



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2023 – 05:41 AM EDT

PDB ID : 4V88
Title : The structure of the eukaryotic ribosome at 3.0 Å resolution.
Authors : Ben-Shem, A.; Garreau de Loubresse, N.; Melnikov, S.; Jenner, L.; Yusupova, G.; Yusupov, M.
Deposited on : 2011-10-11
Resolution : 3.00 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

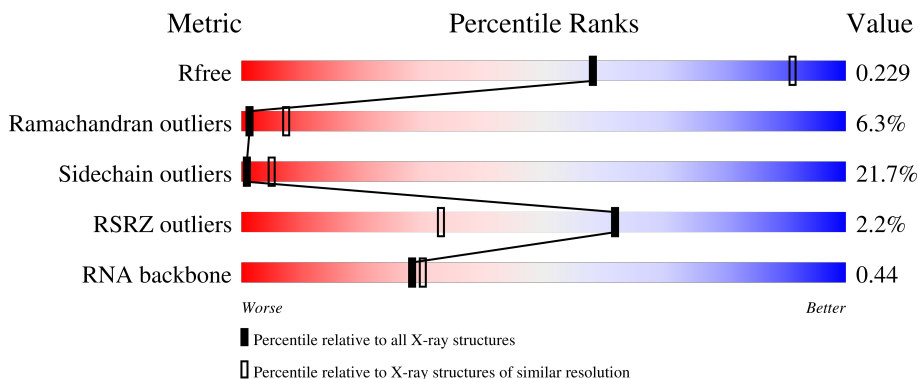
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





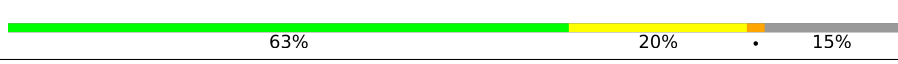
The reported resolution of this entry is 3.00 Å.

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.








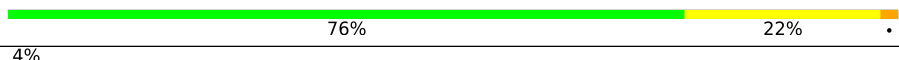

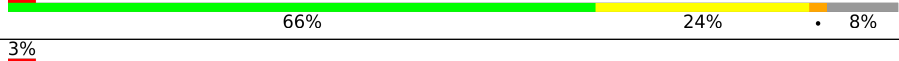

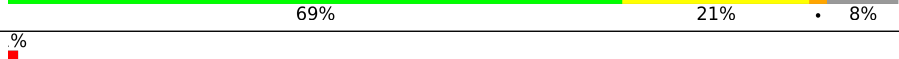
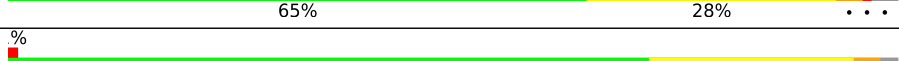
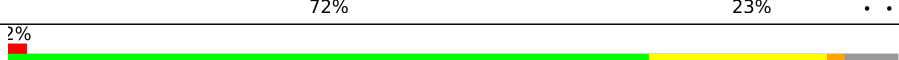
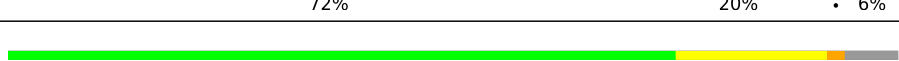
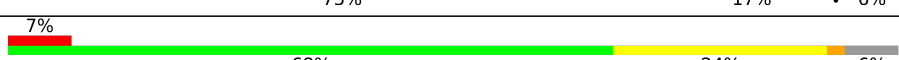
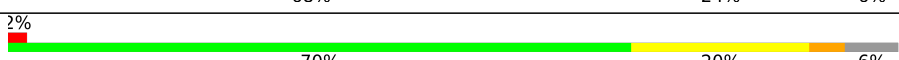
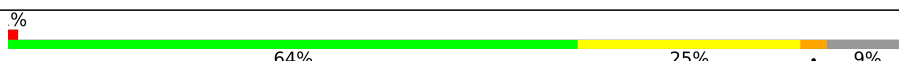
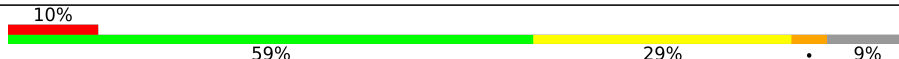
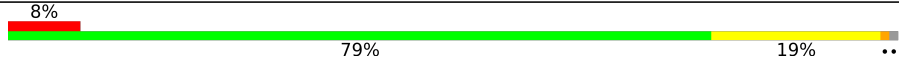



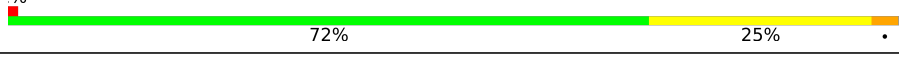
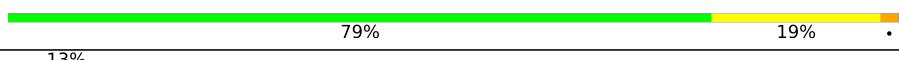
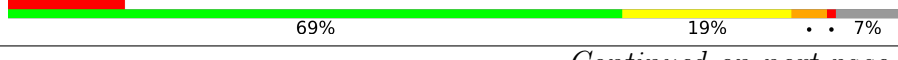

| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 2092 (3.00-3.00) |
| Ramachandran outliers | 138981 | 2333 (3.00-3.00) |
| Sidechain outliers | 138945 | 2336 (3.00-3.00) |
| RSRZ outliers | 127900 | 1990 (3.00-3.00) |
| RNA backbone | 3102 | 1173 (3.30-2.70) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 | A2 | 1800 |  |
| 2 | AA | 252 |  |
| 2 | CA | 252 |  |
| 3 | AB | 255 |  |
| 3 | CB | 255 |  |





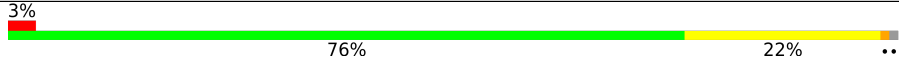
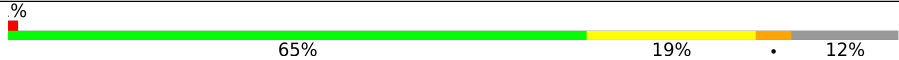
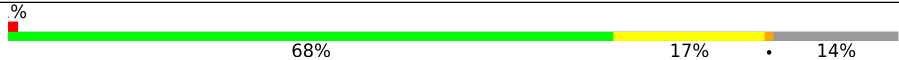
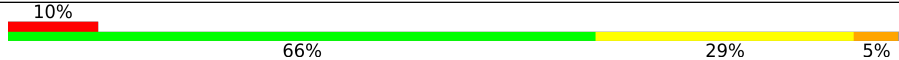
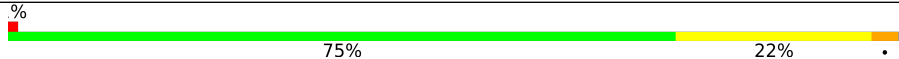
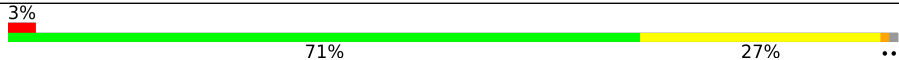
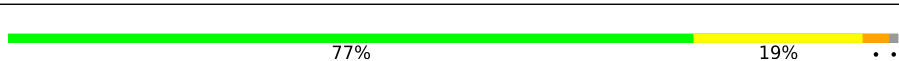
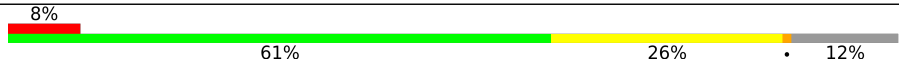


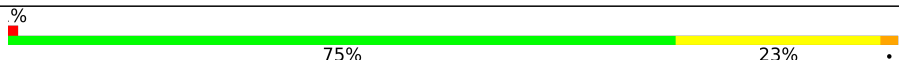
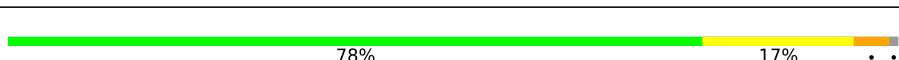
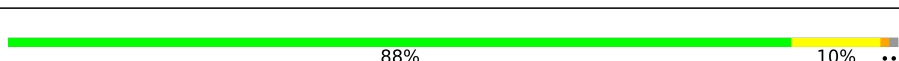
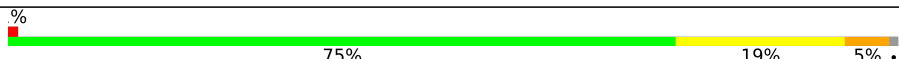
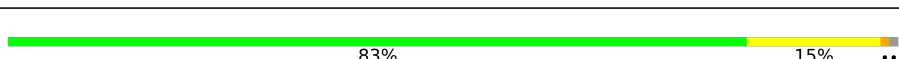

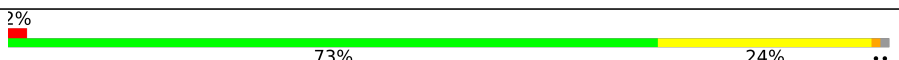
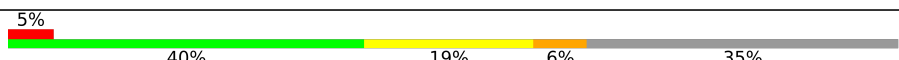
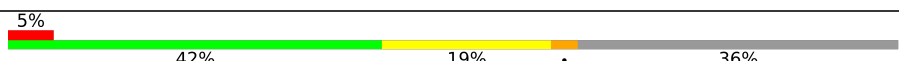
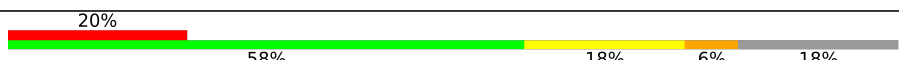
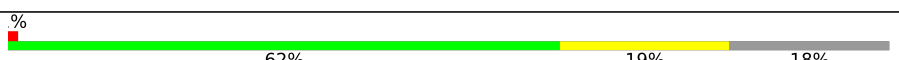
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 4 | AC | 254 |  % 64% 20% 15% 2% |
| 4 | CC | 254 |  2% 65% 17% 15% 2% |
| 5 | AD | 240 |  3% 71% 20% 7% 3% |
| 5 | CD | 240 |  2% 68% 22% 7% 2% |
| 6 | AE | 261 |  3% 72% 25% 3% 3% |
| 6 | CE | 261 |  76% 22% 2% |
| 7 | AF | 225 |  4% 70% 18% 8% 4% |
| 7 | CF | 225 |  3% 66% 24% 8% 3% |
| 8 | AG | 236 |  3% 76% 17% 7% 3% |
| 8 | CG | 236 |  3% 69% 21% 8% 3% |
| 9 | AH | 190 |  % 65% 28% 7% 1% |
| 9 | CH | 190 |  % 72% 23% 5% 1% |
| 10 | AI | 200 |  2% 72% 20% 6% 2% |
| 10 | CI | 200 |  75% 17% 6% |
| 11 | AJ | 197 |  7% 68% 24% 6% 7% |
| 11 | CJ | 197 |  2% 70% 20% 6% 2% |
| 12 | AK | 105 |  % 64% 25% 9% 1% |
| 12 | CK | 105 |  10% 59% 29% 9% 10% |
| 13 | AL | 156 |  8% 79% 19% 2% 8% |
| 13 | CL | 156 |  6% 67% 25% 6% 6% |
| 14 | AM | 143 |  17% 47% 34% 6% 13% 17% |
| 14 | CM | 143 |  28% 50% 27% 8% 13% 28% |
| 15 | AN | 151 |  % 72% 25% 3% 1% |
| 15 | CN | 151 |  79% 19% 2% |
| 16 | AO | 137 |  13% 69% 19% 7% 13% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 16 | CO | 137 |  % 72% 19% 7% |
| 17 | AP | 142 |  % 65% 18% 13% |
| 17 | CP | 142 |  7% 66% 26% 5% |
| 18 | AQ | 143 |  8% 69% 27% .. |
| 18 | CQ | 143 |  3% 76% 22% .. |
| 19 | AR | 136 |  % 65% 19% 12% |
| 19 | CR | 136 |  % 68% 17% 14% |
| 20 | AS | 146 |  10% 66% 29% 5% |
| 20 | CS | 146 |  % 75% 22% .. |
| 21 | AT | 144 |  3% 71% 27% .. |
| 21 | CT | 144 |  % 77% 19% .. |
| 22 | AU | 121 |  8% 61% 26% 12% |
| 22 | CU | 121 |  10% 55% 31% 5% 9% |
| 23 | AV | 87 |  % 72% 23% 5% |
| 23 | CV | 87 |  % 75% 23% . |
| 24 | AW | 130 |  % 78% 17% .. |
| 24 | CW | 130 |  % 88% 10% .. |
| 25 | AX | 145 |  % 75% 19% 5% . |
| 25 | CX | 145 |  % 83% 15% .. |
| 26 | AY | 135 |  2% 72% 24% .. |
| 26 | CY | 135 |  2% 73% 24% .. |
| 27 | AZ | 108 |  5% 40% 19% 6% 35% |
| 27 | CZ | 108 |  5% 42% 19% . 36% |
| 28 | Aa | 119 |  20% 58% 18% 6% 18% |
| 28 | Ca | 119 |  % 62% 19% 18% |



















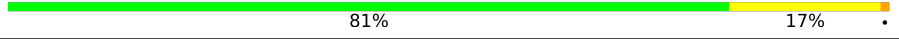






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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------------------|
| 29 | Ab | 82 | 4% 83% 15% .. |
| 29 | Cb | 82 | 73% 26% . |
| 30 | Ac | 67 | 4% 60% 34% 6% |
| 30 | Cc | 67 | 9% 64% 28% 6% |
| 31 | Ad | 56 | 4% 75% 16% 5% |
| 31 | Cd | 56 | 5% 68% 23% 5% |
| 32 | Ae | 63 | 16% 81% 13% 5% |
| 32 | Ce | 63 | 6% 67% 27% 5% |
| 33 | Af | 152 | 3% 33% 11% .. 53% |
| 33 | Cf | 152 | 7% 37% 11% .. 50% |
| 34 | Ag | 319 | 3% 85% 14% . |
| 34 | Cg | 319 | 5% 85% 14% . |
| 35 | Ah | 273 | 2% 47% 9% . 42% |
| 36 | A1 | 3396 | % 37% 46% 10% 7% |
| 36 | A5 | 3396 | % 35% 48% 10% 7% |
| 37 | A3 | 121 | 55% 36% 8% |
| 37 | A7 | 121 | 45% 45% 9% |
| 38 | A4 | 158 | % 39% 52% 9% |
| 38 | A8 | 158 | % 48% 42% 10% |
| 39 | BA | 254 | 84% 13% .. |
| 39 | DA | 254 | 3% 81% 17% .. |
| 40 | BB | 387 | 75% 22% . |
| 40 | DB | 387 | 79% 18% . |
| 41 | BC | 362 | 74% 24% . |
| 41 | DC | 362 | 75% 21% . |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 42 | BD | 297 |  % 75% 23% . |
| 42 | DD | 297 |  % 80% 18% .. |
| 43 | BE | 176 |  74% 13% . 11% |
| 43 | DE | 176 |  % 73% 15% . 11% |
| 44 | BF | 244 |  77% 11% . 9% |
| 44 | DF | 244 |  76% 14% . 9% |
| 45 | BG | 256 |  71% 18% . 9% |
| 45 | DG | 256 |  % 68% 21% . 10% |
| 46 | BH | 191 |  % 75% 24% . |
| 46 | DH | 191 |  % 78% 20% . |
| 47 | BI | 221 |  76% 18% . 5% |
| 47 | DI | 221 |  2% 71% 23% . . |
| 48 | BJ | 174 |  % 68% 25% 5% . |
| 48 | DJ | 174 |  72% 21% . . . |
| 49 | BL | 199 |  75% 19% . . |
| 49 | DL | 199 |  76% 19% . . |
| 50 | BM | 138 |  77% 20% .. |
| 50 | DM | 138 |  80% 17% .. |
| 51 | BN | 204 |  81% 17% . |
| 51 | DN | 204 |  79% 18% . |
| 52 | BO | 219 |  75% 21% . . . |
| 52 | DO | 219 |  % 71% 20% 9% . |
| 53 | BP | 184 |  4% 76% 23% .. |
| 53 | DP | 184 |  70% 12% . 16% |
| 54 | BQ | 186 |  82% 15% .. |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 54 | DQ | 186 | 79% 19% .. |
| 55 | BR | 189 | 78% 21% .. |
| 55 | DR | 189 | 79% 21% .. |
| 56 | BS | 172 | 83% 13% .. |
| 56 | DS | 172 | 79% 19% . |
| 57 | BT | 160 | 75% 22% .. |
| 57 | DT | 160 | 80% 19% .. |
| 58 | BU | 121 | 65% 16% . 17% |
| 58 | DU | 121 | 60% 21% 19% |
| 59 | BV | 137 | 86% 12% .. |
| 59 | DV | 137 | 90% 8% .. |
| 60 | BW | 155 | 51% 12% . 37% |
| 60 | DW | 155 | 73% 13% . 13% |
| 61 | BX | 142 | 66% 18% . 15% |
| 61 | DX | 142 | 65% 18% . 15% |
| 62 | BY | 127 | 78% 20% .. |
| 62 | DY | 127 | 76% 21% .. |
| 63 | BZ | 136 | 74% 24% .. |
| 63 | DZ | 136 | 74% 21% 5% . |
| 64 | Ba | 149 | 79% 14% 6% . |
| 64 | Da | 149 | 75% 22% ... |
| 65 | Bb | 59 | 73% 25% . |
| 65 | Db | 59 | 71% 24% .. |
| 66 | Bc | 105 | 75% 16% . 8% |
| 66 | Dc | 105 | 78% 16% . 5% |



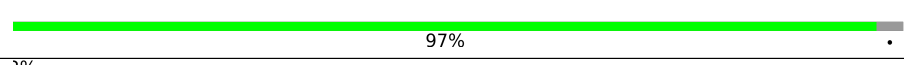
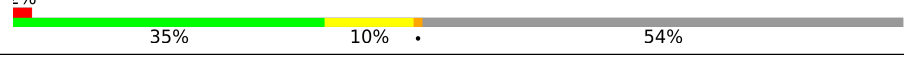
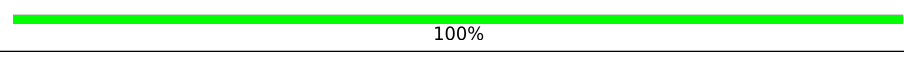
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---------------------|
| 67 | Bd | 113 | 3% 75% 19% . . |
| 67 | Dd | 113 | 73% 21% . . |
| 68 | Be | 130 | 2% 75% 21% . . . |
| 68 | De | 130 | 2% 76% 19% . . . |
| 69 | Bf | 107 | % 85% 10% . . |
| 69 | Df | 107 | 85% 12% . . |
| 70 | Bg | 121 | 2% 69% 20% . 7% |
| 70 | Dg | 121 | 2% 70% 21% . 7% |
| 71 | Bh | 120 | % 72% 26% . . |
| 71 | Dh | 120 | % 76% 22% . . |
| 72 | Bi | 100 | 66% 31% . . |
| 72 | Di | 100 | % 67% 28% . . |
| 73 | Bj | 88 | % 74% 23% . . |
| 73 | Dj | 88 | 2% 74% 25% . |
| 74 | Bk | 78 | 72% 27% . |
| 74 | Dk | 78 | % 76% 23% . |
| 75 | Bl | 51 | 78% 18% . . |
| 75 | Dl | 51 | 2% 75% 22% . . |
| 76 | Bm | 128 | 2% 31% 8% . 59% |
| 76 | Dm | 128 | % 30% 9% . 59% |
| 77 | Bn | 25 | 4% 68% 24% 8% |
| 77 | Dn | 25 | 72% 20% 8% |
| 78 | Bo | 106 | % 74% 23% . . |
| 78 | Do | 106 | 2% 82% 16% . . |
| 79 | Bp | 92 | 79% 18% . . |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 79 | Dp | 92 |  |
| 80 | A6 | 1800 |  |
| 81 | Ch | 273 |  |
| 82 | DK | 155 |  |
| 83 | Dq | 312 |  |
| 84 | Dr | 47 |  |
| 85 | Ds | 46 |  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 86 | OHX | A1 | 3753 | - | - | - | X |
| 86 | OHX | A1 | 3779 | - | - | - | X |
| 86 | OHX | A1 | 3805 | - | - | - | X |
| 86 | OHX | A1 | 3814 | - | - | - | X |
| 86 | OHX | A1 | 3815 | - | - | - | X |
| 86 | OHX | A2 | 2051 | - | - | - | X |
| 86 | OHX | A5 | 3768 | - | - | - | X |
| 86 | OHX | A5 | 3780 | - | - | - | X |
| 86 | OHX | A5 | 3792 | - | - | - | X |
| 86 | OHX | A5 | 3810 | - | - | - | X |
| 86 | OHX | A5 | 3819 | - | - | - | X |
| 86 | OHX | A6 | 2083 | - | - | - | X |
| 86 | OHX | A6 | 2086 | - | - | - | X |
| 86 | OHX | A6 | 2090 | - | - | - | X |
| 86 | OHX | A6 | 2095 | - | - | - | X |
| 86 | OHX | A8 | 218 | - | - | - | X |
| 86 | OHX | BI | 303 | - | - | - | X |
| 86 | OHX | CP | 202 | - | - | - | X |
| 87 | MG | A1 | 3848 | - | - | - | X |
| 87 | MG | A1 | 3909 | - | - | - | X |
| 87 | MG | A1 | 3912 | - | - | - | X |
| 87 | MG | A1 | 3919 | - | - | - | X |
| 87 | MG | A1 | 3922 | - | - | - | X |
| 87 | MG | A1 | 3928 | - | - | - | X |
| 87 | MG | A1 | 3978 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 87 | MG | A1 | 3990 | - | - | - | X |
| 87 | MG | A1 | 4014 | - | - | - | X |
| 87 | MG | A1 | 4059 | - | - | - | X |
| 87 | MG | A1 | 4086 | - | - | - | X |
| 87 | MG | A1 | 4135 | - | - | - | X |
| 87 | MG | A1 | 4144 | - | - | - | X |
| 87 | MG | A1 | 4150 | - | - | - | X |
| 87 | MG | A1 | 4155 | - | - | - | X |
| 87 | MG | A1 | 4187 | - | - | - | X |
| 87 | MG | A1 | 4201 | - | - | - | X |
| 87 | MG | A1 | 4226 | - | - | - | X |
| 87 | MG | A1 | 4232 | - | - | - | X |
| 87 | MG | A1 | 4248 | - | - | - | X |
| 87 | MG | A1 | 4263 | - | - | - | X |
| 87 | MG | A1 | 4269 | - | - | - | X |
| 87 | MG | A1 | 4273 | - | - | - | X |
| 87 | MG | A1 | 4277 | - | - | - | X |
| 87 | MG | A1 | 4282 | - | - | - | X |
| 87 | MG | A1 | 4298 | - | - | - | X |
| 87 | MG | A1 | 4299 | - | - | - | X |
| 87 | MG | A1 | 4302 | - | - | - | X |
| 87 | MG | A1 | 4310 | - | - | - | X |
| 87 | MG | A1 | 4316 | - | - | - | X |
| 87 | MG | A1 | 4326 | - | - | - | X |
| 87 | MG | A1 | 4329 | - | - | - | X |
| 87 | MG | A1 | 4333 | - | - | - | X |
| 87 | MG | A1 | 4337 | - | - | - | X |
| 87 | MG | A1 | 4339 | - | - | - | X |
| 87 | MG | A1 | 4360 | - | - | - | X |
| 87 | MG | A1 | 4368 | - | - | - | X |
| 87 | MG | A1 | 4374 | - | - | - | X |
| 87 | MG | A1 | 4376 | - | - | - | X |
| 87 | MG | A1 | 4385 | - | - | - | X |
| 87 | MG | A1 | 4387 | - | - | - | X |
| 87 | MG | A1 | 4407 | - | - | - | X |
| 87 | MG | A1 | 4408 | - | - | - | X |
| 87 | MG | A1 | 4419 | - | - | - | X |
| 87 | MG | A1 | 4420 | - | - | - | X |
| 87 | MG | A1 | 4432 | - | - | - | X |
| 87 | MG | A1 | 4440 | - | - | - | X |
| 87 | MG | A1 | 4444 | - | - | - | X |
| 87 | MG | A1 | 4447 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 87 | MG | A1 | 4451 | - | - | - | X |
| 87 | MG | A1 | 4453 | - | - | - | X |
| 87 | MG | A1 | 4462 | - | - | - | X |
| 87 | MG | A1 | 4480 | - | - | - | X |
| 87 | MG | A1 | 4495 | - | - | - | X |
| 87 | MG | A1 | 4501 | - | - | - | X |
| 87 | MG | A1 | 4503 | - | - | - | X |
| 87 | MG | A1 | 4504 | - | - | - | X |
| 87 | MG | A2 | 2170 | - | - | - | X |
| 87 | MG | A2 | 2194 | - | - | - | X |
| 87 | MG | A2 | 2196 | - | - | - | X |
| 87 | MG | A2 | 2209 | - | - | - | X |
| 87 | MG | A2 | 2210 | - | - | - | X |
| 87 | MG | A2 | 2211 | - | - | - | X |
| 87 | MG | A2 | 2222 | - | - | - | X |
| 87 | MG | A2 | 2225 | - | - | - | X |
| 87 | MG | A2 | 2241 | - | - | - | X |
| 87 | MG | A2 | 2256 | - | - | - | X |
| 87 | MG | A3 | 220 | - | - | - | X |
| 87 | MG | A3 | 230 | - | - | - | X |
| 87 | MG | A4 | 220 | - | - | - | X |
| 87 | MG | A4 | 245 | - | - | - | X |
| 87 | MG | A5 | 3408 | - | - | - | X |
| 87 | MG | A5 | 3826 | - | - | - | X |
| 87 | MG | A5 | 3862 | - | - | - | X |
| 87 | MG | A5 | 3887 | - | - | - | X |
| 87 | MG | A5 | 3989 | - | - | - | X |
| 87 | MG | A5 | 4022 | - | - | - | X |
| 87 | MG | A5 | 4081 | - | - | - | X |
| 87 | MG | A5 | 4084 | - | - | - | X |
| 87 | MG | A5 | 4135 | - | - | - | X |
| 87 | MG | A5 | 4155 | - | - | - | X |
| 87 | MG | A5 | 4177 | - | - | - | X |
| 87 | MG | A5 | 4202 | - | - | - | X |
| 87 | MG | A5 | 4217 | - | - | - | X |
| 87 | MG | A5 | 4250 | - | - | - | X |
| 87 | MG | A5 | 4254 | - | - | - | X |
| 87 | MG | A5 | 4256 | - | - | - | X |
| 87 | MG | A5 | 4264 | - | - | - | X |
| 87 | MG | A5 | 4265 | - | - | - | X |
| 87 | MG | A5 | 4273 | - | - | - | X |
| 87 | MG | A5 | 4279 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 87 | MG | A5 | 4283 | - | - | - | X |
| 87 | MG | A5 | 4285 | - | - | - | X |
| 87 | MG | A5 | 4309 | - | - | - | X |
| 87 | MG | A5 | 4317 | - | - | - | X |
| 87 | MG | A5 | 4337 | - | - | - | X |
| 87 | MG | A5 | 4345 | - | - | - | X |
| 87 | MG | A5 | 4349 | - | - | - | X |
| 87 | MG | A5 | 4353 | - | - | - | X |
| 87 | MG | A5 | 4372 | - | - | - | X |
| 87 | MG | A5 | 4374 | - | - | - | X |
| 87 | MG | A5 | 4375 | - | - | - | X |
| 87 | MG | A5 | 4379 | - | - | - | X |
| 87 | MG | A5 | 4382 | - | - | - | X |
| 87 | MG | A5 | 4402 | - | - | - | X |
| 87 | MG | A5 | 4409 | - | - | - | X |
| 87 | MG | A5 | 4410 | - | - | - | X |
| 87 | MG | A5 | 4414 | - | - | - | X |
| 87 | MG | A5 | 4424 | - | - | - | X |
| 87 | MG | A5 | 4432 | - | - | - | X |
| 87 | MG | A5 | 4440 | - | - | - | X |
| 87 | MG | A5 | 4464 | - | - | - | X |
| 87 | MG | A5 | 4476 | - | - | - | X |
| 87 | MG | A5 | 4477 | - | - | - | X |
| 87 | MG | A5 | 4482 | - | - | - | X |
| 87 | MG | A5 | 4485 | - | - | - | X |
| 87 | MG | A5 | 4486 | - | - | - | X |
| 87 | MG | A5 | 4488 | - | - | - | X |
| 87 | MG | A5 | 4491 | - | - | - | X |
| 87 | MG | A5 | 4492 | - | - | - | X |
| 87 | MG | A5 | 4510 | - | - | - | X |
| 87 | MG | A5 | 4511 | - | - | - | X |
| 87 | MG | A5 | 4514 | - | - | - | X |
| 87 | MG | A5 | 4515 | - | - | - | X |
| 87 | MG | A5 | 4518 | - | - | - | X |
| 87 | MG | A5 | 4529 | - | - | - | X |
| 87 | MG | A5 | 4541 | - | - | - | X |
| 87 | MG | A5 | 4549 | - | - | - | X |
| 87 | MG | A5 | 4554 | - | - | - | X |
| 87 | MG | A5 | 4561 | - | - | - | X |
| 87 | MG | A5 | 4569 | - | - | - | X |
| 87 | MG | A5 | 4575 | - | - | - | X |
| 87 | MG | A5 | 4579 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 87 | MG | A6 | 2157 | - | - | - | X |
| 87 | MG | A6 | 2158 | - | - | - | X |
| 87 | MG | A6 | 2196 | - | - | - | X |
| 87 | MG | A6 | 2244 | - | - | - | X |
| 87 | MG | A6 | 2246 | - | - | - | X |
| 87 | MG | A6 | 2250 | - | - | - | X |
| 87 | MG | A6 | 2259 | - | - | - | X |
| 87 | MG | A6 | 2262 | - | - | - | X |
| 87 | MG | A6 | 2278 | - | - | - | X |
| 87 | MG | A6 | 2281 | - | - | - | X |
| 87 | MG | A6 | 2284 | - | - | - | X |
| 87 | MG | A6 | 2287 | - | - | - | X |
| 87 | MG | A6 | 2288 | - | - | - | X |
| 87 | MG | A6 | 2296 | - | - | - | X |
| 87 | MG | A6 | 2299 | - | - | - | X |
| 87 | MG | A6 | 2316 | - | - | - | X |
| 87 | MG | A6 | 2317 | - | - | - | X |
| 87 | MG | A6 | 2320 | - | - | - | X |
| 87 | MG | A6 | 2321 | - | - | - | X |
| 87 | MG | A6 | 2322 | - | - | - | X |
| 87 | MG | A6 | 2329 | - | - | - | X |
| 87 | MG | A6 | 2332 | - | - | - | X |
| 87 | MG | A6 | 2333 | - | - | - | X |
| 87 | MG | A6 | 2335 | - | - | - | X |
| 87 | MG | A6 | 2336 | - | - | - | X |
| 87 | MG | A6 | 2338 | - | - | - | X |
| 87 | MG | A7 | 227 | - | - | - | X |
| 87 | MG | A7 | 228 | - | - | - | X |
| 87 | MG | A7 | 229 | - | - | - | X |
| 87 | MG | A8 | 235 | - | - | - | X |
| 87 | MG | BA | 306 | - | - | - | X |
| 87 | MG | BI | 307 | - | - | - | X |
| 87 | MG | BO | 205 | - | - | - | X |
| 87 | MG | BP | 211 | - | - | - | X |
| 87 | MG | BQ | 202 | - | - | - | X |
| 87 | MG | BV | 205 | - | - | - | X |
| 87 | MG | Ba | 207 | - | - | - | X |
| 87 | MG | Ba | 208 | - | - | - | X |
| 87 | MG | Be | 201 | - | - | - | X |
| 87 | MG | Bj | 107 | - | - | - | X |
| 87 | MG | Bl | 4500 | - | - | - | X |
| 87 | MG | CL | 204 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|------------|-------------|--------------|------------|------------------|-----------------|----------------|-------------------------|
| 87 | MG | CP | 203 | - | - | - | X |
| 87 | MG | DB | 414 | - | - | - | X |
| 87 | MG | DC | 405 | - | - | - | X |
| 87 | MG | DH | 202 | - | - | - | X |
| 87 | MG | DH | 203 | - | - | - | X |
| 87 | MG | DO | 207 | - | - | - | X |
| 87 | MG | Db | 102 | - | - | - | X |
| 87 | MG | De | 203 | - | - | - | X |

2 Entry composition [i](#)

There are 89 unique types of molecules in this entry. The entry contains 416785 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 18S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| | | | Total | C | N | O | P | | | |
| 1 | A2 | 1781 | 37835 | 16910 | 6661 | 12482 | 1782 | 0 | 1 | 0 |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 12 | AK | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 772 | 499 | 126 | 145 | 2 | | | |
| 12 | CK | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 761 | 490 | 125 | 144 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 13 | AL | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1213 | 774 | 230 | 206 | 3 | | | |
| 13 | CL | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1168 | 747 | 221 | 197 | 3 | | | |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 32 | Ae | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 475 | 299 | 98 | 77 | 1 | | | |
| 32 | Ce | 62 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 491 | 309 | 101 | 80 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 33 | Af | 71 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 516 | 328 | 93 | 91 | 4 | | | |
| 33 | Cf | 76 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 544 | 346 | 98 | 96 | 4 | | | |

There are 45 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| Af | 82 | UNK | LYS | SEE REMARK 999 | UNP P05759 |
| Af | 83 | UNK | LYS | SEE REMARK 999 | UNP P05759 |
| Af | 84 | UNK | VAL | SEE REMARK 999 | UNP P05759 |
| Af | 85 | UNK | TYR | SEE REMARK 999 | UNP P05759 |
| Af | 86 | UNK | THR | SEE REMARK 999 | UNP P05759 |
| Af | 87 | UNK | THR | SEE REMARK 999 | UNP P05759 |
| Af | 88 | UNK | PRO | SEE REMARK 999 | UNP P05759 |
| Af | 89 | UNK | LYS | SEE REMARK 999 | UNP P05759 |
| Af | 90 | UNK | LYS | SEE REMARK 999 | UNP P05759 |
| Af | 91 | UNK | ILE | SEE REMARK 999 | UNP P05759 |
| Af | 92 | UNK | LYS | SEE REMARK 999 | UNP P05759 |
| Af | 93 | UNK | HIS | SEE REMARK 999 | UNP P05759 |
| Af | 94 | UNK | LYS | SEE REMARK 999 | UNP P05759 |
| Af | 95 | UNK | HIS | SEE REMARK 999 | UNP P05759 |
| Af | 96 | UNK | LYS | SEE REMARK 999 | UNP P05759 |
| Af | 97 | UNK | LYS | SEE REMARK 999 | UNP P05759 |
| Af | 98 | UNK | VAL | SEE REMARK 999 | UNP P05759 |
| Af | 99 | UNK | LYS | SEE REMARK 999 | UNP P05759 |
| Af | 100 | UNK | LEU | SEE REMARK 999 | UNP P05759 |
| Af | 101 | UNK | ALA | SEE REMARK 999 | UNP P05759 |
| Cf | 77 | UNK | GLY | SEE REMARK 999 | UNP P05759 |
| Cf | 78 | UNK | LYS | SEE REMARK 999 | UNP P05759 |
| Cf | 79 | UNK | LYS | SEE REMARK 999 | UNP P05759 |
| Cf | 80 | UNK | ARG | SEE REMARK 999 | UNP P05759 |
| Cf | 81 | UNK | LYS | SEE REMARK 999 | UNP P05759 |
| Cf | 82 | UNK | LYS | SEE REMARK 999 | UNP P05759 |
| Cf | 83 | UNK | LYS | SEE REMARK 999 | UNP P05759 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| Cf | 84 | UNK | VAL | SEE REMARK 999 | UNP P05759 |
| Cf | 85 | UNK | TYR | SEE REMARK 999 | UNP P05759 |
| Cf | 86 | UNK | THR | SEE REMARK 999 | UNP P05759 |
| Cf | 87 | UNK | THR | SEE REMARK 999 | UNP P05759 |
| Cf | 88 | UNK | PRO | SEE REMARK 999 | UNP P05759 |
| Cf | 89 | UNK | LYS | SEE REMARK 999 | UNP P05759 |
| Cf | 90 | UNK | LYS | SEE REMARK 999 | UNP P05759 |
| Cf | 91 | UNK | ILE | SEE REMARK 999 | UNP P05759 |
| Cf | 92 | UNK | LYS | SEE REMARK 999 | UNP P05759 |
| Cf | 93 | UNK | HIS | SEE REMARK 999 | UNP P05759 |
| Cf | 94 | UNK | LYS | SEE REMARK 999 | UNP P05759 |
| Cf | 95 | UNK | HIS | SEE REMARK 999 | UNP P05759 |
| Cf | 96 | UNK | LYS | SEE REMARK 999 | UNP P05759 |
| Cf | 97 | UNK | LYS | SEE REMARK 999 | UNP P05759 |
| Cf | 98 | UNK | VAL | SEE REMARK 999 | UNP P05759 |
| Cf | 99 | UNK | LYS | SEE REMARK 999 | UNP P05759 |
| Cf | 100 | UNK | LEU | SEE REMARK 999 | UNP P05759 |
| Cf | 101 | UNK | ALA | SEE REMARK 999 | UNP P05759 |

- Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein (ASC1, RACK1).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 34 | Ag | 318 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2437 | 1541 | 418 | 470 | 8 | | | |
| 34 | Cg | 318 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2442 | 1544 | 418 | 472 | 8 | | | |

- Molecule 35 is a protein called Suppressor protein STM1.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 35 | Ah | 159 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1105 | 653 | 221 | 231 | | | |

There are 38 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| Ah | 9 | UNK | GLY | SEE REMARK 999 | UNP P39015 |
| Ah | 10 | UNK | ASN | SEE REMARK 999 | UNP P39015 |
| Ah | 11 | UNK | ASP | SEE REMARK 999 | UNP P39015 |
| Ah | 12 | UNK | VAL | SEE REMARK 999 | UNP P39015 |
| Ah | 13 | UNK | GLU | SEE REMARK 999 | UNP P39015 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| Ah | 14 | UNK | ASP | SEE REMARK 999 | UNP P39015 |
| Ah | 15 | UNK | ALA | SEE REMARK 999 | UNP P39015 |
| Ah | 16 | UNK | ASP | SEE REMARK 999 | UNP P39015 |
| Ah | 17 | UNK | VAL | SEE REMARK 999 | UNP P39015 |
| Ah | 18 | UNK | VAL | SEE REMARK 999 | UNP P39015 |
| Ah | 19 | UNK | VAL | SEE REMARK 999 | UNP P39015 |
| Ah | 20 | UNK | LEU | SEE REMARK 999 | UNP P39015 |
| Ah | 151 | UNK | LEU | SEE REMARK 999 | UNP P39015 |
| Ah | 152 | UNK | GLN | SEE REMARK 999 | UNP P39015 |
| Ah | 153 | UNK | ASP | SEE REMARK 999 | UNP P39015 |
| Ah | 154 | UNK | TYR | SEE REMARK 999 | UNP P39015 |
| Ah | 155 | UNK | LEU | SEE REMARK 999 | UNP P39015 |
| Ah | 156 | UNK | ASN | SEE REMARK 999 | UNP P39015 |
| Ah | 157 | UNK | GLN | SEE REMARK 999 | UNP P39015 |
| Ah | 158 | UNK | GLN | SEE REMARK 999 | UNP P39015 |
| Ah | 159 | UNK | ALA | SEE REMARK 999 | UNP P39015 |
| Ah | 160 | UNK | ASN | SEE REMARK 999 | UNP P39015 |
| Ah | 161 | UNK | ASN | SEE REMARK 999 | UNP P39015 |
| Ah | 162 | UNK | GLN | SEE REMARK 999 | UNP P39015 |
| Ah | 163 | UNK | PHE | SEE REMARK 999 | UNP P39015 |
| Ah | 164 | UNK | ASN | SEE REMARK 999 | UNP P39015 |
| Ah | 165 | UNK | LYS | SEE REMARK 999 | UNP P39015 |
| Ah | 166 | UNK | VAL | SEE REMARK 999 | UNP P39015 |
| Ah | 167 | UNK | PRO | SEE REMARK 999 | UNP P39015 |
| Ah | 168 | UNK | GLU | SEE REMARK 999 | UNP P39015 |
| Ah | 169 | UNK | ALA | SEE REMARK 999 | UNP P39015 |
| Ah | 170 | UNK | LYS | SEE REMARK 999 | UNP P39015 |
| Ah | 171 | UNK | LYS | SEE REMARK 999 | UNP P39015 |
| Ah | 172 | UNK | VAL | SEE REMARK 999 | UNP P39015 |
| Ah | 173 | UNK | GLU | SEE REMARK 999 | UNP P39015 |
| Ah | 174 | UNK | LEU | SEE REMARK 999 | UNP P39015 |
| Ah | 175 | UNK | ASP | SEE REMARK 999 | UNP P39015 |
| Ah | 176 | UNK | ALA | SEE REMARK 999 | UNP P39015 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| | | | Total | C | N | O | P | | | |
| 36 | A1 | 3149 | 67355 | 30086 | 12142 | 21978 | 3149 | 0 | 0 | 0 |
| 36 | A5 | 3150 | 67376 | 30095 | 12145 | 21987 | 3149 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 37 | A3 | 121 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2579 | 1152 | 461 | 845 | 121 | | | |
| 37 | A7 | 121 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2579 | 1152 | 461 | 845 | 121 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|---------|-------|
| 38 | A4 | 158 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 3353 | 1500 | 586 | 1109 | 158 | | | |
| 38 | A8 | 158 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 3353 | 1500 | 586 | 1109 | 158 | | | |

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 42 | BD | 296 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2375 | 1501 | 414 | 458 | 2 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 42 | DD | 294 | Total 2359 | C 1489 | N 412 | O 456 | S 2 | 0 | 0 | 0 |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 52 | BO | 197 | Total 3119 | C 2008 | N 581 | O 528 | S 2 | 0 | 197 | 0 |
| 52 | DO | 197 | Total 3119 | C 2008 | N 581 | O 528 | S 2 | 0 | 197 | 0 |

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 58 | BU | 100 | Total | C | N | O | 0 | 0 | 0 |
| | | | 796 | 516 | 131 | 149 | | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 58 | DU | 98 | 778 | 505 | 127 | 146 | 0 | 0 | 0 |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 74 | Bk | 77 | Total | C | N | O | 0 | 0 | 0 |
| | | | 612 | 391 | 115 | 106 | | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 74 | Dk | 77 | Total | C | N | O | 0 | 0 | 0 |
| | | | 608 | 388 | 114 | 106 | | | |

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

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

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

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

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

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

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

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

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

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

- Molecule 80 is a RNA chain called 18S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| | | | Total | C | N | O | P | | | |
| 80 | A6 | 1795 | 38021 | 16989 | 6669 | 12567 | 1796 | 0 | 1 | 0 |

- Molecule 81 is a protein called Suppressor protein STM1.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 81 | Ch | 104 | 680 | 403 | 140 | 137 | 0 | 0 | 0 |

There are 41 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| Ch | 119 | UNK | ALA | SEE REMARK 999 | UNP P39015 |
| Ch | 120 | UNK | GLU | SEE REMARK 999 | UNP P39015 |
| Ch | 121 | UNK | LYS | SEE REMARK 999 | UNP P39015 |
| Ch | 122 | UNK | GLU | SEE REMARK 999 | UNP P39015 |
| Ch | 123 | UNK | ALA | SEE REMARK 999 | UNP P39015 |
| Ch | 124 | UNK | GLN | SEE REMARK 999 | UNP P39015 |
| Ch | 125 | UNK | ALA | SEE REMARK 999 | UNP P39015 |
| Ch | 126 | UNK | ASP | SEE REMARK 999 | UNP P39015 |
| Ch | 127 | UNK | ALA | SEE REMARK 999 | UNP P39015 |
| Ch | 128 | UNK | ALA | SEE REMARK 999 | UNP P39015 |
| Ch | 129 | UNK | ALA | SEE REMARK 999 | UNP P39015 |
| Ch | 130 | UNK | GLU | SEE REMARK 999 | UNP P39015 |
| Ch | 131 | UNK | ILE | SEE REMARK 999 | UNP P39015 |
| Ch | 132 | UNK | ALA | SEE REMARK 999 | UNP P39015 |
| Ch | 133 | UNK | GLU | SEE REMARK 999 | UNP P39015 |
| Ch | 134 | UNK | ASP | SEE REMARK 999 | UNP P39015 |
| Ch | 135 | UNK | ALA | SEE REMARK 999 | UNP P39015 |
| Ch | 136 | UNK | ALA | SEE REMARK 999 | UNP P39015 |
| Ch | 137 | UNK | GLU | SEE REMARK 999 | UNP P39015 |
| Ch | 138 | UNK | ALA | SEE REMARK 999 | UNP P39015 |
| Ch | 139 | UNK | GLU | SEE REMARK 999 | UNP P39015 |
| Ch | 155 | UNK | LEU | SEE REMARK 999 | UNP P39015 |
| Ch | 156 | UNK | ASN | SEE REMARK 999 | UNP P39015 |
| Ch | 157 | UNK | GLN | SEE REMARK 999 | UNP P39015 |
| Ch | 158 | UNK | GLN | SEE REMARK 999 | UNP P39015 |
| Ch | 159 | UNK | ALA | SEE REMARK 999 | UNP P39015 |
| Ch | 160 | UNK | ASN | SEE REMARK 999 | UNP P39015 |
| Ch | 161 | UNK | ASN | SEE REMARK 999 | UNP P39015 |
| Ch | 162 | UNK | GLN | SEE REMARK 999 | UNP P39015 |
| Ch | 163 | UNK | PHE | SEE REMARK 999 | UNP P39015 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| Ch | 164 | UNK | ASN | SEE REMARK 999 | UNP P39015 |
| Ch | 165 | UNK | LYS | SEE REMARK 999 | UNP P39015 |
| Ch | 166 | UNK | VAL | SEE REMARK 999 | UNP P39015 |
| Ch | 167 | UNK | PRO | SEE REMARK 999 | UNP P39015 |
| Ch | 168 | UNK | GLU | SEE REMARK 999 | UNP P39015 |
| Ch | 169 | UNK | ALA | SEE REMARK 999 | UNP P39015 |
| Ch | 170 | UNK | LYS | SEE REMARK 999 | UNP P39015 |
| Ch | 171 | UNK | LYS | SEE REMARK 999 | UNP P39015 |
| Ch | 172 | UNK | VAL | SEE REMARK 999 | UNP P39015 |
| Ch | 173 | UNK | GLU | SEE REMARK 999 | UNP P39015 |
| Ch | 174 | UNK | LEU | SEE REMARK 999 | UNP P39015 |

- Molecule 82 is a protein called Ribosomal protein L12.

