5 | 40 | VAL | 2.1 |
| 22 | D7 | 22 | LYS | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 13 | C8 | 116 | LEU | 2.1 |
| 26 | E1 | 85 | TYR | 2.1 |
| 39 | M5 | 66 | VAL | 2.1 |
| 51 | N7 | 37 | PRO | 2.1 |
| 70 | s2 | 193 | VAL | 2.1 |
| 28 | l3 | 311 | PHE | 2.1 |
| 33 | L8 | 94 | PHE | 2.1 |
| 55 | O1 | 39 | PHE | 2.1 |
| 73 | s5 | 137 | ILE | 2.1 |
| 8 | c3 | 67 | THR | 2.1 |
| 39 | m5 | 139 | HIS | 2.1 |
| 41 | M7 | 162 | GLU | 2.1 |
| 58 | o4 | 34 | HIS | 2.1 |
| 5 | c0 | 1 | MET | 2.1 |
| 76 | s8 | 41 | LYS | 2.1 |
| 10 | c5 | 125 | PRO | 2.1 |
| 37 | M3 | 22 | VAL | 2.1 |
| 42 | m8 | 52 | LEU | 2.1 |
| 44 | N0 | 80 | ARG | 2.1 |
| 68 | S0 | 97 | PRO | 2.1 |
| 72 | S4 | 140 | VAL | 2.1 |
| 75 | S7 | 140 | VAL | 2.1 |
| 21 | d6 | 79 | ILE | 2.1 |
| 75 | s7 | 60 | ILE | 2.1 |
| 79 | SR | 186 | PHE | 2.1 |
| 48 | n4 | 92 | GLU | 2.1 |
| 6 | C1 | 24 | LYS | 2.1 |
| 11 | C6 | 91 | ALA | 2.1 |
| 12 | C7 | 35 | CYS | 2.1 |
| 33 | L8 | 163 | VAL | 2.1 |
| 50 | n6 | 35 | LEU | 2.1 |
| 74 | s6 | 77 | LEU | 2.1 |
| 77 | S9 | 128 | LEU | 2.1 |
| 2 | 6 | 1151 | A | 2.1 |
| 4 | 4 | 80 | A | 2.1 |
| 72 | S4 | 54 | TYR | 2.1 |
| 73 | S5 | 61 | TYR | 2.1 |
| 5 | C0 | 76 | LEU | 2.1 |
| 5 | c0 | 67 | THR | 2.1 |
| 42 | m8 | 179 | ARG | 2.1 |
| 43 | M9 | 189 | ALA | 2.1 |
| 44 | n0 | 31 | ALA | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 74 | S6 | 177 | ARG | 2.1 |
| 78 | SM | 51 | ARG | 2.1 |
| 32 | L7 | 205 | PHE | 2.1 |
| 71 | S3 | 79 | TYR | 2.1 |
| 75 | S7 | 142 | TYR | 2.1 |
| 2 | 2 | 1523 | G | 2.1 |
| 39 | M5 | 52 | GLY | 2.1 |
| 42 | m8 | 79 | LYS | 2.1 |
| 51 | N7 | 20 | GLY | 2.1 |
| 62 | o8 | 74 | LYS | 2.1 |
| 6 | C1 | 153 | PHE | 2.1 |
| 12 | C7 | 58 | MET | 2.1 |
| 21 | d6 | 18 | VAL | 2.1 |
| 36 | m1 | 54 | VAL | 2.1 |
| 42 | m8 | 101 | VAL | 2.1 |
| 73 | S5 | 156 | ARG | 2.1 |
| 14 | C9 | 14 | PHE | 2.1 |
| 30 | L5 | 109 | THR | 2.1 |
| 39 | M5 | 139 | HIS | 2.1 |
| 66 | q2 | 23 | HIS | 2.1 |
| 75 | S7 | 58 | LEU | 2.1 |
| 76 | s8 | 58 | LEU | 2.1 |
| 79 | SR | 243 | LEU | 2.1 |