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

- Molecule 83 is a protein called 60S acidic ribosomal protein P0.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 83 | Dq | 143 | 1077 | 687 | 192 | 195 | 3 | 0 | 0 | 0 |

There are 23 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| Dq | 199 | UNK | SER | SEE REMARK 999 | UNP P05317 |
| Dq | 200 | UNK | SER | SEE REMARK 999 | UNP P05317 |
| Dq | 201 | UNK | ILE | SEE REMARK 999 | UNP P05317 |
| Dq | 202 | UNK | LEU | SEE REMARK 999 | UNP P05317 |
| Dq | 203 | UNK | ASP | SEE REMARK 999 | UNP P05317 |
| Dq | 204 | UNK | ILE | SEE REMARK 999 | UNP P05317 |
| Dq | 205 | UNK | THR | SEE REMARK 999 | UNP P05317 |
| Dq | 206 | UNK | ASP | SEE REMARK 999 | UNP P05317 |
| Dq | 207 | UNK | GLU | SEE REMARK 999 | UNP P05317 |
| Dq | 208 | UNK | GLU | SEE REMARK 999 | UNP P05317 |
| Dq | 209 | UNK | LEU | SEE REMARK 999 | UNP P05317 |
| Dq | 210 | UNK | VAL | SEE REMARK 999 | UNP P05317 |
| Dq | 211 | UNK | SER | SEE REMARK 999 | UNP P05317 |
| Dq | 212 | UNK | HIS | SEE REMARK 999 | UNP P05317 |
| Dq | 213 | UNK | PHE | SEE REMARK 999 | UNP P05317 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| Dq | 214 | UNK | VAL | SEE REMARK 999 | UNP P05317 |
| Dq | 215 | UNK | SER | SEE REMARK 999 | UNP P05317 |
| Dq | 216 | UNK | ALA | SEE REMARK 999 | UNP P05317 |
| Dq | 217 | UNK | VAL | SEE REMARK 999 | UNP P05317 |
| Dq | 218 | UNK | SER | SEE REMARK 999 | UNP P05317 |
| Dq | 219 | UNK | THR | SEE REMARK 999 | UNP P05317 |
| Dq | 220 | UNK | ILE | SEE REMARK 999 | UNP P05317 |
| Dq | 221 | UNK | ALA | SEE REMARK 999 | UNP P05317 |

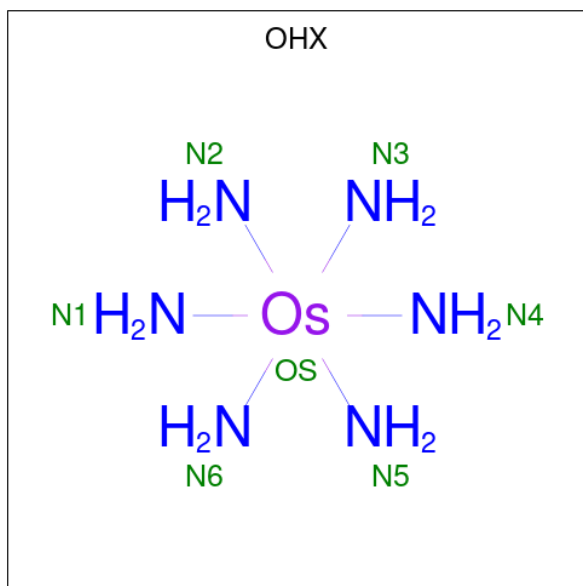
- Molecule 84 is a protein called Ribosomal protein P1 alpha.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 84 | Dr | 47 | 235 | 141 | 47 | 47 | 0 | 0 | 0 |

- Molecule 85 is a protein called Ribosomal protein P2 beta.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 85 | Ds | 46 | 230 | 138 | 46 | 46 | 0 | 0 | 0 |

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



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A2 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | AC | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | AI | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | AL | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | AN | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | AP | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | Ad | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | Ag | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|------------|--------------|-----------------|--------------|---|----|----------------|----------------|
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A1 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A3 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A3 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A4 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | BA | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | BB | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | BB | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | BC | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | BD | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | BI | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | BI | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | BI | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | BI | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | BN | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | BO | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | BP | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | BP | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | BR | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | BT | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | Bb | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | Bf | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | Bj | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | Bj | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | Bj | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | Bo | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 6 | 5 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86 | A6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 86 | A6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A6 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | CB | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | CG | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | CG | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | CI | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | CJ | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | CL | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | CN | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | CP | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | CP | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | CS | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | CY | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | CY | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | Cd | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | Cg | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|------------|--------------|-----------------|--------------|--------|---------|----------------|----------------|
| 86 | A5 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 86 | A5 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 86 | A5 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 86 | A5 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 86 | A5 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 86 | A5 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 86 | A5 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 86 | A5 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 86 | A5 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 86 | A5 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 86 | A5 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 86 | A5 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 86 | A5 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 86 | A5 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 86 | A5 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 86 | A5 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 86 | A5 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 86 | A5 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 86 | A5 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 86 | A5 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |
| 86 | A5 | 1 | Total 7 | N 6 | Os 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A5 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A7 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A7 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A7 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A7 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A7 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A7 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A7 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A7 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A7 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A7 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A7 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A7 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A7 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A7 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A8 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | A8 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A8 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A8 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A8 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A8 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A8 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A8 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A8 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A8 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A8 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A8 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A8 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A8 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A8 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A8 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A8 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A8 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A8 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | A8 | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | DA | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | DB | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | DB | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| | | | Total | N | Os | | |
| 86 | DC | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | DC | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | DD | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | DG | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | DH | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | DI | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | DI | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | DJ | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | DM | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | DO | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | DP | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | DQ | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | DR | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | DV | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | Db | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | De | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | Df | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | Dg | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | Dh | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | Dj | 1 | 7 | 6 | 1 | 0 | 0 |
| 86 | Do | 1 | 7 | 6 | 1 | 0 | 0 |

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 87 | A2 | 171 | Total 171 | Mg 171 | 0 | 0 |
| 87 | AB | 2 | Total 2 | Mg 2 | 0 | 0 |
| 87 | AC | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | AE | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | AI | 2 | Total 2 | Mg 2 | 0 | 0 |
| 87 | AJ | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | AL | 2 | Total 2 | Mg 2 | 0 | 0 |
| 87 | AN | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | AP | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | AS | 2 | Total 2 | Mg 2 | 0 | 0 |
| 87 | AX | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | Aa | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | Ad | 3 | Total 3 | Mg 3 | 0 | 0 |
| 87 | Af | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | A1 | 695 | Total 695 | Mg 695 | 0 | 0 |
| 87 | A3 | 19 | Total 19 | Mg 19 | 0 | 0 |
| 87 | A4 | 34 | Total 34 | Mg 34 | 0 | 0 |
| 87 | BA | 5 | Total 5 | Mg 5 | 0 | 0 |
| 87 | BB | 4 | Total 4 | Mg 4 | 0 | 0 |
| 87 | BC | 6 | Total 6 | Mg 6 | 0 | 0 |
| 87 | BD | 1 | Total 1 | Mg 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 87 | BE | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | BF | 2 | Total 2 | Mg 2 | 0 | 0 |
| 87 | BG | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | BI | 4 | Total 4 | Mg 4 | 0 | 0 |
| 87 | BJ | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | BL | 5 | Total 5 | Mg 5 | 0 | 0 |
| 87 | BN | 6 | Total 6 | Mg 6 | 0 | 0 |
| 87 | BO | 8 | Total 8 | Mg 8 | 0 | 0 |
| 87 | BP | 10 | Total 10 | Mg 10 | 0 | 0 |
| 87 | BQ | 4 | Total 4 | Mg 4 | 0 | 0 |
| 87 | BR | 4 | Total 4 | Mg 4 | 0 | 0 |
| 87 | BS | 2 | Total 2 | Mg 2 | 0 | 0 |
| 87 | BT | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | BV | 5 | Total 5 | Mg 5 | 0 | 0 |
| 87 | BY | 2 | Total 2 | Mg 2 | 0 | 0 |
| 87 | Ba | 8 | Total 8 | Mg 8 | 0 | 0 |
| 87 | Bd | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | Be | 2 | Total 2 | Mg 2 | 0 | 0 |
| 87 | Bf | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | Bg | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | Bj | 7 | Total 7 | Mg 7 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 87 | Bl | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | Bm | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | Bo | 3 | Total 3 | Mg 3 | 0 | 0 |
| 87 | A6 | 239 | Total 239 | Mg 239 | 0 | 0 |
| 87 | CB | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | CE | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | CF | 2 | Total 2 | Mg 2 | 0 | 0 |
| 87 | CG | 2 | Total 2 | Mg 2 | 0 | 0 |
| 87 | CI | 2 | Total 2 | Mg 2 | 0 | 0 |
| 87 | CL | 3 | Total 3 | Mg 3 | 0 | 0 |
| 87 | CP | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | CQ | 2 | Total 2 | Mg 2 | 0 | 0 |
| 87 | CS | 2 | Total 2 | Mg 2 | 0 | 0 |
| 87 | CX | 2 | Total 2 | Mg 2 | 0 | 0 |
| 87 | CY | 2 | Total 2 | Mg 2 | 0 | 0 |
| 87 | CZ | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | Ca | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | Cd | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | Ch | 2 | Total 2 | Mg 2 | 0 | 0 |
| 87 | A5 | 763 | Total 763 | Mg 763 | 0 | 0 |
| 87 | A7 | 26 | Total 26 | Mg 26 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 87 | A8 | 20 | Total 20 | Mg 20 | 0 | 0 |
| 87 | DA | 4 | Total 4 | Mg 4 | 0 | 0 |
| 87 | DB | 13 | Total 13 | Mg 13 | 0 | 0 |
| 87 | DC | 5 | Total 5 | Mg 5 | 0 | 0 |
| 87 | DD | 7 | Total 7 | Mg 7 | 0 | 0 |
| 87 | DF | 4 | Total 4 | Mg 4 | 0 | 0 |
| 87 | DG | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | DH | 2 | Total 2 | Mg 2 | 0 | 0 |
| 87 | DJ | 2 | Total 2 | Mg 2 | 0 | 0 |
| 87 | DL | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | DM | 2 | Total 2 | Mg 2 | 0 | 0 |
| 87 | DN | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | DO | 8 | Total 8 | Mg 8 | 0 | 0 |
| 87 | DP | 7 | Total 7 | Mg 7 | 0 | 0 |
| 87 | DQ | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | DR | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | DS | 4 | Total 4 | Mg 4 | 0 | 0 |
| 87 | DT | 3 | Total 3 | Mg 3 | 0 | 0 |
| 87 | DV | 3 | Total 3 | Mg 3 | 0 | 0 |
| 87 | DW | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | DY | 2 | Total 2 | Mg 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 87 | Da | 4 | Total 4 | Mg 4 | 0 | 0 |
| 87 | Db | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | Dd | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | De | 2 | Total 2 | Mg 2 | 0 | 0 |
| 87 | Df | 4 | Total 4 | Mg 4 | 0 | 0 |
| 87 | Dg | 2 | Total 2 | Mg 2 | 0 | 0 |
| 87 | Dj | 3 | Total 3 | Mg 3 | 0 | 0 |
| 87 | Di | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | Dm | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | Dn | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | Do | 1 | Total 1 | Mg 1 | 0 | 0 |
| 87 | Dp | 3 | Total 3 | Mg 3 | 0 | 0 |
| 87 | Dq | 1 | Total 1 | Mg 1 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 88 | Aa | 1 | Total 1 | Zn 1 | 0 | 0 |
| 88 | Ab | 1 | Total 1 | Zn 1 | 0 | 0 |
| 88 | Ad | 1 | Total 1 | Zn 1 | 0 | 0 |
| 88 | Af | 1 | Total 1 | Zn 1 | 0 | 0 |
| 88 | Bj | 1 | Total 1 | Zn 1 | 0 | 0 |
| 88 | Bm | 1 | Total 1 | Zn 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 88 | Bo | 1 | Total Zn 1 1 | 0 | 0 |
| 88 | Bp | 1 | Total Zn 1 1 | 0 | 0 |
| 88 | Ca | 1 | Total Zn 1 1 | 0 | 0 |
| 88 | Cb | 1 | Total Zn 1 1 | 0 | 0 |
| 88 | Cd | 1 | Total Zn 1 1 | 0 | 0 |
| 88 | Cf | 1 | Total Zn 1 1 | 0 | 0 |
| 88 | Dj | 1 | Total Zn 1 1 | 0 | 0 |
| 88 | Dm | 1 | Total Zn 1 1 | 0 | 0 |
| 88 | Do | 1 | Total Zn 1 1 | 0 | 0 |
| 88 | Dp | 1 | Total Zn 1 1 | 0 | 0 |

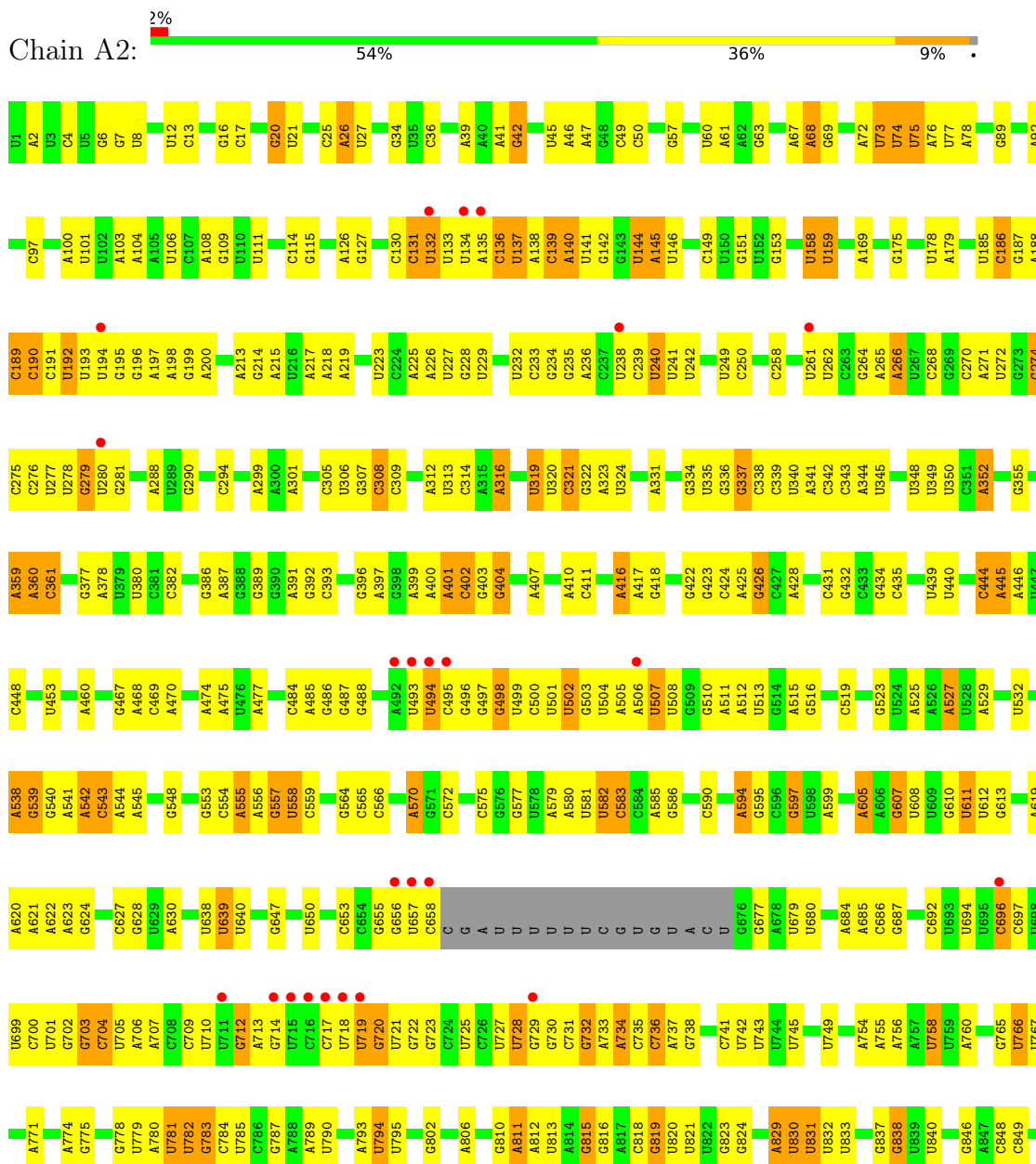
- Molecule 89 is water.

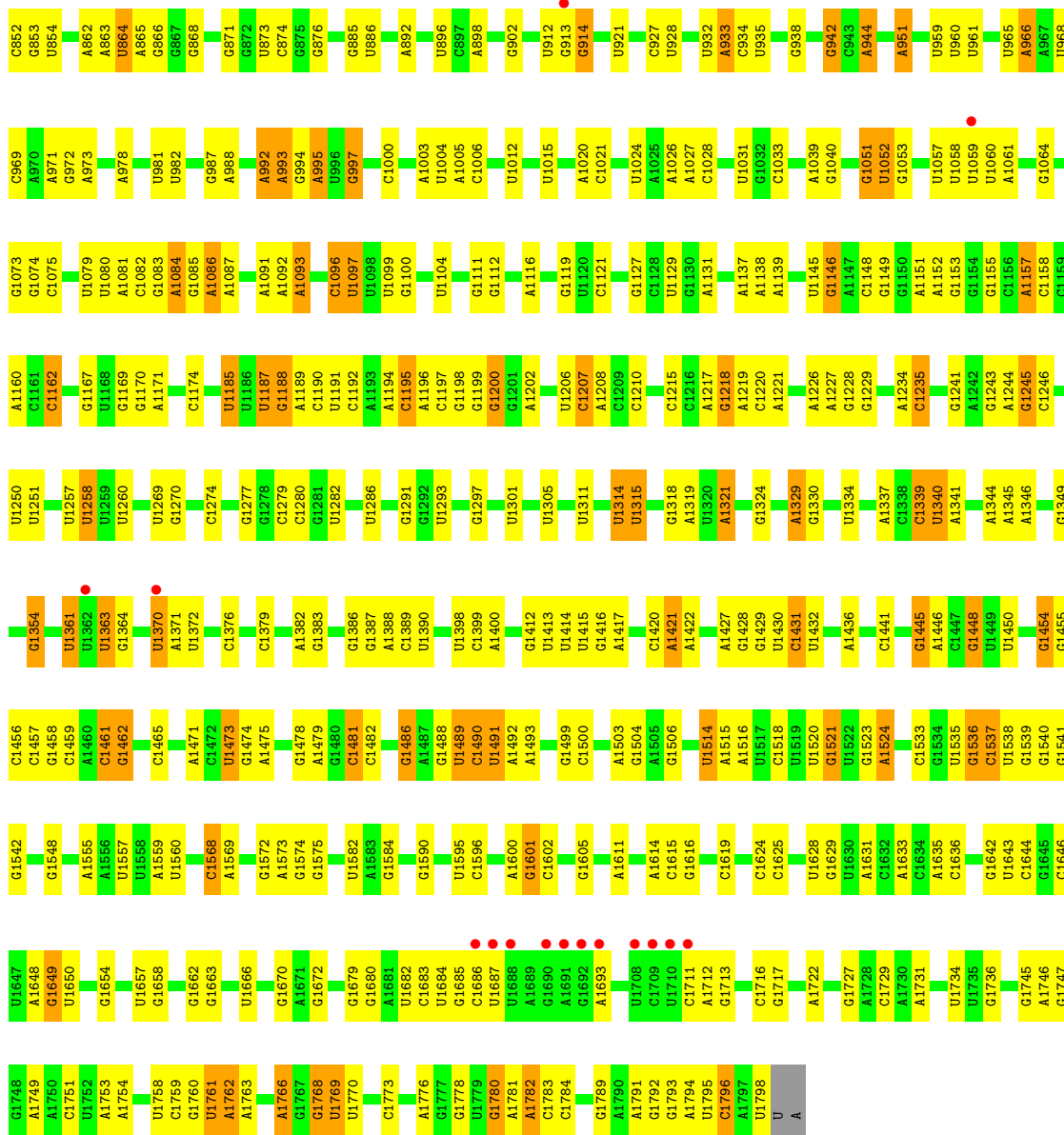
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 89 | CI | 1 | Total O 1 1 | 0 | 0 |
| 89 | DB | 1 | Total O 1 1 | 0 | 0 |

3 Residue-property plots

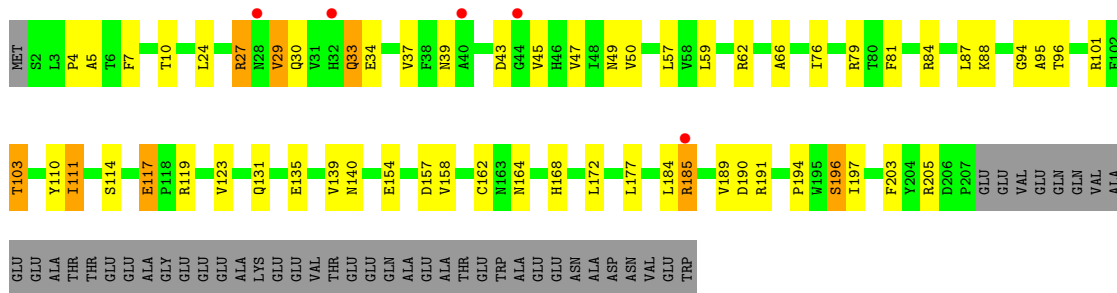
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 18S RIBOSOMAL RNA

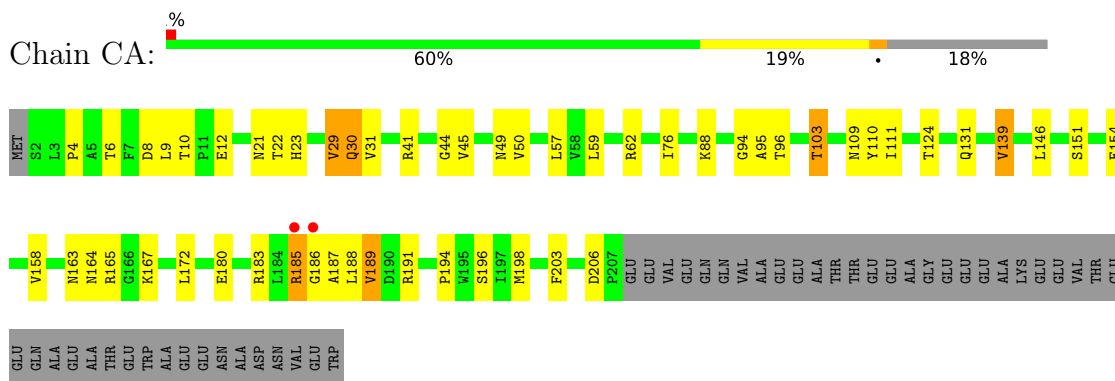




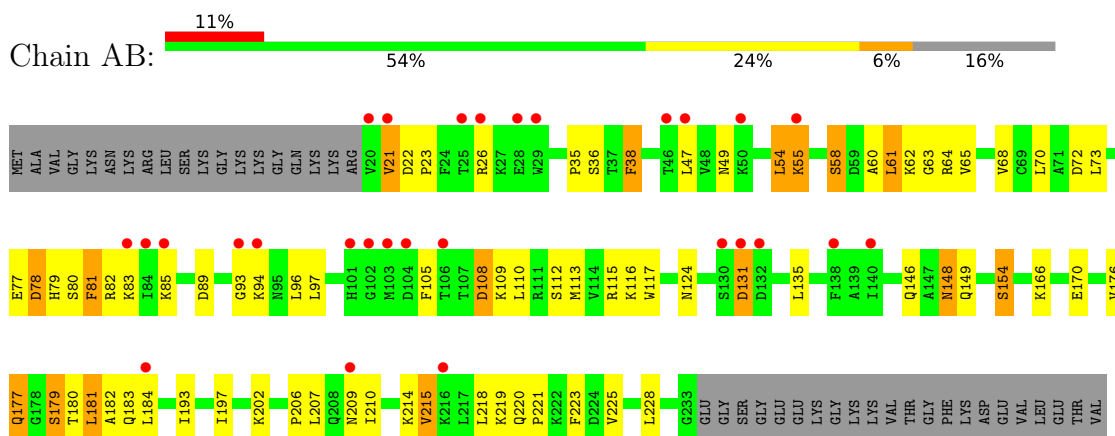
• Molecule 2: 40S ribosomal protein S0-A



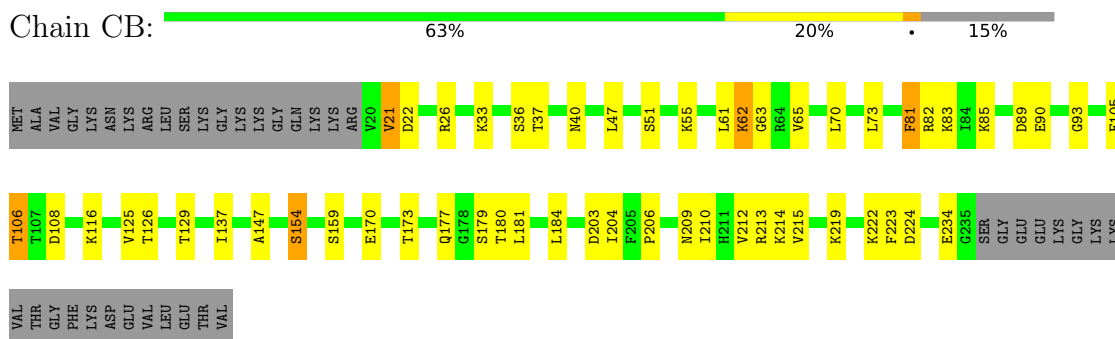
• Molecule 2: 40S ribosomal protein S0-A



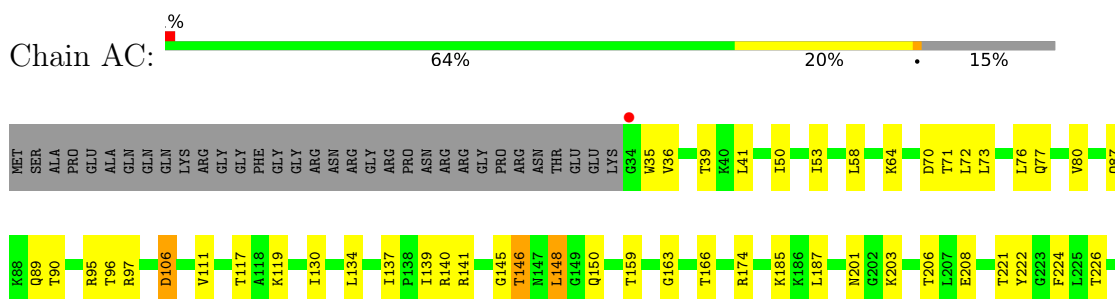
- Molecule 3: 40S ribosomal protein S1-A



- Molecule 3: 40S ribosomal protein S1-A

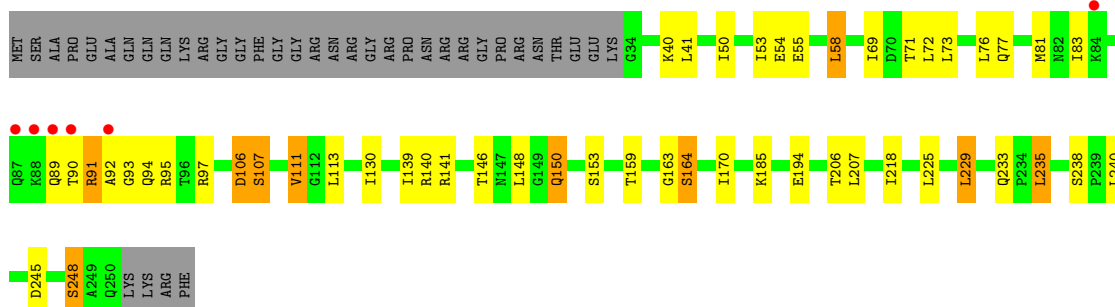


- Molecule 4: 40S ribosomal protein S2

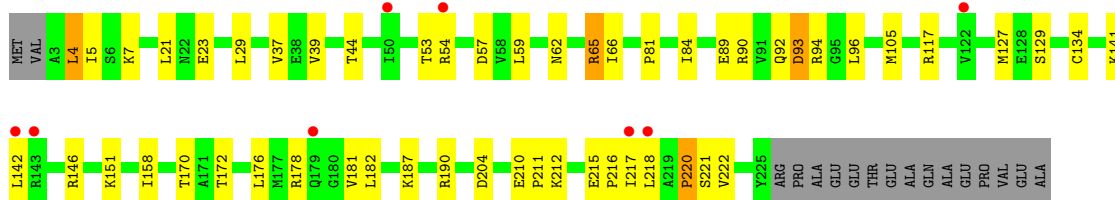
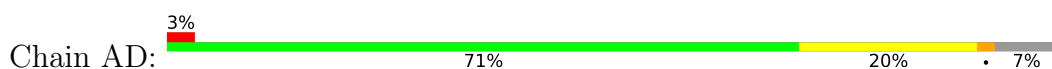




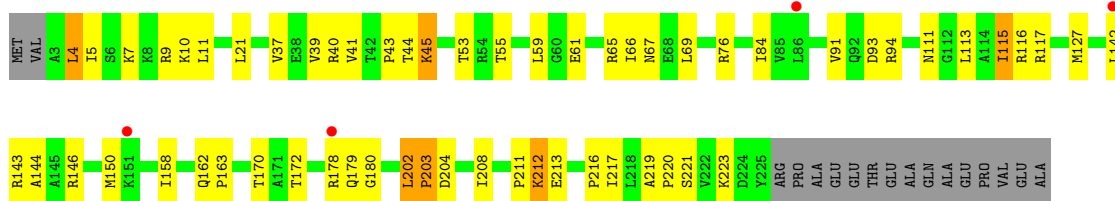
- Molecule 4: 40S ribosomal protein S2



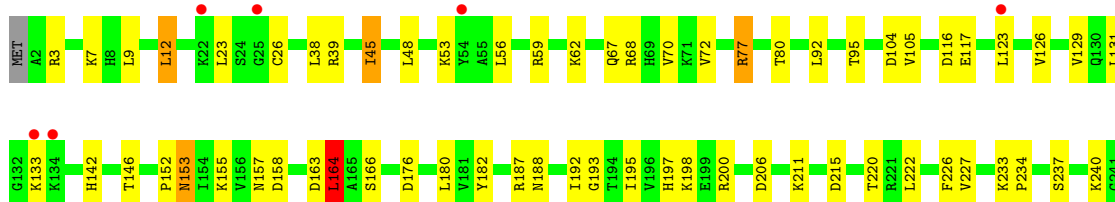
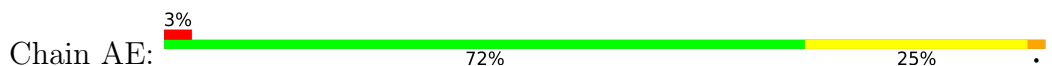
- Molecule 5: 40S ribosomal protein S3



- Molecule 5: 40S ribosomal protein S3



- Molecule 6: 40S ribosomal protein S4-A





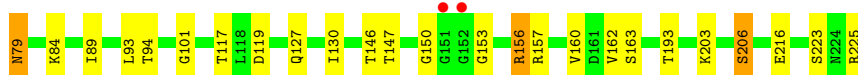
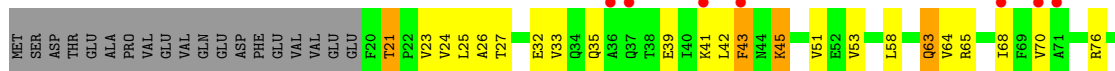
- Molecule 6: 40S ribosomal protein S4-A

Chain CE: 76% 22%



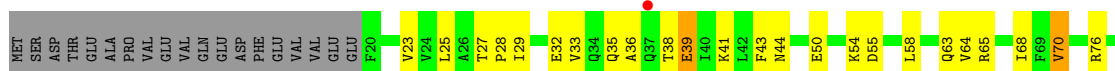
- Molecule 7: 40S ribosomal protein S5

Chain AF: 4% 70% 18% 8%



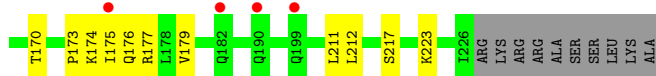
- Molecule 7: 40S ribosomal protein S5

Chain CF: 3% 66% 24% 8%



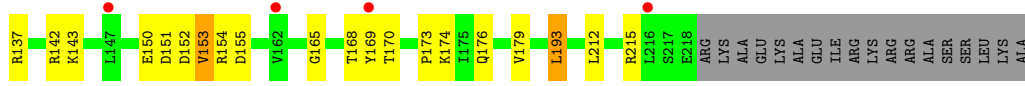
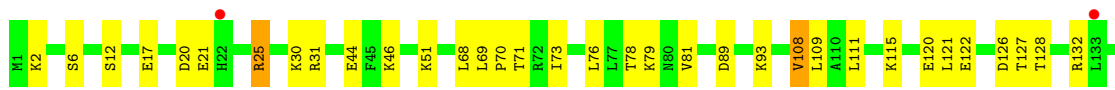
- Molecule 8: 40S ribosomal protein S6-A

Chain AG: 3% 76% 17%

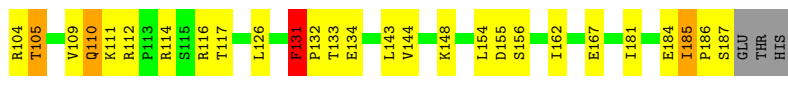
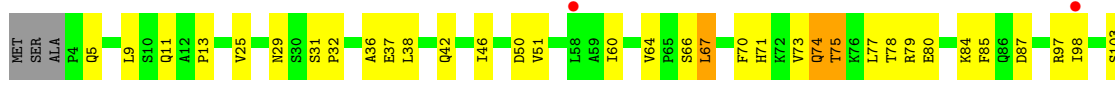


- Molecule 8: 40S ribosomal protein S6-A

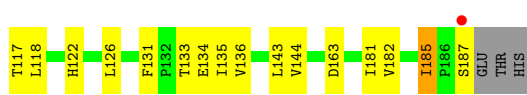
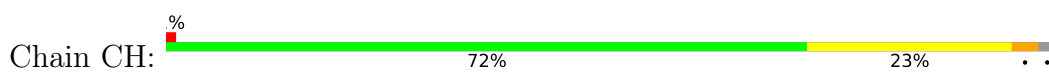
Chain CG: 3% 69% 21% 8%



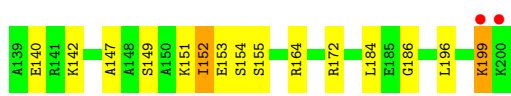
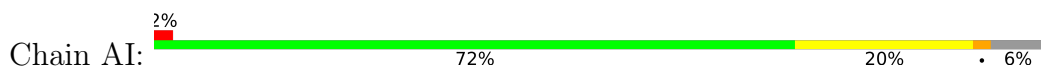
• Molecule 9: 40S ribosomal protein S7-A



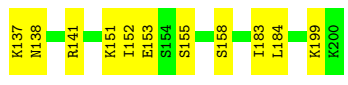
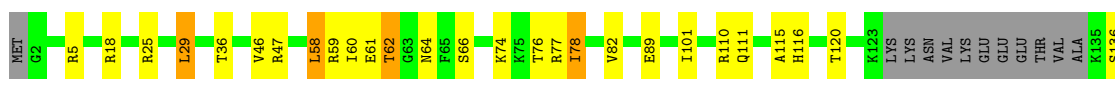
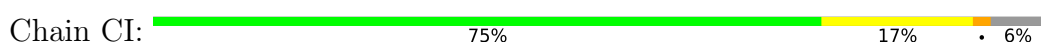
• Molecule 9: 40S ribosomal protein S7-A



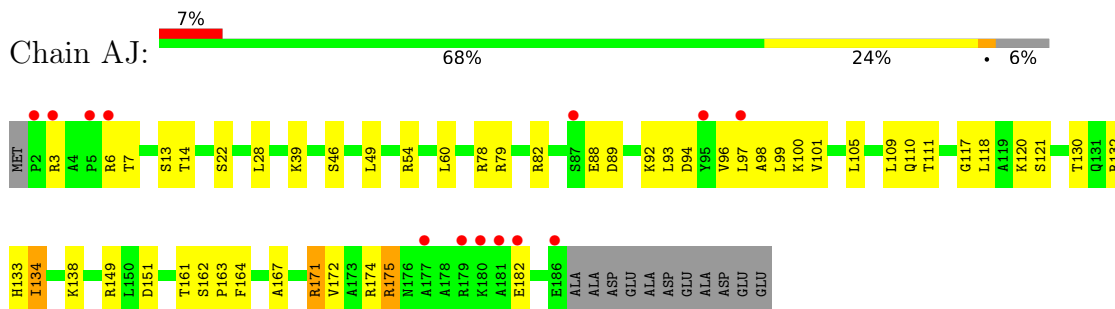
• Molecule 10: 40S ribosomal protein S8-A



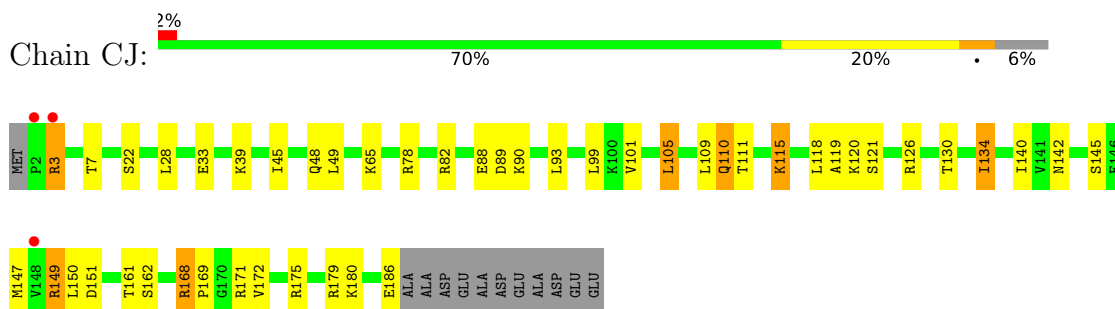
• Molecule 10: 40S ribosomal protein S8-A



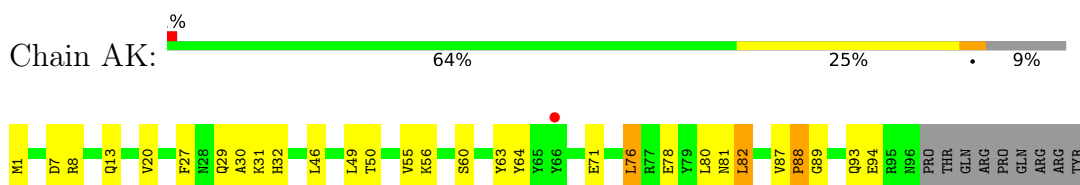
- Molecule 11: 40S ribosomal protein S9-A



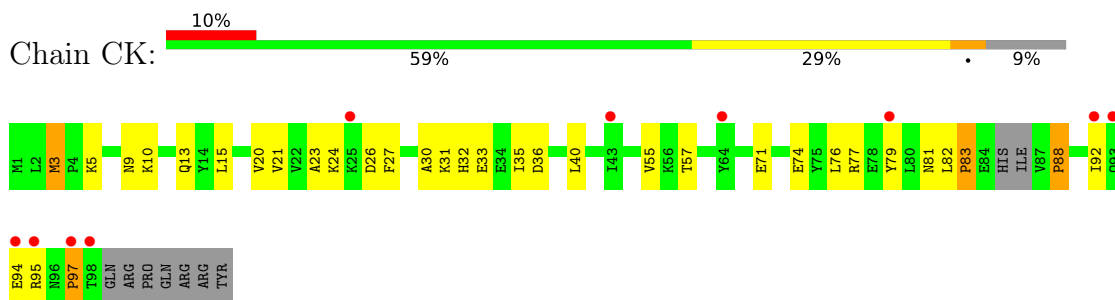
- Molecule 11: 40S ribosomal protein S9-A



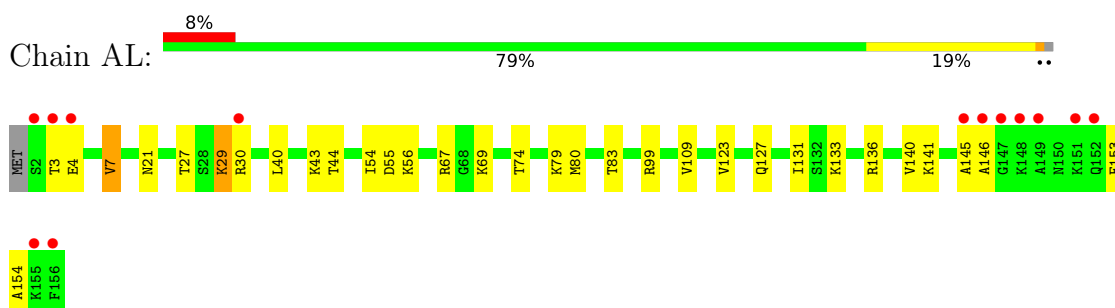
- Molecule 12: 40S ribosomal protein S10-A



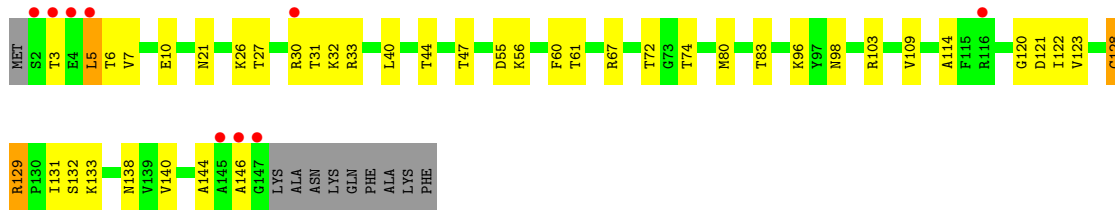
- Molecule 12: 40S ribosomal protein S10-A



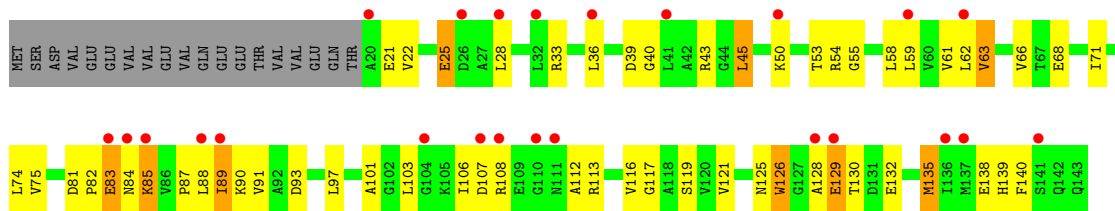
- Molecule 13: 40S ribosomal protein S11-A



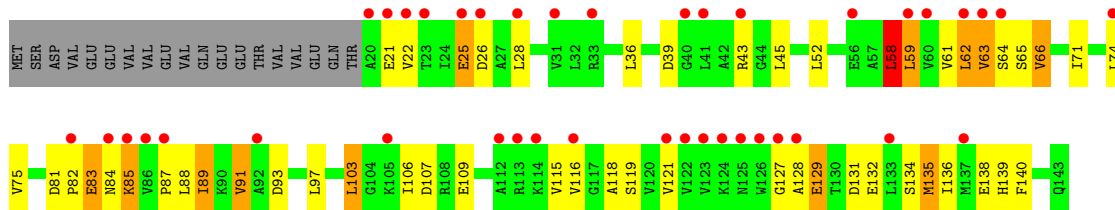
• Molecule 13: 40S ribosomal protein S11-A



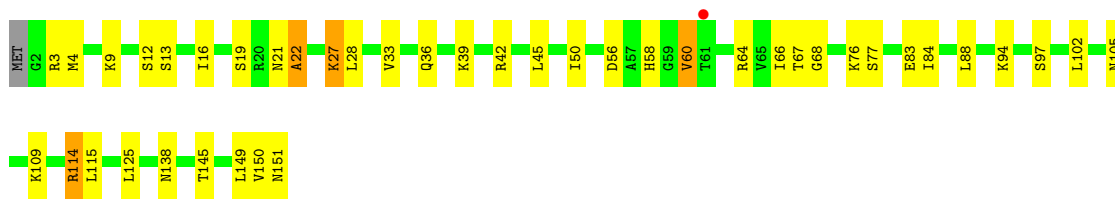
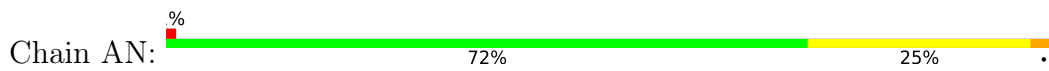
• Molecule 14: 40S ribosomal protein S12



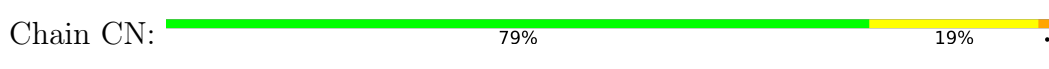
• Molecule 14: 40S ribosomal protein S12



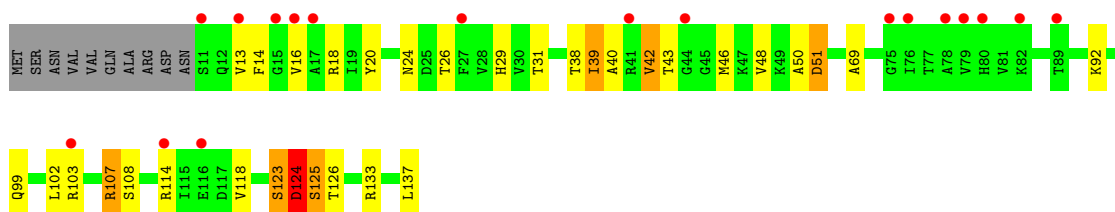
• Molecule 15: 40S ribosomal protein S13



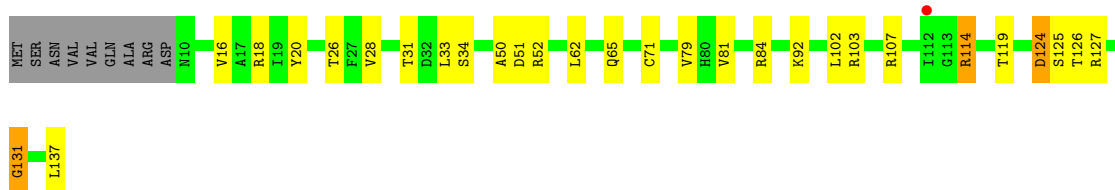
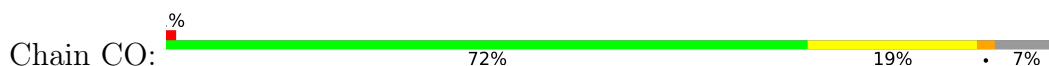
• Molecule 15: 40S ribosomal protein S13



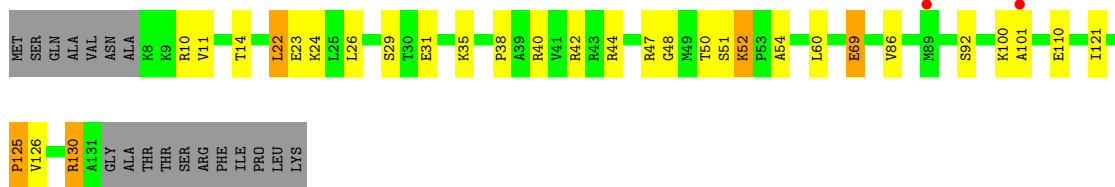
- Molecule 16: 40S ribosomal protein S14-A



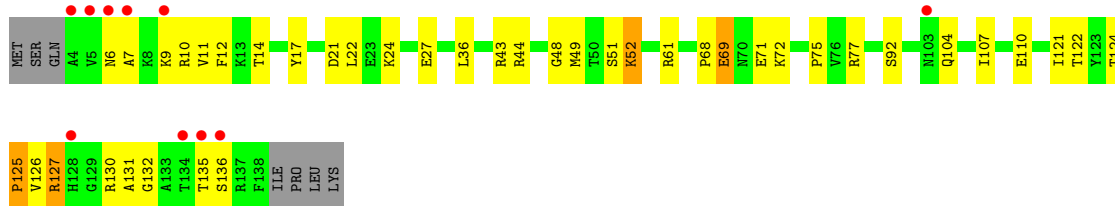
- Molecule 16: 40S ribosomal protein S14-A



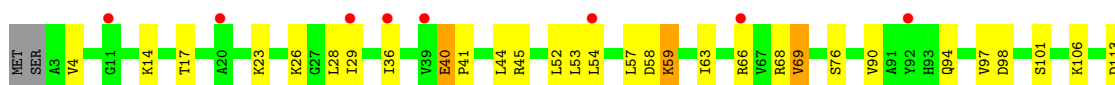
- Molecule 17: 40S ribosomal protein S15



- Molecule 17: 40S ribosomal protein S15

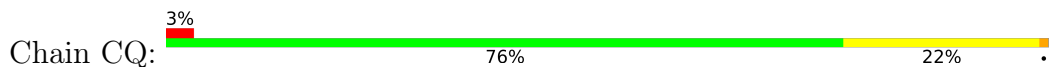


- Molecule 18: 40S ribosomal protein S16-A





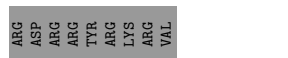
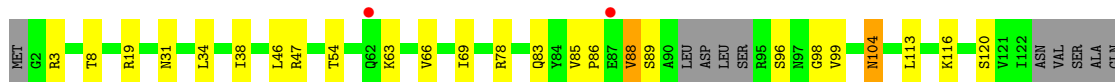
- Molecule 18: 40S ribosomal protein S16-A



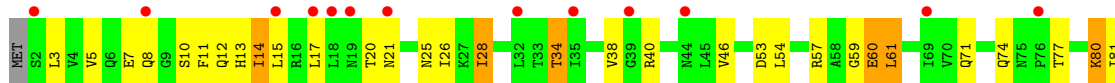
- Molecule 19: 40S ribosomal protein S17-A



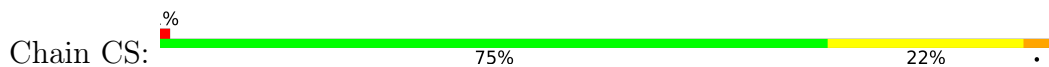
- Molecule 19: 40S ribosomal protein S17-A



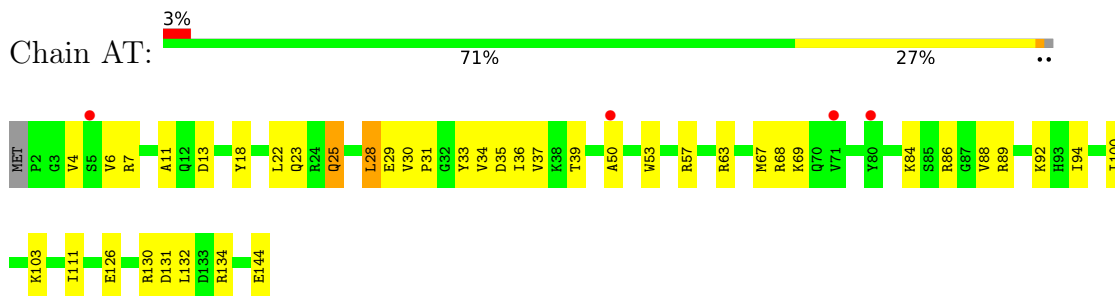
- Molecule 20: 40S ribosomal protein S18-A



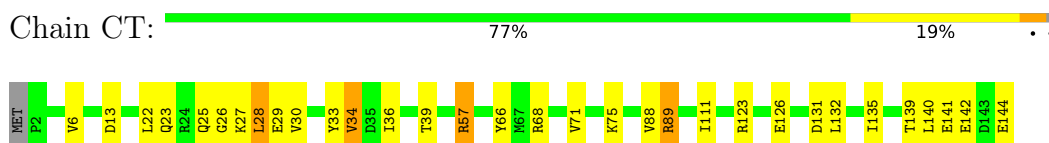
- Molecule 20: 40S ribosomal protein S18-A



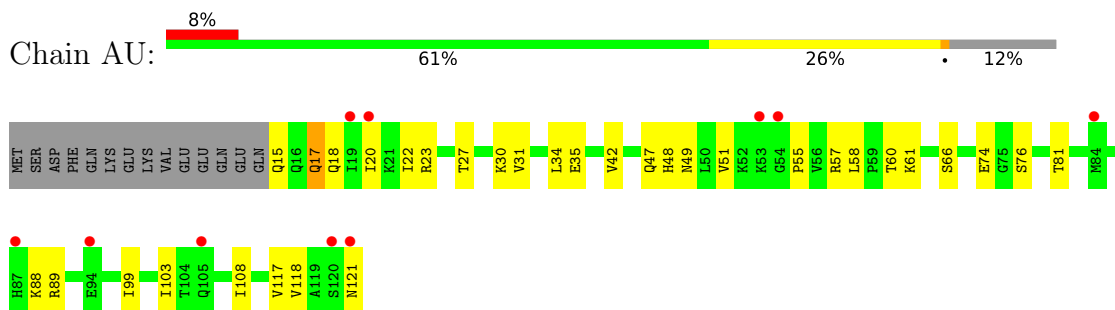
- Molecule 21: 40S ribosomal protein S19-A



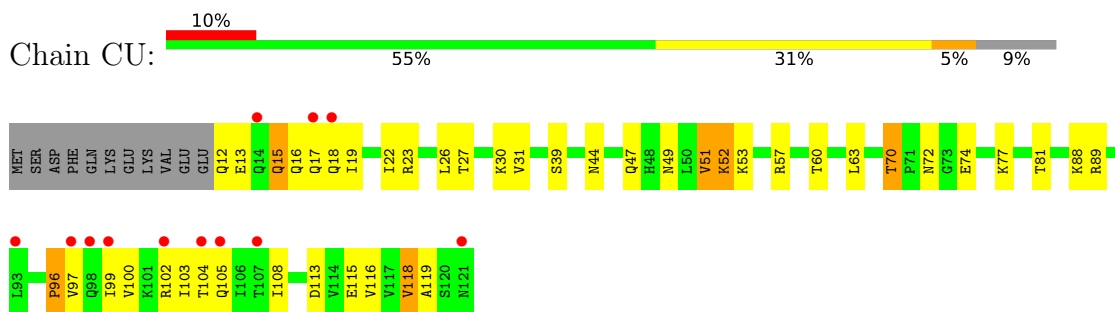
- Molecule 21: 40S ribosomal protein S19-A



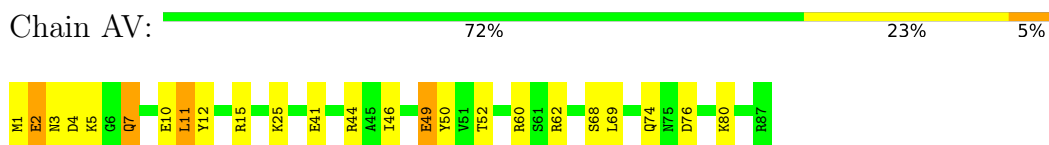
- Molecule 22: 40S ribosomal protein S20



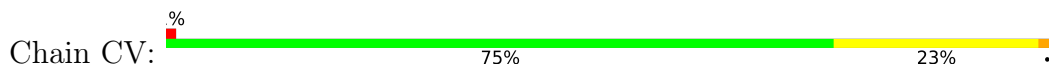
- Molecule 22: 40S ribosomal protein S20



- Molecule 23: 40S ribosomal protein S21-A



- Molecule 23: 40S ribosomal protein S21-A





- Molecule 24: 40S ribosomal protein S22-A

Chain AW: 78% 17% ..