| 66 | q2 | 26 | THR | 2.1 |
| 9 | c4 | 112 | ILE | 2.1 |
| 32 | L7 | 209 | ASN | 2.1 |
| 36 | M1 | 118 | PRO | 2.1 |
| 58 | o4 | 89 | ILE | 2.1 |
| 14 | c9 | 27 | LYS | 2.1 |
| 33 | l8 | 133 | LYS | 2.1 |
| 72 | S4 | 128 | LYS | 2.1 |
| 75 | S7 | 179 | LYS | 2.1 |
| 78 | SM | 83 | LYS | 2.1 |
| 23 | D8 | 55 | VAL | 2.1 |
| 30 | l5 | 170 | GLY | 2.1 |
| 10 | C5 | 36 | LEU | 2.1 |
| 36 | M1 | 148 | VAL | 2.1 |
| 42 | M8 | 104 | LEU | 2.1 |
| 68 | s0 | 73 | VAL | 2.1 |
| 69 | s1 | 73 | LEU | 2.1 |
| 71 | S3 | 41 | VAL | 2.1 |
| 74 | s6 | 157 | VAL | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 79 | SR | 172 | ALA | 2.1 |
| 11 | c6 | 87 | LYS | 2.1 |
| 13 | c8 | 53 | ASP | 2.1 |
| 15 | D0 | 108 | ILE | 2.1 |
| 28 | L3 | 322 | ILE | 2.1 |
| 69 | s1 | 79 | HIS | 2.1 |
| 79 | SR | 205 | SER | 2.1 |
| 72 | S4 | 71 | LYS | 2.1 |
| 36 | m1 | 132 | ASN | 2.1 |
| 62 | o8 | 28 | ASN | 2.1 |
| 6 | C1 | 135 | VAL | 2.1 |
| 10 | c5 | 116 | LEU | 2.1 |
| 11 | C6 | 19 | VAL | 2.1 |
| 28 | l3 | 87 | VAL | 2.1 |
| 44 | n0 | 135 | VAL | 2.1 |
| 72 | s4 | 139 | VAL | 2.1 |
| 78 | sM | 88 | ARG | 2.1 |
| 32 | L7 | 243 | MET | 2.1 |
| 54 | o0 | 70 | PHE | 2.1 |
| 63 | O9 | 2 | ALA | 2.1 |
| 76 | s8 | 109 | PHE | 2.1 |
| 28 | L3 | 367 | LYS | 2.1 |
| 72 | S4 | 69 | HIS | 2.1 |
| 5 | C0 | 26 | ASP | 2.1 |
| 49 | n5 | 112 | THR | 2.1 |
| 9 | c4 | 137 | LEU | 2.1 |
| 34 | L9 | 27 | VAL | 2.1 |
| 45 | n1 | 40 | VAL | 2.1 |
| 45 | n1 | 94 | GLU | 2.1 |
| 49 | N5 | 107 | VAL | 2.1 |
| 72 | S4 | 92 | LEU | 2.1 |
| 77 | s9 | 85 | VAL | 2.1 |
| 77 | s9 | 128 | LEU | 2.1 |
| 79 | SR | 138 | GLY | 2.1 |
| 18 | d3 | 12 | ALA | 2.1 |
| 20 | D5 | 59 | TYR | 2.1 |
| 49 | N5 | 63 | ILE | 2.1 |
| 1 | 5 | 3156 | U | 2.1 |
| 9 | c4 | 44 | GLY | 2.1 |
| 11 | c6 | 126 | PRO | 2.1 |
| 28 | L3 | 382 | THR | 2.1 |
| 29 | l4 | 188 | ARG | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 58 | O4 | 40 | THR | 2.1 |
| 75 | s7 | 96 | ARG | 2.1 |
| 15 | D0 | 62 | VAL | 2.1 |
| 21 | d6 | 84 | VAL | 2.1 |
| 23 | D8 | 28 | VAL | 2.1 |
| 30 | L5 | 201 | GLY | 2.1 |
| 42 | m8 | 62 | VAL | 2.1 |
| 72 | S4 | 123 | LEU | 2.1 |
| 73 | S5 | 161 | ASP | 2.1 |
| 14 | C9 | 54 | PHE | 2.1 |
| 22 | d7 | 50 | ALA | 2.1 |
| 39 | m5 | 130 | PHE | 2.1 |
| 73 | S5 | 48 | PHE | 2.1 |
| 73 | s5 | 155 | ALA | 2.1 |
| 75 | s7 | 70 | PHE | 2.1 |
| 79 | SR | 257 | ALA | 2.1 |
| 69 | s1 | 219 | LYS | 2.1 |
| 22 | D7 | 51 | GLN | 2.1 |
| 42 | M8 | 174 | ARG | 2.1 |
| 17 | d2 | 129 | VAL | 2.1 |
| 17 | D2 | 120 | HIS | 2.1 |
| 45 | N1 | 33 | VAL | 2.1 |
| 73 | S5 | 132 | VAL | 2.1 |
| 18 | D3 | 116 | ASP | 2.1 |
| 26 | e1 | 86 | THR | 2.1 |
| 1 | 1 | 1764 | U | 2.1 |
| 2 | 2 | 1414 | U | 2.1 |
| 4 | 8 | 36 | G | 2.1 |
| 39 | m5 | 204 | LYS | 2.1 |
| 70 | s2 | 118 | ALA | 2.1 |
| 63 | O9 | 51 | ILE | 2.1 |
| 76 | S8 | 35 | ASN | 2.1 |
| 77 | S9 | 142 | ASN | 2.1 |
| 11 | C6 | 8 | GLN | 2.1 |
| 19 | D4 | 61 | ARG | 2.1 |
| 11 | c6 | 88 | GLY | 2.1 |
| 53 | N9 | 54 | LEU | 2.1 |
| 70 | S2 | 208 | GLU | 2.1 |
| 79 | SR | 154 | VAL | 2.1 |
| 39 | M5 | 21 | PHE | 2.1 |
| 58 | O4 | 93 | PHE | 2.1 |
| 70 | S2 | 85 | PRO | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 72 | s4 | 86 | PHE | 2.1 |
| 79 | SR | 295 | SER | 2.1 |
| 11 | C6 | 110 | THR | 2.1 |
| 45 | n1 | 75 | ILE | 2.1 |
| 49 | n5 | 88 | MET | 2.1 |
| 69 | s1 | 45 | LYS | 2.1 |
| 74 | s6 | 74 | LYS | 2.1 |
| 78 | sM | 87 | THR | 2.1 |
| 29 | l4 | 280 | ILE | 2.1 |
| 70 | s2 | 178 | ILE | 2.1 |
| 73 | s5 | 77 | TYR | 2.1 |
| 14 | C9 | 70 | GLN | 2.1 |
| 51 | n7 | 14 | VAL | 2.1 |
| 59 | o5 | 104 | GLN | 2.1 |
| 75 | S7 | 180 | GLN | 2.1 |
| 19 | D4 | 85 | PHE | 2.1 |
| 28 | L3 | 12 | GLY | 2.1 |
| 8 | c3 | 23 | PRO | 2.0 |
| 14 | C9 | 64 | HIS | 2.0 |
| 30 | l5 | 164 | LYS | 2.0 |
| 75 | s7 | 43 | PHE | 2.1 |
| 79 | sR | 192 | PHE | 2.1 |
| 8 | C3 | 124 | ARG | 2.0 |
| 20 | d5 | 100 | ILE | 2.0 |
| 21 | D6 | 36 | ILE | 2.0 |
| 49 | n5 | 90 | ALA | 2.0 |
| 39 | M5 | 203 | ARG | 2.0 |
| 74 | S6 | 155 | ASP | 2.0 |
| 77 | s9 | 17 | ARG | 2.0 |
| 7 | C2 | 103 | LEU | 2.0 |