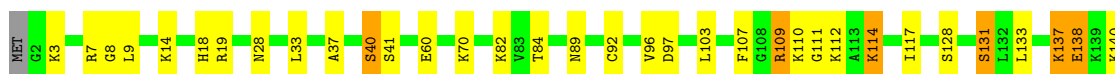
- Molecule 24: 40S ribosomal protein S22-A

Chain CW: 88% 10% ..



- Molecule 25: 40S ribosomal protein S23-A

Chain AX: 75% 19% 5% ..



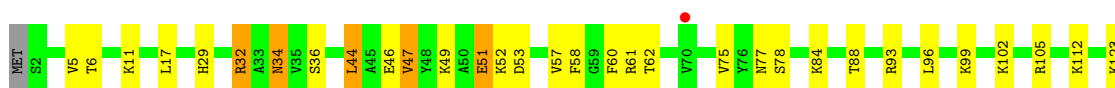
- Molecule 25: 40S ribosomal protein S23-A

Chain CX: 83% 15% ..



- Molecule 26: 40S ribosomal protein S24-A

Chain AY: 72% 24% ..

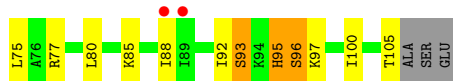
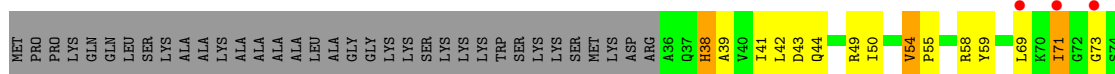


- Molecule 26: 40S ribosomal protein S24-A

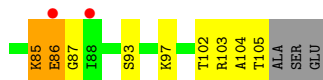
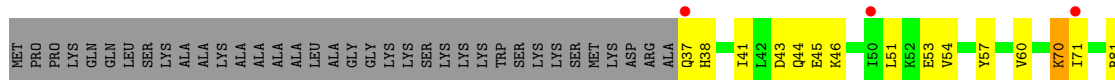
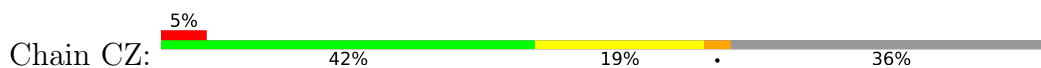
Chain CY: 73% 24% ..



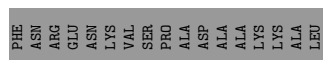
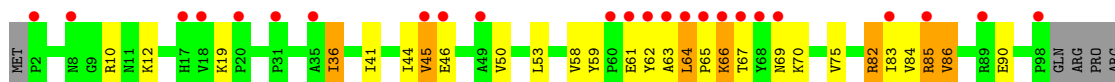
• Molecule 27: 40S ribosomal protein S25-A



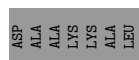
• Molecule 27: 40S ribosomal protein S25-A



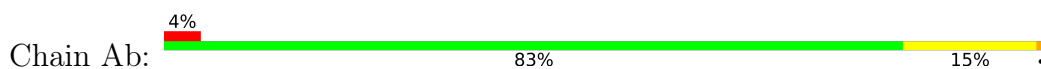
• Molecule 28: 40S ribosomal protein S26-A

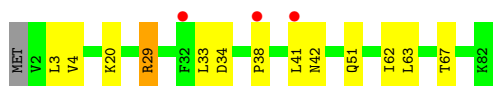


• Molecule 28: 40S ribosomal protein S26-A



• Molecule 29: 40S ribosomal protein S27-A

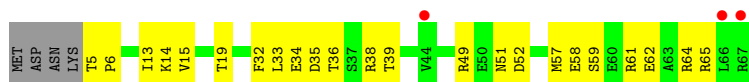




- Molecule 29: 40S ribosomal protein S27-A



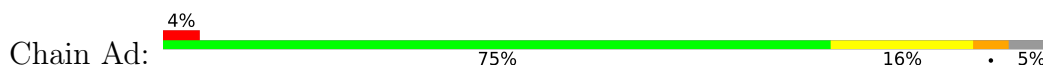
- Molecule 30: 40S ribosomal protein S28-A



- Molecule 30: 40S ribosomal protein S28-A



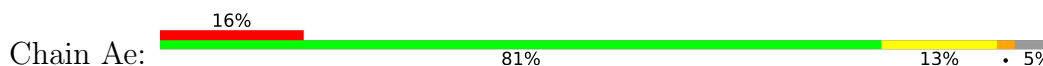
- Molecule 31: 40S ribosomal protein S29-A



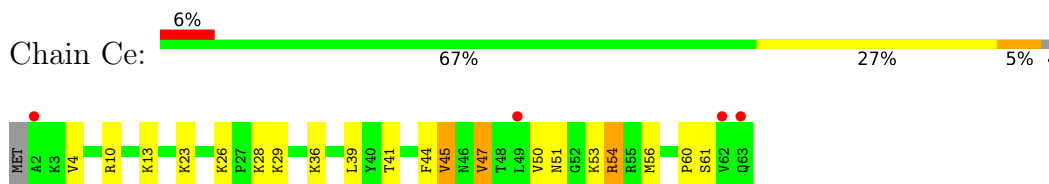
- Molecule 31: 40S ribosomal protein S29-A



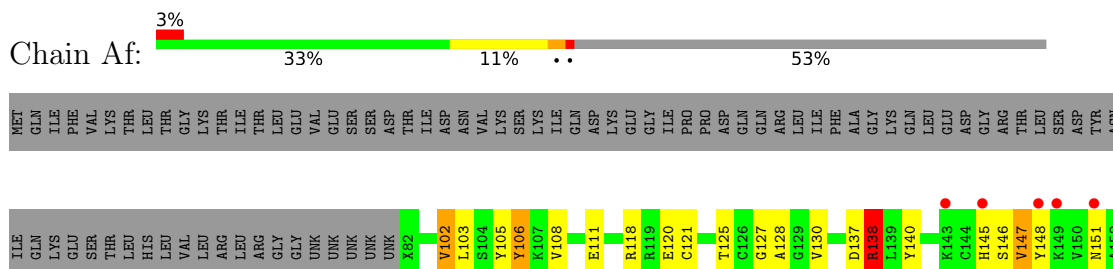
- Molecule 32: 40S ribosomal protein S30-A



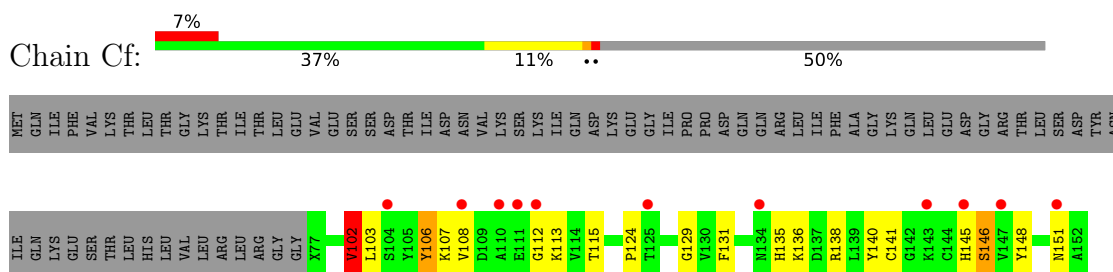
- Molecule 32: 40S ribosomal protein S30-A



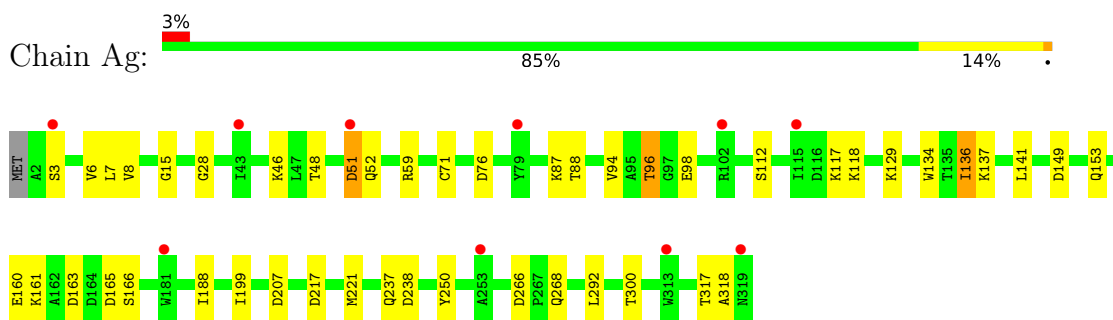
- Molecule 33: 40S ribosomal protein S31



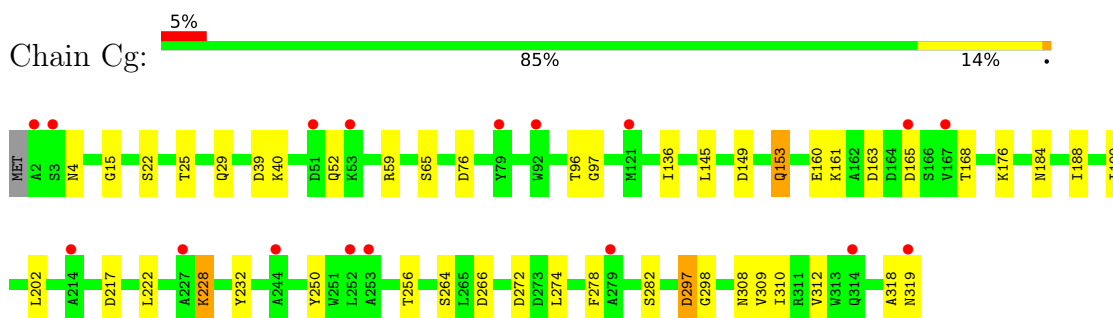
- Molecule 33: 40S ribosomal protein S31



- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein (ASC1, RACK1)



- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein (ASC1, RACK1)



- Molecule 35: Suppressor protein STM1



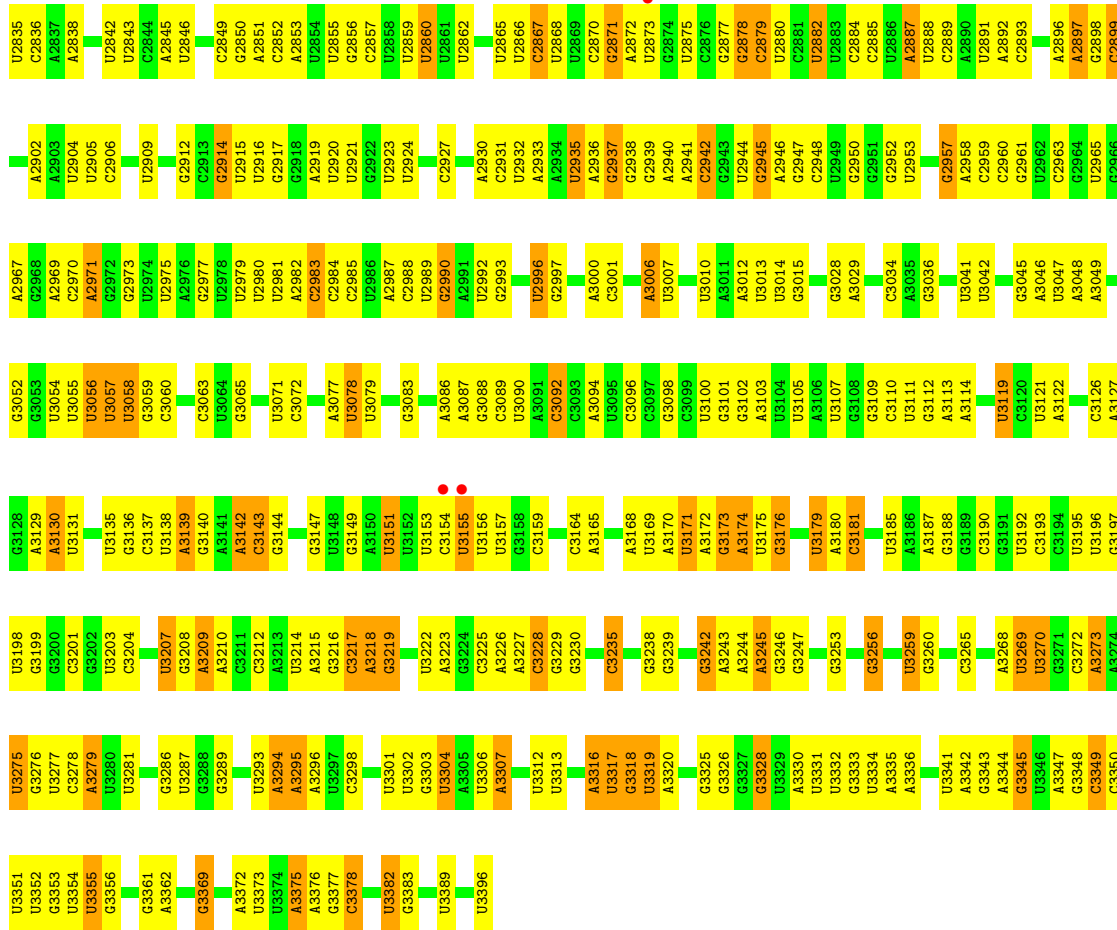
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|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|--|
| MET | SER | ASN | PRO | LYS | PHE | ASP | LEU | LEU | X9 | S28 | K34 | K46 | A47 | R51 | P52 | R53 | I61 | K64 | T65 | R68 | D75 | D78 | T82 | K83 | K84 | S85 | I86 | T87 | R88 | R89 | H94 | S95 | R96 | T97 | T100 | D101 | T102 | K105 | D112 | E130 | D134 | E139 | D140 | | | | | | | | | |
| GLY | LYS | PRO | C73 | THR | ALA | GLN | LEU | SER | X151 | K176 | GLU | ARG | ILE | GLY | GLU | THR | ALA | GLU | LYS | TVR | VAL | PRO | ALA | ASN | VAL | THR | LYS | VAL | GLN | ASN | THR | LEU | ILE | ASP | VAL | LEU | ASN | PHE | ALA | THR | PHE | VAL | GLU | ASN | ASN | THR | ARG | LYS | ASN | PHE | GLY | |
| ASP | ARG | ASN | ASN | ASN | THR | ASN | ASN | PHE | ASN | ASN | ARG | GLY | GLY | GLY | GLY | ALA | ARG | LYS | GLY | ASN | ASN | ALA | THR | ALA | ASN | THR | THR | GLN | LYS | ASN | ARG | ASN | ILE | ASP | VAL | SER | LEU | LEU | PRO | SER | LEU | ALA | ALA | | | | | | | | | |

● Molecule 36: 25S rRNA

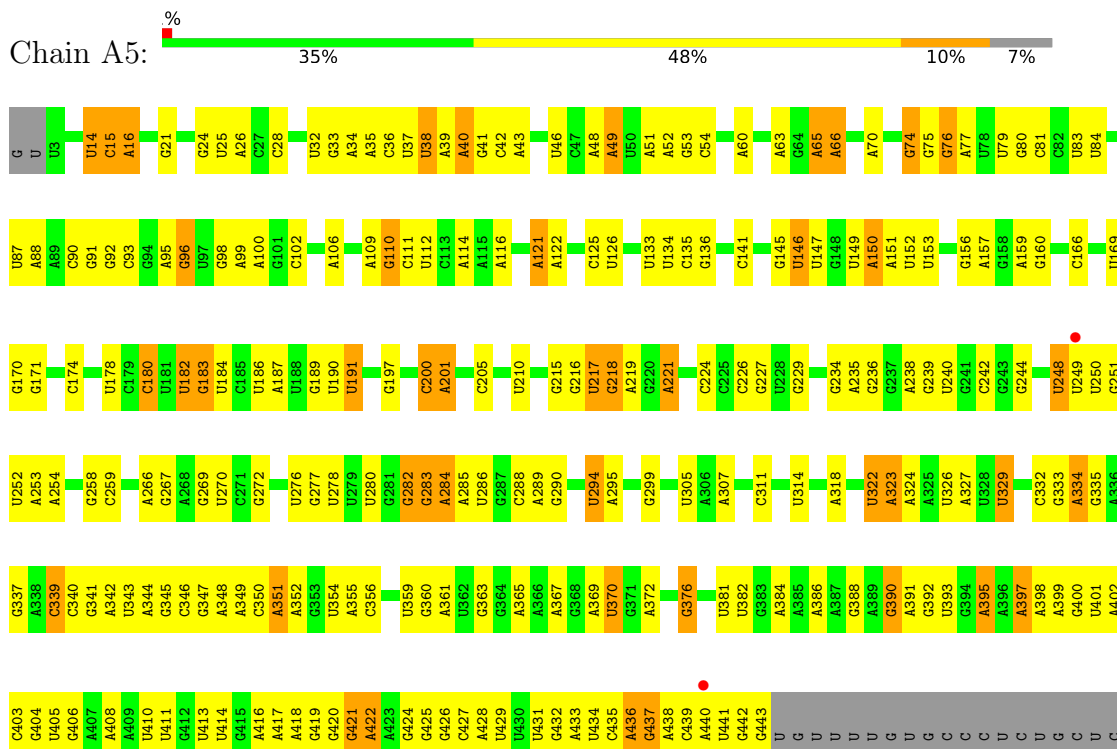


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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| G | U | U3 | A13 | A14 | C15 | A16 | G17 | G18 | U19 | A20 | G21 | G22 | A23 | G24 | U25 | A26 | C27 | C28 | C29 | G30 | C31 | U32 | G33 | A34 | A35 | C36 | U37 | U38 | G39 | A39 | A40 | G41 | C42 | A43 | G44 | U44 | U45 | U46 | C47 | A48 | A49 | U50 | A51 | A52 | G53 | C54 | G55 | G56 | A57 | G58 | G59 | A60 | A61 | A62 | A63 | G64 | A65 | A66 | A67 | C68 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
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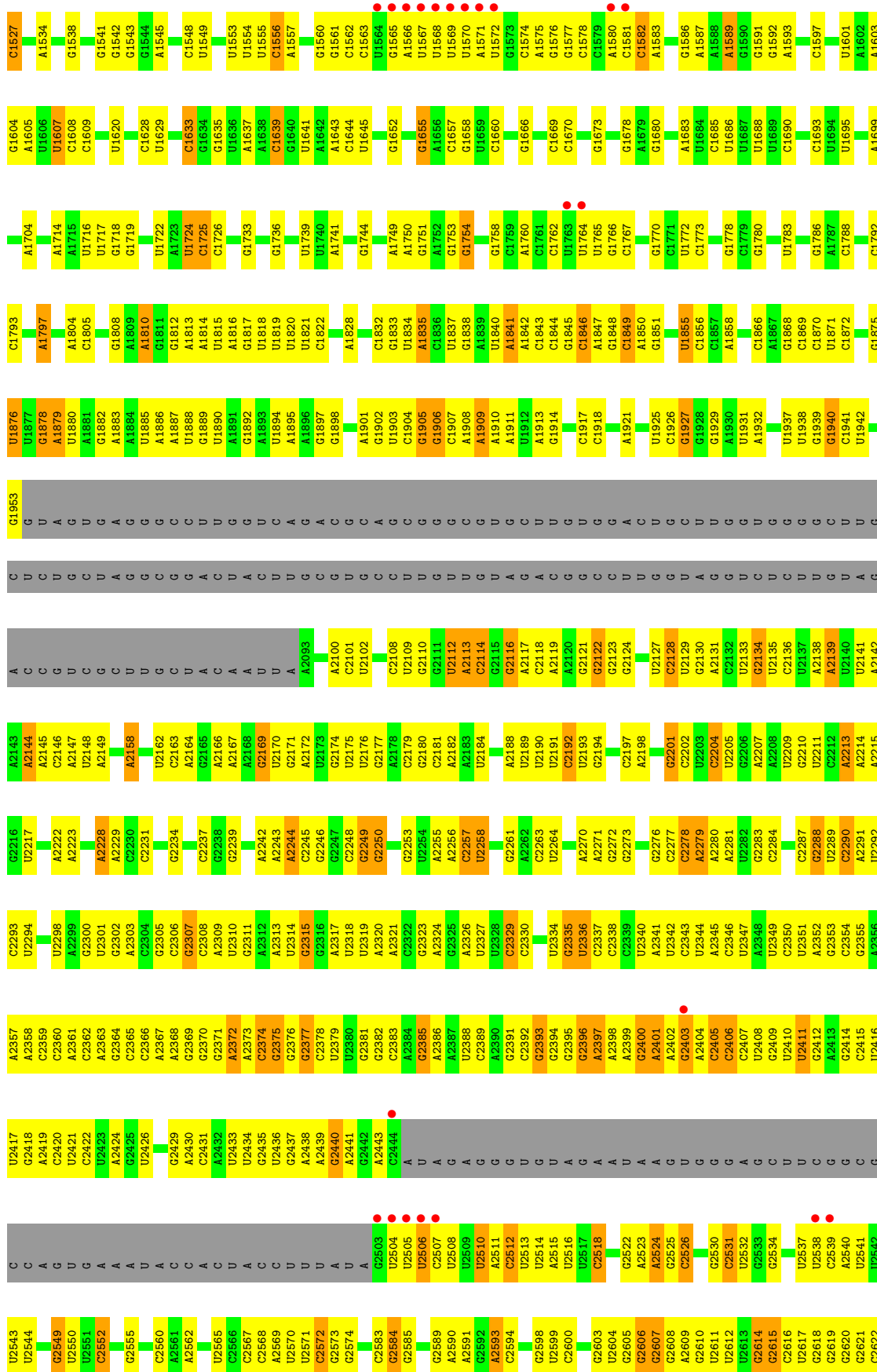
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| C1762 | G1640 | U1553 | A1481 | C1411 | A1350 | C1279 | A1203 | G1139 | A1065 | U987 | U922 | A858 | A786 |
| U1763 | A1643 | U1554 | A1482 | G1414 | U1351 | C1280 | A1204 | G1140 | U1071 | U988 | C923 | G859 | G787 |
| U1764 | U1555 | C1556 | U1483 | G1415 | A1352 | G1281 | G1209 | C1141 | G1072 | A989 | G924 | G860 | C788 |
| G1766 | C1644 | U1557 | U1484 | C1416 | U1353 | G1285 | U1210 | G1142 | U1073 | G994 | G925 | C861 | A789 |
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| | | G1560 | A1487 | A1419 | G1357 | | G1213 | C1146 | C1076 | A929 | C929 | G864 | C792 |
| | | G1561 | A1489 | C1420 | C1358 | C1292 | U1214 | G1147 | A998 | U930 | U930 | G867 | C793 |
| | | C1562 | A1490 | G1421 | U1359 | U1293 | U1215 | G1148 | A999 | G999 | G931 | G868 | U794 |
| | | C1563 | G1491 | G1422 | C1360 | U1294 | C1216 | G1149 | G999 | C1000 | U932 | G869 | U795 |
| | | G1492 | G1492 | G1422 | A1361 | A1294 | A1217 | A1149 | A1080 | U932 | U932 | G870 | U796 |
| | | G1493 | G1493 | U1425 | U1362 | G1295 | U1217 | A1150 | U1081 | A933 | A933 | G871 | U797 |
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| | | U1567 | C1496 | | C1364 | C1298 | G1222 | A1153 | A1083 | A936 | A936 | C873 | G800 |
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| | | U1582 | U1508 | | C1376 | G1310 | U1237 | G1167 | G1019 | C949 | C949 | U889 | G812 |
| | | U1583 | A1509 | | G1377 | G1311 | C1238 | A1167 | A1102 | U950 | G950 | U889 | G813 |
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| | | G1585 | U1511 | | G1379 | G1313 | U1240 | A1169 | A1104 | A952 | A952 | G891 | U815 |
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| | | U1606 | U1522 | | A1393 | A1331 | U1252 | U1180 | G1117 | U826 | G964 | G902 | G826 |
| | | U1607 | U1523 | | A1394 | A1332 | U1253 | U1181 | C1118 | U829 | A965 | U903 | U829 |
| | | C1608 | G1524 | | G1395 | A1333 | U1254 | A1182 | C1119 | A830 | U966 | A904 | A830 |
| | | G1610 | U1526 | | C1396 | A1334 | U1255 | C1183 | C1120 | G831 | A967 | U905 | A831 |
| | | C1615 | A1527 | | U1398 | U1334 | G1262 | A1184 | U1121 | G832 | G968 | G907 | G832 |
| | | U1616 | G1528 | | A1399 | C1335 | U1263 | G1186 | U1122 | U835 | C969 | G908 | U835 |
| | | G1616 | U1529 | | G1400 | A1336 | U1264 | C1187 | U1123 | A836 | A970 | G909 | A836 |
| | | U1617 | A1537 | | A1401 | A1337 | G1265 | U1189 | U1124 | U837 | G971 | G910 | U837 |
| | | U1746 | G1543 | | C1402 | C1338 | U1266 | U1190 | U1125 | G910 | A972 | G910 | G910 |
| | | G1747 | U1546 | | C1403 | G1340 | G1267 | U1191 | G1126 | C911 | A973 | C911 | A843 |
| | | A1750 | A1547 | | G1404 | U1342 | U1268 | C1192 | G1127 | G912 | G974 | G912 | A847 |
| | | U1624 | G1548 | | U1405 | C1342 | A1270 | A1192 | A1130 | A914 | C975 | A914 | A847 |
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| | | U1629 | A1551 | | A1407 | G1345 | C1272 | A1197 | C1132 | C849 | A980 | A916 | C849 |
| | | U1634 | U1550 | | G1408 | G1346 | A1273 | C1198 | U1133 | U850 | A980 | A917 | U850 |
| | | | C1551 | | U1549 | U1347 | A1274 | C1189 | A1057 | U851 | C982 | A918 | C851 |
| | | | U1551 | | G1409 | U1347 | | A1200 | U1060 | U854 | A983 | U919 | G854 |
| | | | U1552 | | U1478 | G1409 | | A1201 | A1060 | A920 | G984 | A920 | G857 |
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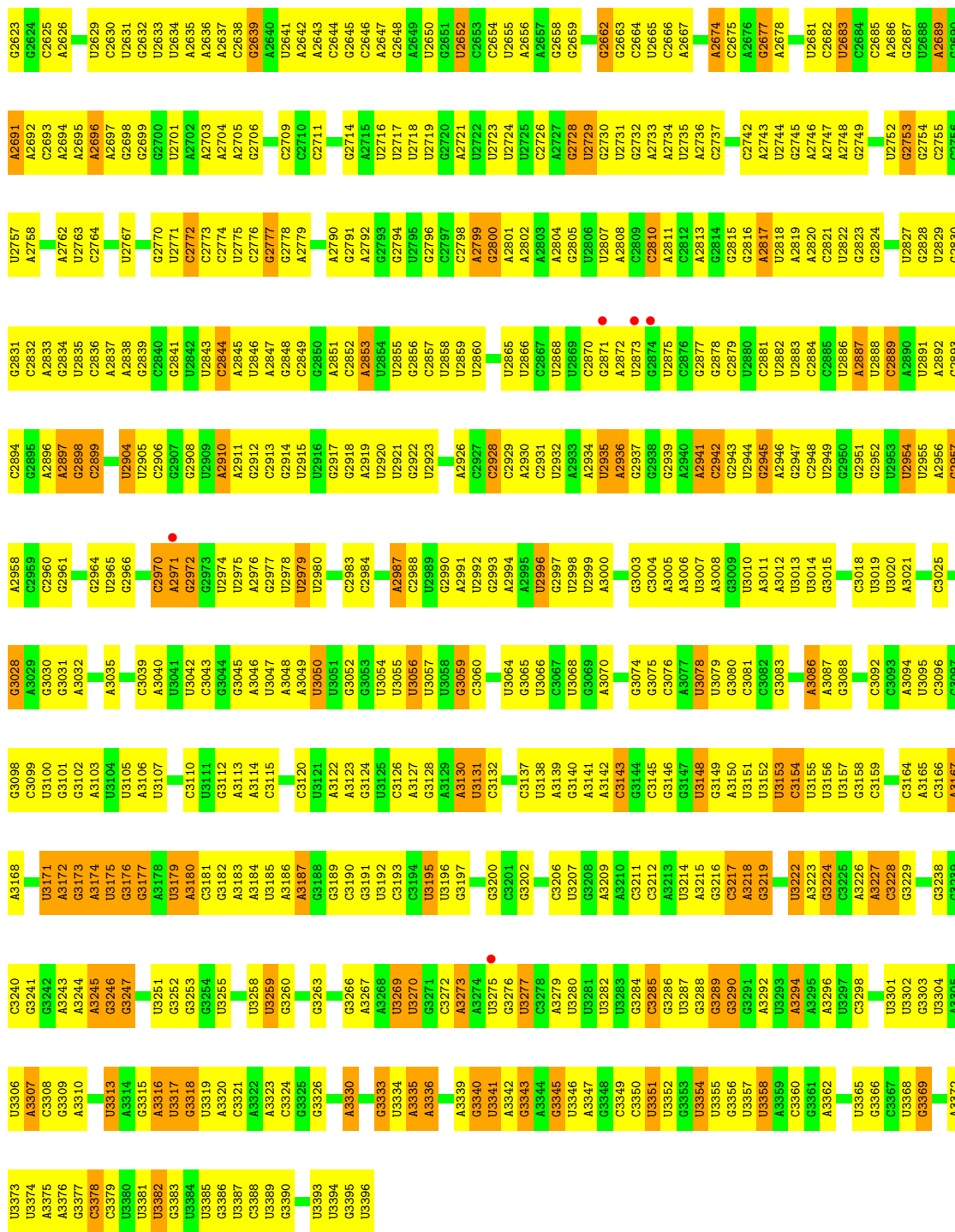


● Molecule 36: 25S rRNA

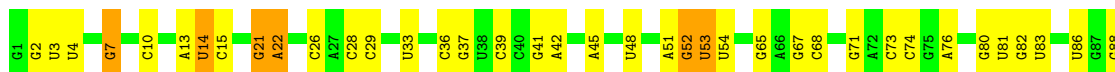


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| U1457 | U1462 | A1330 | A1244 | U1173 | G1112 | G1029 | U966 | U905 | C839 | U768 | U681 | A619 | U | |
| U1458 | A1460 | U1331 | A1245 | C1174 | G1113 | U1033 | A967 | A906 | G840 | G769 | G692 | U620 | G | |
| C1459 | A1460 | A1332 | G1246 | C1175 | G1114 | U1032 | G968 | G907 | C841 | U770 | G688 | A621 | U | |
| A1461 | A1461 | C1335 | U1247 | G1176 | G1115 | U1033 | C969 | G909 | A842 | U771 | U689 | A622 | G | |
| A1462 | A1463 | U1336 | C1248 | G1177 | G1116 | U1034 | A970 | G910 | G843 | U772 | G693 | U623 | G | |
| U1463 | U1463 | A1337 | U1258 | G1178 | G1117 | G1035 | G971 | G911 | A843 | U773 | A690 | G624 | G | |
| G1466 | C1403 | C1338 | A1259 | A1179 | C1118 | A1040 | A972 | C911 | G844 | G779 | A691 | G625 | U | |
| A1467 | C1402 | C1339 | G1262 | U1180 | C1119 | A1041 | A973 | G912 | G845 | A780 | A692 | U626 | A | |
| A1468 | U1405 | A1341 | G1263 | U1181 | C1120 | U1041 | A974 | A913 | A846 | A780 | A693 | U627 | G | |
| C1469 | A1406 | C1342 | G1264 | C1183 | U1121 | U1042 | C975 | A914 | A847 | U782 | A628 | A628 | G | |
| G1473 | A1407 | A1343 | U1265 | A1184 | U1123 | U1044 | U976 | G916 | A848 | A783 | U629 | G652 | G | |
| G1476 | G1408 | G1346 | G1266 | C1187 | U1124 | C1045 | U979 | A917 | C851 | G785 | A630 | U631 | G | |
| A1477 | G1409 | U1347 | U1267 | U1189 | U1125 | A1046 | A980 | C918 | U852 | A786 | U632 | G632 | A | |
| G1480 | U1411 | U1348 | A1270 | C1188 | G1126 | A1047 | U981 | U919 | G857 | G787 | G633 | U633 | A | |
| A1481 | G1412 | U1349 | G1281 | U1189 | U1127 | A1048 | C982 | A920 | U859 | A705 | U634 | C634 | U | |
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| U1491 | C1426 | G1362 | A1294 | C1199 | U1135 | U1060 | A992 | C928 | G867 | A716 | U642 | U642 | U | |
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| C1496 | U1430 | U1366 | A1304 | U1209 | G1139 | U1065 | A996 | A933 | U872 | G721 | A646 | C577 | U | |
| G1500 | G1431 | U1367 | U1305 | G1209 | U1140 | A1080 | A997 | A934 | U873 | G722 | A647 | A578 | G | |
| U1501 | C1432 | U1368 | G1306 | U1210 | G1141 | U1081 | A998 | U935 | U874 | G725 | C648 | G493 | G | |
| A1502 | A1433 | A1369 | G1307 | U1211 | G1142 | U1082 | G999 | U936 | U875 | G726 | C649 | G494 | U | |
| A1503 | G1434 | G1370 | A1308 | G1212 | U1143 | U1083 | C1000 | A937 | U876 | U727 | C650 | C580 | U | |
| A1504 | A1435 | G1371 | A1309 | G1213 | U1144 | U1084 | G1001 | G938 | U877 | G728 | G651 | C581 | U | |
| C1505 | U1436 | G1372 | G1310 | U1214 | G1145 | A1085 | A1002 | C939 | G878 | A734 | G652 | G584 | U | |
| A1506 | G1437 | A1373 | G1311 | U1215 | G1146 | U1086 | A1003 | G940 | U879 | C734 | G653 | A585 | U | |
| G1507 | U1438 | G1374 | C1312 | C1216 | U1148 | U1087 | U1004 | G941 | U880 | A735 | C654 | A586 | U | |
| C1508 | A1439 | G1375 | G1313 | U1220 | G1149 | U1088 | U1007 | U942 | C881 | A736 | C655 | U508 | U | |
| A1509 | G1440 | C1376 | C1314 | U1220 | U1150 | A1088 | U1008 | U943 | U882 | A657 | G656 | U509 | U | |
| G1510 | U1441 | G1377 | U1315 | A1221 | U1151 | U1089 | G1009 | U944 | A883 | G657 | G588 | G510 | U | |
| U1511 | U1442 | U1378 | C1316 | G1222 | G1152 | U1090 | A1010 | C945 | A884 | U741 | A658 | G511 | U | |
| U1512 | G1443 | G1379 | A1317 | A1223 | U1153 | G1087 | G1010 | U946 | A884 | C742 | G659 | G591 | U | |
| G1513 | G1444 | U1380 | A1318 | C1232 | C1161 | U1088 | C1017 | C947 | G887 | A744 | A660 | A592 | U | |
| A1514 | U1445 | A1381 | G1319 | U1232 | G1162 | A1088 | C1018 | C948 | A888 | C745 | G661 | A592 | U | |
| A1515 | A1446 | G1382 | C1320 | G1233 | U1163 | U1099 | G1018 | C949 | U889 | G745 | C593 | A516 | U | |
| C1516 | G1447 | G1383 | G1321 | U1236 | G1164 | U1100 | G1019 | U950 | C890 | C749 | A666 | A516 | U | |
| G1517 | U1448 | U1384 | U1322 | G1237 | A1165 | G1101 | U1014 | C951 | C891 | G749 | A666 | G517 | U | |
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| G1450 | G1450 | A1386 | U1324 | C1238 | U1167 | U1103 | C1016 | U953 | U892 | A751 | G600 | A519 | U | |
| C1451 | U1451 | G1387 | U1325 | C1239 | U1168 | G1104 | C1017 | U954 | C893 | C752 | U669 | A520 | U | |
| U1524 | C1452 | A1388 | A1326 | A1240 | U1169 | C1107 | G1018 | U955 | G894 | C753 | G604 | A521 | U | |
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| | | | | | | | C1023 | U960 | U899 | U759 | C675 | U612 | C526 | U |
| | | | | | | | U1024 | C961 | G900 | G760 | C676 | U613 | G530 | U |
| | | | | | | | A1025 | A962 | G901 | C765 | A677 | G614 | G531 | U |
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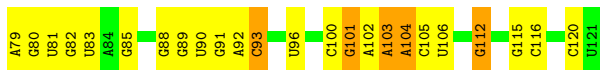
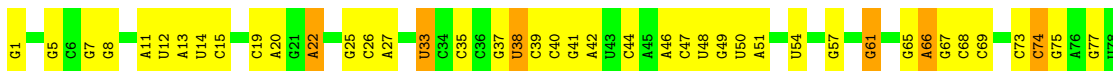


• Molecule 37: 5S rRNA

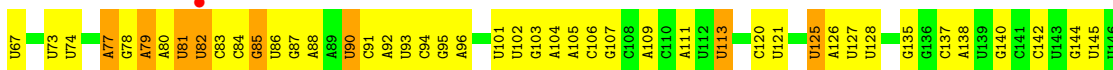




- Molecule 37: 5S rRNA



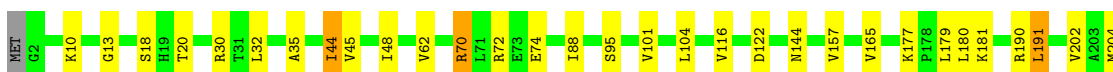
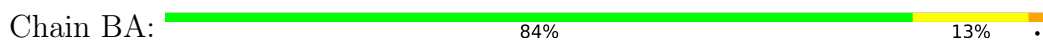
- Molecule 38: 5.8S rRNA



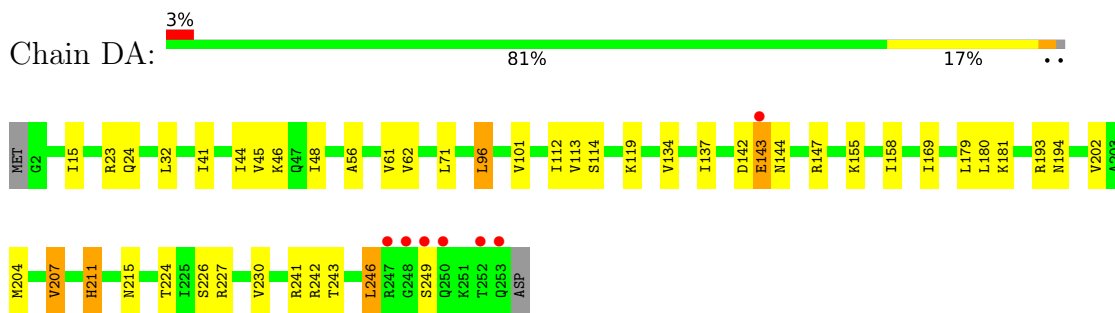
- Molecule 38: 5.8S rRNA



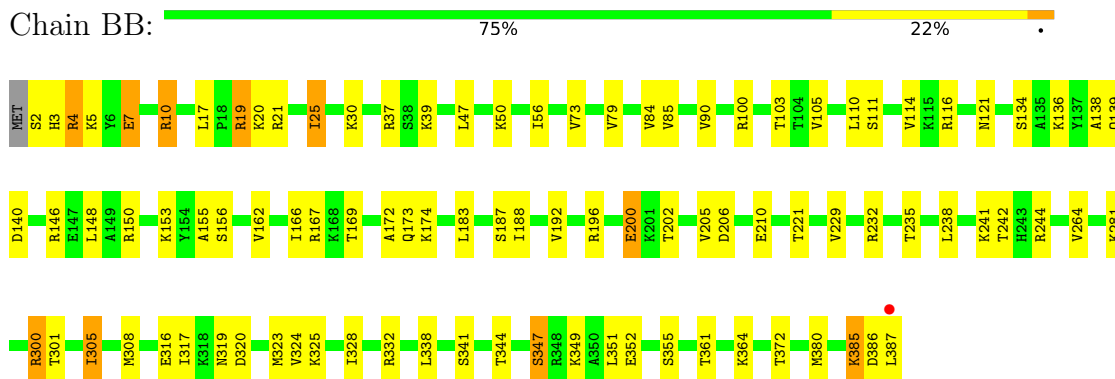
- Molecule 39: 60S ribosomal protein L2-A



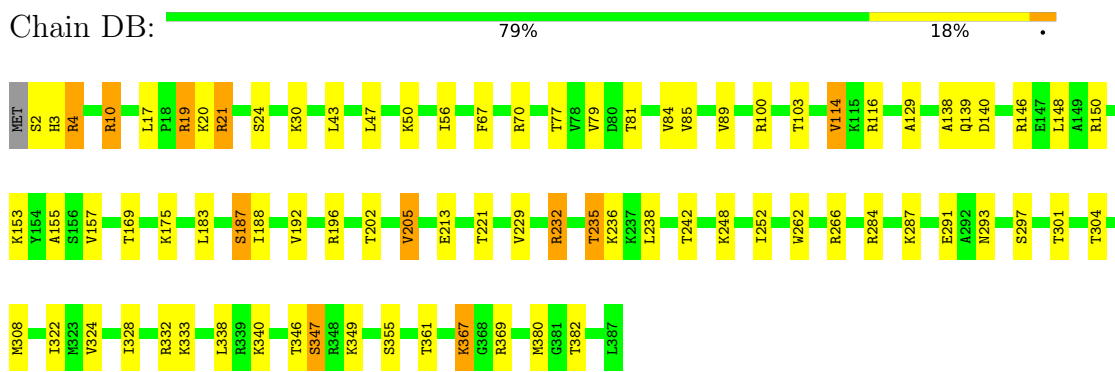
- Molecule 39: 60S ribosomal protein L2-A



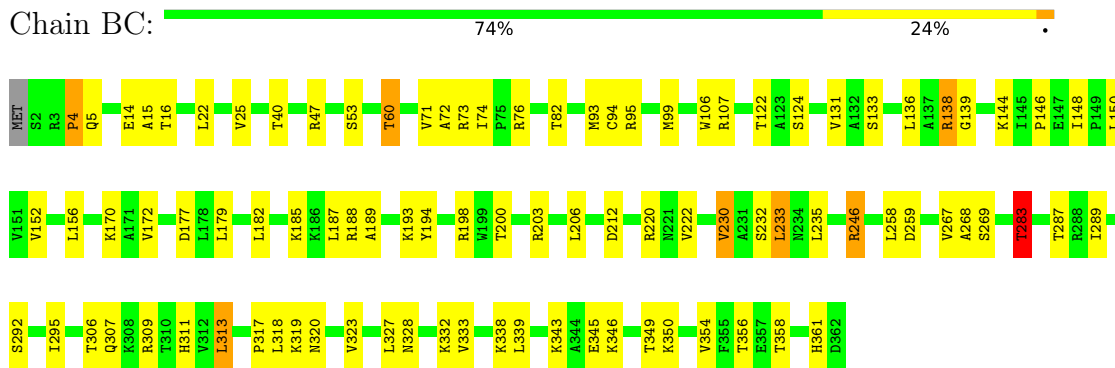
• Molecule 40: 60S ribosomal protein L3




• Molecule 40: 60S ribosomal protein L3



• Molecule 41: 60S ribosomal protein L4-A




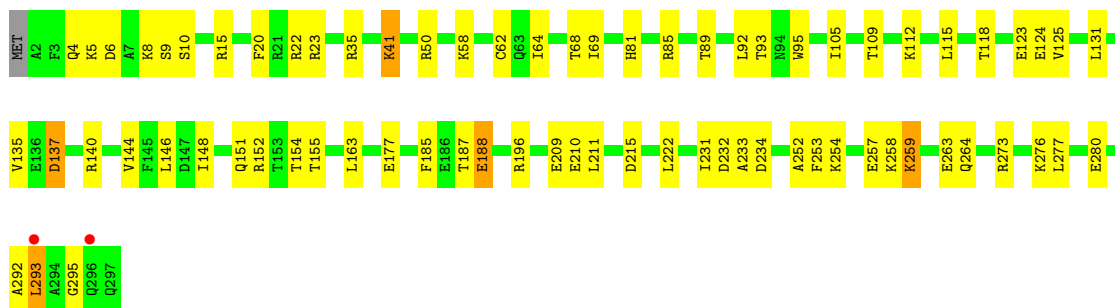
• Molecule 41: 60S ribosomal protein L4-A

Chain DC:  75% 21%




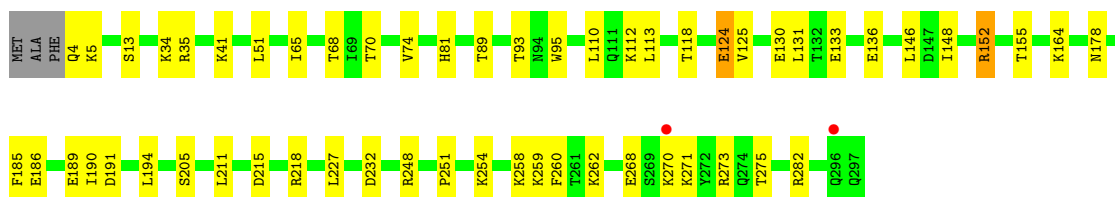
• Molecule 42: 60S ribosomal protein L5

Chain BD:  75% 23%




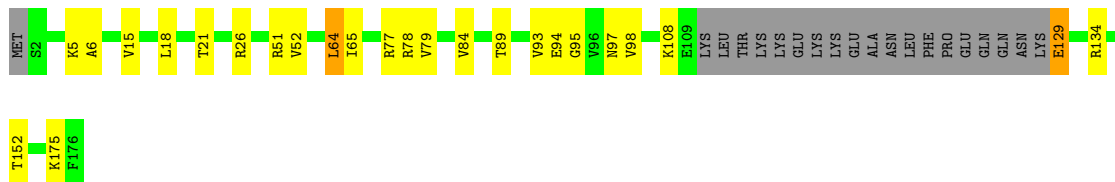
• Molecule 42: 60S ribosomal protein L5

Chain DD:  80% 18%




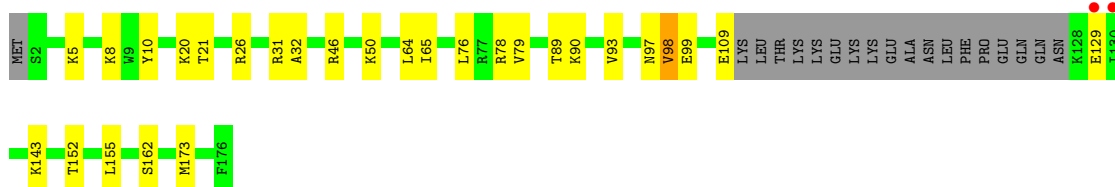
• Molecule 43: 60S ribosomal protein L6-A

Chain BE:  74% 13% 11%

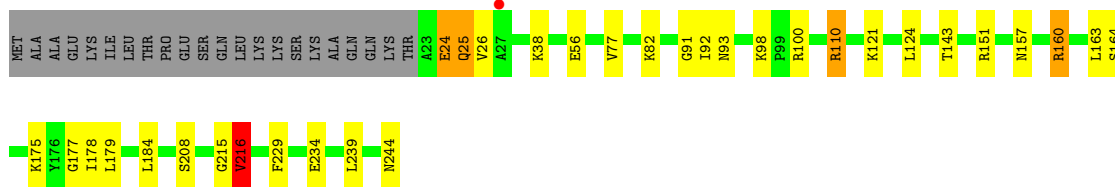
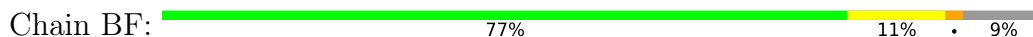


• Molecule 43: 60S ribosomal protein L6-A

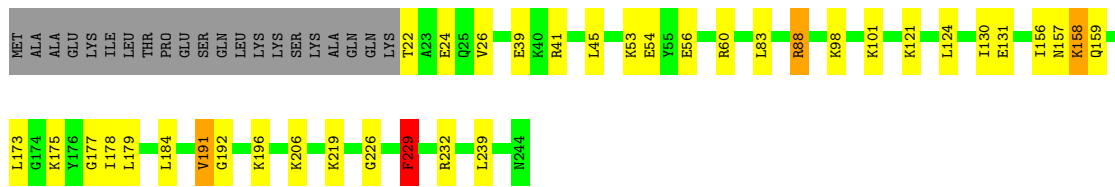
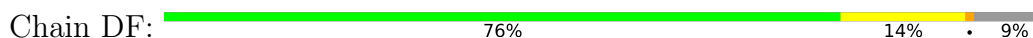
Chain DE:  73% 15% 11%



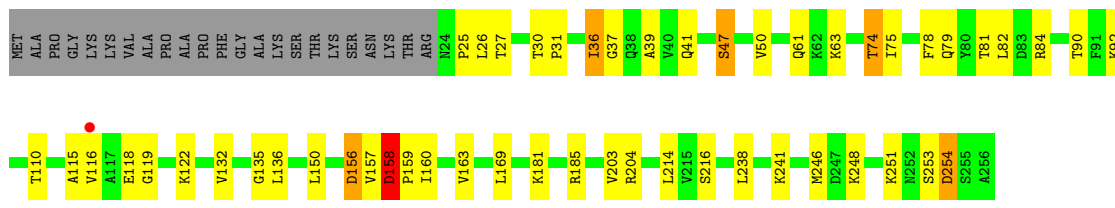
• Molecule 44: 60S ribosomal protein L7-A



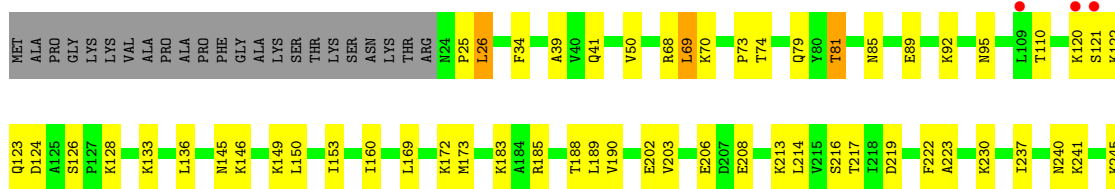
• Molecule 44: 60S ribosomal protein L7-A

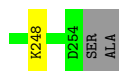


• Molecule 45: 60S ribosomal protein L8-A

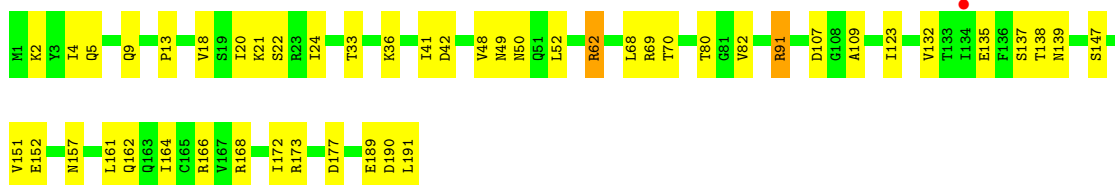
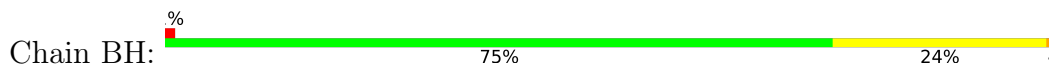


• Molecule 45: 60S ribosomal protein L8-A

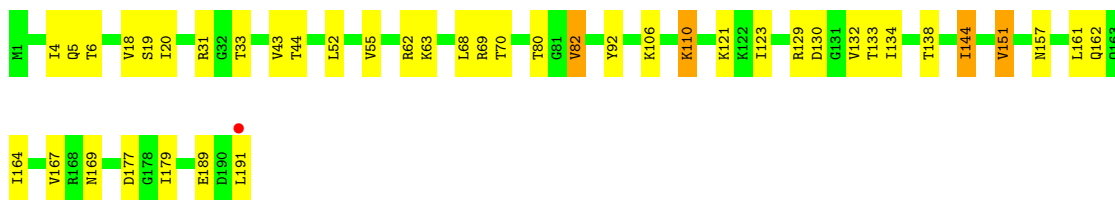
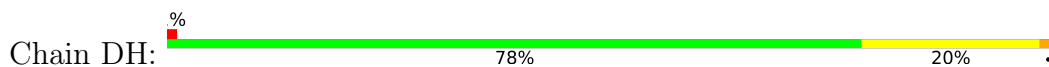




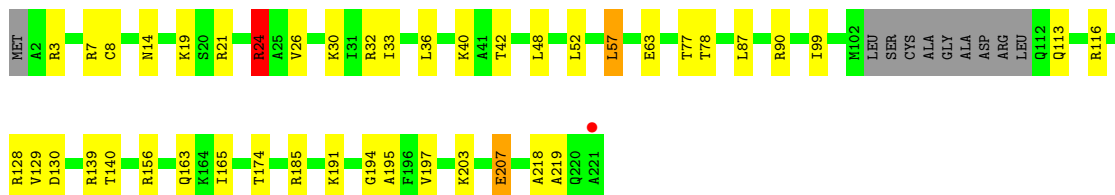
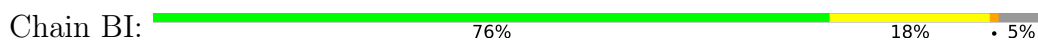
- Molecule 46: 60S ribosomal protein L9-A



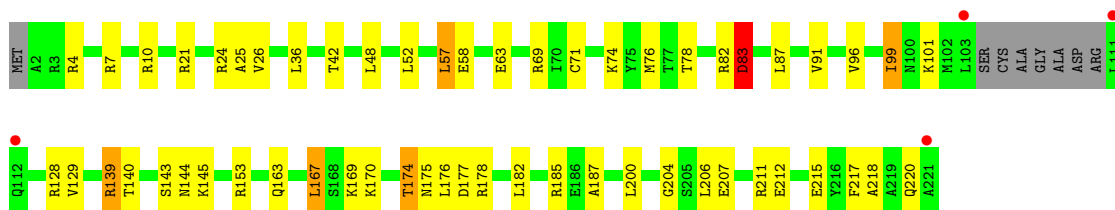
- Molecule 46: 60S ribosomal protein L9-A



- Molecule 47: 60S ribosomal protein L10

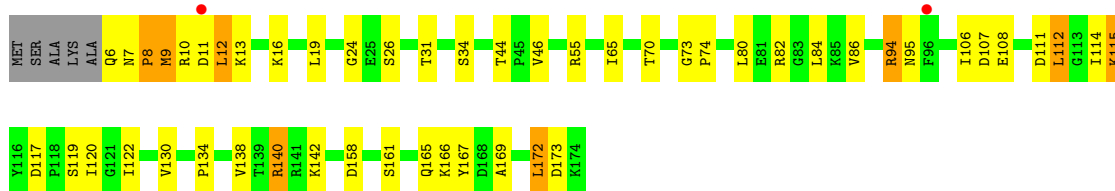


- Molecule 47: 60S ribosomal protein L10



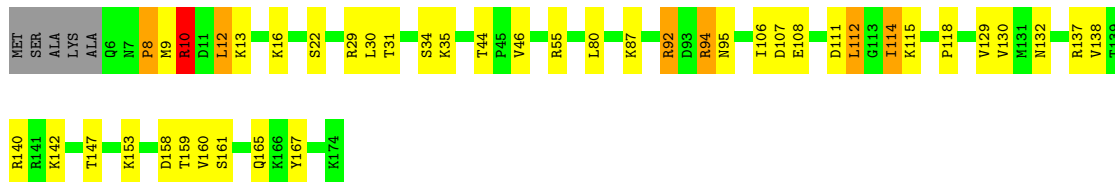
- Molecule 48: 60S ribosomal protein L11-A





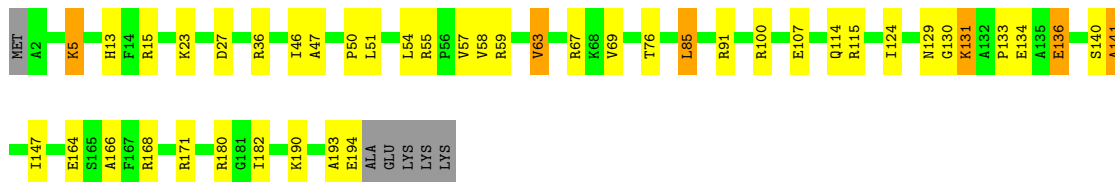
- Molecule 48: 60S ribosomal protein L11-A

Chain DJ: 72% 21% . . .



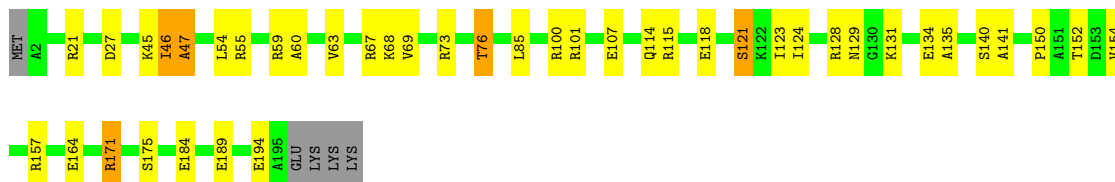
- Molecule 49: 60S ribosomal protein L13-A

Chain BL: 75% 19% . .



- Molecule 49: 60S ribosomal protein L13-A

Chain DL: 76% 19% . .



- Molecule 50: 60S ribosomal protein L14-A

Chain BM: 77% 20% . .



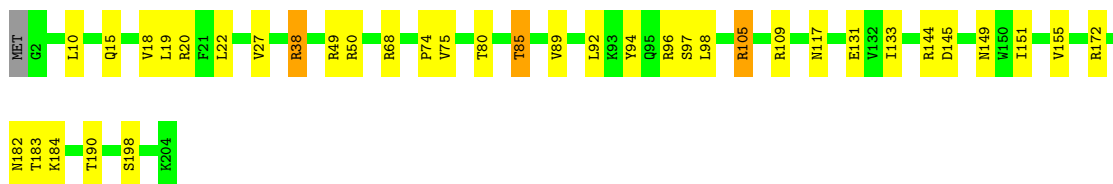
- Molecule 50: 60S ribosomal protein L14-A

Chain DM: 80% 17% . .



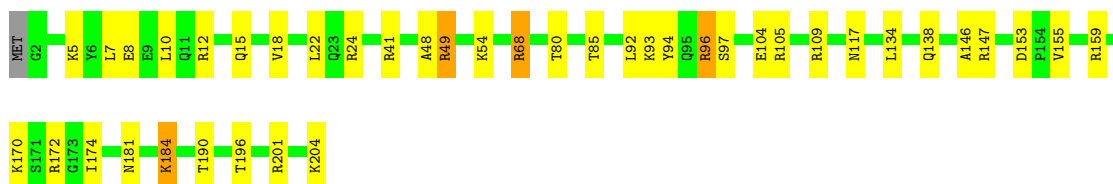
- Molecule 51: 60S ribosomal protein L15-A

Chain BN: 81% 17%



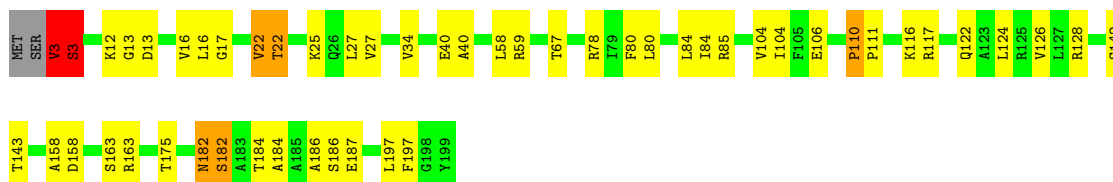
- Molecule 51: 60S ribosomal protein L15-A

Chain DN: 79% 18%



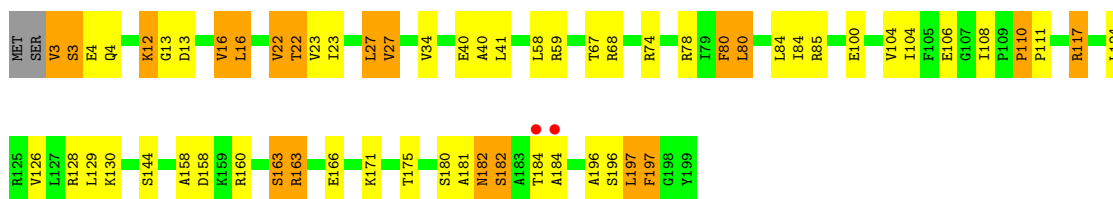
- Molecule 52: 60S ribosomal protein L16-A, 60S ribosomal protein L16-B

Chain BO: 75% 21%



- Molecule 52: 60S ribosomal protein L16-A, 60S ribosomal protein L16-B

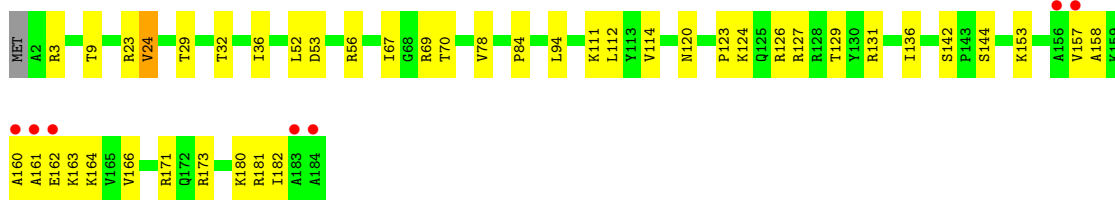
Chain DO: 71% 20% 9%



- Molecule 53: 60S ribosomal protein L17-A

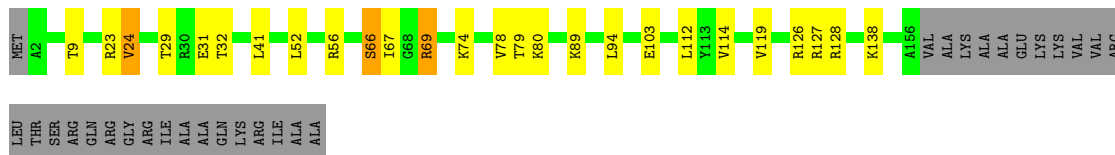
Chain BP: 4% 76% 20%





- Molecule 53: 60S ribosomal protein L17-A

Chain DP: 70% 12% 16%



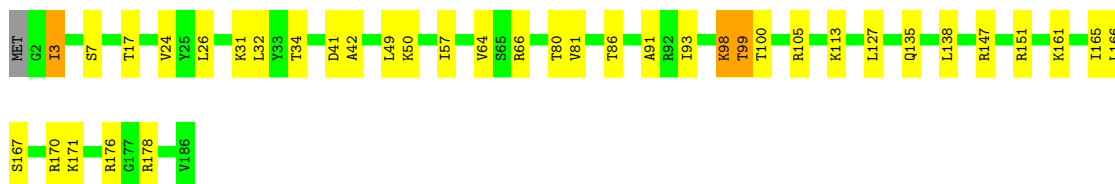
- Molecule 54: 60S ribosomal protein L18-A

Chain BQ: 82% 15% ..



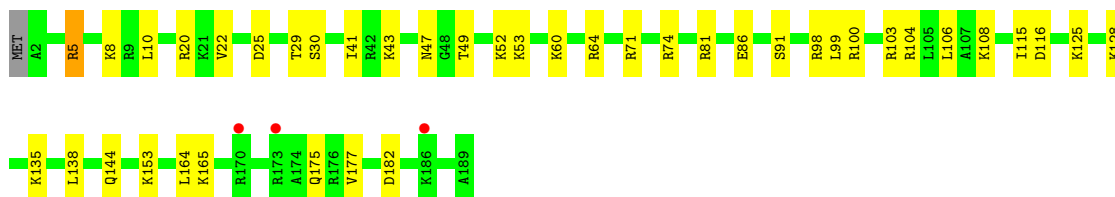
- Molecule 54: 60S ribosomal protein L18-A

Chain DQ: 79% 19% ..

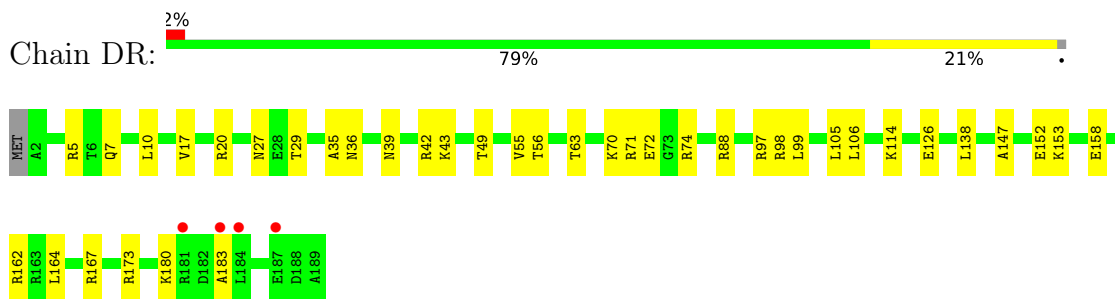


- Molecule 55: 60S ribosomal protein L19-A

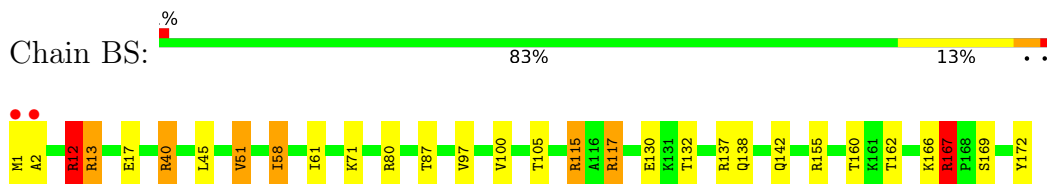
Chain BR: 2% 78% 21% ..



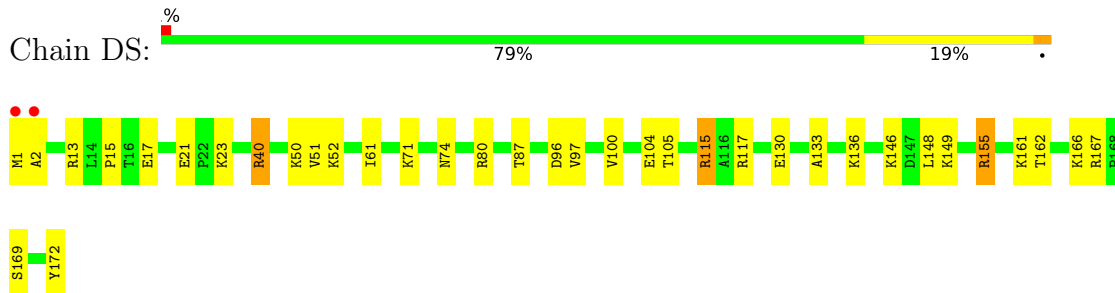
- Molecule 55: 60S ribosomal protein L19-A



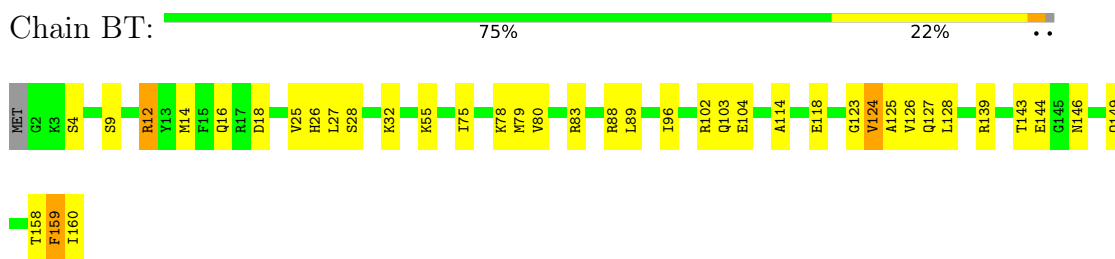
- Molecule 56: 60S ribosomal protein L20-A



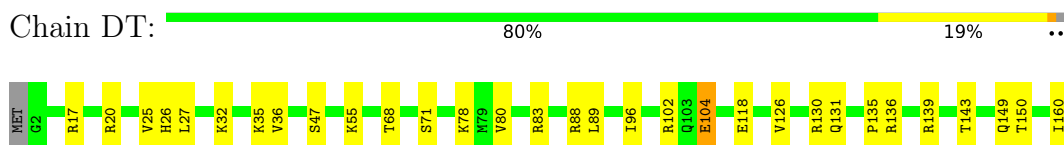
- Molecule 56: 60S ribosomal protein L20-A



- Molecule 57: 60S ribosomal protein L21-A

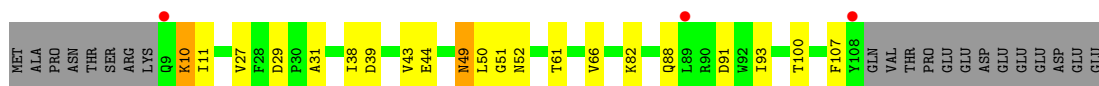


- Molecule 57: 60S ribosomal protein L21-A

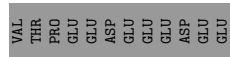


- Molecule 58: 60S ribosomal protein L22-A

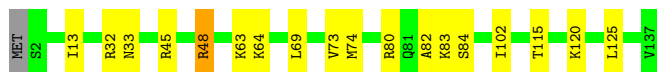




• Molecule 58: 60S ribosomal protein L22-A



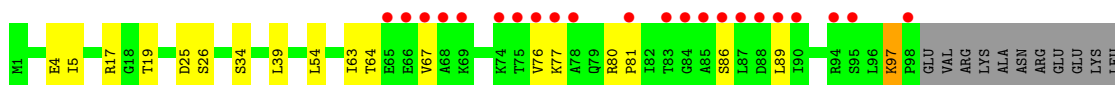
• Molecule 59: 60S ribosomal protein L23-A



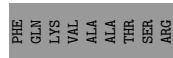
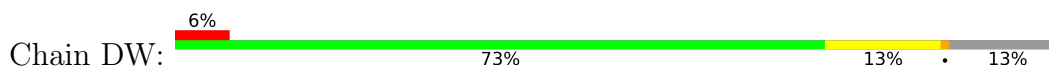
• Molecule 59: 60S ribosomal protein L23-A



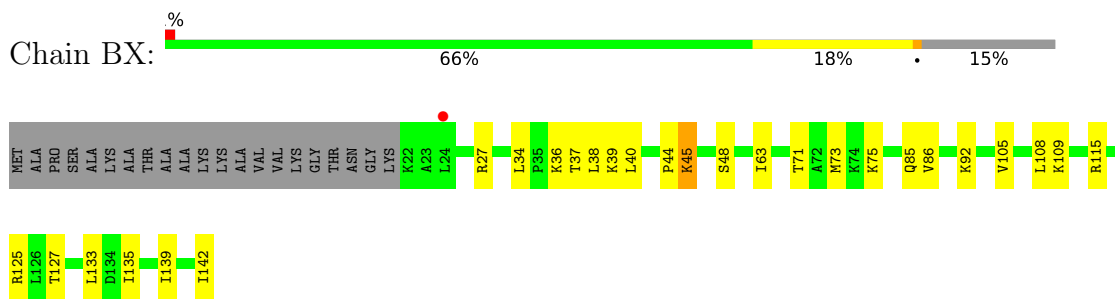
• Molecule 60: 60S ribosomal protein L24-A



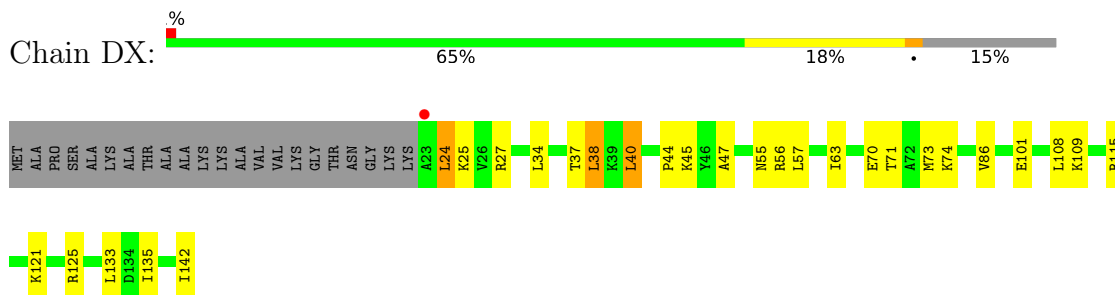
• Molecule 60: 60S ribosomal protein L24-A



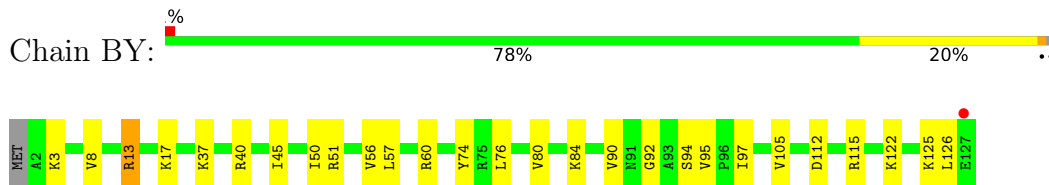
• Molecule 61: 60S ribosomal protein L25



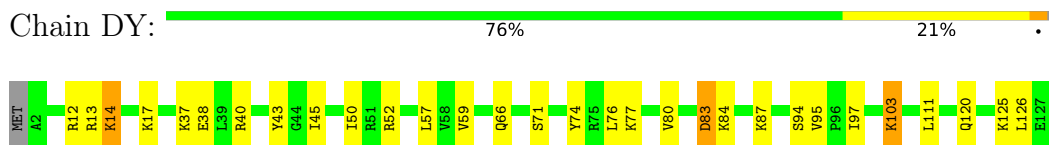
- Molecule 61: 60S ribosomal protein L25



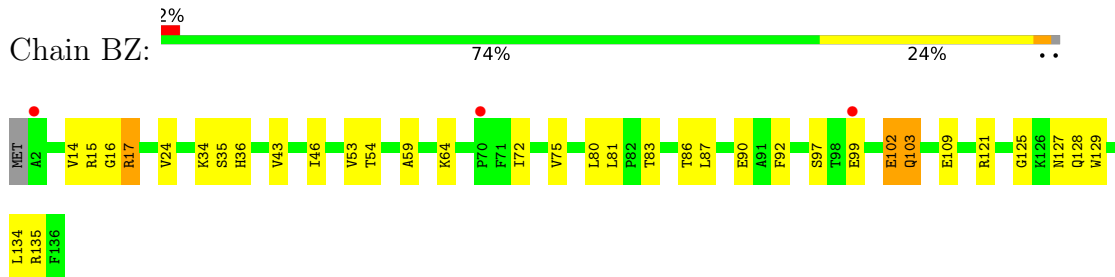
- Molecule 62: 60S ribosomal protein L26-A



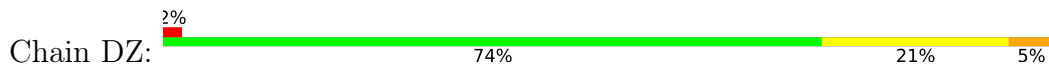
- Molecule 62: 60S ribosomal protein L26-A

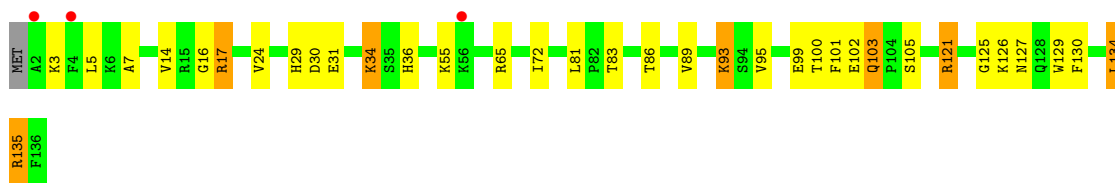


- Molecule 63: 60S ribosomal protein L27-A

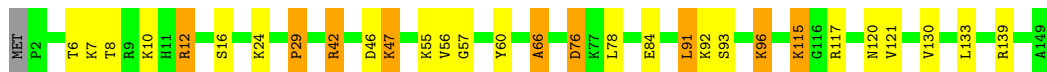
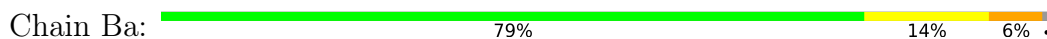


- Molecule 63: 60S ribosomal protein L27-A

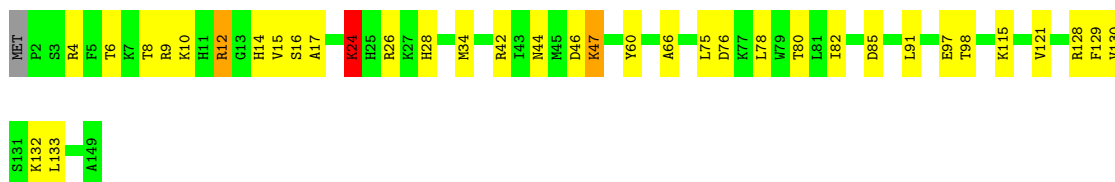
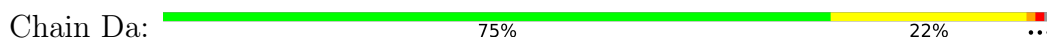




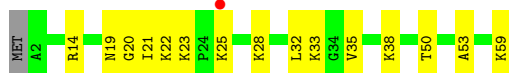
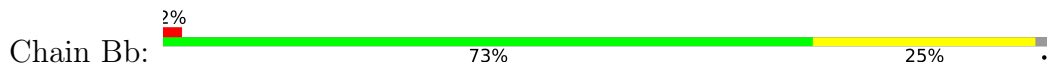
• Molecule 64: 60S ribosomal protein L28



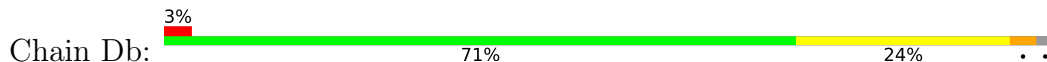
• Molecule 64: 60S ribosomal protein L28



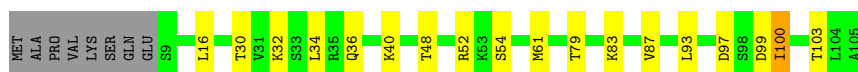
• Molecule 65: 60S ribosomal protein L29



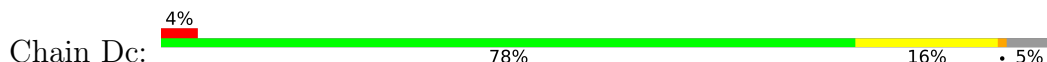
• Molecule 65: 60S ribosomal protein L29

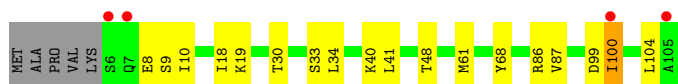


• Molecule 66: 60S ribosomal protein L30

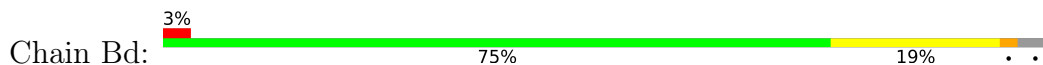


• Molecule 66: 60S ribosomal protein L30

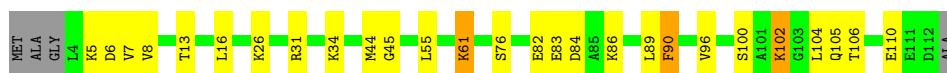




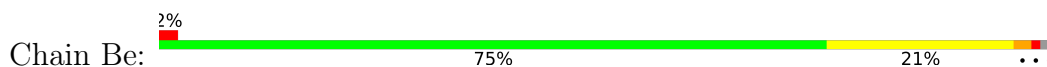
- Molecule 67: 60S ribosomal protein L31-A



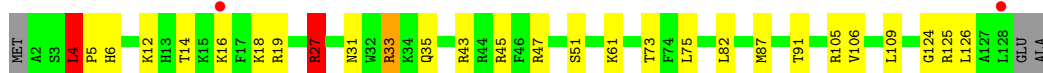
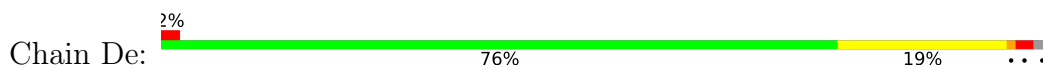
- Molecule 67: 60S ribosomal protein L31-A



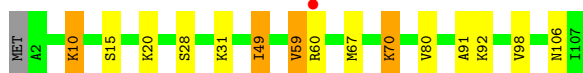
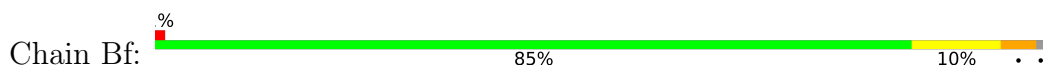
- Molecule 68: 60S ribosomal protein L32



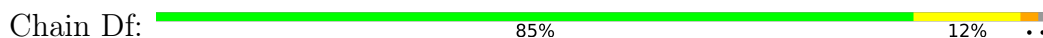
- Molecule 68: 60S ribosomal protein L32



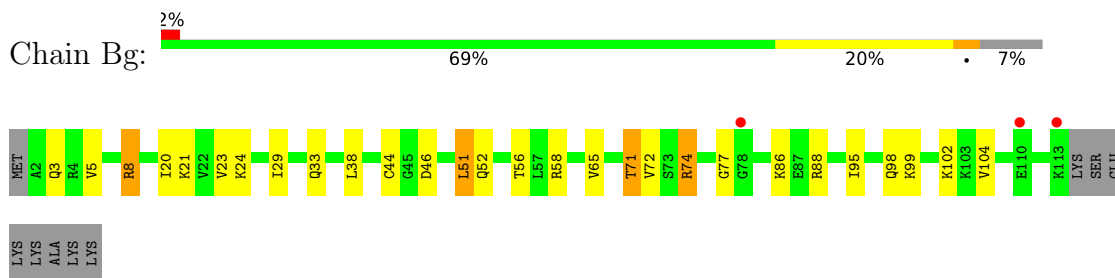
- Molecule 69: 60S ribosomal protein L33-A



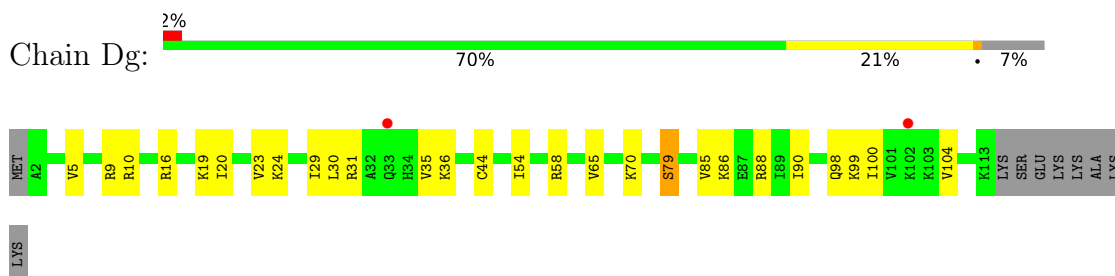
- Molecule 69: 60S ribosomal protein L33-A



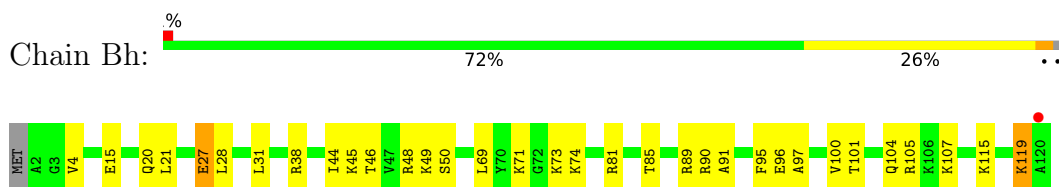
- Molecule 70: 60S ribosomal protein L34-A



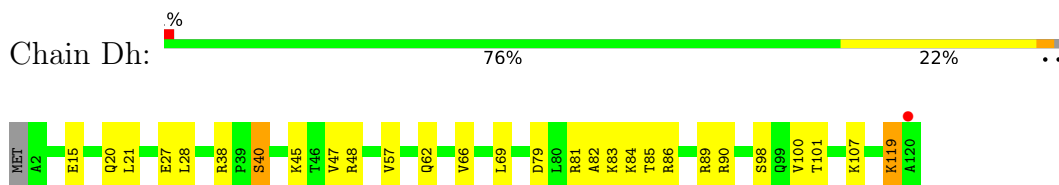
- Molecule 70: 60S ribosomal protein L34-A



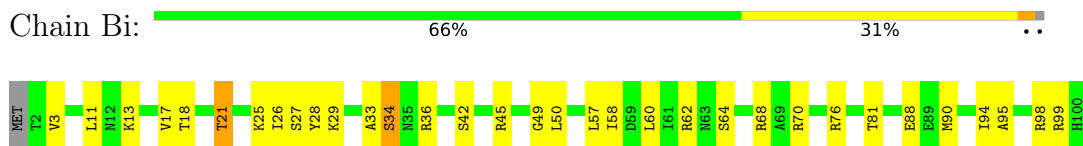
- Molecule 71: 60S ribosomal protein L35-A



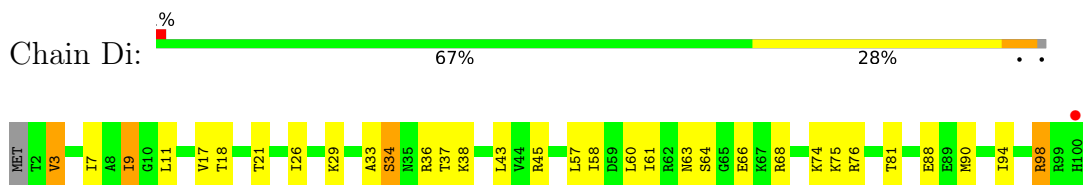
- Molecule 71: 60S ribosomal protein L35-A



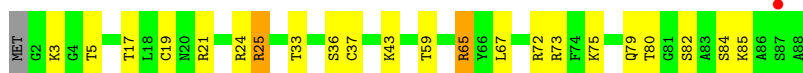
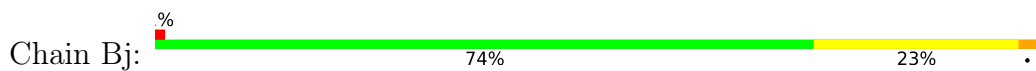
- Molecule 72: 60S ribosomal protein L36-A



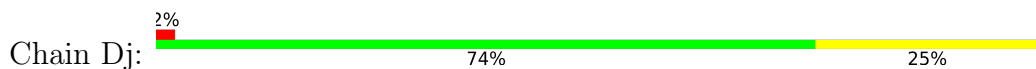
- Molecule 72: 60S ribosomal protein L36-A



- Molecule 73: 60S ribosomal protein L37-A



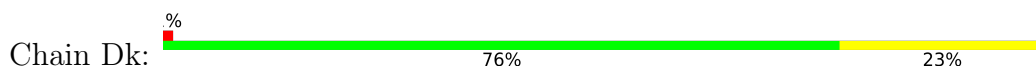
- Molecule 73: 60S ribosomal protein L37-A



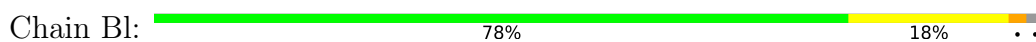
- Molecule 74: 60S ribosomal protein L38



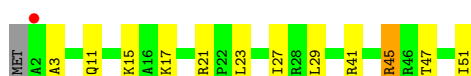
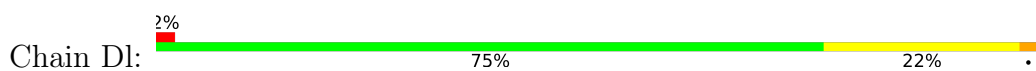
- Molecule 74: 60S ribosomal protein L38



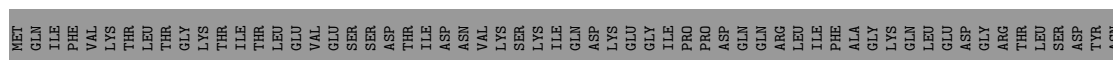
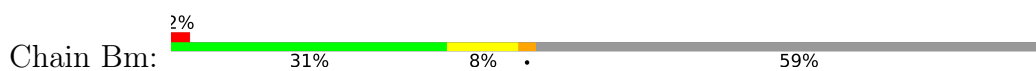
- Molecule 75: 60S ribosomal protein L39

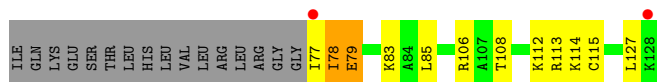


- Molecule 75: 60S ribosomal protein L39

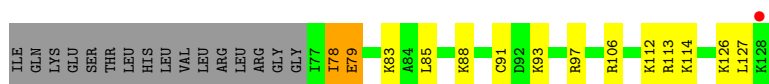
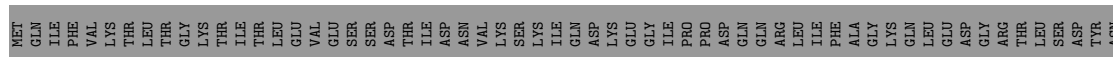
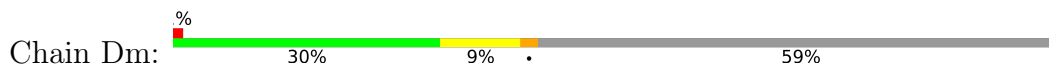


- Molecule 76: 60S ribosomal protein L40

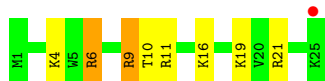




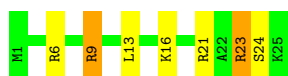
- Molecule 76: 60S ribosomal protein L40



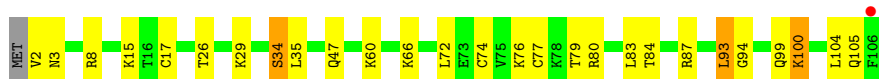
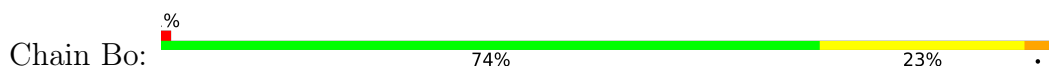
- Molecule 77: 60S ribosomal protein L41-A



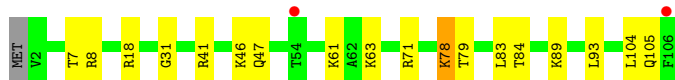
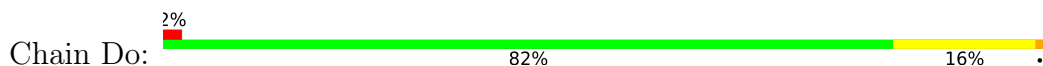
- Molecule 77: 60S ribosomal protein L41-A



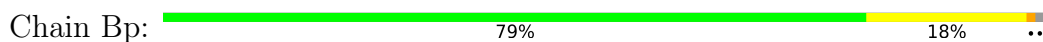
- Molecule 78: 60S ribosomal protein L42-A



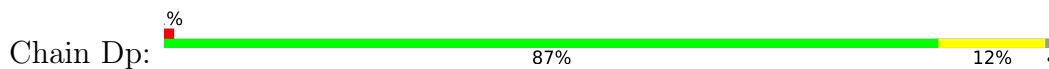
- Molecule 78: 60S ribosomal protein L42-A