| 37 | m3 | 97 | VAL | 2.0 |
| 49 | n5 | 111 | ASN | 2.0 |
| 69 | s1 | 88 | VAL | 2.0 |
| 79 | SR | 301 | LEU | 2.0 |
| 6 | c1 | 13 | PHE | 2.0 |
| 7 | C2 | 117 | GLY | 2.0 |
| 7 | c2 | 29 | LYS | 2.0 |
| 66 | Q2 | 31 | GLY | 2.0 |
| 76 | S8 | 113 | PHE | 2.0 |
| 7 | C2 | 82 | PRO | 2.0 |
| 69 | S1 | 211 | HIS | 2.0 |
| 72 | S4 | 15 | PRO | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 79 | sR | 190 | ALA | 2.0 |
| 6 | C1 | 27 | THR | 2.0 |
| 10 | c5 | 123 | TYR | 2.0 |
| 58 | o4 | 8 | ARG | 2.0 |
| 70 | s2 | 198 | THR | 2.0 |
| 36 | M1 | 80 | LEU | 2.0 |
| 39 | m5 | 60 | VAL | 2.0 |
| 52 | n8 | 123 | VAL | 2.0 |
| 74 | s6 | 147 | LEU | 2.0 |
| 22 | d7 | 72 | LYS | 2.0 |
| 33 | l8 | 43 | LYS | 2.0 |
| 69 | s1 | 145 | LYS | 2.0 |
| 73 | s5 | 128 | ASN | 2.0 |
| 78 | sM | 57 | ASN | 2.0 |
| 1 | 5 | 1838 | G | 2.0 |
| 7 | c2 | 20 | ALA | 2.0 |
| 1 | 5 | 1017 | C | 2.0 |
| 54 | O0 | 44 | ILE | 2.0 |
| 17 | d2 | 52 | TYR | 2.0 |
| 52 | n8 | 109 | TYR | 2.0 |
| 25 | E0 | 50 | VAL | 2.0 |
| 46 | N2 | 65 | VAL | 2.0 |
| 1 | 1 | 1570 | U | 2.0 |
| 26 | E1 | 107 | LYS | 2.0 |
| 27 | L2 | 63 | PHE | 2.0 |
| 39 | M5 | 93 | LYS | 2.0 |
| 66 | Q2 | 13 | LYS | 2.0 |
| 79 | SR | 42 | LEU | 2.0 |
| 32 | L7 | 91 | GLY | 2.0 |
| 44 | n0 | 63 | GLN | 2.0 |
| 11 | c6 | 137 | ARG | 2.0 |
| 30 | l5 | 139 | PRO | 2.0 |
| 37 | M3 | 18 | TRP | 2.0 |
| 71 | S3 | 116 | ARG | 2.0 |
| 13 | C8 | 45 | LEU | 2.0 |
| 55 | o1 | 108 | VAL | 2.0 |
| 73 | s5 | 132 | VAL | 2.0 |
| 74 | s6 | 111 | LEU | 2.0 |
| 2 | 2 | 279 | G | 2.0 |
| 14 | c9 | 25 | GLN | 2.0 |
| 34 | L9 | 85 | GLY | 2.0 |
| 72 | S4 | 25 | GLY | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 17 | D2 | 68 | ARG | 2.0 |
| 52 | n8 | 26 | ARG | 2.0 |
| 51 | N7 | 77 | TYR | 2.0 |
| 68 | s0 | 195 | TRP | 2.0 |
| 75 | S7 | 135 | ILE | 2.0 |
| 79 | sR | 172 | ALA | 2.0 |
| 6 | c1 | 20 | PHE | 2.0 |
| 8 | c3 | 53 | LEU | 2.0 |
| 21 | D6 | 72 | HIS | 2.0 |
| 24 | d9 | 16 | LYS | 2.0 |
| 28 | L3 | 79 | VAL | 2.0 |
| 29 | l4 | 219 | LEU | 2.0 |
| 37 | M3 | 14 | PHE | 2.0 |
| 39 | m5 | 140 | LYS | 2.0 |
| 39 | M5 | 125 | SER | 2.0 |
| 52 | n8 | 47 | LYS | 2.0 |
| 68 | S0 | 102 | PHE | 2.0 |
| 73 | s5 | 84 | LYS | 2.0 |
| 2 | 2 | 793 | A | 2.0 |
| 30 | L5 | 59 | ASP | 2.0 |
| 45 | n1 | 38 | ASP | 2.0 |
| 72 | S4 | 199 | GLU | 2.0 |
| 11 | c6 | 91 | ALA | 2.0 |
| 42 | M8 | 93 | ILE | 2.0 |
| 49 | n5 | 27 | ARG | 2.0 |
| 55 | o1 | 14 | ILE | 2.0 |
| 59 | o5 | 114 | ARG | 2.0 |
| 69 | S1 | 193 | ILE | 2.0 |
| 72 | S4 | 148 | ARG | 2.0 |
| 75 | s7 | 47 | ARG | 2.0 |
| 79 | SR | 114 | ASP | 2.0 |
| 6 | C1 | 125 | VAL | 2.0 |
| 10 | C5 | 98 | ASN | 2.0 |
| 15 | D0 | 55 | PRO | 2.0 |
| 5 | C0 | 60 | SER | 2.0 |
| 6 | c1 | 42 | PHE | 2.0 |
| 33 | l8 | 200 | LEU | 2.0 |
| 36 | m1 | 174 | LYS | 2.0 |
| 71 | S3 | 141 | LYS | 2.0 |
| 74 | s6 | 136 | LYS | 2.0 |
| 1 | 1 | 1552 | G | 2.0 |
| 22 | d7 | 19 | HIS | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 50 | N6 | 72 | SER | 2.0 |
| 7 | C2 | 96 | GLN | 2.0 |
| 11 | c6 | 9 | THR | 2.0 |
| 19 | D4 | 121 | THR | 2.0 |
| 21 | d6 | 10 | ARG | 2.0 |
| 17 | D2 | 83 | ILE | 2.0 |
| 30 | L5 | 64 | ILE | 2.0 |
| 30 | L5 | 297 | GLN | 2.0 |
| 66 | q2 | 10 | THR | 2.0 |
| 66 | q2 | 30 | ALA | 2.0 |
| 71 | s3 | 50 | ILE | 2.0 |
| 72 | S4 | 80 | THR | 2.0 |
| 7 | C2 | 37 | VAL | 2.0 |
| 15 | D0 | 97 | VAL | 2.0 |
| 17 | D2 | 119 | LYS | 2.0 |
| 19 | D4 | 96 | LEU | 2.0 |
| 28 | L3 | 338 | LEU | 2.0 |
| 32 | L7 | 117 | VAL | 2.0 |
| 33 | l8 | 163 | VAL | 2.0 |
| 33 | L8 | 151 | VAL | 2.0 |
| 42 | m8 | 155 | MET | 2.0 |
| 70 | s2 | 197 | TYR | 2.0 |
| 72 | S4 | 126 | VAL | 2.0 |
| 72 | S4 | 134 | LYS | 2.0 |
| 72 | s4 | 208 | VAL | 2.0 |
| 74 | S6 | 136 | LYS | 2.0 |
| 69 | S1 | 81 | PHE | 2.0 |
| 19 | d4 | 120 | GLY | 2.0 |
| 26 | E1 | 118 | ARG | 2.0 |
| 48 | n4 | 80 | ARG | 2.0 |
| 55 | O1 | 11 | GLU | 2.0 |
| 71 | S3 | 214 | GLU | 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](#)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers [i](#)

There are no such residues in this entry.