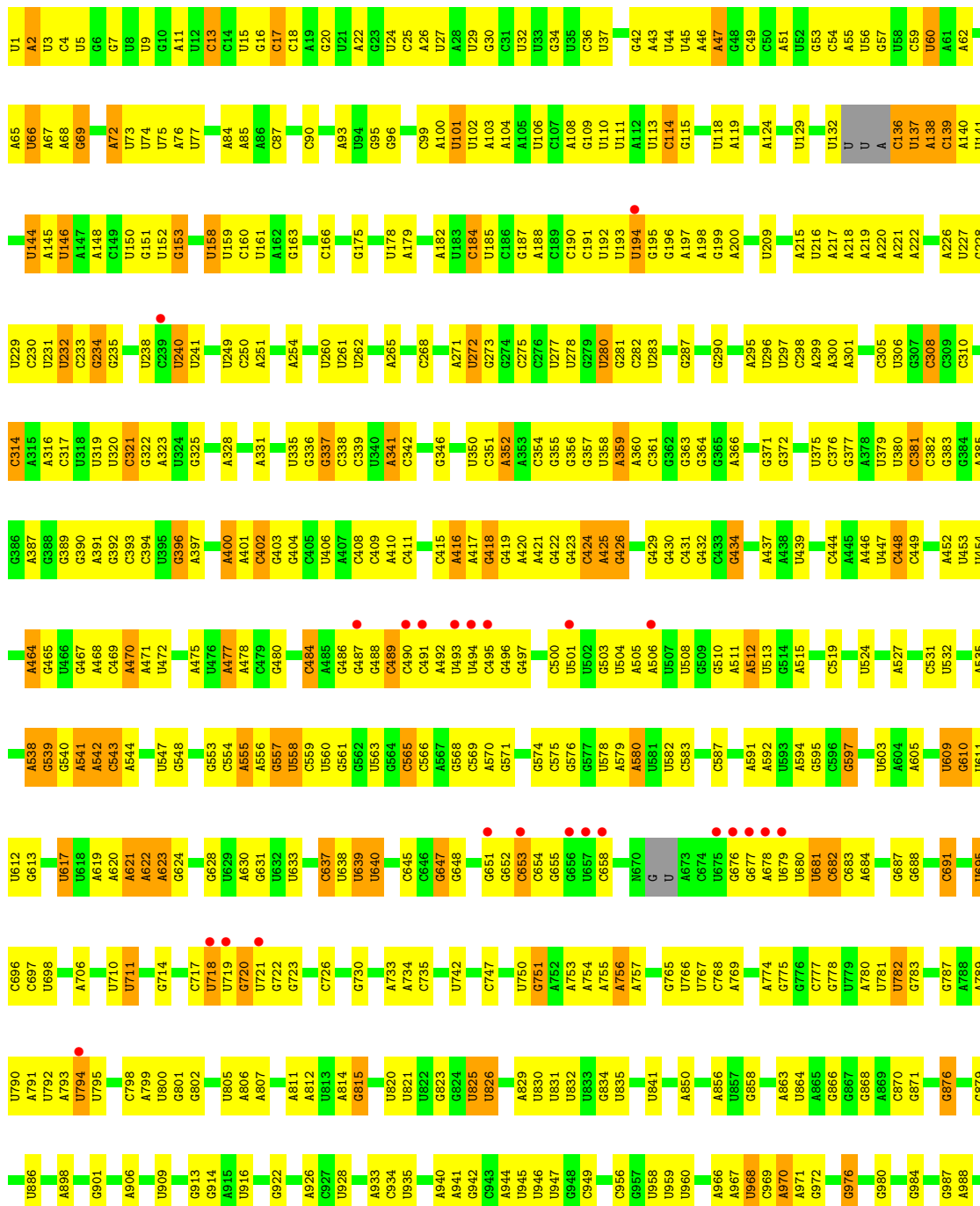
- Molecule 79: 60S ribosomal protein L43-A

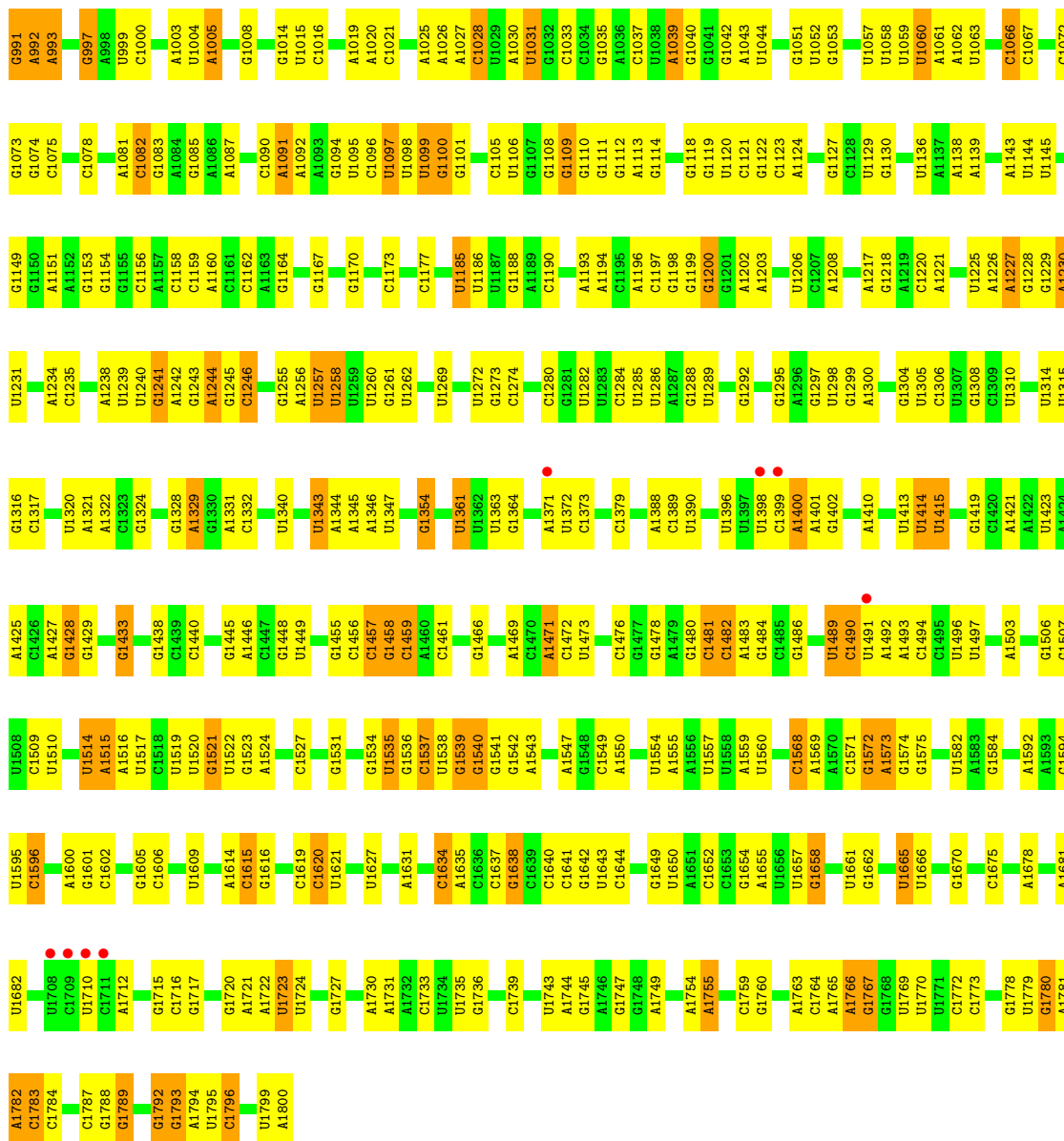


• Molecule 79: 60S ribosomal protein L43-A

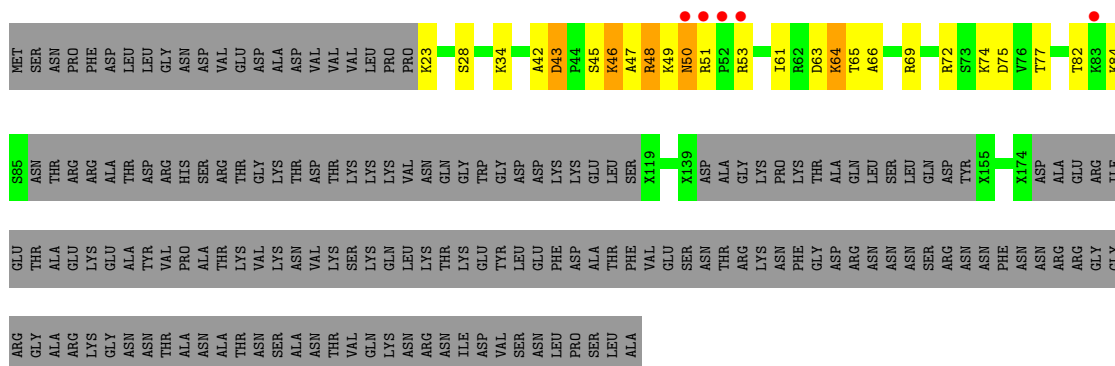


• Molecule 80: 18S rRNA



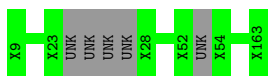


● Molecule 81: Suppressor protein STM1




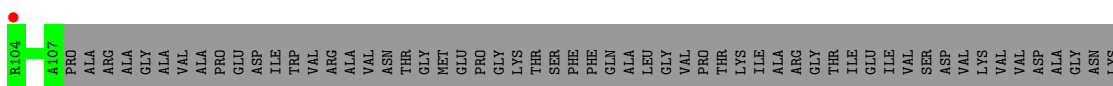
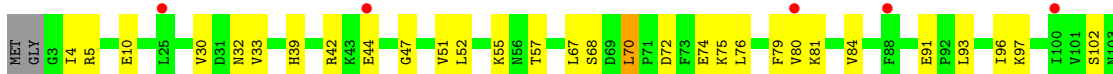
- Molecule 82: Ribosomal protein L12

Chain DK:  97%



- Molecule 83: 60S acidic ribosomal protein P0

Chain Dq:  2% 35% 10% 54%

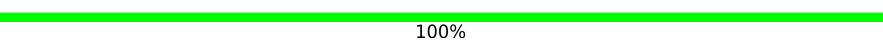


- Molecule 84: Ribosomal protein P1 alpha

Chain Dr:  100%

There are no outlier residues recorded for this chain.

- Molecule 85: Ribosomal protein P2 beta

Chain Ds:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 436.43Å 288.22Å 305.08Å 90.00° 98.99° 90.00° | Depositor |
| Resolution (Å) | 300.00 – 3.00 301.33 – 2.90 | Depositor EDS |
| % Data completeness (in resolution range) | 100.0 (300.00-3.00) 99.9 (301.33-2.90) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.52 (at 2.91Å) | Xtrriage |
| Refinement program | PHENIX | Depositor |
| R, R_{free} | 0.181 , 0.229 0.189 , 0.229 | Depositor DCC |
| R_{free} test set | 32787 reflections (2.00%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 68.6 | Xtrriage |
| Anisotropy | 0.203 | Xtrriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.29 , 74.8 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$ | Xtrriage |
| Estimated twinning fraction | No twinning to report. | Xtrriage |
| F_o, F_c correlation | 0.94 | EDS |
| Total number of atoms | 416785 | wwPDB-VP |
| Average B, all atoms (Å ²) | 80.0 | wwPDB-VP |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% 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: ZN, OHX, MG

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | A2 | 0.92 | 36/42128 (0.1%) | 1.49 | 822/65642 (1.3%) |
| 2 | AA | 0.54 | 0/1617 | 0.80 | 0/2215 |
| 2 | CA | 0.64 | 0/1623 | 0.88 | 0/2222 |
| 3 | AB | 0.45 | 0/1735 | 0.81 | 0/2335 |
| 3 | CB | 0.61 | 0/1748 | 0.80 | 1/2352 (0.0%) |
| 4 | AC | 0.60 | 0/1665 | 0.77 | 0/2263 |
| 4 | CC | 0.70 | 0/1665 | 0.93 | 6/2263 (0.3%) |
| 5 | AD | 0.59 | 0/1759 | 0.74 | 0/2368 |
| 5 | CD | 0.54 | 0/1759 | 0.76 | 1/2368 (0.0%) |
| 6 | AE | 0.57 | 0/2109 | 0.86 | 1/2839 (0.0%) |
| 6 | CE | 0.70 | 0/2109 | 0.94 | 2/2839 (0.1%) |
| 7 | AF | 0.49 | 0/1629 | 0.72 | 0/2202 |
| 7 | CF | 0.62 | 0/1629 | 0.86 | 2/2202 (0.1%) |
| 8 | AG | 0.55 | 0/1823 | 0.75 | 0/2439 |
| 8 | CG | 0.68 | 0/1779 | 0.87 | 2/2379 (0.1%) |
| 9 | AH | 0.52 | 0/1506 | 0.77 | 0/2028 |
| 9 | CH | 0.59 | 0/1516 | 0.85 | 0/2043 |
| 10 | AI | 0.68 | 0/1514 | 0.89 | 3/2021 (0.1%) |
| 10 | CI | 0.75 | 0/1514 | 0.99 | 2/2021 (0.1%) |
| 11 | AJ | 0.59 | 0/1519 | 0.81 | 1/2035 (0.0%) |
| 11 | CJ | 0.70 | 0/1519 | 0.91 | 3/2035 (0.1%) |
| 12 | AK | 0.55 | 0/789 | 0.83 | 3/1067 (0.3%) |
| 12 | CK | 0.51 | 0/776 | 0.83 | 3/1047 (0.3%) |
| 13 | AL | 0.70 | 0/1239 | 0.81 | 0/1673 |
| 13 | CL | 0.76 | 0/1194 | 0.98 | 5/1610 (0.3%) |
| 14 | AM | 0.49 | 0/898 | 0.76 | 0/1220 |
| 14 | CM | 0.44 | 0/898 | 0.77 | 2/1220 (0.2%) |
| 15 | AN | 0.61 | 0/1215 | 0.83 | 3/1638 (0.2%) |
| 15 | CN | 0.67 | 0/1215 | 0.89 | 1/1638 (0.1%) |
| 16 | AO | 0.48 | 0/901 | 0.82 | 1/1217 (0.1%) |
| 16 | CO | 0.70 | 0/960 | 0.92 | 0/1290 |
| 17 | AP | 0.60 | 0/998 | 0.86 | 2/1341 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | CP | 0.57 | 0/1060 | 0.83 | 0/1426 |
| 18 | AQ | 0.56 | 0/1125 | 0.85 | 3/1510 (0.2%) |
| 18 | CQ | 0.66 | 0/1131 | 0.85 | 1/1518 (0.1%) |
| 19 | AR | 0.54 | 0/935 | 0.82 | 0/1254 |
| 19 | CR | 0.60 | 0/914 | 0.86 | 0/1224 |
| 20 | AS | 0.59 | 0/1211 | 0.80 | 0/1628 |
| 20 | CS | 0.63 | 0/1211 | 0.92 | 3/1628 (0.2%) |
| 21 | AT | 0.57 | 0/1130 | 0.81 | 0/1517 |
| 21 | CT | 0.66 | 0/1130 | 0.86 | 3/1517 (0.2%) |
| 22 | AU | 0.55 | 0/865 | 0.76 | 0/1169 |
| 22 | CU | 0.62 | 0/892 | 0.86 | 0/1205 |
| 23 | AV | 0.52 | 0/693 | 0.75 | 0/935 |
| 23 | CV | 0.65 | 0/693 | 0.86 | 0/935 |
| 24 | AW | 0.65 | 0/1038 | 0.86 | 3/1395 (0.2%) |
| 24 | CW | 0.81 | 0/1038 | 0.89 | 1/1395 (0.1%) |
| 25 | AX | 0.72 | 0/1139 | 0.91 | 2/1518 (0.1%) |
| 25 | CX | 0.86 | 0/1139 | 0.99 | 3/1518 (0.2%) |
| 26 | AY | 0.56 | 0/1087 | 0.77 | 1/1449 (0.1%) |
| 26 | CY | 0.65 | 0/1087 | 0.84 | 0/1449 |
| 27 | AZ | 0.49 | 0/571 | 0.85 | 1/768 (0.1%) |
| 27 | CZ | 0.51 | 0/566 | 0.80 | 1/761 (0.1%) |
| 28 | Aa | 0.54 | 0/782 | 0.77 | 0/1047 |
| 28 | Ca | 0.63 | 0/782 | 0.84 | 0/1047 |
| 29 | Ab | 0.53 | 0/620 | 0.82 | 1/838 (0.1%) |
| 29 | Cb | 0.55 | 0/620 | 0.87 | 0/838 |
| 30 | Ac | 0.43 | 0/499 | 0.72 | 0/670 |
| 30 | Cc | 0.53 | 0/499 | 0.84 | 0/670 |
| 31 | Ad | 0.71 | 1/452 (0.2%) | 0.94 | 1/600 (0.2%) |
| 31 | Cd | 0.77 | 1/452 (0.2%) | 0.94 | 1/600 (0.2%) |
| 32 | Ae | 0.50 | 0/483 | 0.71 | 0/643 |
| 32 | Ce | 0.62 | 0/499 | 0.89 | 1/665 (0.2%) |
| 33 | Af | 0.53 | 0/404 | 0.99 | 2/542 (0.4%) |
| 33 | Cf | 0.46 | 0/404 | 0.84 | 0/542 |
| 34 | Ag | 0.49 | 0/2490 | 0.70 | 0/3389 |
| 34 | Cg | 0.51 | 0/2495 | 0.69 | 0/3395 |
| 35 | Ah | 0.86 | 2/925 (0.2%) | 0.87 | 2/1240 (0.2%) |
| 36 | A1 | 1.42 | 515/75394 (0.7%) | 1.91 | 3591/117545 (3.1%) |
| 36 | A5 | 1.46 | 607/75414 (0.8%) | 1.88 | 3500/117575 (3.0%) |
| 37 | A3 | 1.15 | 5/2883 (0.2%) | 1.59 | 68/4491 (1.5%) |
| 37 | A7 | 1.38 | 13/2883 (0.5%) | 1.80 | 121/4491 (2.7%) |
| 38 | A4 | 1.31 | 18/3746 (0.5%) | 1.79 | 159/5832 (2.7%) |
| 38 | A8 | 1.16 | 4/3746 (0.1%) | 1.70 | 130/5832 (2.2%) |
| 39 | BA | 0.84 | 0/1948 | 1.01 | 5/2617 (0.2%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 39 | DA | 0.87 | 1/1946 (0.1%) | 1.05 | 4/2614 (0.2%) |
| 40 | BB | 0.92 | 3/3146 (0.1%) | 1.05 | 11/4228 (0.3%) |
| 40 | DB | 1.02 | 4/3146 (0.1%) | 1.11 | 13/4228 (0.3%) |
| 41 | BC | 0.96 | 3/2800 (0.1%) | 1.14 | 17/3790 (0.4%) |
| 41 | DC | 0.87 | 0/2800 | 1.07 | 11/3790 (0.3%) |
| 42 | BD | 0.71 | 2/2425 (0.1%) | 0.87 | 1/3271 (0.0%) |
| 42 | DD | 0.89 | 1/2408 (0.0%) | 0.96 | 3/3248 (0.1%) |
| 43 | BE | 0.88 | 0/1260 | 1.02 | 3/1694 (0.2%) |
| 43 | DE | 0.90 | 1/1269 (0.1%) | 1.00 | 3/1705 (0.2%) |
| 44 | BF | 0.96 | 1/1821 (0.1%) | 1.06 | 7/2451 (0.3%) |
| 44 | DF | 0.99 | 1/1828 (0.1%) | 1.04 | 6/2461 (0.2%) |
| 45 | BG | 0.64 | 0/1836 | 0.82 | 1/2481 (0.0%) |
| 45 | DG | 0.64 | 0/1795 | 0.81 | 1/2429 (0.0%) |
| 46 | BH | 0.80 | 0/1539 | 0.97 | 5/2073 (0.2%) |
| 46 | DH | 0.97 | 2/1539 (0.1%) | 1.01 | 1/2073 (0.0%) |
| 47 | BI | 0.90 | 2/1741 (0.1%) | 0.97 | 5/2335 (0.2%) |
| 47 | DI | 0.92 | 1/1758 (0.1%) | 1.08 | 12/2358 (0.5%) |
| 48 | BJ | 0.65 | 0/1374 | 0.85 | 1/1842 (0.1%) |
| 48 | DJ | 0.81 | 1/1374 (0.1%) | 0.99 | 4/1842 (0.2%) |
| 49 | BL | 0.89 | 0/1568 | 1.02 | 8/2106 (0.4%) |
| 49 | DL | 0.82 | 0/1573 | 1.04 | 6/2113 (0.3%) |
| 50 | BM | 0.88 | 0/1068 | 0.91 | 0/1438 |
| 50 | DM | 0.95 | 0/1074 | 1.01 | 4/1446 (0.3%) |
| 51 | BN | 0.88 | 0/1757 | 1.05 | 5/2354 (0.2%) |
| 51 | DN | 0.83 | 1/1757 (0.1%) | 1.00 | 6/2354 (0.3%) |
| 52 | BO | 0.92 | 10/3160 (0.3%) | 1.16 | 10/4208 (0.2%) |
| 52 | DO | 0.98 | 11/3159 (0.3%) | 1.02 | 25/4205 (0.6%) |
| 53 | BP | 0.97 | 2/1443 (0.1%) | 1.02 | 3/1944 (0.2%) |
| 53 | DP | 1.05 | 1/1250 (0.1%) | 1.09 | 5/1683 (0.3%) |
| 54 | BQ | 0.98 | 0/1465 | 1.13 | 8/1965 (0.4%) |
| 54 | DQ | 0.89 | 1/1465 (0.1%) | 1.12 | 8/1965 (0.4%) |
| 55 | BR | 0.71 | 1/1538 (0.1%) | 0.87 | 1/2050 (0.0%) |
| 55 | DR | 0.78 | 1/1538 (0.1%) | 0.87 | 3/2050 (0.1%) |
| 56 | BS | 0.89 | 0/1481 | 1.06 | 9/1990 (0.5%) |
| 56 | DS | 1.02 | 0/1481 | 1.09 | 7/1990 (0.4%) |
| 57 | BT | 0.93 | 0/1300 | 0.98 | 1/1743 (0.1%) |
| 57 | DT | 1.01 | 2/1300 (0.2%) | 1.01 | 1/1743 (0.1%) |
| 58 | BU | 0.52 | 0/812 | 0.70 | 0/1099 |
| 58 | DU | 0.56 | 0/794 | 0.77 | 0/1076 |
| 59 | BV | 0.86 | 0/1018 | 1.03 | 3/1369 (0.2%) |
| 59 | DV | 0.98 | 0/1018 | 1.09 | 4/1369 (0.3%) |
| 60 | BW | 0.68 | 0/712 | 0.86 | 1/958 (0.1%) |
| 60 | DW | 0.80 | 0/1052 | 0.90 | 1/1398 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|--------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 61 | BX | 0.73 | 0/979 | 0.87 | 0/1321 |
| 61 | DX | 0.72 | 0/974 | 0.86 | 0/1314 |
| 62 | BY | 0.78 | 0/1004 | 1.10 | 5/1341 (0.4%) |
| 62 | DY | 0.79 | 1/1004 (0.1%) | 0.98 | 2/1341 (0.1%) |
| 63 | BZ | 0.59 | 0/1118 | 0.81 | 1/1497 (0.1%) |
| 63 | DZ | 0.55 | 0/1118 | 0.83 | 2/1497 (0.1%) |
| 64 | Ba | 0.97 | 2/1204 (0.2%) | 1.16 | 7/1612 (0.4%) |
| 64 | Da | 0.94 | 2/1204 (0.2%) | 1.14 | 9/1612 (0.6%) |
| 65 | Bb | 0.83 | 0/473 | 0.85 | 0/629 |
| 65 | Db | 0.91 | 0/473 | 1.14 | 1/629 (0.2%) |
| 66 | Bc | 0.59 | 0/751 | 0.73 | 0/1008 |
| 66 | Dc | 0.61 | 0/775 | 0.77 | 0/1040 |
| 67 | Bd | 0.73 | 0/890 | 0.89 | 1/1196 (0.1%) |
| 67 | Dd | 0.94 | 2/897 (0.2%) | 0.95 | 1/1205 (0.1%) |
| 68 | Be | 1.02 | 2/1041 (0.2%) | 1.19 | 9/1394 (0.6%) |
| 68 | De | 1.03 | 0/1041 | 1.27 | 11/1394 (0.8%) |
| 69 | Bf | 1.19 | 4/868 (0.5%) | 1.08 | 2/1168 (0.2%) |
| 69 | Df | 1.12 | 1/868 (0.1%) | 1.09 | 3/1168 (0.3%) |
| 70 | Bg | 0.70 | 0/890 | 0.98 | 4/1189 (0.3%) |
| 70 | Dg | 0.72 | 0/890 | 0.92 | 0/1189 |
| 71 | Bh | 0.83 | 0/978 | 0.94 | 2/1301 (0.2%) |
| 71 | Dh | 0.67 | 0/974 | 0.80 | 0/1297 |
| 72 | Bi | 0.77 | 0/778 | 0.98 | 1/1034 (0.1%) |
| 72 | Di | 0.67 | 0/777 | 0.85 | 0/1033 |
| 73 | Bj | 0.98 | 2/696 (0.3%) | 1.19 | 6/923 (0.7%) |
| 73 | Dj | 0.87 | 0/696 | 1.04 | 3/923 (0.3%) |
| 74 | Bk | 0.59 | 0/618 | 0.75 | 0/826 |
| 74 | Dk | 0.50 | 0/614 | 0.70 | 0/822 |
| 75 | Bl | 0.90 | 1/443 (0.2%) | 1.07 | 1/588 (0.2%) |
| 75 | Dl | 0.90 | 0/443 | 1.02 | 1/588 (0.2%) |
| 76 | Bm | 0.89 | 1/423 (0.2%) | 0.97 | 1/562 (0.2%) |
| 76 | Dm | 1.08 | 2/423 (0.5%) | 1.13 | 1/562 (0.2%) |
| 77 | Bn | 0.78 | 0/234 | 1.18 | 2/300 (0.7%) |
| 77 | Dn | 0.90 | 0/234 | 1.15 | 1/300 (0.3%) |
| 78 | Bo | 0.87 | 1/860 (0.1%) | 0.97 | 2/1136 (0.2%) |
| 78 | Do | 0.83 | 0/860 | 0.88 | 1/1136 (0.1%) |
| 79 | Bp | 0.80 | 0/701 | 0.96 | 1/934 (0.1%) |
| 79 | Dp | 0.86 | 0/701 | 0.98 | 1/934 (0.1%) |
| 80 | A6 | 1.13 | 97/42174 (0.2%) | 1.61 | 1103/65711 (1.7%) |
| 81 | Ch | 0.64 | 0/480 | 0.85 | 0/642 |
| 83 | Dq | 0.54 | 0/977 | 0.75 | 1/1313 (0.1%) |
| All | All | 1.11 | 1373/432157 (0.3%) | 1.51 | 9884/634038 (1.6%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2 | CA | 0 | 1 |
| 3 | AB | 0 | 1 |
| 5 | CD | 0 | 1 |
| 7 | CF | 0 | 2 |
| 9 | AH | 0 | 1 |
| 11 | CJ | 0 | 3 |
| 13 | AL | 0 | 1 |
| 16 | AO | 0 | 1 |
| 16 | CO | 0 | 1 |
| 17 | CP | 0 | 1 |
| 18 | CQ | 0 | 1 |
| 19 | AR | 0 | 2 |
| 22 | CU | 0 | 1 |
| 25 | CX | 0 | 1 |
| 27 | AZ | 0 | 3 |
| 27 | CZ | 0 | 2 |
| 29 | Ab | 0 | 1 |
| 33 | Af | 0 | 2 |
| 33 | Cf | 0 | 2 |
| 35 | Ah | 0 | 1 |
| 36 | A1 | 0 | 3 |
| 36 | A5 | 0 | 1 |
| 39 | DA | 0 | 2 |
| 40 | BB | 0 | 1 |
| 41 | BC | 0 | 1 |
| 41 | DC | 0 | 1 |
| 42 | DD | 0 | 1 |
| 43 | BE | 0 | 2 |
| 43 | DE | 0 | 1 |
| 44 | BF | 0 | 1 |
| 44 | DF | 0 | 2 |
| 45 | BG | 0 | 3 |
| 46 | BH | 0 | 1 |
| 48 | BJ | 0 | 1 |
| 52 | BO | 0 | 2 |
| 52 | DO | 0 | 2 |
| 56 | DS | 0 | 1 |
| 57 | BT | 0 | 1 |
| 59 | DV | 0 | 1 |

Continued on next page...

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 62 | DY | 0 | 1 |
| 63 | DZ | 0 | 1 |
| 64 | Da | 0 | 3 |
| 65 | Bb | 0 | 2 |
| 65 | Db | 0 | 1 |
| 67 | Bd | 0 | 1 |
| 78 | Bo | 0 | 1 |
| All | All | 0 | 67 |

All (1373) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|--------|--------|-------------|----------|
| 52 | BO | 3[A] | VAL | C-N | 26.80 | 1.95 | 1.34 |
| 36 | A1 | 2777 | G | C5-C6 | -23.22 | 1.19 | 1.42 |
| 52 | DO | 197[B] | PHE | C-N | -21.96 | 0.93 | 1.33 |
| 52 | DO | 182[B] | SER | C-N | 18.04 | 1.75 | 1.34 |
| 36 | A5 | 1152 | G | N9-C8 | 15.01 | 1.48 | 1.37 |
| 36 | A5 | 1152 | G | N9-C4 | -14.78 | 1.26 | 1.38 |
| 52 | BO | 197[B] | PHE | C-N | -14.63 | 1.06 | 1.33 |
| 35 | Ah | 134 | ASP | CG-OD1 | 13.92 | 1.57 | 1.25 |
| 36 | A5 | 1152 | G | C2-N3 | -13.38 | 1.22 | 1.32 |
| 36 | A1 | 3242 | G | N9-C4 | -13.12 | 1.27 | 1.38 |
| 36 | A1 | 2777 | G | C8-N7 | -13.09 | 1.23 | 1.30 |
| 35 | Ah | 134 | ASP | CG-OD2 | 12.58 | 1.54 | 1.25 |
| 36 | A1 | 3242 | G | C2-N3 | -11.79 | 1.23 | 1.32 |
| 52 | DO | 23[B] | ILE | C-N | -11.03 | 1.08 | 1.34 |
| 80 | A6 | 337 | G | C2-N2 | 10.65 | 1.45 | 1.34 |
| 36 | A1 | 2993 | G | N9-C4 | -10.48 | 1.29 | 1.38 |
| 52 | BO | 13[B] | ASP | C-N | 10.23 | 1.57 | 1.34 |
| 40 | BB | 7 | GLU | CG-CD | 9.97 | 1.67 | 1.51 |
| 52 | DO | 3[B] | SER | C-N | 9.61 | 1.56 | 1.34 |
| 52 | BO | 40[B] | ALA | C-N | -9.49 | 1.12 | 1.34 |
| 36 | A5 | 3216 | G | N7-C5 | -9.44 | 1.33 | 1.39 |
| 36 | A1 | 2714 | G | N9-C4 | -9.34 | 1.30 | 1.38 |
| 36 | A1 | 942 | U | C2-N3 | -9.30 | 1.31 | 1.37 |
| 36 | A1 | 39 | A | N7-C5 | -9.25 | 1.33 | 1.39 |
| 40 | BB | 7 | GLU | CB-CG | 9.23 | 1.69 | 1.52 |
| 36 | A1 | 2777 | G | C5-C4 | -9.20 | 1.31 | 1.38 |
| 36 | A1 | 2278 | C | C2-O2 | -9.19 | 1.16 | 1.24 |
| 36 | A5 | 2941 | A | N9-C4 | -9.16 | 1.32 | 1.37 |
| 80 | A6 | 163 | G | N9-C4 | -9.06 | 1.30 | 1.38 |
| 36 | A5 | 2914 | G | P-OP2 | -9.06 | 1.33 | 1.49 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-------|------|-------|-------|-------------|----------|
| 36 | A5 | 1434 | G | N7-C5 | -9.05 | 1.33 | 1.39 |
| 36 | A5 | 1449 | A | N9-C4 | -9.03 | 1.32 | 1.37 |
| 36 | A1 | 1377 | G | N1-C2 | -8.96 | 1.30 | 1.37 |
| 36 | A5 | 652 | G | N1-C2 | -8.88 | 1.30 | 1.37 |
| 80 | A6 | 337 | G | C8-N7 | -8.88 | 1.25 | 1.30 |
| 36 | A1 | 2714 | G | N9-C8 | 8.83 | 1.44 | 1.37 |
| 36 | A5 | 1450 | G | C8-N7 | -8.74 | 1.25 | 1.30 |
| 36 | A1 | 3181 | C | N3-C4 | -8.72 | 1.27 | 1.33 |
| 36 | A5 | 953 | G | C5-C4 | -8.71 | 1.32 | 1.38 |
| 36 | A1 | 2419 | A | N9-C4 | -8.68 | 1.32 | 1.37 |
| 36 | A5 | 367 | A | N9-C4 | -8.65 | 1.32 | 1.37 |
| 36 | A1 | 1592 | G | C6-O6 | -8.58 | 1.16 | 1.24 |
| 52 | DO | 80[B] | LEU | C-N | 8.57 | 1.53 | 1.34 |
| 36 | A1 | 2867 | C | N3-C4 | -8.51 | 1.27 | 1.33 |
| 52 | BO | 22[B] | THR | C-N | 8.49 | 1.53 | 1.34 |
| 36 | A1 | 2777 | G | N1-C2 | -8.48 | 1.30 | 1.37 |
| 36 | A5 | 3088 | G | C6-O6 | -8.43 | 1.16 | 1.24 |
| 36 | A5 | 2278 | C | C2-O2 | -8.32 | 1.17 | 1.24 |
| 36 | A1 | 49 | A | N9-C4 | -8.26 | 1.32 | 1.37 |
| 36 | A5 | 2899 | C | N3-C4 | -8.26 | 1.28 | 1.33 |
| 80 | A6 | 1652 | C | N3-C4 | -8.23 | 1.28 | 1.33 |
| 36 | A1 | 2800 | G | P-OP1 | -8.20 | 1.35 | 1.49 |
| 36 | A5 | 2191 | U | C4-C5 | -8.19 | 1.36 | 1.43 |
| 36 | A5 | 1178 | G | P-OP2 | -8.17 | 1.35 | 1.49 |
| 80 | A6 | 65 | A | N9-C4 | -8.17 | 1.32 | 1.37 |
| 1 | A2 | 553 | G | C6-N1 | 8.12 | 1.45 | 1.39 |
| 36 | A5 | 1887 | A | N9-C4 | -8.12 | 1.32 | 1.37 |
| 36 | A1 | 2356 | A | N9-C4 | -8.11 | 1.32 | 1.37 |
| 80 | A6 | 337 | G | N1-C2 | 8.08 | 1.44 | 1.37 |
| 36 | A5 | 2393 | G | C8-N7 | -8.08 | 1.26 | 1.30 |
| 36 | A5 | 2726 | C | N3-C4 | -8.06 | 1.28 | 1.33 |
| 80 | A6 | 337 | G | C2-N3 | 8.06 | 1.39 | 1.32 |
| 36 | A5 | 2817 | A | P-OP1 | -8.02 | 1.35 | 1.49 |
| 36 | A5 | 1152 | G | C5-C6 | -7.99 | 1.34 | 1.42 |
| 36 | A5 | 2830 | G | C6-N1 | -7.98 | 1.33 | 1.39 |
| 36 | A5 | 2280 | A | N9-C4 | -7.97 | 1.33 | 1.37 |
| 36 | A5 | 3216 | G | N9-C8 | -7.97 | 1.32 | 1.37 |
| 36 | A5 | 1849 | C | N3-C4 | -7.97 | 1.28 | 1.33 |
| 39 | DA | 211 | HIS | C-O | 7.97 | 1.38 | 1.23 |
| 36 | A5 | 2314 | U | N3-C4 | 7.95 | 1.45 | 1.38 |
| 36 | A1 | 2777 | G | N7-C5 | -7.94 | 1.34 | 1.39 |
| 36 | A5 | 1152 | G | N3-C4 | -7.91 | 1.29 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|-------|-------|-------------|----------|
| 36 | A5 | 3114 | A | N9-C4 | -7.89 | 1.33 | 1.37 |
| 36 | A1 | 3242 | G | N3-C4 | -7.88 | 1.29 | 1.35 |
| 36 | A5 | 3245 | A | N9-C4 | -7.88 | 1.33 | 1.37 |
| 36 | A5 | 1311 | G | C5-C4 | -7.86 | 1.32 | 1.38 |
| 36 | A5 | 953 | G | N7-C5 | -7.84 | 1.34 | 1.39 |
| 36 | A1 | 652 | G | N1-C2 | -7.83 | 1.31 | 1.37 |
| 36 | A5 | 917 | A | N7-C5 | -7.80 | 1.34 | 1.39 |
| 38 | A4 | 12 | A | N3-C4 | -7.80 | 1.30 | 1.34 |
| 36 | A1 | 2836 | C | N3-C4 | -7.79 | 1.28 | 1.33 |
| 80 | A6 | 163 | G | N3-C4 | -7.77 | 1.30 | 1.35 |
| 75 | B1 | 2 | ALA | CA-CB | -7.77 | 1.36 | 1.52 |
| 36 | A5 | 519 | A | N7-C5 | -7.75 | 1.34 | 1.39 |
| 36 | A5 | 2703 | A | N7-C5 | -7.74 | 1.34 | 1.39 |
| 36 | A5 | 631 | U | C2-N3 | -7.71 | 1.32 | 1.37 |
| 36 | A5 | 2945 | G | P-O5' | -7.71 | 1.52 | 1.59 |
| 80 | A6 | 1595 | U | C2-N3 | -7.70 | 1.32 | 1.37 |
| 36 | A5 | 1902 | G | C5-C4 | -7.69 | 1.32 | 1.38 |
| 36 | A1 | 816 | A | N3-C4 | 7.67 | 1.39 | 1.34 |
| 36 | A1 | 317 | A | N7-C5 | -7.66 | 1.34 | 1.39 |
| 36 | A1 | 1164 | G | C6-N1 | -7.66 | 1.34 | 1.39 |
| 36 | A5 | 41 | G | P-OP1 | -7.66 | 1.35 | 1.49 |
| 57 | DT | 104 | GLU | CB-CG | 7.65 | 1.66 | 1.52 |
| 36 | A1 | 966 | U | C4-O4 | -7.65 | 1.17 | 1.23 |
| 36 | A5 | 345 | G | N1-C2 | -7.64 | 1.31 | 1.37 |
| 36 | A5 | 1434 | G | N9-C8 | -7.63 | 1.32 | 1.37 |
| 36 | A5 | 2804 | A | N9-C4 | -7.62 | 1.33 | 1.37 |
| 36 | A1 | 1492 | G | N9-C4 | 7.62 | 1.44 | 1.38 |
| 36 | A5 | 2314 | U | C2-N3 | 7.60 | 1.43 | 1.37 |
| 36 | A5 | 1301 | A | N7-C5 | -7.59 | 1.34 | 1.39 |
| 36 | A5 | 970 | A | N9-C4 | -7.58 | 1.33 | 1.37 |
| 36 | A1 | 963 | G | N7-C5 | -7.56 | 1.34 | 1.39 |
| 80 | A6 | 542 | A | N7-C5 | -7.55 | 1.34 | 1.39 |
| 36 | A5 | 3006 | A | N3-C4 | -7.55 | 1.30 | 1.34 |
| 36 | A5 | 2335 | G | N3-C4 | -7.54 | 1.30 | 1.35 |
| 36 | A5 | 2272 | G | C5-C4 | -7.54 | 1.33 | 1.38 |
| 52 | DO | 84[B] | ILE | C-N | 7.54 | 1.51 | 1.34 |
| 80 | A6 | 1773 | C | C4-N4 | 7.53 | 1.40 | 1.33 |
| 52 | BO | 182[B] | SER | C-N | -7.53 | 1.16 | 1.34 |
| 36 | A1 | 895 | A | N9-C8 | 7.53 | 1.43 | 1.37 |
| 36 | A1 | 1507 | G | N9-C8 | -7.52 | 1.32 | 1.37 |
| 36 | A1 | 970 | A | N9-C4 | -7.51 | 1.33 | 1.37 |
| 36 | A1 | 2952 | G | N9-C4 | -7.51 | 1.31 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-------|------|-------|-------|-------------|----------|
| 36 | A1 | 282 | G | N7-C5 | -7.50 | 1.34 | 1.39 |
| 36 | A5 | 1307 | G | P-O5' | -7.48 | 1.52 | 1.59 |
| 54 | DQ | 171 | LYS | CE-NZ | 7.47 | 1.67 | 1.49 |
| 36 | A1 | 659 | G | N1-C2 | -7.43 | 1.31 | 1.37 |
| 36 | A5 | 960 | U | N1-C2 | 7.43 | 1.45 | 1.38 |
| 36 | A5 | 2191 | U | C4-O4 | -7.43 | 1.17 | 1.23 |
| 36 | A1 | 2919 | A | N9-C4 | -7.41 | 1.33 | 1.37 |
| 36 | A5 | 934 | G | P-OP1 | -7.40 | 1.36 | 1.49 |
| 36 | A1 | 1886 | A | N9-C4 | -7.40 | 1.33 | 1.37 |
| 41 | BC | 94 | CYS | CB-SG | -7.40 | 1.69 | 1.82 |
| 80 | A6 | 1535 | U | C2-N3 | -7.39 | 1.32 | 1.37 |
| 36 | A5 | 1303 | A | C5-C4 | -7.39 | 1.33 | 1.38 |
| 36 | A1 | 35 | A | N9-C4 | -7.39 | 1.33 | 1.37 |
| 36 | A5 | 2134 | G | N1-C2 | -7.39 | 1.31 | 1.37 |
| 36 | A1 | 2777 | G | N9-C4 | -7.38 | 1.32 | 1.38 |
| 36 | A5 | 1902 | G | P-OP1 | -7.36 | 1.36 | 1.49 |
| 36 | A5 | 953 | G | N9-C8 | -7.36 | 1.32 | 1.37 |
| 36 | A5 | 2948 | C | N3-C4 | -7.35 | 1.28 | 1.33 |
| 36 | A1 | 2697 | A | C6-N6 | -7.34 | 1.28 | 1.33 |
| 36 | A5 | 2385 | G | N9-C4 | -7.32 | 1.32 | 1.38 |
| 36 | A5 | 3245 | A | C5-C6 | -7.32 | 1.34 | 1.41 |
| 36 | A5 | 1443 | G | C2-N3 | -7.31 | 1.26 | 1.32 |
| 69 | Bf | 70 | LYS | CE-NZ | 7.29 | 1.67 | 1.49 |
| 36 | A1 | 929 | A | N3-C4 | -7.29 | 1.30 | 1.34 |
| 36 | A5 | 1374 | G | N1-C2 | -7.29 | 1.31 | 1.37 |
| 36 | A1 | 644 | G | N7-C5 | -7.28 | 1.34 | 1.39 |
| 36 | A1 | 2611 | U | C4-O4 | -7.28 | 1.17 | 1.23 |
| 78 | Bo | 77 | CYS | CB-SG | -7.28 | 1.69 | 1.82 |
| 36 | A1 | 799 | G | N3-C4 | -7.27 | 1.30 | 1.35 |
| 36 | A5 | 345 | G | C6-N1 | -7.27 | 1.34 | 1.39 |
| 36 | A5 | 2919 | A | C6-N1 | -7.26 | 1.30 | 1.35 |
| 36 | A5 | 1515 | A | C5-C6 | -7.24 | 1.34 | 1.41 |
| 52 | BO | 27[B] | VAL | C-N | 7.24 | 1.50 | 1.34 |
| 36 | A1 | 637 | C | N1-C6 | -7.23 | 1.32 | 1.37 |
| 36 | A1 | 644 | G | C6-O6 | 7.23 | 1.30 | 1.24 |
| 36 | A1 | 1308 | A | P-OP2 | -7.22 | 1.36 | 1.49 |
| 36 | A1 | 660 | A | C6-N6 | -7.21 | 1.28 | 1.33 |
| 36 | A5 | 3122 | A | N3-C4 | -7.21 | 1.30 | 1.34 |
| 36 | A5 | 2141 | U | P-OP2 | -7.20 | 1.36 | 1.49 |
| 36 | A5 | 2943 | G | N7-C5 | -7.18 | 1.34 | 1.39 |
| 36 | A1 | 816 | A | N9-C4 | 7.17 | 1.42 | 1.37 |
| 36 | A1 | 1430 | U | P-OP1 | -7.17 | 1.36 | 1.49 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 36 | A1 | 339 | C | N3-C4 | -7.17 | 1.28 | 1.33 |
| 36 | A1 | 2679 | A | N9-C4 | -7.16 | 1.33 | 1.37 |
| 36 | A5 | 2949 | U | P-OP1 | -7.16 | 1.36 | 1.49 |
| 36 | A5 | 1849 | C | C2-N3 | -7.15 | 1.30 | 1.35 |
| 37 | A7 | 85 | G | N1-C2 | -7.15 | 1.32 | 1.37 |
| 36 | A5 | 2364 | G | C6-N1 | -7.14 | 1.34 | 1.39 |
| 1 | A2 | 377 | G | N9-C4 | -7.14 | 1.32 | 1.38 |
| 36 | A5 | 644 | G | N7-C5 | -7.13 | 1.34 | 1.39 |
| 36 | A5 | 1430 | U | P-OP1 | -7.12 | 1.36 | 1.49 |
| 80 | A6 | 609 | U | N3-C4 | -7.09 | 1.32 | 1.38 |
| 36 | A5 | 1112 | A | N7-C5 | -7.08 | 1.35 | 1.39 |
| 36 | A5 | 2837 | A | C5-C4 | -7.07 | 1.33 | 1.38 |
| 36 | A1 | 661 | G | N7-C5 | -7.07 | 1.35 | 1.39 |
| 36 | A5 | 2689 | A | N3-C4 | -7.07 | 1.30 | 1.34 |
| 36 | A1 | 1304 | A | N9-C4 | -7.07 | 1.33 | 1.37 |
| 36 | A1 | 1099 | A | N9-C4 | -7.06 | 1.33 | 1.37 |
| 36 | A5 | 1159 | A | N9-C4 | -7.05 | 1.33 | 1.37 |
| 37 | A7 | 96 | U | C2-O2 | -7.05 | 1.16 | 1.22 |
| 38 | A8 | 20 | U | C4-O4 | -7.05 | 1.18 | 1.23 |
| 80 | A6 | 100 | A | P-OP2 | -7.04 | 1.36 | 1.49 |
| 36 | A1 | 631 | U | C2-O2 | -7.03 | 1.16 | 1.22 |
| 36 | A5 | 1110 | U | C4-O4 | -7.03 | 1.18 | 1.23 |
| 36 | A5 | 420 | G | N7-C5 | -7.03 | 1.35 | 1.39 |
| 36 | A5 | 2364 | G | N3-C4 | -7.02 | 1.30 | 1.35 |
| 36 | A1 | 2640 | A | C6-N1 | -7.01 | 1.30 | 1.35 |
| 37 | A3 | 89 | G | N7-C5 | -7.01 | 1.35 | 1.39 |
| 36 | A1 | 889 | U | C2-N3 | -7.00 | 1.32 | 1.37 |
| 36 | A5 | 1887 | A | N7-C5 | -7.00 | 1.35 | 1.39 |
| 36 | A5 | 726 | G | C5-C6 | -7.00 | 1.35 | 1.42 |
| 64 | Ba | 24 | LYS | CE-NZ | 6.99 | 1.66 | 1.49 |
| 36 | A1 | 1301 | A | N7-C5 | -6.98 | 1.35 | 1.39 |
| 80 | A6 | 397 | A | N9-C4 | -6.97 | 1.33 | 1.37 |
| 36 | A5 | 3180 | A | N3-C4 | -6.97 | 1.30 | 1.34 |
| 80 | A6 | 1744 | A | N9-C4 | -6.95 | 1.33 | 1.37 |
| 36 | A5 | 1200 | A | N3-C4 | -6.95 | 1.30 | 1.34 |
| 36 | A5 | 2361 | A | N9-C4 | 6.95 | 1.42 | 1.37 |
| 80 | A6 | 1105 | C | N1-C6 | -6.95 | 1.32 | 1.37 |
| 36 | A5 | 2887 | A | P-OP2 | -6.95 | 1.37 | 1.49 |
| 36 | A1 | 148 | G | N7-C5 | -6.94 | 1.35 | 1.39 |
| 36 | A5 | 2434 | U | N3-C4 | -6.94 | 1.32 | 1.38 |
| 38 | A4 | 28 | C | N3-C4 | -6.93 | 1.29 | 1.33 |
| 36 | A1 | 2279 | A | C5-C6 | -6.93 | 1.34 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|--------|-------|-------------|----------|
| 36 | A5 | 971 | G | C5-C4 | -6.93 | 1.33 | 1.38 |
| 36 | A1 | 3227 | A | N9-C4 | -6.92 | 1.33 | 1.37 |
| 36 | A5 | 2335 | G | C6-N1 | -6.91 | 1.34 | 1.39 |
| 36 | A5 | 2399 | A | N9-C4 | -6.91 | 1.33 | 1.37 |
| 36 | A5 | 1901 | A | N7-C5 | -6.89 | 1.35 | 1.39 |
| 36 | A5 | 2138 | A | N7-C5 | -6.89 | 1.35 | 1.39 |
| 36 | A1 | 658 | G | C8-N7 | -6.88 | 1.26 | 1.30 |
| 36 | A5 | 1184 | A | N9-C4 | -6.88 | 1.33 | 1.37 |
| 36 | A1 | 2394 | G | C5-C4 | -6.88 | 1.33 | 1.38 |
| 36 | A1 | 3130 | A | N7-C5 | -6.88 | 1.35 | 1.39 |
| 36 | A1 | 1153 | A | N7-C5 | -6.88 | 1.35 | 1.39 |
| 36 | A5 | 2336 | U | C2-N3 | -6.87 | 1.32 | 1.37 |
| 36 | A1 | 970 | A | N3-C4 | -6.86 | 1.30 | 1.34 |
| 36 | A5 | 2836 | C | C4-C5 | 6.86 | 1.48 | 1.43 |
| 1 | A2 | 1456 | C | N3-C4 | -6.85 | 1.29 | 1.33 |
| 36 | A1 | 66 | A | N9-C4 | -6.84 | 1.33 | 1.37 |
| 36 | A5 | 334 | A | C5-C4 | -6.84 | 1.33 | 1.38 |
| 36 | A5 | 340 | C | P-OP1 | -6.83 | 1.37 | 1.49 |
| 36 | A1 | 2376 | G | N9-C8 | -6.83 | 1.33 | 1.37 |
| 80 | A6 | 1503 | A | N9-C8 | 6.82 | 1.43 | 1.37 |
| 36 | A1 | 1117 | G | C5-C4 | -6.82 | 1.33 | 1.38 |
| 36 | A1 | 2692 | A | N9-C4 | 6.82 | 1.42 | 1.37 |
| 36 | A5 | 1592 | G | N1-C2 | -6.82 | 1.32 | 1.37 |
| 36 | A1 | 345 | G | N9-C8 | -6.82 | 1.33 | 1.37 |
| 36 | A5 | 1042 | U | C2-N3 | -6.82 | 1.32 | 1.37 |
| 36 | A1 | 1928 | G | C2-N3 | -6.80 | 1.27 | 1.32 |
| 36 | A5 | 429 | U | C2-N3 | -6.79 | 1.32 | 1.37 |
| 36 | A1 | 1114 | U | C2-N3 | -6.79 | 1.33 | 1.37 |
| 36 | A5 | 986 | U | C4-C5 | -6.78 | 1.37 | 1.43 |
| 47 | BI | 14 | ASN | CG-ND2 | 6.75 | 1.49 | 1.32 |
| 36 | A5 | 2636 | A | C6-N1 | -6.75 | 1.30 | 1.35 |
| 36 | A5 | 1449 | A | P-OP2 | -6.75 | 1.37 | 1.49 |
| 52 | BO | 184[B] | ALA | C-N | 6.75 | 1.49 | 1.34 |
| 36 | A5 | 3316 | A | N9-C4 | -6.74 | 1.33 | 1.37 |
| 36 | A5 | 930 | U | C4-O4 | -6.74 | 1.18 | 1.23 |
| 80 | A6 | 1600 | A | N9-C4 | -6.73 | 1.33 | 1.37 |
| 36 | A5 | 1178 | G | C2-N3 | -6.73 | 1.27 | 1.32 |
| 37 | A7 | 81 | U | C4-O4 | -6.72 | 1.18 | 1.23 |
| 36 | A1 | 2816 | G | C5-C4 | -6.72 | 1.33 | 1.38 |
| 80 | A6 | 1119 | G | C6-N1 | -6.71 | 1.34 | 1.39 |
| 36 | A5 | 1592 | G | C6-N1 | -6.71 | 1.34 | 1.39 |
| 1 | A2 | 1455 | G | C6-O6 | 6.71 | 1.30 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|-------|-------|-------------|----------|
| 36 | A1 | 922 | U | P-OP2 | -6.71 | 1.37 | 1.49 |
| 1 | A2 | 992 | A | C2-N3 | -6.70 | 1.27 | 1.33 |
| 36 | A1 | 2188 | A | N9-C4 | -6.69 | 1.33 | 1.37 |
| 36 | A5 | 2395 | G | C5-C4 | -6.69 | 1.33 | 1.38 |
| 36 | A5 | 847 | A | N9-C4 | -6.69 | 1.33 | 1.37 |
| 36 | A1 | 874 | U | C2-N3 | -6.68 | 1.33 | 1.37 |
| 36 | A1 | 912 | G | C5-C4 | -6.68 | 1.33 | 1.38 |
| 36 | A5 | 3137 | C | N1-C6 | 6.68 | 1.41 | 1.37 |
| 1 | A2 | 553 | G | C6-O6 | 6.67 | 1.30 | 1.24 |
| 36 | A5 | 2912 | G | N7-C5 | -6.67 | 1.35 | 1.39 |
| 36 | A1 | 1887 | A | N9-C4 | -6.67 | 1.33 | 1.37 |
| 36 | A1 | 2409 | G | N3-C4 | -6.66 | 1.30 | 1.35 |
| 80 | A6 | 163 | G | C5-C6 | -6.66 | 1.35 | 1.42 |
| 36 | A5 | 1371 | G | C6-N1 | -6.66 | 1.34 | 1.39 |
| 36 | A1 | 910 | G | N7-C5 | -6.66 | 1.35 | 1.39 |
| 36 | A1 | 1326 | A | N9-C4 | -6.66 | 1.33 | 1.37 |
| 36 | A1 | 2657 | A | N7-C5 | -6.65 | 1.35 | 1.39 |
| 36 | A5 | 1319 | G | N7-C5 | -6.65 | 1.35 | 1.39 |
| 36 | A1 | 3216 | G | N7-C5 | -6.65 | 1.35 | 1.39 |
| 37 | A7 | 85 | G | C6-N1 | -6.65 | 1.34 | 1.39 |
| 36 | A1 | 654 | C | N1-C6 | -6.64 | 1.33 | 1.37 |
| 36 | A5 | 2911 | A | N7-C5 | -6.64 | 1.35 | 1.39 |
| 36 | A5 | 3006 | A | N9-C4 | -6.63 | 1.33 | 1.37 |
| 36 | A5 | 1301 | A | C5-C6 | -6.63 | 1.35 | 1.41 |
| 36 | A1 | 653 | A | C6-N6 | -6.63 | 1.28 | 1.33 |
| 36 | A1 | 30 | G | C6-N1 | -6.63 | 1.34 | 1.39 |
| 36 | A1 | 195 | U | C2-O2 | -6.63 | 1.16 | 1.22 |
| 36 | A1 | 2601 | A | N9-C4 | -6.62 | 1.33 | 1.37 |
| 36 | A1 | 85 | A | N9-C4 | -6.62 | 1.33 | 1.37 |
| 36 | A1 | 2617 | U | N3-C4 | -6.62 | 1.32 | 1.38 |
| 80 | A6 | 1773 | C | N3-C4 | 6.61 | 1.38 | 1.33 |
| 36 | A5 | 3209 | A | C5-C4 | 6.61 | 1.43 | 1.38 |
| 80 | A6 | 1773 | C | C2-N3 | 6.61 | 1.41 | 1.35 |
| 80 | A6 | 1119 | G | N7-C5 | -6.60 | 1.35 | 1.39 |
| 36 | A1 | 1307 | G | N1-C2 | -6.60 | 1.32 | 1.37 |
| 36 | A1 | 45 | A | N7-C5 | -6.60 | 1.35 | 1.39 |
| 36 | A5 | 2693 | C | C2-N3 | -6.59 | 1.30 | 1.35 |
| 52 | DO | 158[B] | ASP | C-N | 6.59 | 1.49 | 1.34 |
| 36 | A1 | 643 | U | N1-C2 | -6.59 | 1.32 | 1.38 |
| 36 | A1 | 1481 | A | N7-C5 | -6.59 | 1.35 | 1.39 |
| 36 | A1 | 3222 | U | C2-N3 | -6.59 | 1.33 | 1.37 |
| 36 | A5 | 3362 | A | N3-C4 | -6.59 | 1.30 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-------|------|---------|-------|-------------|----------|
| 36 | A1 | 942 | U | N3-C4 | -6.58 | 1.32 | 1.38 |
| 80 | A6 | 351 | C | N1-C6 | -6.58 | 1.33 | 1.37 |
| 36 | A5 | 2853 | A | N9-C4 | -6.58 | 1.33 | 1.37 |
| 36 | A1 | 1154 | A | N7-C5 | -6.58 | 1.35 | 1.39 |
| 80 | A6 | 337 | G | N7-C5 | -6.58 | 1.35 | 1.39 |
| 36 | A5 | 2918 | G | N7-C5 | -6.58 | 1.35 | 1.39 |
| 36 | A5 | 267 | G | C8-N7 | -6.56 | 1.27 | 1.30 |
| 36 | A5 | 859 | G | N1-C2 | -6.56 | 1.32 | 1.37 |
| 52 | DO | 22[B] | THR | C-N | 6.56 | 1.49 | 1.34 |
| 36 | A5 | 1429 | G | C6-N1 | -6.56 | 1.34 | 1.39 |
| 80 | A6 | 53 | G | C6-N1 | -6.54 | 1.34 | 1.39 |
| 36 | A5 | 1515 | A | C6-N1 | -6.54 | 1.30 | 1.35 |
| 36 | A5 | 91 | G | N3-C4 | -6.53 | 1.30 | 1.35 |
| 36 | A1 | 931 | C | N3-C4 | -6.53 | 1.29 | 1.33 |
| 36 | A5 | 642 | U | N3-C4 | -6.53 | 1.32 | 1.38 |
| 36 | A5 | 1142 | G | N7-C5 | -6.53 | 1.35 | 1.39 |
| 36 | A1 | 2899 | C | N1-C6 | -6.52 | 1.33 | 1.37 |
| 36 | A1 | 965 | A | N3-C4 | -6.52 | 1.30 | 1.34 |
| 36 | A5 | 942 | U | P-OP1 | -6.51 | 1.37 | 1.49 |
| 36 | A5 | 1849 | C | N1-C6 | -6.51 | 1.33 | 1.37 |
| 36 | A5 | 1307 | G | C3'-O3' | 6.50 | 1.51 | 1.42 |
| 36 | A5 | 1833 | G | N1-C2 | -6.50 | 1.32 | 1.37 |
| 36 | A5 | 3106 | A | N7-C5 | -6.49 | 1.35 | 1.39 |
| 36 | A5 | 1490 | A | N7-C5 | -6.49 | 1.35 | 1.39 |
| 36 | A1 | 3306 | U | C4-C5 | 6.49 | 1.49 | 1.43 |
| 36 | A1 | 884 | A | N9-C4 | -6.48 | 1.33 | 1.37 |
| 1 | A2 | 1200 | G | C6-N1 | 6.48 | 1.44 | 1.39 |
| 36 | A1 | 1394 | A | N7-C5 | -6.47 | 1.35 | 1.39 |
| 36 | A1 | 3129 | A | N9-C4 | -6.47 | 1.33 | 1.37 |
| 36 | A5 | 637 | C | C2-O2 | -6.45 | 1.18 | 1.24 |
| 36 | A1 | 417 | A | N9-C4 | -6.45 | 1.33 | 1.37 |
| 36 | A5 | 1487 | G | N1-C2 | -6.45 | 1.32 | 1.37 |
| 36 | A1 | 2606 | G | N9-C8 | -6.44 | 1.33 | 1.37 |
| 36 | A5 | 1841 | A | N7-C5 | -6.44 | 1.35 | 1.39 |
| 36 | A5 | 1370 | G | N1-C2 | -6.43 | 1.32 | 1.37 |
| 36 | A1 | 2679 | A | N3-C4 | -6.43 | 1.30 | 1.34 |
| 36 | A5 | 813 | G | N7-C5 | -6.42 | 1.35 | 1.39 |
| 36 | A1 | 2355 | G | N7-C5 | -6.42 | 1.35 | 1.39 |
| 36 | A1 | 2376 | G | N7-C5 | -6.42 | 1.35 | 1.39 |
| 36 | A1 | 511 | G | C6-N1 | -6.41 | 1.35 | 1.39 |
| 36 | A5 | 420 | G | C5-C4 | -6.41 | 1.33 | 1.38 |
| 36 | A5 | 2123 | G | C5-C4 | -6.41 | 1.33 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 80 | A6 | 101 | U | P-OP2 | -6.40 | 1.38 | 1.49 |
| 36 | A5 | 2323 | G | C6-N1 | -6.40 | 1.35 | 1.39 |
| 36 | A5 | 2987 | A | N7-C5 | -6.40 | 1.35 | 1.39 |
| 36 | A1 | 1152 | G | P-O5' | -6.40 | 1.53 | 1.59 |
| 36 | A1 | 812 | G | N7-C5 | -6.40 | 1.35 | 1.39 |
| 36 | A5 | 2147 | A | C5-C6 | -6.39 | 1.35 | 1.41 |
| 36 | A5 | 1143 | A | N9-C4 | -6.39 | 1.34 | 1.37 |
| 36 | A5 | 1117 | G | C5-C4 | -6.39 | 1.33 | 1.38 |
| 36 | A1 | 895 | A | C5-C4 | 6.39 | 1.43 | 1.38 |
| 36 | A1 | 878 | G | P-OP2 | -6.39 | 1.38 | 1.49 |
| 36 | A1 | 2364 | G | N9-C4 | -6.39 | 1.32 | 1.38 |
| 36 | A5 | 802 | C | N1-C6 | -6.39 | 1.33 | 1.37 |
| 1 | A2 | 992 | A | N9-C4 | -6.38 | 1.34 | 1.37 |
| 68 | Be | 41 | VAL | CB-CG1 | -6.37 | 1.39 | 1.52 |
| 80 | A6 | 366 | A | N9-C4 | -6.37 | 1.34 | 1.37 |
| 36 | A1 | 1606 | U | C2-N3 | -6.37 | 1.33 | 1.37 |
| 36 | A1 | 2726 | C | N3-C4 | -6.37 | 1.29 | 1.33 |
| 36 | A5 | 2816 | G | C5-C4 | -6.36 | 1.33 | 1.38 |
| 36 | A1 | 364 | G | N9-C4 | -6.36 | 1.32 | 1.38 |
| 1 | A2 | 1754 | A | N9-C4 | -6.35 | 1.34 | 1.37 |
| 36 | A1 | 701 | G | C6-O6 | -6.35 | 1.18 | 1.24 |
| 36 | A5 | 3102 | G | C6-N1 | -6.34 | 1.35 | 1.39 |
| 36 | A1 | 628 | A | N9-C4 | -6.34 | 1.34 | 1.37 |
| 36 | A5 | 342 | A | N9-C4 | -6.33 | 1.34 | 1.37 |
| 36 | A1 | 2368 | A | C6-N1 | -6.33 | 1.31 | 1.35 |
| 36 | A1 | 1130 | A | N7-C5 | -6.33 | 1.35 | 1.39 |
| 36 | A5 | 2937 | G | N9-C8 | -6.32 | 1.33 | 1.37 |
| 36 | A1 | 2952 | G | C5-C6 | -6.32 | 1.36 | 1.42 |
| 36 | A1 | 940 | G | C6-N1 | -6.31 | 1.35 | 1.39 |
| 36 | A5 | 1406 | A | N3-C4 | -6.31 | 1.31 | 1.34 |
| 36 | A1 | 2983 | C | N3-C4 | -6.31 | 1.29 | 1.33 |
| 36 | A1 | 3362 | A | N7-C5 | -6.30 | 1.35 | 1.39 |
| 38 | A4 | 10 | A | C6-N6 | -6.29 | 1.28 | 1.33 |
| 36 | A1 | 2958 | A | C6-N6 | -6.29 | 1.28 | 1.33 |
| 36 | A1 | 3130 | A | C6-N1 | -6.28 | 1.31 | 1.35 |
| 36 | A1 | 646 | A | N7-C5 | -6.28 | 1.35 | 1.39 |
| 36 | A1 | 1180 | A | C6-N1 | -6.28 | 1.31 | 1.35 |
| 38 | A4 | 13 | A | C6-N6 | -6.27 | 1.28 | 1.33 |
| 36 | A5 | 2905 | U | C2-N3 | -6.26 | 1.33 | 1.37 |
| 36 | A5 | 2128 | C | N1-C6 | -6.26 | 1.33 | 1.37 |
| 57 | DT | 32 | LYS | CD-CE | 6.26 | 1.66 | 1.51 |
| 80 | A6 | 400 | A | N9-C4 | 6.26 | 1.41 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 36 | A5 | 1913 | A | C5-C6 | -6.26 | 1.35 | 1.41 |
| 36 | A1 | 1434 | G | N9-C8 | -6.25 | 1.33 | 1.37 |
| 80 | A6 | 1503 | A | C5-C4 | 6.25 | 1.43 | 1.38 |
| 36 | A1 | 2800 | G | N9-C4 | -6.24 | 1.32 | 1.38 |
| 36 | A5 | 1902 | G | N9-C8 | -6.24 | 1.33 | 1.37 |
| 36 | A5 | 2291 | A | N3-C4 | -6.24 | 1.31 | 1.34 |
| 36 | A5 | 2856 | G | N9-C8 | -6.24 | 1.33 | 1.37 |
| 36 | A5 | 1449 | A | C5-C6 | -6.23 | 1.35 | 1.41 |
| 36 | A1 | 2977 | G | C5-C4 | -6.23 | 1.33 | 1.38 |
| 36 | A1 | 1150 | A | N3-C4 | -6.23 | 1.31 | 1.34 |
| 36 | A1 | 1372 | C | N3-C4 | -6.23 | 1.29 | 1.33 |
| 69 | Bf | 10 | LYS | CD-CE | 6.22 | 1.66 | 1.51 |
| 36 | A5 | 876 | A | N3-C4 | -6.22 | 1.31 | 1.34 |
| 36 | A5 | 953 | G | N9-C4 | -6.22 | 1.32 | 1.38 |
| 52 | BO | 3[B] | SER | C-N | 6.22 | 1.48 | 1.34 |
| 36 | A5 | 2194 | G | C5-C4 | -6.21 | 1.33 | 1.38 |
| 36 | A5 | 2754 | G | P-OP1 | -6.21 | 1.38 | 1.49 |
| 36 | A5 | 3182 | G | C6-N1 | -6.21 | 1.35 | 1.39 |
| 36 | A5 | 1487 | G | C6-N1 | -6.21 | 1.35 | 1.39 |
| 36 | A1 | 2421 | U | C4-O4 | -6.21 | 1.18 | 1.23 |
| 36 | A1 | 2800 | G | N3-C4 | -6.21 | 1.31 | 1.35 |
| 53 | DP | 66 | SER | C-O | 6.21 | 1.35 | 1.23 |
| 69 | Bf | 70 | LYS | CD-CE | 6.21 | 1.66 | 1.51 |
| 36 | A5 | 795 | G | C5-C4 | -6.20 | 1.34 | 1.38 |
| 36 | A5 | 884 | A | C8-N7 | 6.20 | 1.35 | 1.31 |
| 36 | A5 | 2737 | C | N1-C6 | -6.20 | 1.33 | 1.37 |
| 1 | A2 | 49 | C | P-OP2 | -6.20 | 1.38 | 1.49 |
| 36 | A1 | 2383 | C | N3-C4 | 6.20 | 1.38 | 1.33 |
| 36 | A1 | 2993 | G | N3-C4 | -6.20 | 1.31 | 1.35 |
| 36 | A5 | 2314 | U | C4-O4 | 6.19 | 1.28 | 1.23 |
| 36 | A5 | 3172 | A | C8-N7 | -6.19 | 1.27 | 1.31 |
| 37 | A7 | 91 | G | N9-C8 | -6.19 | 1.33 | 1.37 |
| 36 | A1 | 1846 | C | P-O5' | -6.19 | 1.53 | 1.59 |
| 36 | A5 | 2823 | G | N7-C5 | -6.19 | 1.35 | 1.39 |
| 36 | A5 | 1835 | A | P-OP1 | -6.18 | 1.38 | 1.49 |
| 36 | A5 | 2858 | U | N3-C4 | -6.18 | 1.32 | 1.38 |
| 36 | A5 | 872 | U | C4-O4 | -6.18 | 1.18 | 1.23 |
| 1 | A2 | 1241 | G | N9-C8 | 6.17 | 1.42 | 1.37 |
| 36 | A5 | 1369 | A | P-OP2 | -6.17 | 1.38 | 1.49 |
| 36 | A5 | 1847 | A | N9-C4 | -6.17 | 1.34 | 1.37 |
| 36 | A1 | 347 | G | C5-C4 | -6.17 | 1.34 | 1.38 |
| 36 | A1 | 1055 | A | N9-C4 | -6.17 | 1.34 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 36 | A1 | 1307 | G | C3'-O3' | 6.17 | 1.50 | 1.42 |
| 36 | A1 | 584 | G | C5-C4 | -6.17 | 1.34 | 1.38 |
| 40 | DB | 367 | LYS | CE-NZ | 6.16 | 1.64 | 1.49 |
| 36 | A5 | 421 | G | C6-N1 | -6.16 | 1.35 | 1.39 |
| 36 | A1 | 2800 | G | C5-C4 | -6.16 | 1.34 | 1.38 |
| 36 | A5 | 1152 | G | C8-N7 | 6.15 | 1.34 | 1.30 |
| 80 | A6 | 1097 | U | C3'-O3' | 6.15 | 1.50 | 1.42 |
| 36 | A1 | 857 | G | N1-C2 | -6.14 | 1.32 | 1.37 |
| 36 | A5 | 218 | G | P-O5' | -6.14 | 1.53 | 1.59 |
| 36 | A1 | 668 | G | N3-C4 | -6.14 | 1.31 | 1.35 |
| 36 | A5 | 2881 | C | C2-O2 | -6.14 | 1.19 | 1.24 |
| 36 | A1 | 1434 | G | N7-C5 | -6.14 | 1.35 | 1.39 |
| 36 | A5 | 1851 | G | N9-C8 | -6.13 | 1.33 | 1.37 |
| 36 | A5 | 3006 | A | N7-C5 | -6.13 | 1.35 | 1.39 |
| 36 | A1 | 2169 | G | C5-C6 | 6.13 | 1.48 | 1.42 |
| 36 | A5 | 649 | A | C5-C6 | -6.13 | 1.35 | 1.41 |
| 36 | A5 | 363 | G | C5-C4 | -6.13 | 1.34 | 1.38 |
| 43 | DE | 90 | LYS | CD-CE | 6.13 | 1.66 | 1.51 |
| 64 | Da | 24 | LYS | CE-NZ | 6.13 | 1.64 | 1.49 |
| 36 | A5 | 1169 | A | N9-C4 | -6.13 | 1.34 | 1.37 |
| 36 | A1 | 279 | U | C4-O4 | -6.12 | 1.18 | 1.23 |
| 36 | A1 | 1164 | G | N3-C4 | -6.12 | 1.31 | 1.35 |
| 38 | A4 | 82 | U | P-O5' | 6.12 | 1.65 | 1.59 |
| 36 | A5 | 434 | U | C2-N3 | -6.12 | 1.33 | 1.37 |
| 36 | A1 | 2853 | A | N7-C5 | -6.11 | 1.35 | 1.39 |
| 36 | A5 | 2848 | G | N7-C5 | -6.11 | 1.35 | 1.39 |
| 37 | A7 | 96 | U | C4-O4 | -6.11 | 1.18 | 1.23 |
| 36 | A5 | 659 | G | N7-C5 | -6.10 | 1.35 | 1.39 |
| 36 | A5 | 1797 | A | N7-C5 | -6.10 | 1.35 | 1.39 |
| 36 | A1 | 1336 | U | C2-N3 | -6.10 | 1.33 | 1.37 |
| 36 | A1 | 1902 | G | C8-N7 | -6.10 | 1.27 | 1.30 |
| 36 | A5 | 2830 | G | N3-C4 | -6.10 | 1.31 | 1.35 |
| 36 | A1 | 670 | C | N3-C4 | -6.09 | 1.29 | 1.33 |
| 36 | A1 | 1433 | A | N7-C5 | -6.09 | 1.35 | 1.39 |
| 36 | A1 | 1103 | A | N9-C4 | 6.08 | 1.41 | 1.37 |
| 36 | A1 | 921 | A | N7-C5 | -6.08 | 1.35 | 1.39 |
| 36 | A5 | 2372 | A | N3-C4 | -6.08 | 1.31 | 1.34 |
| 36 | A1 | 426 | G | N1-C2 | -6.08 | 1.32 | 1.37 |
| 36 | A1 | 3006 | A | N9-C4 | -6.07 | 1.34 | 1.37 |
| 36 | A1 | 34 | A | N9-C4 | -6.07 | 1.34 | 1.37 |
| 36 | A5 | 2975 | U | C4-O4 | -6.07 | 1.18 | 1.23 |
| 36 | A5 | 3308 | C | N3-C4 | -6.07 | 1.29 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 36 | A1 | 359 | U | C4-O4 | -6.07 | 1.18 | 1.23 |
| 36 | A1 | 2138 | A | N7-C5 | -6.07 | 1.35 | 1.39 |
| 36 | A1 | 3209 | A | C6-N1 | 6.07 | 1.39 | 1.35 |
| 36 | A5 | 2377 | G | N9-C8 | -6.07 | 1.33 | 1.37 |
| 36 | A1 | 1467 | A | C6-N1 | -6.07 | 1.31 | 1.35 |
| 38 | A4 | 12 | A | N9-C4 | -6.06 | 1.34 | 1.37 |
| 36 | A5 | 3102 | G | N1-C2 | -6.06 | 1.32 | 1.37 |
| 36 | A5 | 859 | G | C6-N1 | -6.06 | 1.35 | 1.39 |
| 36 | A5 | 2733 | A | N9-C4 | -6.05 | 1.34 | 1.37 |
| 36 | A5 | 1174 | G | C5-C4 | -6.05 | 1.34 | 1.38 |
| 36 | A1 | 2827 | U | C2-N3 | -6.05 | 1.33 | 1.37 |
| 36 | A5 | 2915 | U | C2-O2 | -6.05 | 1.17 | 1.22 |
| 36 | A5 | 1490 | A | C5-C6 | -6.04 | 1.35 | 1.41 |
| 36 | A1 | 800 | G | C2-N3 | -6.04 | 1.27 | 1.32 |
| 36 | A5 | 1454 | A | C6-N6 | -6.03 | 1.29 | 1.33 |
| 40 | DB | 262 | TRP | CB-CG | -6.03 | 1.39 | 1.50 |
| 36 | A1 | 857 | G | C6-O6 | -6.03 | 1.18 | 1.24 |
| 36 | A5 | 2948 | C | C4-N4 | -6.02 | 1.28 | 1.33 |
| 36 | A1 | 348 | A | P-OP1 | -6.02 | 1.38 | 1.49 |
| 36 | A5 | 2341 | A | N3-C4 | 6.02 | 1.38 | 1.34 |
| 36 | A1 | 1149 | G | N3-C4 | -6.01 | 1.31 | 1.35 |
| 36 | A1 | 2147 | A | N7-C5 | -6.01 | 1.35 | 1.39 |
| 36 | A5 | 1504 | A | C6-N1 | -6.01 | 1.31 | 1.35 |
| 36 | A5 | 2980 | U | C2-O2 | -6.01 | 1.17 | 1.22 |
| 36 | A1 | 347 | G | N9-C4 | -6.00 | 1.33 | 1.38 |
| 36 | A1 | 576 | C | N1-C6 | -6.00 | 1.33 | 1.37 |
| 36 | A5 | 744 | A | N9-C4 | -6.00 | 1.34 | 1.37 |
| 36 | A5 | 2214 | A | P-OP2 | -6.00 | 1.38 | 1.49 |
| 36 | A5 | 2704 | A | N7-C5 | -6.00 | 1.35 | 1.39 |
| 36 | A5 | 2857 | C | C4-N4 | -6.00 | 1.28 | 1.33 |
| 36 | A5 | 3008 | A | N9-C4 | -5.99 | 1.34 | 1.37 |
| 36 | A5 | 1149 | G | C5-C4 | -5.99 | 1.34 | 1.38 |
| 36 | A5 | 3005 | A | C6-N1 | -5.98 | 1.31 | 1.35 |
| 36 | A5 | 1332 | A | C5-C4 | -5.98 | 1.34 | 1.38 |
| 36 | A5 | 2730 | G | N9-C4 | -5.98 | 1.33 | 1.38 |
| 36 | A1 | 189 | G | N7-C5 | -5.97 | 1.35 | 1.39 |
| 36 | A5 | 2188 | A | N3-C4 | -5.97 | 1.31 | 1.34 |
| 36 | A5 | 647 | A | N3-C4 | -5.97 | 1.31 | 1.34 |
| 36 | A5 | 1152 | G | N1-C2 | 5.96 | 1.42 | 1.37 |
| 36 | A5 | 2706 | G | C5-C4 | -5.96 | 1.34 | 1.38 |
| 36 | A1 | 1796 | G | C6-N1 | -5.96 | 1.35 | 1.39 |
| 36 | A1 | 3054 | U | C2-N3 | -5.95 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 36 | A1 | 2244 | A | N3-C4 | -5.95 | 1.31 | 1.34 |
| 80 | A6 | 538 | A | N9-C4 | 5.95 | 1.41 | 1.37 |
| 37 | A7 | 89 | G | C5-C4 | -5.95 | 1.34 | 1.38 |
| 36 | A1 | 3344 | A | N7-C5 | -5.95 | 1.35 | 1.39 |
| 1 | A2 | 1782 | A | C6-N1 | -5.94 | 1.31 | 1.35 |
| 42 | BD | 41 | LYS | CE-NZ | 5.94 | 1.64 | 1.49 |
| 36 | A5 | 416 | A | N7-C5 | -5.94 | 1.35 | 1.39 |
| 36 | A1 | 2278 | C | N1-C6 | 5.94 | 1.40 | 1.37 |
| 36 | A1 | 826 | G | C6-N1 | -5.93 | 1.35 | 1.39 |
| 36 | A5 | 1837 | U | P-OP2 | -5.93 | 1.38 | 1.49 |
| 36 | A1 | 1507 | G | C8-N7 | -5.93 | 1.27 | 1.30 |
| 36 | A5 | 3335 | A | N9-C4 | -5.93 | 1.34 | 1.37 |
| 73 | Bj | 19 | CYS | CB-SG | -5.92 | 1.72 | 1.81 |
| 36 | A5 | 348 | A | P-OP1 | -5.92 | 1.38 | 1.49 |
| 36 | A5 | 1449 | A | N7-C5 | -5.92 | 1.35 | 1.39 |
| 36 | A1 | 2983 | C | C4-C5 | 5.92 | 1.47 | 1.43 |
| 36 | A1 | 378 | A | N7-C5 | -5.92 | 1.35 | 1.39 |
| 38 | A8 | 111 | A | N9-C4 | -5.92 | 1.34 | 1.37 |
| 37 | A3 | 101 | G | N3-C4 | -5.92 | 1.31 | 1.35 |
| 36 | A5 | 1138 | U | C4-O4 | -5.91 | 1.19 | 1.23 |
| 36 | A1 | 2642 | A | N9-C4 | -5.91 | 1.34 | 1.37 |
| 69 | Bf | 10 | LYS | CE-NZ | 5.91 | 1.63 | 1.49 |
| 36 | A1 | 1515 | A | N7-C5 | -5.91 | 1.35 | 1.39 |
| 36 | A5 | 345 | G | C5-C4 | -5.91 | 1.34 | 1.38 |
| 36 | A1 | 635 | G | P-OP2 | -5.90 | 1.39 | 1.49 |
| 41 | BC | 194 | TYR | CD1-CE1 | -5.90 | 1.30 | 1.39 |
| 36 | A5 | 2524 | A | C5-C4 | 5.90 | 1.42 | 1.38 |
| 36 | A5 | 784 | A | C5-C6 | -5.89 | 1.35 | 1.41 |
| 36 | A5 | 857 | G | C6-O6 | -5.89 | 1.18 | 1.24 |
| 36 | A5 | 2335 | G | C5-C4 | -5.89 | 1.34 | 1.38 |
| 36 | A1 | 2811 | A | N3-C4 | -5.89 | 1.31 | 1.34 |
| 80 | A6 | 392 | G | N1-C2 | -5.89 | 1.33 | 1.37 |
| 36 | A1 | 584 | G | N7-C5 | -5.89 | 1.35 | 1.39 |
| 36 | A1 | 3057 | U | N3-C4 | -5.89 | 1.33 | 1.38 |
| 36 | A5 | 868 | C | N1-C6 | -5.88 | 1.33 | 1.37 |
| 36 | A5 | 3227 | A | N3-C4 | -5.88 | 1.31 | 1.34 |
| 38 | A4 | 96 | A | N9-C4 | -5.88 | 1.34 | 1.37 |
| 80 | A6 | 1723 | U | C2-O2 | -5.88 | 1.17 | 1.22 |
| 36 | A5 | 922 | U | P-OP2 | -5.88 | 1.39 | 1.49 |
| 36 | A5 | 2278 | C | N1-C6 | 5.87 | 1.40 | 1.37 |
| 36 | A1 | 1127 | G | N7-C5 | -5.87 | 1.35 | 1.39 |
| 36 | A5 | 577 | C | N1-C6 | -5.87 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 36 | A5 | 3000 | A | N9-C4 | -5.86 | 1.34 | 1.37 |
| 36 | A1 | 2798 | C | P-OP1 | -5.86 | 1.39 | 1.49 |
| 36 | A1 | 2640 | A | C5-C4 | -5.86 | 1.34 | 1.38 |
| 36 | A5 | 1203 | A | C5-C6 | -5.86 | 1.35 | 1.41 |
| 36 | A5 | 1149 | G | N9-C8 | -5.85 | 1.33 | 1.37 |
| 36 | A5 | 3010 | U | C2-N3 | -5.85 | 1.33 | 1.37 |
| 36 | A5 | 931 | C | C4-N4 | -5.85 | 1.28 | 1.33 |
| 36 | A1 | 367 | A | N9-C4 | -5.85 | 1.34 | 1.37 |
| 36 | A1 | 1375 | G | C5-C4 | -5.85 | 1.34 | 1.38 |
| 36 | A1 | 2409 | G | N7-C5 | -5.84 | 1.35 | 1.39 |
| 36 | A5 | 2946 | A | C6-N1 | -5.84 | 1.31 | 1.35 |
| 36 | A5 | 3047 | U | C2-N3 | -5.84 | 1.33 | 1.37 |
| 36 | A1 | 1902 | G | N1-C2 | 5.83 | 1.42 | 1.37 |
| 36 | A5 | 2884 | C | C2-O2 | -5.83 | 1.19 | 1.24 |
| 80 | A6 | 553 | G | N7-C5 | -5.83 | 1.35 | 1.39 |
| 80 | A6 | 17 | C | C4-N4 | -5.83 | 1.28 | 1.33 |
| 36 | A5 | 1429 | G | N9-C8 | -5.83 | 1.33 | 1.37 |
| 36 | A5 | 1332 | A | C6-N1 | -5.82 | 1.31 | 1.35 |
| 36 | A5 | 2971 | A | N9-C4 | 5.82 | 1.41 | 1.37 |
| 36 | A5 | 1172 | G | N1-C2 | -5.82 | 1.33 | 1.37 |
| 36 | A1 | 2413 | A | C5-C6 | -5.81 | 1.35 | 1.41 |
| 80 | A6 | 1765 | A | N9-C4 | -5.81 | 1.34 | 1.37 |
| 1 | A2 | 1291 | G | N3-C4 | -5.81 | 1.31 | 1.35 |
| 36 | A1 | 747 | A | N3-C4 | -5.81 | 1.31 | 1.34 |
| 36 | A5 | 1156 | C | C4-N4 | -5.81 | 1.28 | 1.33 |
| 36 | A1 | 909 | G | C5-C4 | -5.81 | 1.34 | 1.38 |
| 36 | A5 | 2977 | G | C6-N1 | -5.80 | 1.35 | 1.39 |
| 36 | A1 | 3114 | A | N3-C4 | -5.80 | 1.31 | 1.34 |
| 80 | A6 | 1655 | A | N3-C4 | -5.80 | 1.31 | 1.34 |
| 36 | A1 | 338 | A | N7-C5 | -5.80 | 1.35 | 1.39 |
| 80 | A6 | 1322 | A | N3-C4 | -5.79 | 1.31 | 1.34 |
| 36 | A1 | 1145 | G | C5-C4 | -5.79 | 1.34 | 1.38 |
| 37 | A3 | 95 | A | C6-N1 | -5.79 | 1.31 | 1.35 |
| 36 | A5 | 1903 | U | C4-O4 | 5.79 | 1.28 | 1.23 |
| 36 | A5 | 1308 | A | N9-C8 | -5.79 | 1.33 | 1.37 |
| 36 | A1 | 345 | G | C5-C4 | -5.79 | 1.34 | 1.38 |
| 36 | A5 | 2915 | U | C2-N3 | -5.78 | 1.33 | 1.37 |
| 36 | A5 | 3095 | U | C4-O4 | -5.78 | 1.19 | 1.23 |
| 36 | A1 | 99 | A | N7-C5 | -5.78 | 1.35 | 1.39 |
| 36 | A1 | 1429 | G | N9-C8 | -5.78 | 1.33 | 1.37 |
| 36 | A1 | 799 | G | N9-C4 | -5.78 | 1.33 | 1.38 |
| 36 | A5 | 2732 | G | C6-N1 | -5.78 | 1.35 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 36 | A1 | 2827 | U | N3-C4 | -5.77 | 1.33 | 1.38 |
| 36 | A5 | 805 | G | N7-C5 | 5.77 | 1.42 | 1.39 |
| 36 | A5 | 2612 | U | C2-N3 | -5.77 | 1.33 | 1.37 |
| 36 | A5 | 2960 | C | C4-N4 | -5.77 | 1.28 | 1.33 |
| 36 | A5 | 1305 | U | N1-C6 | -5.77 | 1.32 | 1.38 |
| 36 | A5 | 369 | A | C6-N6 | -5.77 | 1.29 | 1.33 |
| 36 | A5 | 518 | G | C5-C4 | -5.77 | 1.34 | 1.38 |
| 36 | A5 | 3245 | A | N7-C5 | -5.77 | 1.35 | 1.39 |
| 36 | A1 | 2341 | A | N9-C4 | -5.76 | 1.34 | 1.37 |
| 36 | A5 | 1127 | G | C5-C4 | -5.76 | 1.34 | 1.38 |
| 36 | A1 | 624 | G | N7-C5 | -5.76 | 1.35 | 1.39 |
| 1 | A2 | 992 | A | N9-C8 | 5.76 | 1.42 | 1.37 |
| 36 | A5 | 3005 | A | N7-C5 | -5.76 | 1.35 | 1.39 |
| 36 | A1 | 1592 | G | N7-C5 | -5.76 | 1.35 | 1.39 |
| 36 | A5 | 1208 | U | N3-C4 | -5.76 | 1.33 | 1.38 |
| 36 | A5 | 2401 | A | N9-C4 | 5.76 | 1.41 | 1.37 |
| 36 | A5 | 2412 | G | N1-C2 | -5.76 | 1.33 | 1.37 |
| 36 | A1 | 2621 | G | N3-C4 | -5.75 | 1.31 | 1.35 |
| 80 | A6 | 1388 | A | N3-C4 | -5.75 | 1.31 | 1.34 |
| 36 | A5 | 2367 | A | N9-C4 | 5.75 | 1.41 | 1.37 |
| 36 | A1 | 1156 | C | N3-C4 | -5.75 | 1.29 | 1.33 |
| 36 | A5 | 1112 | A | C6-N1 | -5.75 | 1.31 | 1.35 |
| 36 | A1 | 1197 | A | C6-N1 | -5.75 | 1.31 | 1.35 |
| 36 | A5 | 100 | A | N9-C4 | -5.75 | 1.34 | 1.37 |
| 36 | A1 | 421 | G | N1-C2 | -5.74 | 1.33 | 1.37 |
| 36 | A1 | 1171 | G | N7-C5 | -5.74 | 1.35 | 1.39 |
| 36 | A1 | 1592 | G | C5-C6 | -5.74 | 1.36 | 1.42 |
| 80 | A6 | 331 | A | N9-C4 | -5.74 | 1.34 | 1.37 |
| 36 | A5 | 1213 | G | N1-C2 | -5.74 | 1.33 | 1.37 |
| 36 | A5 | 2858 | U | C2-N3 | -5.74 | 1.33 | 1.37 |
| 36 | A1 | 851 | C | C4-C5 | -5.74 | 1.38 | 1.43 |
| 36 | A5 | 1365 | G | C6-N1 | -5.74 | 1.35 | 1.39 |
| 36 | A1 | 50 | U | C4-O4 | -5.74 | 1.19 | 1.23 |
| 36 | A5 | 1462 | A | N9-C4 | -5.74 | 1.34 | 1.37 |
| 36 | A5 | 2957 | G | C8-N7 | -5.74 | 1.27 | 1.30 |
| 36 | A1 | 2415 | C | C4-N4 | -5.73 | 1.28 | 1.33 |
| 36 | A1 | 3273 | A | N7-C5 | -5.73 | 1.35 | 1.39 |
| 36 | A5 | 1898 | G | C5-C4 | -5.73 | 1.34 | 1.38 |
| 36 | A1 | 909 | G | N9-C8 | -5.73 | 1.33 | 1.37 |
| 36 | A5 | 1450 | G | C5-C4 | -5.73 | 1.34 | 1.38 |
| 36 | A5 | 2921 | U | C4-O4 | -5.73 | 1.19 | 1.23 |
| 36 | A5 | 2860 | U | C4-O4 | 5.72 | 1.28 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-------|------|-------|-------|-------------|----------|
| 52 | DO | 40[B] | ALA | C-N | -5.72 | 1.20 | 1.34 |
| 36 | A5 | 883 | A | P-OP1 | 5.72 | 1.58 | 1.49 |
| 36 | A5 | 953 | G | N3-C4 | -5.72 | 1.31 | 1.35 |
| 36 | A5 | 1477 | A | N3-C4 | -5.72 | 1.31 | 1.34 |
| 42 | BD | 62 | CYS | CB-SG | -5.71 | 1.72 | 1.81 |
| 36 | A5 | 339 | C | N3-C4 | -5.71 | 1.29 | 1.33 |
| 36 | A5 | 2375 | G | C6-N1 | -5.71 | 1.35 | 1.39 |
| 36 | A1 | 3174 | A | C8-N7 | 5.71 | 1.35 | 1.31 |
| 36 | A5 | 428 | A | N7-C5 | -5.71 | 1.35 | 1.39 |
| 1 | A2 | 1560 | U | N3-C4 | -5.71 | 1.33 | 1.38 |
| 36 | A5 | 2888 | U | C2-N3 | -5.71 | 1.33 | 1.37 |
| 36 | A1 | 636 | C | C4-N4 | -5.71 | 1.28 | 1.33 |
| 1 | A2 | 993 | A | N7-C5 | -5.71 | 1.35 | 1.39 |
| 36 | A1 | 421 | G | C6-O6 | -5.71 | 1.19 | 1.24 |
| 36 | A1 | 3114 | A | N9-C4 | -5.71 | 1.34 | 1.37 |
| 36 | A5 | 1910 | A | C5-C4 | -5.70 | 1.34 | 1.38 |
| 36 | A5 | 326 | U | C4-O4 | -5.70 | 1.19 | 1.23 |
| 36 | A5 | 1189 | C | N1-C6 | -5.70 | 1.33 | 1.37 |
| 36 | A1 | 803 | C | C4-N4 | -5.70 | 1.28 | 1.33 |
| 36 | A1 | 867 | G | C5-C4 | -5.70 | 1.34 | 1.38 |
| 36 | A1 | 1874 | A | N7-C5 | -5.70 | 1.35 | 1.39 |
| 80 | A6 | 357 | G | N9-C8 | -5.70 | 1.33 | 1.37 |
| 36 | A5 | 1338 | C | N1-C6 | -5.69 | 1.33 | 1.37 |
| 36 | A5 | 1849 | C | C4-C5 | -5.69 | 1.38 | 1.43 |
| 36 | A1 | 635 | G | C5-C4 | -5.69 | 1.34 | 1.38 |
| 36 | A5 | 2888 | U | C4-C5 | -5.69 | 1.38 | 1.43 |
| 36 | A5 | 2350 | C | N1-C6 | -5.69 | 1.33 | 1.37 |
| 36 | A1 | 1330 | A | C5-C6 | -5.69 | 1.35 | 1.41 |
| 36 | A1 | 701 | G | C6-N1 | -5.68 | 1.35 | 1.39 |
| 36 | A5 | 2646 | C | N1-C6 | -5.68 | 1.33 | 1.37 |
| 36 | A1 | 1910 | A | N9-C4 | -5.68 | 1.34 | 1.37 |
| 36 | A5 | 652 | G | C5-C4 | -5.68 | 1.34 | 1.38 |
| 36 | A5 | 876 | A | N1-C2 | -5.68 | 1.29 | 1.34 |
| 1 | A2 | 1555 | A | N3-C4 | -5.68 | 1.31 | 1.34 |
| 36 | A1 | 2944 | U | C4-O4 | -5.68 | 1.19 | 1.23 |
| 36 | A1 | 963 | G | C5-C6 | -5.67 | 1.36 | 1.42 |
| 36 | A1 | 1911 | A | C5-C6 | -5.67 | 1.35 | 1.41 |
| 36 | A5 | 924 | G | C2-N3 | -5.67 | 1.28 | 1.32 |
| 36 | A5 | 2134 | G | C6-N1 | -5.67 | 1.35 | 1.39 |
| 38 | A8 | 54 | A | N9-C4 | -5.67 | 1.34 | 1.37 |
| 36 | A1 | 187 | A | N9-C4 | 5.67 | 1.41 | 1.37 |
| 37 | A7 | 39 | C | N3-C4 | -5.67 | 1.29 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 36 | A1 | 2418 | G | O3'-P | 5.67 | 1.68 | 1.61 |
| 80 | A6 | 1537 | C | N3-C4 | 5.67 | 1.38 | 1.33 |
| 36 | A5 | 984 | G | N7-C5 | -5.67 | 1.35 | 1.39 |
| 36 | A5 | 2361 | A | N7-C5 | -5.67 | 1.35 | 1.39 |
| 36 | A5 | 200 | C | N3-C4 | -5.66 | 1.29 | 1.33 |
| 36 | A1 | 2213 | A | N7-C5 | -5.66 | 1.35 | 1.39 |
| 36 | A1 | 2946 | A | N9-C4 | -5.66 | 1.34 | 1.37 |
| 36 | A5 | 1145 | G | N3-C4 | -5.66 | 1.31 | 1.35 |
| 36 | A1 | 1664 | G | C6-N1 | -5.66 | 1.35 | 1.39 |
| 36 | A5 | 2892 | A | C6-N1 | -5.65 | 1.31 | 1.35 |
| 31 | Cd | 7 | TRP | CB-CG | 5.65 | 1.60 | 1.50 |
| 38 | A4 | 103 | G | N9-C4 | 5.65 | 1.42 | 1.38 |
| 80 | A6 | 423 | G | C6-N1 | -5.64 | 1.35 | 1.39 |
| 36 | A5 | 39 | A | N3-C4 | -5.64 | 1.31 | 1.34 |
| 36 | A5 | 1370 | G | C6-N1 | -5.64 | 1.35 | 1.39 |
| 36 | A5 | 2340 | U | C4-O4 | -5.63 | 1.19 | 1.23 |
| 36 | A1 | 780 | A | N3-C4 | -5.63 | 1.31 | 1.34 |
| 36 | A1 | 1180 | A | N3-C4 | -5.63 | 1.31 | 1.34 |
| 36 | A1 | 2794 | G | C6-N1 | -5.63 | 1.35 | 1.39 |
| 36 | A5 | 3039 | C | N1-C6 | -5.63 | 1.33 | 1.37 |
| 1 | A2 | 865 | A | C6-N1 | -5.63 | 1.31 | 1.35 |
| 36 | A1 | 44 | U | C4-O4 | -5.63 | 1.19 | 1.23 |
| 36 | A1 | 822 | G | C2-N3 | -5.63 | 1.28 | 1.32 |
| 36 | A1 | 2130 | G | C6-N1 | -5.63 | 1.35 | 1.39 |
| 36 | A5 | 900 | G | C6-N1 | -5.63 | 1.35 | 1.39 |
| 36 | A5 | 2147 | A | N7-C5 | -5.63 | 1.35 | 1.39 |
| 1 | A2 | 1746 | A | N9-C4 | -5.63 | 1.34 | 1.37 |
| 36 | A1 | 2315 | G | C6-N1 | -5.63 | 1.35 | 1.39 |
| 36 | A1 | 2393 | G | C8-N7 | -5.63 | 1.27 | 1.30 |
| 36 | A5 | 1043 | C | N3-C4 | -5.62 | 1.30 | 1.33 |
| 62 | DY | 38 | GLU | CG-CD | 5.62 | 1.60 | 1.51 |
| 36 | A1 | 1150 | A | N9-C4 | -5.62 | 1.34 | 1.37 |
| 36 | A5 | 657 | A | N3-C4 | -5.62 | 1.31 | 1.34 |
| 36 | A1 | 92 | G | C6-O6 | -5.62 | 1.19 | 1.24 |
| 36 | A1 | 2326 | A | N9-C4 | -5.62 | 1.34 | 1.37 |
| 36 | A5 | 1370 | G | N9-C8 | -5.62 | 1.33 | 1.37 |
| 36 | A5 | 2419 | A | C6-N1 | -5.61 | 1.31 | 1.35 |
| 36 | A5 | 2647 | A | N3-C4 | -5.61 | 1.31 | 1.34 |
| 76 | Bm | 115 | CYS | CB-SG | -5.61 | 1.72 | 1.81 |
| 36 | A5 | 2810 | C | N1-C6 | -5.61 | 1.33 | 1.37 |
| 36 | A5 | 1099 | A | C6-N1 | -5.61 | 1.31 | 1.35 |
| 36 | A1 | 1173 | U | C4-O4 | -5.60 | 1.19 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 36 | A1 | 2846 | U | N3-C4 | -5.60 | 1.33 | 1.38 |
| 36 | A5 | 1320 | C | C4-C5 | -5.60 | 1.38 | 1.43 |
| 52 | DO | 4[B] | GLN | C-N | -5.60 | 1.23 | 1.34 |
| 80 | A6 | 542 | A | C5-C6 | -5.60 | 1.36 | 1.41 |
| 36 | A5 | 2148 | U | C4-O4 | -5.60 | 1.19 | 1.23 |
| 36 | A1 | 649 | A | C6-N1 | -5.60 | 1.31 | 1.35 |
| 36 | A1 | 365 | A | N7-C5 | -5.59 | 1.35 | 1.39 |
| 36 | A5 | 1414 | G | C6-N1 | -5.59 | 1.35 | 1.39 |
| 36 | A5 | 1434 | G | C5-C4 | -5.59 | 1.34 | 1.38 |
| 36 | A1 | 1396 | C | C4-N4 | -5.59 | 1.28 | 1.33 |
| 47 | BI | 8 | CYS | CB-SG | -5.59 | 1.72 | 1.81 |
| 36 | A1 | 2946 | A | C5-C6 | -5.58 | 1.36 | 1.41 |
| 36 | A5 | 3218 | A | N9-C4 | -5.58 | 1.34 | 1.37 |
| 36 | A5 | 2382 | G | N7-C5 | -5.58 | 1.35 | 1.39 |
| 36 | A5 | 817 | A | C4'-C3' | -5.58 | 1.47 | 1.52 |
| 36 | A5 | 1309 | U | N1-C2 | -5.58 | 1.33 | 1.38 |
| 36 | A5 | 2626 | A | N9-C8 | -5.58 | 1.33 | 1.37 |
| 36 | A5 | 3088 | G | C5-C6 | -5.58 | 1.36 | 1.42 |
| 36 | A1 | 307 | A | N7-C5 | -5.57 | 1.35 | 1.39 |
| 36 | A5 | 559 | A | N7-C5 | -5.57 | 1.35 | 1.39 |
| 36 | A5 | 3374 | U | C4-O4 | -5.57 | 1.19 | 1.23 |
| 36 | A5 | 3013 | U | C2-N3 | -5.57 | 1.33 | 1.37 |
| 36 | A5 | 2302 | G | N1-C2 | -5.57 | 1.33 | 1.37 |
| 36 | A1 | 1305 | U | C4-O4 | -5.57 | 1.19 | 1.23 |
| 36 | A1 | 3226 | A | N9-C4 | -5.57 | 1.34 | 1.37 |
| 36 | A1 | 1459 | C | N3-C4 | -5.56 | 1.30 | 1.33 |
| 36 | A1 | 2957 | G | N9-C8 | -5.56 | 1.33 | 1.37 |
| 36 | A5 | 2301 | U | C2-O2 | -5.56 | 1.17 | 1.22 |
| 36 | A1 | 2647 | A | N3-C4 | -5.56 | 1.31 | 1.34 |
| 36 | A1 | 2728 | G | C5-C4 | -5.56 | 1.34 | 1.38 |
| 36 | A5 | 640 | U | C2-N3 | -5.56 | 1.33 | 1.37 |
| 36 | A5 | 2323 | G | N1-C2 | -5.56 | 1.33 | 1.37 |
| 36 | A5 | 657 | A | N9-C4 | -5.56 | 1.34 | 1.37 |
| 36 | A5 | 2860 | U | P-OP2 | -5.56 | 1.39 | 1.49 |
| 36 | A1 | 1510 | G | C6-N1 | -5.56 | 1.35 | 1.39 |
| 36 | A1 | 2605 | G | C5-C4 | -5.55 | 1.34 | 1.38 |
| 36 | A1 | 2909 | U | C2-N3 | 5.55 | 1.41 | 1.37 |
| 80 | A6 | 1118 | G | N3-C4 | -5.55 | 1.31 | 1.35 |
| 36 | A5 | 1433 | A | N7-C5 | -5.55 | 1.35 | 1.39 |
| 36 | A1 | 1668 | G | C6-N1 | -5.55 | 1.35 | 1.39 |
| 36 | A1 | 2880 | U | C2-N3 | 5.55 | 1.41 | 1.37 |
| 36 | A5 | 49 | A | C5-C4 | -5.55 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 36 | A1 | 2640 | A | N3-C4 | -5.55 | 1.31 | 1.34 |
| 36 | A5 | 949 | C | N3-C4 | -5.55 | 1.30 | 1.33 |
| 36 | A5 | 2823 | G | C5-C4 | -5.55 | 1.34 | 1.38 |
| 36 | A1 | 659 | G | N7-C5 | -5.54 | 1.35 | 1.39 |
| 36 | A1 | 1432 | C | C2-O2 | -5.54 | 1.19 | 1.24 |
| 36 | A5 | 1413 | G | C6-N1 | -5.54 | 1.35 | 1.39 |
| 1 | A2 | 577 | G | C5-C6 | -5.54 | 1.36 | 1.42 |
| 36 | A5 | 2609 | A | C5-C4 | -5.54 | 1.34 | 1.38 |
| 80 | A6 | 1478 | G | N7-C5 | -5.54 | 1.35 | 1.39 |
| 36 | A5 | 824 | C | N3-C4 | -5.54 | 1.30 | 1.33 |
| 36 | A5 | 987 | U | C2-O2 | -5.54 | 1.17 | 1.22 |
| 36 | A1 | 1446 | A | N9-C8 | -5.53 | 1.33 | 1.37 |
| 36 | A5 | 2932 | U | C2-N3 | -5.52 | 1.33 | 1.37 |
| 36 | A5 | 3052 | G | N1-C2 | -5.52 | 1.33 | 1.37 |
| 36 | A1 | 953 | G | C2-N3 | -5.52 | 1.28 | 1.32 |
| 36 | A1 | 2750 | U | C2-N3 | -5.52 | 1.33 | 1.37 |
| 80 | A6 | 1749 | A | N3-C4 | 5.52 | 1.38 | 1.34 |
| 36 | A5 | 891 | G | N9-C4 | -5.52 | 1.33 | 1.38 |
| 36 | A1 | 86 | G | C6-N1 | -5.52 | 1.35 | 1.39 |
| 36 | A5 | 1875 | G | C6-N1 | -5.52 | 1.35 | 1.39 |
| 36 | A5 | 2164 | A | N7-C5 | -5.52 | 1.35 | 1.39 |
| 36 | A5 | 420 | G | N9-C8 | -5.52 | 1.33 | 1.37 |
| 36 | A5 | 1432 | C | N1-C6 | -5.52 | 1.33 | 1.37 |
| 36 | A5 | 899 | U | C4-O4 | -5.52 | 1.19 | 1.23 |
| 36 | A5 | 1174 | G | C8-N7 | -5.52 | 1.27 | 1.30 |
| 36 | A5 | 1901 | A | N9-C8 | -5.52 | 1.33 | 1.37 |
| 36 | A5 | 2908 | G | C2-N3 | -5.52 | 1.28 | 1.32 |
| 36 | A1 | 1592 | G | N3-C4 | 5.51 | 1.39 | 1.35 |
| 36 | A1 | 1369 | A | N7-C5 | -5.51 | 1.35 | 1.39 |
| 36 | A5 | 2391 | G | C6-O6 | -5.51 | 1.19 | 1.24 |
| 36 | A1 | 2169 | G | N7-C5 | 5.51 | 1.42 | 1.39 |
| 36 | A1 | 1153 | A | N3-C4 | -5.50 | 1.31 | 1.34 |
| 36 | A1 | 2971 | A | N9-C4 | 5.50 | 1.41 | 1.37 |
| 41 | BC | 106 | TRP | CB-CG | -5.50 | 1.40 | 1.50 |
| 36 | A5 | 421 | G | N1-C2 | -5.50 | 1.33 | 1.37 |
| 36 | A5 | 1177 | G | N7-C5 | -5.50 | 1.35 | 1.39 |
| 36 | A5 | 1330 | A | N3-C4 | -5.50 | 1.31 | 1.34 |
| 36 | A5 | 1443 | G | N3-C4 | -5.50 | 1.31 | 1.35 |
| 36 | A5 | 2419 | A | P-O5' | 5.50 | 1.65 | 1.59 |
| 36 | A5 | 2920 | U | P-OP1 | -5.50 | 1.39 | 1.49 |
| 36 | A5 | 2904 | U | C2-N3 | -5.50 | 1.33 | 1.37 |
| 36 | A1 | 1379 | G | C6-N1 | -5.50 | 1.35 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 38 | A4 | 73 | U | C4-O4 | -5.50 | 1.19 | 1.23 |
| 36 | A5 | 2417 | U | C4-O4 | 5.50 | 1.28 | 1.23 |
| 36 | A5 | 3184 | A | N9-C4 | -5.50 | 1.34 | 1.37 |
| 36 | A1 | 670 | C | N1-C6 | -5.50 | 1.33 | 1.37 |
| 36 | A5 | 344 | A | N9-C8 | -5.50 | 1.33 | 1.37 |
| 36 | A5 | 706 | A | C5-C4 | -5.49 | 1.34 | 1.38 |
| 36 | A5 | 1195 | A | N1-C2 | -5.49 | 1.29 | 1.34 |
| 36 | A1 | 2385 | G | N9-C4 | -5.49 | 1.33 | 1.38 |
| 40 | DB | 349 | LYS | CD-CE | 5.49 | 1.65 | 1.51 |
| 36 | A1 | 3344 | A | C5-C6 | -5.49 | 1.36 | 1.41 |
| 36 | A5 | 2987 | A | C6-N1 | -5.49 | 1.31 | 1.35 |
| 36 | A1 | 1126 | G | C5-C4 | -5.49 | 1.34 | 1.38 |
| 37 | A7 | 5 | G | N9-C8 | -5.49 | 1.34 | 1.37 |
| 36 | A1 | 2434 | U | N3-C4 | -5.49 | 1.33 | 1.38 |
| 36 | A5 | 360 | G | N9-C8 | -5.48 | 1.34 | 1.37 |
| 36 | A5 | 1911 | A | C5-C6 | -5.48 | 1.36 | 1.41 |
| 1 | A2 | 1084 | A | N3-C4 | -5.48 | 1.31 | 1.34 |
| 36 | A1 | 1395 | G | C5-C4 | -5.48 | 1.34 | 1.38 |
| 38 | A4 | 25 | G | C6-N1 | -5.48 | 1.35 | 1.39 |
| 36 | A5 | 2122 | G | C5-C4 | -5.48 | 1.34 | 1.38 |
| 36 | A1 | 867 | G | N3-C4 | -5.48 | 1.31 | 1.35 |
| 1 | A2 | 542 | A | N9-C4 | -5.48 | 1.34 | 1.37 |
| 36 | A1 | 48 | A | C5-C4 | -5.48 | 1.34 | 1.38 |
| 36 | A1 | 1394 | A | N9-C8 | -5.48 | 1.33 | 1.37 |
| 36 | A5 | 1319 | G | N9-C8 | -5.48 | 1.34 | 1.37 |
| 36 | A1 | 789 | A | N3-C4 | -5.48 | 1.31 | 1.34 |
| 38 | A4 | 10 | A | N7-C5 | -5.48 | 1.35 | 1.39 |
| 36 | A1 | 282 | G | C5-C4 | -5.47 | 1.34 | 1.38 |
| 80 | A6 | 1118 | G | C5-C4 | -5.47 | 1.34 | 1.38 |
| 36 | A5 | 2744 | U | C2-N3 | -5.47 | 1.33 | 1.37 |
| 36 | A5 | 889 | U | C4-O4 | -5.47 | 1.19 | 1.23 |
| 36 | A1 | 2367 | A | C8-N7 | -5.47 | 1.27 | 1.31 |
| 36 | A1 | 3042 | U | N3-C4 | -5.47 | 1.33 | 1.38 |
| 36 | A5 | 3088 | G | N7-C5 | -5.47 | 1.35 | 1.39 |
| 36 | A1 | 339 | C | N1-C6 | -5.46 | 1.33 | 1.37 |
| 36 | A5 | 635 | G | P-OP2 | -5.46 | 1.39 | 1.49 |
| 36 | A1 | 369 | A | C6-N6 | -5.46 | 1.29 | 1.33 |
| 36 | A1 | 1369 | A | N9-C4 | -5.46 | 1.34 | 1.37 |
| 36 | A1 | 2817 | A | C6-N1 | -5.46 | 1.31 | 1.35 |
| 36 | A1 | 2611 | U | N3-C4 | -5.46 | 1.33 | 1.38 |
| 80 | A6 | 341 | A | N3-C4 | -5.46 | 1.31 | 1.34 |
| 36 | A5 | 834 | U | C4-O4 | -5.46 | 1.19 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 36 | A5 | 2941 | A | N9-C8 | -5.46 | 1.33 | 1.37 |
| 36 | A1 | 1197 | A | C5-C6 | -5.46 | 1.36 | 1.41 |
| 36 | A5 | 1147 | G | N9-C8 | -5.46 | 1.34 | 1.37 |
| 36 | A1 | 885 | U | C2-N3 | -5.45 | 1.33 | 1.37 |
| 80 | A6 | 418 | G | N7-C5 | -5.45 | 1.35 | 1.39 |
| 80 | A6 | 1670 | G | C5-C4 | -5.45 | 1.34 | 1.38 |
| 36 | A5 | 1324 | U | C2-N3 | -5.45 | 1.33 | 1.37 |
| 80 | A6 | 314 | C | C2-O2 | -5.45 | 1.19 | 1.24 |
| 36 | A5 | 1301 | A | N9-C8 | -5.45 | 1.33 | 1.37 |
| 36 | A5 | 2824 | G | N7-C5 | -5.45 | 1.35 | 1.39 |
| 36 | A1 | 672 | A | C6-N1 | 5.45 | 1.39 | 1.35 |
| 36 | A1 | 1122 | U | N3-C4 | -5.45 | 1.33 | 1.38 |
| 36 | A5 | 354 | U | C2-N3 | -5.45 | 1.33 | 1.37 |
| 36 | A5 | 3107 | U | C2-N3 | -5.45 | 1.33 | 1.37 |
| 80 | A6 | 1109 | G | C6-N1 | -5.45 | 1.35 | 1.39 |
| 36 | A5 | 1130 | A | N1-C2 | -5.45 | 1.29 | 1.34 |
| 1 | A2 | 553 | G | N1-C2 | 5.44 | 1.42 | 1.37 |
| 36 | A5 | 522 | A | P-O5' | -5.44 | 1.54 | 1.59 |
| 36 | A5 | 1492 | G | C2-N3 | 5.44 | 1.37 | 1.32 |
| 80 | A6 | 553 | G | C6-O6 | 5.44 | 1.29 | 1.24 |
| 36 | A1 | 1858 | A | N7-C5 | -5.44 | 1.35 | 1.39 |
| 36 | A5 | 3096 | C | N1-C6 | -5.44 | 1.33 | 1.37 |
| 36 | A1 | 2286 | U | N3-C4 | -5.44 | 1.33 | 1.38 |
| 36 | A1 | 2867 | C | C2-N3 | -5.44 | 1.31 | 1.35 |
| 36 | A5 | 2336 | U | C2-O2 | -5.44 | 1.17 | 1.22 |
| 36 | A1 | 1147 | G | N1-C2 | -5.44 | 1.33 | 1.37 |
| 36 | A1 | 2737 | C | N1-C2 | -5.44 | 1.34 | 1.40 |
| 36 | A5 | 2198 | A | N9-C4 | -5.44 | 1.34 | 1.37 |
| 36 | A1 | 656 | A | N7-C5 | -5.43 | 1.35 | 1.39 |
| 36 | A5 | 2717 | U | C2-N3 | -5.43 | 1.33 | 1.37 |
| 36 | A1 | 899 | U | C2-N3 | -5.43 | 1.33 | 1.37 |
| 36 | A1 | 2147 | A | N9-C4 | -5.43 | 1.34 | 1.37 |
| 36 | A5 | 2342 | U | C2-N3 | -5.43 | 1.33 | 1.37 |
| 1 | A2 | 331 | A | N9-C4 | -5.43 | 1.34 | 1.37 |
| 36 | A1 | 1169 | A | P-O5' | -5.43 | 1.54 | 1.59 |
| 36 | A5 | 2397 | A | C5-C6 | 5.43 | 1.46 | 1.41 |
| 36 | A5 | 2912 | G | N9-C8 | -5.43 | 1.34 | 1.37 |
| 36 | A5 | 3273 | A | N9-C4 | -5.43 | 1.34 | 1.37 |
| 36 | A5 | 1845 | G | C5-C4 | -5.42 | 1.34 | 1.38 |
| 36 | A5 | 36 | C | N1-C2 | -5.42 | 1.34 | 1.40 |
| 68 | Be | 8 | LYS | CD-CE | 5.42 | 1.64 | 1.51 |
| 36 | A5 | 1320 | C | C4-N4 | -5.42 | 1.29 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 36 | A5 | 2611 | U | P-OP1 | -5.42 | 1.39 | 1.49 |
| 36 | A1 | 867 | G | N7-C5 | -5.42 | 1.35 | 1.39 |
| 36 | A1 | 2372 | A | N3-C4 | -5.41 | 1.31 | 1.34 |
| 36 | A5 | 2128 | C | C4-N4 | -5.41 | 1.29 | 1.33 |
| 36 | A5 | 2336 | U | N3-C4 | -5.41 | 1.33 | 1.38 |
| 36 | A5 | 2775 | U | C2-N3 | -5.41 | 1.33 | 1.37 |
| 36 | A1 | 1122 | U | C4-O4 | -5.41 | 1.19 | 1.23 |
| 36 | A1 | 2177 | G | N7-C5 | -5.41 | 1.36 | 1.39 |
| 36 | A1 | 1307 | G | C5-C4 | -5.40 | 1.34 | 1.38 |
| 36 | A5 | 1908 | A | C6-N1 | -5.40 | 1.31 | 1.35 |
| 36 | A1 | 912 | G | C8-N7 | -5.40 | 1.27 | 1.30 |
| 36 | A1 | 984 | G | N7-C5 | -5.40 | 1.36 | 1.39 |
| 36 | A1 | 2345 | A | C6-N1 | -5.40 | 1.31 | 1.35 |
| 36 | A1 | 1446 | A | N7-C5 | -5.40 | 1.36 | 1.39 |
| 36 | A1 | 1151 | U | C4-O4 | 5.40 | 1.27 | 1.23 |
| 36 | A5 | 39 | A | C5-C4 | -5.39 | 1.34 | 1.38 |
| 36 | A5 | 365 | A | N7-C5 | -5.39 | 1.36 | 1.39 |
| 36 | A1 | 1124 | U | C5-C6 | -5.39 | 1.29 | 1.34 |
| 36 | A1 | 426 | G | C8-N7 | -5.39 | 1.27 | 1.30 |
| 36 | A1 | 2400 | G | N9-C4 | -5.39 | 1.33 | 1.38 |
| 37 | A3 | 88 | G | C6-N1 | -5.39 | 1.35 | 1.39 |
| 80 | A6 | 1670 | G | N7-C5 | -5.39 | 1.36 | 1.39 |
| 36 | A5 | 3307 | A | C2-N3 | -5.39 | 1.28 | 1.33 |
| 37 | A7 | 88 | G | N1-C2 | -5.39 | 1.33 | 1.37 |
| 36 | A1 | 2699 | G | N1-C2 | -5.39 | 1.33 | 1.37 |
| 36 | A1 | 3296 | A | C6-N1 | -5.39 | 1.31 | 1.35 |
| 36 | A5 | 2834 | G | C2-N3 | -5.39 | 1.28 | 1.32 |
| 36 | A1 | 1117 | G | P-OP1 | -5.39 | 1.39 | 1.49 |
| 1 | A2 | 377 | G | C6-N1 | 5.38 | 1.43 | 1.39 |
| 36 | A1 | 647 | A | C6-N6 | -5.38 | 1.29 | 1.33 |
| 36 | A1 | 2309 | A | N9-C4 | -5.38 | 1.34 | 1.37 |
| 36 | A5 | 2365 | C | N3-C4 | -5.38 | 1.30 | 1.33 |
| 36 | A5 | 831 | G | N7-C5 | -5.38 | 1.36 | 1.39 |
| 36 | A1 | 1164 | G | N1-C2 | -5.38 | 1.33 | 1.37 |
| 36 | A5 | 631 | U | N3-C4 | -5.38 | 1.33 | 1.38 |
| 36 | A5 | 1086 | C | C4-C5 | -5.38 | 1.38 | 1.43 |
| 36 | A5 | 41 | G | N9-C4 | -5.38 | 1.33 | 1.38 |
| 36 | A5 | 417 | A | N7-C5 | -5.38 | 1.36 | 1.39 |
| 36 | A5 | 1327 | C | N3-C4 | -5.38 | 1.30 | 1.33 |
| 36 | A1 | 3136 | G | C6-N1 | -5.37 | 1.35 | 1.39 |
| 36 | A5 | 895 | A | N3-C4 | -5.37 | 1.31 | 1.34 |
| 1 | A2 | 538 | A | N3-C4 | 5.37 | 1.38 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 36 | A1 | 46 | U | C2-N3 | -5.37 | 1.33 | 1.37 |
| 36 | A1 | 423 | A | N3-C4 | -5.37 | 1.31 | 1.34 |
| 36 | A1 | 2737 | C | N1-C6 | -5.37 | 1.33 | 1.37 |
| 36 | A5 | 1895 | A | N3-C4 | -5.37 | 1.31 | 1.34 |
| 37 | A7 | 66 | A | P-OP2 | -5.37 | 1.39 | 1.49 |
| 1 | A2 | 555 | A | N9-C4 | 5.37 | 1.41 | 1.37 |
| 36 | A1 | 2357 | A | N7-C5 | -5.37 | 1.36 | 1.39 |
| 36 | A1 | 2919 | A | N7-C5 | -5.37 | 1.36 | 1.39 |
| 36 | A1 | 1337 | A | N9-C4 | 5.37 | 1.41 | 1.37 |
| 38 | A8 | 25 | G | N1-C2 | -5.37 | 1.33 | 1.37 |
| 36 | A5 | 755 | A | C6-N1 | -5.36 | 1.31 | 1.35 |
| 36 | A1 | 1145 | G | C6-N1 | -5.36 | 1.35 | 1.39 |
| 36 | A1 | 626 | U | C2-N3 | -5.36 | 1.33 | 1.37 |
| 36 | A1 | 718 | G | N9-C8 | 5.36 | 1.41 | 1.37 |
| 36 | A5 | 508 | U | C5-C6 | -5.36 | 1.29 | 1.34 |
| 36 | A5 | 3112 | G | C5-C4 | -5.36 | 1.34 | 1.38 |
| 36 | A1 | 1170 | A | N3-C4 | 5.36 | 1.38 | 1.34 |
| 36 | A1 | 2828 | G | C6-N1 | -5.36 | 1.35 | 1.39 |
| 36 | A1 | 2920 | U | C2-N3 | -5.36 | 1.34 | 1.37 |
| 44 | BF | 234 | GLU | CD-OE2 | 5.36 | 1.31 | 1.25 |
| 80 | A6 | 1600 | A | C5-C4 | 5.36 | 1.42 | 1.38 |
| 36 | A5 | 864 | G | C5-C4 | -5.36 | 1.34 | 1.38 |
| 36 | A5 | 1296 | C | N3-C4 | -5.35 | 1.30 | 1.33 |
| 53 | BP | 124 | LYS | CE-NZ | 5.35 | 1.62 | 1.49 |
| 36 | A5 | 363 | G | N3-C4 | -5.35 | 1.31 | 1.35 |
| 36 | A5 | 2974 | U | C2-N3 | -5.35 | 1.34 | 1.37 |
| 40 | DB | 287 | LYS | CD-CE | 5.35 | 1.64 | 1.51 |
| 36 | A5 | 1833 | G | C6-N1 | -5.35 | 1.35 | 1.39 |
| 36 | A1 | 37 | U | N1-C2 | -5.35 | 1.33 | 1.38 |
| 36 | A1 | 938 | C | C4-N4 | -5.35 | 1.29 | 1.33 |
| 36 | A1 | 2281 | A | N9-C4 | -5.35 | 1.34 | 1.37 |
| 36 | A1 | 2800 | G | N9-C8 | -5.35 | 1.34 | 1.37 |
| 36 | A5 | 95 | A | C5-C4 | -5.35 | 1.35 | 1.38 |
| 36 | A5 | 666 | A | N3-C4 | -5.34 | 1.31 | 1.34 |
| 36 | A5 | 1338 | C | C4-C5 | -5.34 | 1.38 | 1.43 |
| 36 | A5 | 990 | U | C2-N3 | -5.34 | 1.34 | 1.37 |
| 36 | A1 | 317 | A | C5-C6 | -5.34 | 1.36 | 1.41 |
| 36 | A5 | 2697 | A | N9-C4 | 5.34 | 1.41 | 1.37 |
| 36 | A5 | 3039 | C | C4-C5 | -5.34 | 1.38 | 1.43 |
| 36 | A1 | 658 | G | P-OP2 | -5.34 | 1.39 | 1.49 |
| 36 | A1 | 791 | A | P-O5' | -5.34 | 1.54 | 1.59 |
| 36 | A1 | 3301 | U | C2-N3 | -5.34 | 1.34 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 80 | A6 | 317 | C | N1-C6 | -5.34 | 1.33 | 1.37 |
| 80 | A6 | 1596 | C | N3-C4 | -5.34 | 1.30 | 1.33 |
| 36 | A5 | 784 | A | N7-C5 | -5.34 | 1.36 | 1.39 |
| 36 | A1 | 1537 | A | N7-C5 | -5.34 | 1.36 | 1.39 |
| 36 | A1 | 2397 | A | N3-C4 | 5.34 | 1.38 | 1.34 |
| 36 | A5 | 1415 | U | C2-O2 | -5.33 | 1.17 | 1.22 |
| 36 | A1 | 1893 | A | C6-N1 | -5.33 | 1.31 | 1.35 |
| 36 | A5 | 2395 | G | C6-N1 | -5.33 | 1.35 | 1.39 |
| 36 | A1 | 939 | U | N1-C2 | -5.33 | 1.33 | 1.38 |
| 80 | A6 | 1087 | A | C6-N1 | -5.33 | 1.31 | 1.35 |
| 36 | A1 | 883 | A | P-OP1 | -5.33 | 1.39 | 1.49 |
| 80 | A6 | 314 | C | N3-C4 | -5.33 | 1.30 | 1.33 |
| 80 | A6 | 1119 | G | N3-C4 | -5.33 | 1.31 | 1.35 |
| 36 | A5 | 1902 | G | C6-N1 | -5.33 | 1.35 | 1.39 |
| 36 | A1 | 637 | C | C3'-C2' | -5.32 | 1.46 | 1.52 |
| 36 | A5 | 806 | A | P-OP2 | -5.32 | 1.40 | 1.49 |
| 36 | A5 | 2619 | G | C6-O6 | -5.32 | 1.19 | 1.24 |
| 36 | A5 | 903 | U | C2-N3 | -5.32 | 1.34 | 1.37 |
| 36 | A5 | 1190 | A | C6-N1 | -5.32 | 1.31 | 1.35 |
| 36 | A5 | 2643 | A | C6-N1 | 5.32 | 1.39 | 1.35 |
| 36 | A5 | 3216 | G | C5-C4 | -5.32 | 1.34 | 1.38 |
| 47 | DI | 96 | VAL | CB-CG2 | -5.32 | 1.41 | 1.52 |
| 36 | A5 | 1404 | G | N9-C8 | -5.32 | 1.34 | 1.37 |
| 1 | A2 | 973 | A | N7-C5 | -5.32 | 1.36 | 1.39 |
| 36 | A5 | 2693 | C | N1-C6 | -5.32 | 1.33 | 1.37 |
| 36 | A5 | 2937 | G | C5-C4 | -5.32 | 1.34 | 1.38 |
| 36 | A1 | 592 | A | N3-C4 | 5.32 | 1.38 | 1.34 |
| 36 | A1 | 3180 | A | N3-C4 | -5.32 | 1.31 | 1.34 |
| 36 | A1 | 2958 | A | N9-C8 | -5.31 | 1.33 | 1.37 |
| 36 | A5 | 1840 | U | C2-N3 | -5.31 | 1.34 | 1.37 |
| 36 | A5 | 1851 | G | C8-N7 | -5.31 | 1.27 | 1.30 |
| 36 | A5 | 1425 | U | C2-N3 | -5.31 | 1.34 | 1.37 |
| 36 | A5 | 1468 | A | N7-C5 | -5.31 | 1.36 | 1.39 |
| 36 | A1 | 95 | A | N3-C4 | -5.31 | 1.31 | 1.34 |
| 36 | A1 | 937 | G | C5-C4 | -5.31 | 1.34 | 1.38 |
| 36 | A5 | 290 | G | C6-N1 | -5.31 | 1.35 | 1.39 |
| 36 | A5 | 2204 | C | N3-C4 | -5.31 | 1.30 | 1.33 |
| 36 | A1 | 3209 | A | C5-C4 | 5.30 | 1.42 | 1.38 |
| 36 | A5 | 52 | A | N7-C5 | -5.30 | 1.36 | 1.39 |
| 36 | A5 | 1443 | G | N1-C2 | -5.30 | 1.33 | 1.37 |
| 36 | A5 | 3114 | A | N3-C4 | -5.30 | 1.31 | 1.34 |
| 36 | A1 | 933 | A | C6-N1 | -5.30 | 1.31 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|-------|-------|-------------|----------|
| 36 | A5 | 2632 | G | C8-N7 | 5.30 | 1.34 | 1.30 |
| 36 | A1 | 45 | A | C6-N6 | -5.30 | 1.29 | 1.33 |
| 36 | A5 | 3065 | G | C6-N1 | -5.30 | 1.35 | 1.39 |
| 36 | A1 | 2093 | A | N9-C4 | 5.30 | 1.41 | 1.37 |
| 36 | A1 | 1902 | G | N7-C5 | -5.30 | 1.36 | 1.39 |
| 38 | A4 | 16 | G | C5-C4 | -5.30 | 1.34 | 1.38 |
| 36 | A5 | 2730 | G | N7-C5 | -5.30 | 1.36 | 1.39 |
| 1 | A2 | 582 | U | P-O5' | -5.29 | 1.54 | 1.59 |
| 36 | A1 | 963 | G | C5-C4 | -5.29 | 1.34 | 1.38 |
| 36 | A5 | 2272 | G | C6-N1 | -5.29 | 1.35 | 1.39 |
| 36 | A5 | 3032 | A | N7-C5 | -5.29 | 1.36 | 1.39 |
| 36 | A1 | 815 | G | C6-N1 | -5.29 | 1.35 | 1.39 |
| 36 | A1 | 279 | U | C2-O2 | -5.29 | 1.17 | 1.22 |
| 36 | A5 | 925 | A | N7-C5 | -5.29 | 1.36 | 1.39 |
| 40 | BB | 200 | GLU | CG-CD | 5.29 | 1.59 | 1.51 |
| 36 | A5 | 2434 | U | C2-N3 | -5.29 | 1.34 | 1.37 |
| 36 | A5 | 2734 | A | N9-C4 | -5.29 | 1.34 | 1.37 |
| 36 | A5 | 2376 | G | C6-O6 | -5.29 | 1.19 | 1.24 |
| 36 | A1 | 318 | A | N7-C5 | -5.28 | 1.36 | 1.39 |
| 36 | A1 | 591 | G | C8-N7 | -5.28 | 1.27 | 1.30 |
| 36 | A5 | 1151 | U | C4-O4 | -5.28 | 1.19 | 1.23 |
| 36 | A1 | 2988 | C | C2-O2 | -5.28 | 1.19 | 1.24 |
| 36 | A5 | 818 | C | P-OP1 | -5.28 | 1.40 | 1.49 |
| 36 | A5 | 1115 | G | N7-C5 | -5.28 | 1.36 | 1.39 |
| 36 | A5 | 1888 | U | N1-C6 | -5.28 | 1.33 | 1.38 |
| 36 | A5 | 1362 | G | C6-N1 | -5.28 | 1.35 | 1.39 |
| 36 | A1 | 2821 | C | N3-C4 | 5.28 | 1.37 | 1.33 |
| 36 | A1 | 2939 | G | N7-C5 | -5.28 | 1.36 | 1.39 |
| 36 | A5 | 956 | U | N3-C4 | -5.28 | 1.33 | 1.38 |
| 36 | A5 | 3115 | C | N3-C4 | -5.28 | 1.30 | 1.33 |
| 52 | DO | 196[B] | SER | C-N | -5.28 | 1.22 | 1.34 |
| 64 | Da | 15 | VAL | C-O | 5.28 | 1.33 | 1.23 |
| 80 | A6 | 119 | A | N9-C4 | -5.28 | 1.34 | 1.37 |
| 80 | A6 | 623 | A | N9-C4 | -5.28 | 1.34 | 1.37 |
| 80 | A6 | 377 | G | N1-C2 | -5.27 | 1.33 | 1.37 |
| 36 | A5 | 1409 | G | C6-N1 | -5.27 | 1.35 | 1.39 |
| 36 | A1 | 2816 | G | C6-N1 | -5.27 | 1.35 | 1.39 |
| 36 | A5 | 505 | G | N3-C4 | -5.27 | 1.31 | 1.35 |
| 36 | A5 | 1131 | G | N7-C5 | -5.27 | 1.36 | 1.39 |
| 36 | A5 | 1209 | G | C2-N3 | -5.27 | 1.28 | 1.32 |
| 36 | A5 | 658 | G | N3-C4 | -5.27 | 1.31 | 1.35 |
| 36 | A5 | 994 | G | C5-C4 | -5.27 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 36 | A5 | 1117 | G | N7-C5 | -5.27 | 1.36 | 1.39 |
| 36 | A1 | 91 | G | C8-N7 | 5.27 | 1.34 | 1.30 |
| 36 | A5 | 2191 | U | N3-C4 | -5.26 | 1.33 | 1.38 |
| 36 | A1 | 323 | A | N9-C4 | -5.26 | 1.34 | 1.37 |
| 80 | A6 | 478 | A | N9-C4 | -5.26 | 1.34 | 1.37 |
| 80 | A6 | 1780 | G | N1-C2 | -5.26 | 1.33 | 1.37 |
| 36 | A5 | 798 | G | C6-O6 | -5.26 | 1.19 | 1.24 |
| 36 | A5 | 2341 | A | N9-C8 | -5.26 | 1.33 | 1.37 |
| 36 | A5 | 3070 | A | C6-N1 | -5.26 | 1.31 | 1.35 |
| 36 | A1 | 2983 | C | P-O5' | -5.26 | 1.54 | 1.59 |
| 36 | A5 | 1135 | A | N9-C8 | -5.26 | 1.33 | 1.37 |
| 36 | A1 | 641 | C | N3-C4 | -5.25 | 1.30 | 1.33 |
| 36 | A1 | 2649 | A | C5-C4 | -5.25 | 1.35 | 1.38 |
| 36 | A5 | 2318 | U | N3-C4 | -5.25 | 1.33 | 1.38 |
| 80 | A6 | 1654 | G | N3-C4 | -5.25 | 1.31 | 1.35 |
| 36 | A1 | 289 | A | N7-C5 | -5.25 | 1.36 | 1.39 |
| 36 | A1 | 1492 | G | C6-N1 | -5.25 | 1.35 | 1.39 |
| 36 | A5 | 1838 | G | C5-C4 | -5.25 | 1.34 | 1.38 |
| 36 | A5 | 2706 | G | C8-N7 | -5.25 | 1.27 | 1.30 |
| 80 | A6 | 337 | G | C5-C6 | -5.25 | 1.37 | 1.42 |
| 36 | A5 | 1171 | G | N7-C5 | -5.25 | 1.36 | 1.39 |
| 36 | A1 | 361 | A | C6-N6 | -5.24 | 1.29 | 1.33 |
| 36 | A1 | 653 | A | C5-C6 | -5.24 | 1.36 | 1.41 |
| 36 | A1 | 45 | A | C5-C6 | -5.24 | 1.36 | 1.41 |
| 36 | A1 | 2662 | G | N7-C5 | -5.24 | 1.36 | 1.39 |
| 80 | A6 | 1781 | A | N9-C4 | 5.24 | 1.41 | 1.37 |
| 36 | A5 | 912 | G | N3-C4 | 5.24 | 1.39 | 1.35 |
| 36 | A5 | 1326 | A | C5-C4 | -5.24 | 1.35 | 1.38 |
| 36 | A5 | 2734 | A | N3-C4 | -5.24 | 1.31 | 1.34 |
| 36 | A1 | 2426 | U | C2-O2 | -5.24 | 1.17 | 1.22 |
| 53 | BP | 129 | THR | CB-CG2 | -5.24 | 1.35 | 1.52 |
| 36 | A1 | 805 | G | N7-C5 | 5.24 | 1.42 | 1.39 |
| 36 | A5 | 1515 | A | N7-C5 | -5.24 | 1.36 | 1.39 |
| 44 | DF | 131 | GLU | CD-OE2 | 5.24 | 1.31 | 1.25 |
| 36 | A1 | 2317 | A | C6-N1 | -5.24 | 1.31 | 1.35 |
| 36 | A5 | 2617 | U | C4-O4 | -5.23 | 1.19 | 1.23 |
| 36 | A5 | 433 | A | N9-C4 | -5.23 | 1.34 | 1.37 |
| 36 | A1 | 420 | G | C6-N1 | -5.23 | 1.35 | 1.39 |
| 36 | A5 | 2163 | C | N3-C4 | -5.23 | 1.30 | 1.33 |
| 36 | A5 | 3372 | A | N9-C4 | 5.23 | 1.41 | 1.37 |
| 36 | A1 | 430 | U | N1-C6 | -5.23 | 1.33 | 1.38 |
| 36 | A1 | 2938 | G | C2-N3 | -5.23 | 1.28 | 1.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 80 | A6 | 352 | A | N9-C4 | -5.23 | 1.34 | 1.37 |
| 37 | A3 | 95 | A | C5-C6 | -5.23 | 1.36 | 1.41 |
| 36 | A5 | 2214 | A | N9-C4 | -5.22 | 1.34 | 1.37 |
| 76 | Dm | 79 | GLU | CD-OE1 | 5.22 | 1.31 | 1.25 |
| 80 | A6 | 647 | G | N3-C4 | -5.22 | 1.31 | 1.35 |
| 36 | A5 | 934 | G | C5-C4 | -5.22 | 1.34 | 1.38 |
| 36 | A5 | 2620 | G | N1-C2 | -5.22 | 1.33 | 1.37 |
| 36 | A1 | 673 | U | C4-O4 | -5.22 | 1.19 | 1.23 |
| 36 | A1 | 1124 | U | C4-O4 | -5.22 | 1.19 | 1.23 |
| 36 | A5 | 917 | A | N3-C4 | -5.22 | 1.31 | 1.34 |
| 36 | A1 | 942 | U | N1-C2 | -5.22 | 1.33 | 1.38 |
| 36 | A1 | 1422 | G | C6-N1 | -5.22 | 1.35 | 1.39 |
| 36 | A5 | 658 | G | N9-C4 | -5.22 | 1.33 | 1.38 |
| 36 | A1 | 286 | U | C2-N3 | -5.21 | 1.34 | 1.37 |
| 36 | A5 | 3000 | A | C5-C4 | -5.21 | 1.35 | 1.38 |
| 36 | A1 | 1507 | G | C5-C4 | -5.21 | 1.34 | 1.38 |
| 36 | A5 | 3179 | U | C4-O4 | -5.21 | 1.19 | 1.23 |
| 36 | A1 | 49 | A | N3-C4 | -5.21 | 1.31 | 1.34 |
| 36 | A1 | 278 | U | C2-O2 | -5.21 | 1.17 | 1.22 |
| 36 | A1 | 2626 | A | N9-C4 | 5.21 | 1.41 | 1.37 |
| 80 | A6 | 597 | G | C6-N1 | -5.21 | 1.35 | 1.39 |
| 36 | A1 | 795 | G | C5-C4 | -5.21 | 1.34 | 1.38 |
| 36 | A5 | 1477 | A | C6-N1 | -5.21 | 1.31 | 1.35 |
| 36 | A5 | 645 | A | C8-N7 | -5.21 | 1.27 | 1.31 |
| 80 | A6 | 992 | A | N9-C4 | -5.20 | 1.34 | 1.37 |
| 36 | A5 | 693 | A | N9-C4 | -5.20 | 1.34 | 1.37 |
| 36 | A1 | 1845 | G | C5-C4 | -5.20 | 1.34 | 1.38 |
| 80 | A6 | 1655 | A | C5-C4 | -5.20 | 1.35 | 1.38 |
| 36 | A1 | 106 | A | N9-C4 | -5.20 | 1.34 | 1.37 |
| 36 | A1 | 1304 | A | N9-C8 | -5.20 | 1.33 | 1.37 |
| 36 | A1 | 584 | G | N3-C4 | -5.20 | 1.31 | 1.35 |
| 36 | A5 | 1311 | G | N7-C5 | -5.20 | 1.36 | 1.39 |
| 80 | A6 | 392 | G | C5-C4 | -5.20 | 1.34 | 1.38 |
| 80 | A6 | 592 | A | N3-C4 | -5.20 | 1.31 | 1.34 |
| 36 | A1 | 359 | U | C2-N3 | -5.19 | 1.34 | 1.37 |
| 36 | A5 | 2922 | G | C6-O6 | -5.19 | 1.19 | 1.24 |
| 36 | A1 | 28 | C | C2-N3 | -5.19 | 1.31 | 1.35 |
| 36 | A1 | 345 | G | P-OP2 | -5.19 | 1.40 | 1.49 |
| 36 | A5 | 282 | G | C2-N3 | -5.19 | 1.28 | 1.32 |
| 36 | A5 | 1114 | U | C2-N3 | -5.19 | 1.34 | 1.37 |
| 36 | A1 | 640 | U | N1-C6 | -5.19 | 1.33 | 1.38 |
| 36 | A1 | 1117 | G | N9-C8 | -5.19 | 1.34 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 36 | A1 | 2377 | G | C6-N1 | -5.19 | 1.35 | 1.39 |
| 36 | A5 | 1170 | A | C8-N7 | -5.19 | 1.27 | 1.31 |
| 36 | A5 | 2327 | U | N3-C4 | -5.19 | 1.33 | 1.38 |
| 36 | A5 | 2692 | A | N7-C5 | -5.19 | 1.36 | 1.39 |
| 36 | A5 | 2912 | G | C5-C4 | -5.19 | 1.34 | 1.38 |
| 80 | A6 | 375 | U | C4-O4 | -5.19 | 1.19 | 1.23 |
| 36 | A1 | 3215 | A | N9-C4 | -5.18 | 1.34 | 1.37 |
| 80 | A6 | 434 | G | C6-N1 | -5.18 | 1.35 | 1.39 |
| 80 | A6 | 980 | G | N9-C8 | -5.18 | 1.34 | 1.37 |
| 36 | A5 | 1056 | U | C2-N3 | 5.18 | 1.41 | 1.37 |
| 36 | A5 | 2375 | G | P-OP2 | -5.18 | 1.40 | 1.49 |
| 1 | A2 | 352 | A | N9-C8 | -5.18 | 1.33 | 1.37 |
| 36 | A5 | 835 | G | C5-C4 | -5.18 | 1.34 | 1.38 |
| 36 | A5 | 1116 | G | N9-C8 | -5.18 | 1.34 | 1.37 |
| 36 | A1 | 1170 | A | N9-C4 | 5.18 | 1.41 | 1.37 |
| 36 | A1 | 2277 | C | C4-N4 | -5.18 | 1.29 | 1.33 |
| 36 | A5 | 345 | G | C6-O6 | -5.18 | 1.19 | 1.24 |
| 36 | A5 | 627 | U | C2-N3 | -5.18 | 1.34 | 1.37 |
| 36 | A5 | 1832 | C | N1-C6 | -5.18 | 1.34 | 1.37 |
| 36 | A1 | 826 | G | C5-C4 | -5.18 | 1.34 | 1.38 |
| 38 | A4 | 10 | A | C6-N1 | -5.18 | 1.31 | 1.35 |
| 36 | A5 | 49 | A | N3-C4 | -5.18 | 1.31 | 1.34 |
| 36 | A5 | 884 | A | C5-C6 | -5.18 | 1.36 | 1.41 |
| 36 | A1 | 642 | U | P-O5' | -5.17 | 1.54 | 1.59 |
| 36 | A1 | 2877 | G | N7-C5 | -5.17 | 1.36 | 1.39 |
| 36 | A5 | 2372 | A | C6-N1 | -5.17 | 1.31 | 1.35 |
| 36 | A1 | 1178 | G | N3-C4 | -5.17 | 1.31 | 1.35 |
| 36 | A5 | 649 | A | N7-C5 | -5.17 | 1.36 | 1.39 |
| 36 | A5 | 1607 | U | C3'-O3' | 5.17 | 1.49 | 1.42 |
| 80 | A6 | 1644 | C | N3-C4 | -5.17 | 1.30 | 1.33 |
| 36 | A5 | 284 | A | N9-C4 | 5.17 | 1.41 | 1.37 |
| 36 | A1 | 42 | C | N1-C6 | 5.17 | 1.40 | 1.37 |
| 36 | A5 | 859 | G | C2-N3 | -5.17 | 1.28 | 1.32 |
| 1 | A2 | 474 | A | N9-C4 | -5.17 | 1.34 | 1.37 |
| 36 | A1 | 1497 | C | P-OP2 | 5.17 | 1.57 | 1.49 |
| 36 | A5 | 70 | A | N7-C5 | -5.17 | 1.36 | 1.39 |
| 36 | A5 | 2634 | U | N3-C4 | 5.17 | 1.43 | 1.38 |
| 36 | A1 | 987 | U | C2-O2 | -5.16 | 1.17 | 1.22 |
| 36 | A1 | 2426 | U | C4-O4 | -5.16 | 1.19 | 1.23 |
| 36 | A5 | 2837 | A | N3-C4 | -5.16 | 1.31 | 1.34 |
| 36 | A5 | 2859 | U | C2-N3 | -5.16 | 1.34 | 1.37 |
| 42 | DD | 95 | TRP | CG-CD1 | 5.16 | 1.44 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 36 | A1 | 2278 | C | N3-C4 | -5.16 | 1.30 | 1.33 |
| 36 | A1 | 583 | G | C6-N1 | -5.16 | 1.35 | 1.39 |
| 36 | A5 | 436 | A | C5-C4 | 5.16 | 1.42 | 1.38 |
| 36 | A5 | 1157 | G | N9-C8 | -5.16 | 1.34 | 1.37 |
| 48 | DJ | 8 | PRO | CB-CG | 5.16 | 1.75 | 1.50 |
| 36 | A1 | 1409 | G | C6-N1 | -5.16 | 1.35 | 1.39 |
| 36 | A1 | 1908 | A | P-OP2 | -5.16 | 1.40 | 1.49 |
| 36 | A1 | 3216 | G | N9-C8 | -5.16 | 1.34 | 1.37 |
| 36 | A1 | 795 | G | N1-C2 | -5.16 | 1.33 | 1.37 |
| 36 | A5 | 2414 | G | C5-C4 | -5.16 | 1.34 | 1.38 |
| 36 | A5 | 2858 | U | C2-O2 | -5.16 | 1.17 | 1.22 |
| 36 | A1 | 1202 | A | C6-N1 | -5.15 | 1.31 | 1.35 |
| 36 | A1 | 1741 | A | C5-C6 | -5.15 | 1.36 | 1.41 |
| 36 | A1 | 2595 | A | N9-C8 | 5.15 | 1.41 | 1.37 |
| 36 | A1 | 1450 | G | C2-N3 | -5.15 | 1.28 | 1.32 |
| 38 | A4 | 21 | C | P-O5' | -5.15 | 1.54 | 1.59 |
| 36 | A5 | 984 | G | C6-N1 | -5.15 | 1.35 | 1.39 |
| 36 | A5 | 1151 | U | C2-N3 | -5.15 | 1.34 | 1.37 |
| 36 | A1 | 2364 | G | N3-C4 | -5.15 | 1.31 | 1.35 |
| 36 | A5 | 1208 | U | C2-N3 | -5.14 | 1.34 | 1.37 |
| 36 | A5 | 2172 | A | N9-C4 | -5.14 | 1.34 | 1.37 |
| 36 | A5 | 404 | G | N9-C8 | -5.14 | 1.34 | 1.37 |
| 36 | A1 | 638 | C | C2-O2 | -5.14 | 1.19 | 1.24 |
| 36 | A1 | 2394 | G | C8-N7 | -5.14 | 1.27 | 1.30 |
| 36 | A1 | 2920 | U | C2-O2 | -5.14 | 1.17 | 1.22 |
| 38 | A4 | 48 | A | N7-C5 | -5.14 | 1.36 | 1.39 |
| 36 | A1 | 892 | U | C4-O4 | -5.14 | 1.19 | 1.23 |
| 36 | A1 | 1133 | A | N9-C4 | -5.14 | 1.34 | 1.37 |
| 80 | A6 | 1 | U | N1-C2 | 5.13 | 1.43 | 1.38 |
| 36 | A5 | 3316 | A | N3-C4 | -5.13 | 1.31 | 1.34 |
| 36 | A1 | 832 | G | C6-N1 | -5.13 | 1.35 | 1.39 |
| 36 | A1 | 1480 | G | C8-N7 | -5.13 | 1.27 | 1.30 |
| 46 | DH | 82 | VAL | CB-CG2 | -5.13 | 1.42 | 1.52 |
| 36 | A1 | 1131 | G | C6-N1 | -5.13 | 1.35 | 1.39 |
| 36 | A1 | 1837 | U | P-OP2 | -5.13 | 1.40 | 1.49 |
| 36 | A1 | 1328 | C | N1-C6 | -5.13 | 1.34 | 1.37 |
| 36 | A5 | 609 | G | N3-C4 | -5.13 | 1.31 | 1.35 |
| 36 | A1 | 1841 | A | N9-C4 | 5.13 | 1.41 | 1.37 |
| 80 | A6 | 687 | G | N9-C4 | -5.12 | 1.33 | 1.38 |
| 36 | A5 | 1338 | C | C4-N4 | -5.12 | 1.29 | 1.33 |
| 36 | A1 | 221 | A | N9-C8 | -5.12 | 1.33 | 1.37 |
| 36 | A1 | 951 | A | N9-C4 | -5.12 | 1.34 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 36 | A1 | 2149 | A | C6-N1 | -5.12 | 1.31 | 1.35 |
| 36 | A5 | 1797 | A | C5-C4 | -5.12 | 1.35 | 1.38 |
| 36 | A5 | 2666 | C | N1-C6 | -5.12 | 1.34 | 1.37 |
| 36 | A5 | 2859 | U | N3-C4 | -5.12 | 1.33 | 1.38 |
| 36 | A1 | 73 | C | N1-C6 | -5.12 | 1.34 | 1.37 |
| 36 | A1 | 2642 | A | N3-C4 | -5.12 | 1.31 | 1.34 |
| 36 | A1 | 2877 | G | C6-N1 | -5.12 | 1.35 | 1.39 |
| 36 | A5 | 2865 | U | N1-C2 | 5.12 | 1.43 | 1.38 |
| 36 | A1 | 3319 | U | N1-C2 | 5.11 | 1.43 | 1.38 |
| 36 | A5 | 2928 | C | C4'-C3' | -5.11 | 1.47 | 1.52 |
| 36 | A5 | 2936 | A | C4'-C3' | -5.11 | 1.47 | 1.52 |
| 1 | A2 | 387 | A | N7-C5 | 5.11 | 1.42 | 1.39 |
| 36 | A1 | 159 | A | N9-C4 | -5.11 | 1.34 | 1.37 |
| 36 | A1 | 338 | A | C5-C4 | -5.11 | 1.35 | 1.38 |
| 36 | A5 | 1117 | G | C6-O6 | -5.11 | 1.19 | 1.24 |
| 38 | A4 | 13 | A | C5-C6 | -5.11 | 1.36 | 1.41 |
| 36 | A1 | 835 | G | C5-C4 | -5.11 | 1.34 | 1.38 |
| 36 | A5 | 891 | G | N3-C4 | -5.11 | 1.31 | 1.35 |
| 36 | A5 | 984 | G | N9-C8 | -5.11 | 1.34 | 1.37 |
| 36 | A1 | 1481 | A | P-O5' | -5.10 | 1.54 | 1.59 |
| 36 | A5 | 1179 | A | P-OP2 | -5.10 | 1.40 | 1.49 |
| 36 | A5 | 1886 | A | N3-C4 | -5.10 | 1.31 | 1.34 |
| 36 | A1 | 1431 | G | C6-N1 | -5.10 | 1.35 | 1.39 |
| 36 | A1 | 287 | G | N3-C4 | -5.10 | 1.31 | 1.35 |
| 80 | A6 | 55 | A | C5-C4 | -5.10 | 1.35 | 1.38 |
| 36 | A5 | 1143 | A | N3-C4 | -5.10 | 1.31 | 1.34 |
| 36 | A5 | 1902 | G | C8-N7 | -5.10 | 1.27 | 1.30 |
| 67 | Dd | 61 | LYS | CD-CE | 5.10 | 1.64 | 1.51 |
| 36 | A1 | 1060 | U | C2-N3 | -5.10 | 1.34 | 1.37 |
| 36 | A5 | 38 | U | O3'-P | -5.10 | 1.55 | 1.61 |
| 36 | A1 | 907 | G | N7-C5 | -5.10 | 1.36 | 1.39 |
| 36 | A1 | 952 | A | C5-C6 | -5.10 | 1.36 | 1.41 |
| 36 | A1 | 1845 | G | N7-C5 | -5.10 | 1.36 | 1.39 |
| 36 | A5 | 1898 | G | N9-C8 | -5.10 | 1.34 | 1.37 |
| 36 | A5 | 2243 | A | N3-C4 | -5.09 | 1.31 | 1.34 |
| 36 | A1 | 1305 | U | C2-N3 | -5.09 | 1.34 | 1.37 |
| 36 | A1 | 2160 | G | N7-C5 | -5.09 | 1.36 | 1.39 |
| 36 | A5 | 2934 | A | C6-N1 | -5.09 | 1.31 | 1.35 |
| 36 | A1 | 2888 | U | C4-O4 | -5.09 | 1.19 | 1.23 |
| 36 | A5 | 2371 | G | N1-C2 | -5.09 | 1.33 | 1.37 |
| 64 | Ba | 42 | ARG | CZ-NH2 | 5.09 | 1.39 | 1.33 |
| 52 | BO | 158[B] | ASP | C-N | -5.09 | 1.22 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 36 | A5 | 397 | A | N3-C4 | -5.09 | 1.31 | 1.34 |
| 36 | A5 | 2659 | G | N1-C2 | -5.09 | 1.33 | 1.37 |
| 80 | A6 | 49 | C | P-OP2 | -5.08 | 1.40 | 1.49 |
| 36 | A5 | 2147 | A | C5-C4 | -5.08 | 1.35 | 1.38 |
| 36 | A5 | 2620 | G | C5-C4 | -5.08 | 1.34 | 1.38 |
| 36 | A5 | 2693 | C | N3-C4 | -5.08 | 1.30 | 1.33 |
| 36 | A5 | 999 | G | C5-C4 | -5.08 | 1.34 | 1.38 |
| 36 | A1 | 2987 | A | C6-N1 | -5.08 | 1.31 | 1.35 |
| 1 | A2 | 142 | G | N9-C4 | -5.08 | 1.33 | 1.38 |
| 36 | A1 | 1164 | G | N9-C4 | -5.08 | 1.33 | 1.38 |
| 36 | A5 | 2141 | U | P-OP1 | -5.08 | 1.40 | 1.49 |
| 36 | A1 | 2132 | C | P-OP1 | -5.08 | 1.40 | 1.49 |
| 36 | A1 | 2147 | A | C5-C4 | -5.08 | 1.35 | 1.38 |
| 36 | A5 | 652 | G | N7-C5 | -5.08 | 1.36 | 1.39 |
| 36 | A5 | 1910 | A | C6-N6 | -5.08 | 1.29 | 1.33 |
| 36 | A1 | 679 | U | C2-N3 | -5.07 | 1.34 | 1.37 |
| 80 | A6 | 420 | A | N9-C4 | -5.07 | 1.34 | 1.37 |
| 36 | A5 | 1145 | G | C2-N3 | -5.07 | 1.28 | 1.32 |
| 36 | A1 | 1124 | U | C4-C5 | -5.07 | 1.39 | 1.43 |
| 38 | A4 | 23 | U | C2-N3 | 5.07 | 1.41 | 1.37 |
| 36 | A5 | 656 | A | O3'-P | -5.07 | 1.55 | 1.61 |
| 36 | A5 | 1117 | G | C8-N7 | -5.07 | 1.27 | 1.30 |
| 36 | A1 | 50 | U | N3-C4 | -5.07 | 1.33 | 1.38 |
| 36 | A5 | 987 | U | C4-C5 | 5.07 | 1.48 | 1.43 |
| 36 | A5 | 2302 | G | C6-N1 | -5.07 | 1.36 | 1.39 |
| 36 | A5 | 2922 | G | C5-C6 | -5.07 | 1.37 | 1.42 |
| 36 | A1 | 2370 | G | N7-C5 | -5.06 | 1.36 | 1.39 |
| 36 | A1 | 923 | C | N1-C2 | -5.06 | 1.35 | 1.40 |
| 36 | A5 | 34 | A | N3-C4 | -5.06 | 1.31 | 1.34 |
| 36 | A5 | 3122 | A | N7-C5 | -5.06 | 1.36 | 1.39 |
| 36 | A1 | 1454 | A | N9-C4 | -5.06 | 1.34 | 1.37 |
| 36 | A5 | 1188 | U | C2-N3 | -5.06 | 1.34 | 1.37 |
| 36 | A1 | 1299 | U | C4-O4 | -5.06 | 1.19 | 1.23 |
| 36 | A1 | 1310 | G | N1-C2 | -5.06 | 1.33 | 1.37 |
| 36 | A1 | 1417 | G | C5-C4 | -5.05 | 1.34 | 1.38 |
| 36 | A1 | 3063 | C | N3-C4 | -5.05 | 1.30 | 1.33 |
| 80 | A6 | 539 | G | C5-C4 | 5.05 | 1.41 | 1.38 |
| 36 | A5 | 2372 | A | C3'-O3' | 5.05 | 1.49 | 1.42 |
| 36 | A1 | 2412 | G | N7-C5 | -5.05 | 1.36 | 1.39 |
| 36 | A1 | 2860 | U | P-O5' | -5.05 | 1.54 | 1.59 |
| 36 | A5 | 1188 | U | C5-C6 | -5.05 | 1.29 | 1.34 |
| 36 | A5 | 2717 | U | C2-O2 | -5.05 | 1.17 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 36 | A5 | 2855 | U | C4-O4 | -5.05 | 1.19 | 1.23 |
| 36 | A1 | 960 | U | C2-O2 | 5.05 | 1.26 | 1.22 |
| 36 | A1 | 1165 | A | C6-N6 | -5.05 | 1.29 | 1.33 |
| 36 | A5 | 585 | A | N3-C4 | -5.05 | 1.31 | 1.34 |
| 51 | DN | 94 | TYR | CE1-CZ | 5.05 | 1.45 | 1.38 |
| 76 | Dm | 79 | GLU | CD-OE2 | 5.05 | 1.31 | 1.25 |
| 36 | A1 | 936 | A | C6-N6 | -5.05 | 1.29 | 1.33 |
| 36 | A5 | 2993 | G | N1-C2 | -5.05 | 1.33 | 1.37 |
| 36 | A1 | 3307 | A | C6-N1 | -5.04 | 1.32 | 1.35 |
| 36 | A5 | 2882 | U | C2-O2 | -5.04 | 1.17 | 1.22 |
| 55 | BR | 125 | LYS | CD-CE | 5.04 | 1.63 | 1.51 |
| 36 | A5 | 1295 | G | C6-N1 | -5.04 | 1.36 | 1.39 |
| 46 | DH | 110 | LYS | CD-CE | 5.04 | 1.63 | 1.51 |
| 36 | A1 | 574 | U | C4-O4 | -5.04 | 1.19 | 1.23 |
| 80 | A6 | 335 | U | N1-C2 | -5.04 | 1.34 | 1.38 |
| 36 | A1 | 1852 | G | C6-O6 | 5.04 | 1.28 | 1.24 |
| 80 | A6 | 158 | U | C3'-O3' | 5.04 | 1.49 | 1.42 |
| 36 | A5 | 877 | C | C4-N4 | -5.04 | 1.29 | 1.33 |
| 36 | A5 | 1123 | U | N3-C4 | -5.04 | 1.33 | 1.38 |
| 36 | A5 | 1435 | A | C6-N6 | -5.04 | 1.29 | 1.33 |
| 55 | DR | 72 | GLU | CG-CD | 5.04 | 1.59 | 1.51 |
| 36 | A1 | 345 | G | N7-C5 | -5.04 | 1.36 | 1.39 |
| 36 | A1 | 893 | C | P-OP2 | -5.04 | 1.40 | 1.49 |
| 36 | A1 | 2833 | A | N9-C4 | -5.04 | 1.34 | 1.37 |
| 36 | A5 | 2958 | A | N9-C4 | -5.04 | 1.34 | 1.37 |
| 1 | A2 | 1773 | C | C4-N4 | 5.03 | 1.38 | 1.33 |
| 36 | A5 | 652 | G | N9-C8 | -5.03 | 1.34 | 1.37 |
| 36 | A1 | 198 | A | C6-N1 | -5.03 | 1.32 | 1.35 |
| 36 | A5 | 726 | G | N7-C5 | -5.03 | 1.36 | 1.39 |
| 36 | A5 | 1427 | U | C2-N3 | -5.03 | 1.34 | 1.37 |
| 36 | A1 | 2393 | G | N9-C8 | -5.03 | 1.34 | 1.37 |
| 36 | A1 | 919 | U | C4-O4 | -5.03 | 1.19 | 1.23 |
| 36 | A1 | 1145 | G | C8-N7 | -5.03 | 1.27 | 1.30 |
| 36 | A1 | 3375 | A | N7-C5 | -5.03 | 1.36 | 1.39 |
| 80 | A6 | 1723 | U | C2-N3 | -5.03 | 1.34 | 1.37 |
| 36 | A5 | 1049 | C | C4-N4 | -5.03 | 1.29 | 1.33 |
| 37 | A7 | 88 | G | C2-N3 | -5.03 | 1.28 | 1.32 |
| 36 | A1 | 2302 | G | N1-C2 | -5.02 | 1.33 | 1.37 |
| 36 | A5 | 1299 | U | C4-O4 | -5.02 | 1.19 | 1.23 |
| 36 | A5 | 333 | G | C6-N1 | -5.02 | 1.36 | 1.39 |
| 36 | A5 | 2743 | A | C6-N6 | -5.02 | 1.29 | 1.33 |
| 1 | A2 | 1782 | A | N3-C4 | -5.02 | 1.31 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 31 | Ad | 7 | TRP | CB-CG | 5.02 | 1.59 | 1.50 |
| 36 | A1 | 2919 | A | C6-N1 | -5.02 | 1.32 | 1.35 |
| 80 | A6 | 609 | U | C2-N3 | -5.02 | 1.34 | 1.37 |
| 36 | A5 | 2366 | C | C2-N3 | 5.02 | 1.39 | 1.35 |
| 36 | A1 | 952 | A | N7-C5 | -5.01 | 1.36 | 1.39 |
| 80 | A6 | 47 | A | C5'-C4' | -5.01 | 1.45 | 1.51 |
| 36 | A5 | 106 | A | N9-C4 | -5.01 | 1.34 | 1.37 |
| 67 | Dd | 102 | LYS | CD-CE | 5.01 | 1.63 | 1.51 |
| 36 | A1 | 952 | A | C6-N6 | -5.01 | 1.29 | 1.33 |
| 36 | A1 | 2350 | C | N1-C6 | -5.01 | 1.34 | 1.37 |
| 36 | A1 | 3139 | A | C6-N6 | -5.01 | 1.29 | 1.33 |
| 38 | A4 | 36 | G | N9-C4 | -5.01 | 1.33 | 1.38 |
| 80 | A6 | 1595 | U | N3-C4 | -5.01 | 1.33 | 1.38 |
| 36 | A5 | 282 | G | N3-C4 | -5.01 | 1.31 | 1.35 |
| 36 | A5 | 867 | G | C2-N3 | -5.01 | 1.28 | 1.32 |
| 36 | A5 | 3187 | A | C6-N1 | -5.01 | 1.32 | 1.35 |
| 1 | A2 | 1758 | U | N1-C2 | 5.01 | 1.43 | 1.38 |
| 36 | A1 | 357 | A | N3-C4 | -5.01 | 1.31 | 1.34 |
| 36 | A1 | 413 | U | C4-O4 | -5.01 | 1.19 | 1.23 |
| 36 | A1 | 1056 | U | C4-O4 | -5.01 | 1.19 | 1.23 |
| 80 | A6 | 1602 | C | N3-C4 | -5.01 | 1.30 | 1.33 |
| 36 | A5 | 2190 | U | C2-O2 | -5.01 | 1.17 | 1.22 |
| 80 | A6 | 437 | A | N9-C4 | -5.01 | 1.34 | 1.37 |
| 36 | A1 | 372 | A | N3-C4 | 5.01 | 1.37 | 1.34 |
| 80 | A6 | 163 | G | N9-C8 | 5.01 | 1.41 | 1.37 |
| 36 | A5 | 2375 | G | C6-O6 | -5.01 | 1.19 | 1.24 |
| 36 | A5 | 3245 | A | N1-C2 | 5.01 | 1.38 | 1.34 |
| 73 | Bj | 43 | LYS | CD-CE | 5.00 | 1.63 | 1.51 |
| 36 | A5 | 2930 | A | N3-C4 | 5.00 | 1.37 | 1.34 |
| 36 | A1 | 406 | G | C6-N1 | -5.00 | 1.36 | 1.39 |
| 36 | A1 | 2369 | G | N9-C8 | -5.00 | 1.34 | 1.37 |
| 36 | A5 | 2291 | A | N9-C4 | -5.00 | 1.34 | 1.37 |
| 36 | A5 | 2652 | U | N1-C2 | -5.00 | 1.34 | 1.38 |
| 36 | A5 | 2944 | U | C4-O4 | -5.00 | 1.19 | 1.23 |
| 69 | Df | 91 | ALA | N-CA | 5.00 | 1.56 | 1.46 |
| 36 | A1 | 668 | G | C5-C4 | -5.00 | 1.34 | 1.38 |
| 36 | A1 | 2697 | A | C6-N1 | -5.00 | 1.32 | 1.35 |
| 36 | A5 | 1184 | A | N3-C4 | -5.00 | 1.31 | 1.34 |
| 36 | A5 | 1388 | U | C2-O2 | -5.00 | 1.17 | 1.22 |
| 36 | A5 | 2315 | G | N9-C4 | -5.00 | 1.33 | 1.38 |
| 37 | A7 | 12 | U | C4-O4 | -5.00 | 1.19 | 1.23 |

All (9884) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 36 | A1 | 2777 | G | C4-C5-N7 | 50.47 | 130.99 | 110.80 |
| 36 | A1 | 2777 | G | N9-C4-C5 | -40.53 | 89.19 | 105.40 |
| 36 | A1 | 2777 | G | C5-C6-O6 | -39.10 | 105.14 | 128.60 |
| 52 | BO | 3[A] | VAL | CA-C-N | -39.08 | 31.23 | 117.20 |
| 36 | A5 | 1152 | G | N3-C4-C5 | 33.63 | 145.41 | 128.60 |
| 36 | A1 | 2777 | G | N1-C6-O6 | 32.55 | 139.43 | 119.90 |
| 36 | A1 | 2777 | G | C6-C5-N7 | -32.03 | 111.18 | 130.40 |
| 36 | A5 | 1152 | G | N3-C4-N9 | -31.59 | 107.05 | 126.00 |
| 52 | BO | 3[A] | VAL | C-N-CA | -31.16 | 43.80 | 121.70 |
| 36 | A5 | 1152 | G | N3-C2-N2 | -26.99 | 101.01 | 119.90 |
| 36 | A1 | 2777 | G | C5-N7-C8 | -26.62 | 90.99 | 104.30 |
| 36 | A1 | 3242 | G | N3-C4-N9 | -25.00 | 111.00 | 126.00 |
| 36 | A5 | 1152 | G | C2-N3-C4 | -24.03 | 99.89 | 111.90 |
| 36 | A1 | 2714 | G | N3-C4-C5 | 22.55 | 139.87 | 128.60 |
| 36 | A5 | 922 | U | C5-C6-N1 | -22.08 | 111.66 | 122.70 |
| 36 | A5 | 922 | U | C2-N3-C4 | -21.60 | 114.04 | 127.00 |
| 80 | A6 | 1773 | C | N3-C4-C5 | -21.52 | 113.29 | 121.90 |
| 36 | A1 | 2777 | G | N3-C4-N9 | 20.18 | 138.11 | 126.00 |
| 36 | A5 | 1152 | G | C5-N7-C8 | -20.02 | 94.29 | 104.30 |
| 36 | A1 | 1495 | U | C5-C6-N1 | -19.83 | 112.79 | 122.70 |
| 36 | A1 | 2714 | G | N3-C4-N9 | -19.57 | 114.26 | 126.00 |
| 36 | A5 | 922 | U | N1-C2-N3 | 19.47 | 126.58 | 114.90 |
| 36 | A5 | 1152 | G | C8-N9-C1' | 18.98 | 151.68 | 127.00 |
| 36 | A5 | 3245 | A | C2-N3-C4 | -18.87 | 101.16 | 110.60 |
| 36 | A1 | 2714 | G | C2-N3-C4 | -18.73 | 102.53 | 111.90 |
| 1 | A2 | 553 | G | N1-C6-O6 | 18.62 | 131.07 | 119.90 |
| 36 | A5 | 3245 | A | C5-N7-C8 | -18.61 | 94.59 | 103.90 |
| 36 | A1 | 3242 | G | N3-C4-C5 | 18.44 | 137.82 | 128.60 |
| 1 | A2 | 1200 | G | N1-C6-O6 | 17.86 | 130.61 | 119.90 |
| 36 | A1 | 1492 | G | N3-C4-C5 | -17.61 | 119.79 | 128.60 |
| 80 | A6 | 609 | U | C5-C6-N1 | -17.30 | 114.05 | 122.70 |
| 36 | A5 | 1152 | G | N1-C6-O6 | 17.20 | 130.22 | 119.90 |
| 36 | A1 | 2617 | U | C5-C6-N1 | -16.99 | 114.21 | 122.70 |
| 36 | A5 | 1152 | G | C4-N9-C1' | -16.85 | 104.59 | 126.50 |
| 36 | A5 | 1152 | G | C4-C5-N7 | 16.78 | 117.51 | 110.80 |
| 36 | A1 | 2777 | G | C8-N9-C4 | 16.56 | 113.03 | 106.40 |
| 80 | A6 | 609 | U | C5-C4-O4 | 16.48 | 135.79 | 125.90 |
| 36 | A1 | 2952 | G | C5-C6-O6 | -16.45 | 118.73 | 128.60 |
| 36 | A5 | 1152 | G | N1-C2-N2 | 16.25 | 130.82 | 116.20 |
| 36 | A1 | 1495 | U | C4-C5-C6 | 16.12 | 129.37 | 119.70 |
| 36 | A5 | 922 | U | N1-C2-O2 | -16.09 | 111.53 | 122.80 |
| 36 | A5 | 3245 | A | N7-C8-N9 | 15.82 | 121.71 | 113.80 |
| 80 | A6 | 553 | G | N1-C6-O6 | 15.73 | 129.34 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 80 | A6 | 337 | G | C6-C5-N7 | -15.69 | 120.99 | 130.40 |
| 36 | A5 | 776 | U | C5-C6-N1 | -15.52 | 114.94 | 122.70 |
| 36 | A5 | 2726 | C | C6-N1-C2 | -15.44 | 114.12 | 120.30 |
| 36 | A1 | 1308 | A | N7-C8-N9 | 15.43 | 121.51 | 113.80 |
| 36 | A1 | 517 | G | C8-N9-C4 | -15.42 | 100.23 | 106.40 |
| 36 | A1 | 1495 | U | N1-C2-N3 | 15.31 | 124.09 | 114.90 |
| 36 | A1 | 3242 | G | N3-C2-N2 | -15.29 | 109.20 | 119.90 |
| 36 | A1 | 2846 | U | C5-C4-O4 | 15.27 | 135.06 | 125.90 |
| 36 | A5 | 1450 | G | C5-N7-C8 | 15.24 | 111.92 | 104.30 |
| 36 | A1 | 644 | G | C5-C6-O6 | 15.20 | 137.72 | 128.60 |
| 36 | A1 | 1409 | G | N1-C6-O6 | -15.20 | 110.78 | 119.90 |
| 36 | A1 | 3242 | G | C8-N9-C1' | 15.18 | 146.74 | 127.00 |
| 36 | A1 | 804 | C | N1-C2-O2 | -15.14 | 109.82 | 118.90 |
| 1 | A2 | 577 | G | C4-C5-N7 | 15.02 | 116.81 | 110.80 |
| 36 | A5 | 3245 | A | C4-C5-N7 | 14.99 | 118.19 | 110.70 |
| 80 | A6 | 163 | G | C5-N7-C8 | -14.81 | 96.89 | 104.30 |
| 36 | A5 | 3245 | A | N1-C6-N6 | 14.78 | 127.47 | 118.60 |
| 36 | A1 | 1308 | A | C8-N9-C4 | -14.71 | 99.92 | 105.80 |
| 36 | A1 | 3306 | U | N1-C2-N3 | 14.70 | 123.72 | 114.90 |
| 36 | A1 | 1492 | G | C5-N7-C8 | 14.61 | 111.61 | 104.30 |
| 36 | A5 | 3245 | A | C6-C5-N7 | -14.56 | 122.11 | 132.30 |
| 36 | A1 | 1902 | G | N1-C6-O6 | 14.47 | 128.58 | 119.90 |
| 36 | A1 | 3242 | G | N9-C4-C5 | 14.45 | 111.18 | 105.40 |
| 80 | A6 | 337 | G | C8-N9-C1' | -14.40 | 108.28 | 127.00 |
| 36 | A5 | 1152 | G | C5-C6-O6 | -14.38 | 119.97 | 128.60 |
| 36 | A1 | 2827 | U | C5-C6-N1 | -14.27 | 115.57 | 122.70 |
| 36 | A1 | 1592 | G | C5-C6-N1 | 14.27 | 118.63 | 111.50 |
| 1 | A2 | 1200 | G | C5-C6-O6 | -14.23 | 120.06 | 128.60 |
| 36 | A1 | 2278 | C | N1-C2-O2 | -14.20 | 110.38 | 118.90 |
| 80 | A6 | 163 | G | N3-C4-C5 | 14.20 | 135.70 | 128.60 |
| 80 | A6 | 163 | G | N3-C4-N9 | -14.19 | 117.48 | 126.00 |
| 36 | A1 | 3306 | U | N3-C2-O2 | -14.18 | 112.27 | 122.20 |
| 1 | A2 | 1773 | C | N3-C4-C5 | -14.15 | 116.24 | 121.90 |
| 36 | A5 | 2353 | G | C5-C6-O6 | -14.14 | 120.12 | 128.60 |
| 36 | A1 | 2434 | U | C5-C4-O4 | 14.07 | 134.34 | 125.90 |
| 36 | A1 | 1492 | G | C2-N3-C4 | 14.07 | 118.93 | 111.90 |
| 36 | A5 | 2726 | C | C5-C4-N4 | 14.02 | 130.02 | 120.20 |
| 36 | A5 | 2634 | U | C2-N3-C4 | -13.99 | 118.61 | 127.00 |
| 36 | A1 | 885 | U | C5-C6-N1 | -13.96 | 115.72 | 122.70 |
| 36 | A5 | 2634 | U | C5-C4-O4 | -13.96 | 117.53 | 125.90 |
| 36 | A5 | 776 | U | N1-C2-N3 | 13.95 | 123.27 | 114.90 |
| 36 | A1 | 2298 | U | C5-C6-N1 | -13.92 | 115.74 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 36 | A5 | 1592 | G | N1-C6-O6 | -13.92 | 111.55 | 119.90 |
| 36 | A1 | 2679 | A | C2-N3-C4 | -13.84 | 103.68 | 110.60 |
| 36 | A1 | 709 | A | C8-N9-C4 | 13.83 | 111.33 | 105.80 |
| 36 | A1 | 776 | U | C4-C5-C6 | 13.82 | 128.00 | 119.70 |
| 80 | A6 | 163 | G | C2-N3-C4 | -13.82 | 104.99 | 111.90 |
| 80 | A6 | 609 | U | N3-C4-O4 | -13.74 | 109.78 | 119.40 |
| 36 | A1 | 2278 | C | N1-C2-N3 | 13.64 | 128.75 | 119.20 |
| 36 | A1 | 2617 | U | C5-C4-O4 | 13.48 | 133.99 | 125.90 |
| 36 | A5 | 2245 | C | C6-N1-C2 | -13.44 | 114.93 | 120.30 |
| 36 | A5 | 776 | U | C4-C5-C6 | 13.41 | 127.75 | 119.70 |
| 1 | A2 | 1560 | U | C5-C4-O4 | 13.36 | 133.91 | 125.90 |
| 36 | A5 | 2372 | A | C8-N9-C4 | -13.34 | 100.47 | 105.80 |
| 80 | A6 | 308 | C | C5-C6-N1 | -13.32 | 114.34 | 121.00 |
| 80 | A6 | 337 | G | C4-N9-C1' | 13.31 | 143.80 | 126.50 |
| 36 | A5 | 1450 | G | N7-C8-N9 | -13.30 | 106.45 | 113.10 |
| 36 | A1 | 1216 | C | C6-N1-C2 | -13.27 | 114.99 | 120.30 |
| 1 | A2 | 1773 | C | C6-N1-C2 | -13.23 | 115.01 | 120.30 |
| 36 | A5 | 922 | U | C4-C5-C6 | 13.22 | 127.63 | 119.70 |
| 36 | A1 | 3242 | G | C4-N9-C1' | -13.22 | 109.31 | 126.50 |
| 36 | A1 | 1592 | G | C4-C5-N7 | 13.19 | 116.08 | 110.80 |
| 36 | A1 | 2836 | C | C5-C4-N4 | 13.19 | 129.43 | 120.20 |
| 80 | A6 | 1280 | C | N3-C4-C5 | -13.12 | 116.65 | 121.90 |
| 36 | A5 | 631 | U | N3-C2-O2 | -13.11 | 113.02 | 122.20 |
| 36 | A1 | 2278 | C | C6-N1-C2 | -13.07 | 115.07 | 120.30 |
| 80 | A6 | 1773 | C | N3-C4-N4 | 13.03 | 127.12 | 118.00 |
| 36 | A1 | 2983 | C | C5-C6-N1 | -13.02 | 114.49 | 121.00 |
| 36 | A5 | 2278 | C | N1-C2-O2 | -12.99 | 111.11 | 118.90 |
| 36 | A5 | 2303 | A | C2-N3-C4 | 12.97 | 117.08 | 110.60 |
| 36 | A5 | 2361 | A | C2-N3-C4 | 12.96 | 117.08 | 110.60 |
| 36 | A5 | 3214 | U | C5-C4-O4 | 12.88 | 133.63 | 125.90 |
| 36 | A1 | 1846 | C | N1-C2-O2 | -12.87 | 111.18 | 118.90 |
| 36 | A1 | 1342 | C | N3-C4-C5 | 12.86 | 127.04 | 121.90 |
| 36 | A5 | 2726 | C | N1-C2-N3 | 12.84 | 128.19 | 119.20 |
| 36 | A1 | 2983 | C | C5-C4-N4 | 12.79 | 129.15 | 120.20 |
| 36 | A1 | 3242 | G | N1-C2-N2 | 12.77 | 127.69 | 116.20 |
| 36 | A5 | 1208 | U | N3-C4-O4 | -12.77 | 110.46 | 119.40 |
| 36 | A1 | 1592 | G | N3-C2-N2 | 12.74 | 128.82 | 119.90 |
| 36 | A1 | 2617 | U | N3-C4-O4 | -12.71 | 110.51 | 119.40 |
| 80 | A6 | 453 | U | N3-C2-O2 | -12.70 | 113.31 | 122.20 |
| 1 | A2 | 577 | G | C5-N7-C8 | -12.68 | 97.96 | 104.30 |
| 36 | A5 | 1208 | U | C5-C4-O4 | 12.68 | 133.51 | 125.90 |
| 36 | A5 | 2308 | C | N1-C2-O2 | -12.67 | 111.30 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 36 | A1 | 2617 | U | C2-N3-C4 | -12.66 | 119.40 | 127.00 |
| 36 | A5 | 2327 | U | C5-C6-N1 | -12.66 | 116.37 | 122.70 |
| 36 | A5 | 3214 | U | N3-C2-O2 | -12.64 | 113.35 | 122.20 |
| 36 | A5 | 1152 | G | C4-C5-C6 | -12.63 | 111.22 | 118.80 |
| 36 | A1 | 3269 | U | N3-C2-O2 | -12.62 | 113.37 | 122.20 |
| 68 | De | 43 | ARG | NE-CZ-NH1 | 12.58 | 126.59 | 120.30 |
| 36 | A1 | 3306 | U | C5-C4-O4 | 12.57 | 133.44 | 125.90 |
| 36 | A1 | 1492 | G | C4-C5-N7 | -12.56 | 105.78 | 110.80 |
| 36 | A1 | 2314 | U | N1-C2-N3 | -12.56 | 107.36 | 114.90 |
| 36 | A5 | 2758 | A | C2-N3-C4 | 12.56 | 116.88 | 110.60 |
| 1 | A2 | 1541 | G | N1-C6-O6 | -12.55 | 112.37 | 119.90 |
| 36 | A1 | 709 | A | N7-C8-N9 | -12.51 | 107.54 | 113.80 |
| 36 | A1 | 1911 | A | N1-C6-N6 | 12.50 | 126.10 | 118.60 |
| 80 | A6 | 308 | C | C2-N3-C4 | -12.46 | 113.67 | 119.90 |
| 36 | A1 | 2726 | C | C6-N1-C2 | -12.44 | 115.33 | 120.30 |
| 36 | A5 | 1371 | G | N1-C6-O6 | -12.43 | 112.44 | 119.90 |
| 36 | A1 | 2983 | C | N3-C4-N4 | -12.43 | 109.30 | 118.00 |
| 36 | A1 | 2899 | C | C4-C5-C6 | 12.41 | 123.61 | 117.40 |
| 36 | A5 | 776 | U | N3-C2-O2 | -12.40 | 113.52 | 122.20 |
| 36 | A5 | 1846 | C | C5-C6-N1 | -12.38 | 114.81 | 121.00 |
| 80 | A6 | 1773 | C | C6-N1-C2 | -12.38 | 115.35 | 120.30 |
| 80 | A6 | 337 | G | N9-C4-C5 | -12.38 | 100.45 | 105.40 |
| 36 | A1 | 1904 | C | N1-C2-O2 | -12.36 | 111.48 | 118.90 |
| 36 | A1 | 2836 | C | C4-C5-C6 | 12.35 | 123.58 | 117.40 |
| 36 | A1 | 1495 | U | N1-C2-O2 | -12.35 | 114.16 | 122.80 |
| 36 | A1 | 1902 | G | C5-C6-O6 | -12.34 | 121.19 | 128.60 |
| 36 | A1 | 2952 | G | N1-C6-O6 | 12.32 | 127.29 | 119.90 |
| 36 | A5 | 1434 | G | C5-N7-C8 | 12.31 | 110.46 | 104.30 |
| 36 | A5 | 1450 | G | C4-C5-N7 | -12.30 | 105.88 | 110.80 |
| 36 | A1 | 54 | C | N3-C4-N4 | -12.30 | 109.39 | 118.00 |
| 80 | A6 | 65 | A | C2-N3-C4 | -12.30 | 104.45 | 110.60 |
| 36 | A1 | 3344 | A | N7-C8-N9 | 12.29 | 119.94 | 113.80 |
| 36 | A1 | 1858 | A | C2-N3-C4 | 12.29 | 116.74 | 110.60 |
| 36 | A1 | 672 | A | N1-C6-N6 | 12.28 | 125.97 | 118.60 |
| 37 | A7 | 120 | C | C6-N1-C2 | 12.26 | 125.20 | 120.30 |
| 36 | A5 | 591 | G | C5-C6-O6 | -12.24 | 121.25 | 128.60 |
| 36 | A1 | 295 | A | C8-N9-C4 | -12.24 | 100.90 | 105.80 |
| 36 | A1 | 3362 | A | N1-C6-N6 | 12.21 | 125.93 | 118.60 |
| 36 | A1 | 3362 | A | C6-C5-N7 | -12.16 | 123.79 | 132.30 |
| 36 | A1 | 1902 | G | C6-C5-N7 | -12.14 | 123.12 | 130.40 |
| 62 | BY | 13 | ARG | NE-CZ-NH2 | -12.11 | 114.25 | 120.30 |
| 36 | A1 | 2726 | C | N3-C2-O2 | -12.08 | 113.44 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 36 | A5 | 2340 | U | N3-C4-O4 | -12.06 | 110.96 | 119.40 |
| 36 | A1 | 2846 | U | N3-C2-O2 | -12.02 | 113.79 | 122.20 |
| 36 | A1 | 2952 | G | C4-C5-N7 | 12.01 | 115.60 | 110.80 |
| 80 | A6 | 144 | U | N3-C2-O2 | -12.00 | 113.80 | 122.20 |
| 36 | A5 | 3245 | A | N1-C2-N3 | 12.00 | 135.30 | 129.30 |
| 36 | A1 | 517 | G | N7-C8-N9 | 11.93 | 119.07 | 113.10 |
| 36 | A1 | 1336 | U | N3-C2-O2 | -11.93 | 113.85 | 122.20 |
| 36 | A5 | 1308 | A | N7-C8-N9 | 11.93 | 119.76 | 113.80 |
| 36 | A5 | 2726 | C | C4-C5-C6 | 11.93 | 123.36 | 117.40 |
| 80 | A6 | 553 | G | C6-C5-N7 | -11.92 | 123.25 | 130.40 |
| 36 | A1 | 1495 | U | C2-N3-C4 | -11.91 | 119.85 | 127.00 |
| 36 | A5 | 1056 | U | C4-C5-C6 | 11.91 | 126.85 | 119.70 |
| 1 | A2 | 1200 | G | N3-C2-N2 | -11.91 | 111.56 | 119.90 |
| 36 | A1 | 2617 | U | C4-C5-C6 | 11.89 | 126.83 | 119.70 |
| 36 | A1 | 435 | C | C6-N1-C2 | 11.84 | 125.04 | 120.30 |
| 36 | A1 | 2130 | G | N1-C6-O6 | -11.83 | 112.80 | 119.90 |
| 36 | A5 | 290 | G | N1-C6-O6 | -11.82 | 112.81 | 119.90 |
| 36 | A5 | 966 | U | N3-C2-O2 | -11.77 | 113.96 | 122.20 |
| 36 | A1 | 3306 | U | N3-C4-O4 | -11.76 | 111.17 | 119.40 |
| 36 | A1 | 2617 | U | N1-C2-N3 | 11.75 | 121.95 | 114.90 |
| 80 | A6 | 553 | G | C5-C6-O6 | -11.75 | 121.55 | 128.60 |
| 36 | A1 | 895 | A | C5-N7-C8 | -11.75 | 98.03 | 103.90 |
| 36 | A5 | 667 | C | C6-N1-C2 | 11.72 | 124.99 | 120.30 |
| 36 | A1 | 2777 | G | N3-C2-N2 | 11.72 | 128.10 | 119.90 |
| 36 | A5 | 2278 | C | N1-C2-N3 | 11.71 | 127.40 | 119.20 |
| 1 | A2 | 577 | G | C5-C6-O6 | -11.69 | 121.58 | 128.60 |
| 36 | A5 | 2726 | C | N3-C4-C5 | -11.67 | 117.23 | 121.90 |
| 36 | A1 | 2633 | U | N3-C2-O2 | -11.64 | 114.05 | 122.20 |
| 36 | A5 | 2808 | A | N9-C4-C5 | -11.64 | 101.14 | 105.80 |
| 36 | A1 | 979 | U | C6-N1-C2 | -11.64 | 114.02 | 121.00 |
| 36 | A1 | 942 | U | N3-C4-O4 | -11.61 | 111.27 | 119.40 |
| 36 | A1 | 1156 | C | N3-C4-C5 | 11.59 | 126.54 | 121.90 |
| 36 | A1 | 3344 | A | C6-C5-N7 | -11.58 | 124.19 | 132.30 |
| 36 | A1 | 2679 | A | N1-C2-N3 | 11.57 | 135.09 | 129.30 |
| 80 | A6 | 1773 | C | N1-C2-O2 | -11.56 | 111.96 | 118.90 |
| 80 | A6 | 163 | G | C4-C5-N7 | 11.55 | 115.42 | 110.80 |
| 80 | A6 | 687 | G | N3-C2-N2 | -11.55 | 111.81 | 119.90 |
| 36 | A5 | 1389 | G | C4-C5-N7 | 11.53 | 115.41 | 110.80 |
| 36 | A1 | 2278 | C | C2-N3-C4 | -11.52 | 114.14 | 119.90 |
| 36 | A1 | 2817 | A | C6-N1-C2 | -11.51 | 111.69 | 118.60 |
| 1 | A2 | 1782 | A | N9-C4-C5 | 11.51 | 110.40 | 105.80 |
| 36 | A1 | 2827 | U | N3-C2-O2 | -11.47 | 114.17 | 122.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 80 | A6 | 1027 | A | C8-N9-C4 | -11.47 | 101.21 | 105.80 |
| 36 | A1 | 3362 | A | C5-N7-C8 | -11.46 | 98.17 | 103.90 |
| 36 | A1 | 645 | A | C6-N1-C2 | -11.46 | 111.72 | 118.60 |
| 36 | A1 | 591 | G | C5-C6-O6 | -11.45 | 121.73 | 128.60 |
| 36 | A1 | 2983 | C | C4-C5-C6 | 11.44 | 123.12 | 117.40 |
| 36 | A5 | 1130 | A | C2-N3-C4 | 11.44 | 116.32 | 110.60 |
| 36 | A1 | 1202 | A | C2-N3-C4 | -11.43 | 104.89 | 110.60 |
| 36 | A1 | 3214 | U | N3-C2-O2 | -11.42 | 114.21 | 122.20 |
| 36 | A5 | 1592 | G | N3-C2-N2 | 11.41 | 127.89 | 119.90 |
| 80 | A6 | 609 | U | N3-C2-O2 | -11.40 | 114.22 | 122.20 |
| 36 | A1 | 2413 | A | N1-C2-N3 | -11.36 | 123.62 | 129.30 |
| 36 | A5 | 2899 | C | N3-C2-O2 | -11.35 | 113.96 | 121.90 |
| 36 | A5 | 1797 | A | C5-N7-C8 | 11.34 | 109.57 | 103.90 |
| 1 | A2 | 553 | G | N3-C2-N2 | -11.34 | 111.96 | 119.90 |
| 36 | A1 | 664 | U | C5-C6-N1 | -11.33 | 117.04 | 122.70 |
| 36 | A1 | 2726 | C | N1-C2-N3 | 11.32 | 127.12 | 119.20 |
| 36 | A1 | 1307 | G | N1-C6-O6 | -11.31 | 113.11 | 119.90 |
| 36 | A1 | 963 | G | C5-C6-O6 | -11.31 | 121.81 | 128.60 |
| 80 | A6 | 609 | U | N1-C2-N3 | 11.31 | 121.68 | 114.90 |
| 36 | A1 | 776 | U | C5-C6-N1 | -11.27 | 117.07 | 122.70 |
| 36 | A5 | 2142 | A | C5-C6-N1 | 11.26 | 123.33 | 117.70 |
| 1 | A2 | 393 | C | C6-N1-C2 | 11.25 | 124.80 | 120.30 |
| 36 | A1 | 2353 | G | C5-C6-O6 | -11.24 | 121.86 | 128.60 |
| 36 | A5 | 414 | U | C4-C5-C6 | 11.24 | 126.44 | 119.70 |
| 36 | A1 | 776 | U | N1-C2-N3 | 11.24 | 121.64 | 114.90 |
| 37 | A3 | 81 | U | C5-C4-O4 | -11.23 | 119.16 | 125.90 |
| 80 | A6 | 1600 | A | C2-N3-C4 | -11.23 | 104.99 | 110.60 |
| 1 | A2 | 639 | U | N3-C2-O2 | -11.22 | 114.35 | 122.20 |
| 36 | A1 | 645 | A | C5-C6-N1 | 11.21 | 123.31 | 117.70 |
| 80 | A6 | 1596 | C | N3-C2-O2 | -11.20 | 114.06 | 121.90 |
| 1 | A2 | 1280 | C | N3-C4-C5 | -11.19 | 117.42 | 121.90 |
| 36 | A5 | 3377 | G | C5-C6-O6 | -11.18 | 121.89 | 128.60 |
| 36 | A1 | 2772 | C | C2-N1-C1' | 11.18 | 131.09 | 118.80 |
| 1 | A2 | 1600 | A | C2-N3-C4 | -11.17 | 105.02 | 110.60 |
| 36 | A5 | 2744 | U | N3-C2-O2 | -11.17 | 114.38 | 122.20 |
| 36 | A5 | 1004 | U | N1-C2-O2 | 11.16 | 130.61 | 122.80 |
| 36 | A1 | 1838 | G | N1-C6-O6 | 11.16 | 126.59 | 119.90 |
| 36 | A1 | 3362 | A | N1-C2-N3 | 11.16 | 134.88 | 129.30 |
| 36 | A1 | 895 | A | C8-N9-C4 | -11.15 | 101.34 | 105.80 |
| 1 | A2 | 577 | G | N1-C6-O6 | 11.13 | 126.58 | 119.90 |
| 36 | A5 | 15 | C | C6-N1-C2 | -11.12 | 115.85 | 120.30 |
| 36 | A1 | 895 | A | N7-C8-N9 | 11.12 | 119.36 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 36 | A1 | 1858 | A | N3-C4-C5 | -11.12 | 119.02 | 126.80 |
| 36 | A1 | 3362 | A | C2-N3-C4 | -11.11 | 105.04 | 110.60 |
| 80 | A6 | 639 | U | N3-C2-O2 | -11.11 | 114.42 | 122.20 |
| 36 | A1 | 1741 | A | C2-N3-C4 | -11.11 | 105.04 | 110.60 |
| 36 | A5 | 2278 | C | N3-C4-N4 | -11.08 | 110.25 | 118.00 |
| 38 | A4 | 113 | U | N1-C2-N3 | 11.06 | 121.53 | 114.90 |
| 80 | A6 | 337 | G | N1-C6-O6 | 11.05 | 126.53 | 119.90 |
| 80 | A6 | 1560 | U | N3-C2-O2 | -11.05 | 114.47 | 122.20 |
| 36 | A1 | 2634 | U | C2-N3-C4 | -11.02 | 120.39 | 127.00 |
| 36 | A5 | 2836 | C | C2-N3-C4 | -11.02 | 114.39 | 119.90 |
| 36 | A1 | 2993 | G | N3-C4-N9 | -11.01 | 119.40 | 126.00 |
| 36 | A5 | 3060 | C | N1-C2-O2 | -11.00 | 112.30 | 118.90 |
| 36 | A1 | 2169 | G | N1-C6-O6 | -10.98 | 113.31 | 119.90 |
| 36 | A5 | 3138 | U | N1-C2-O2 | -10.98 | 115.12 | 122.80 |
| 36 | A1 | 3362 | A | N7-C8-N9 | 10.96 | 119.28 | 113.80 |
| 80 | A6 | 1514 | U | C5-C4-O4 | 10.96 | 132.47 | 125.90 |
| 80 | A6 | 1773 | C | C4-C5-C6 | 10.96 | 122.88 | 117.40 |
| 80 | A6 | 453 | U | C5-C4-O4 | 10.93 | 132.46 | 125.90 |
| 80 | A6 | 1745 | G | C5-C6-N1 | 10.93 | 116.97 | 111.50 |
| 1 | A2 | 1782 | A | C8-N9-C4 | -10.91 | 101.43 | 105.80 |
| 36 | A5 | 947 | G | N3-C4-C5 | -10.90 | 123.15 | 128.60 |
| 36 | A5 | 776 | U | C5-C4-O4 | 10.88 | 132.43 | 125.90 |
| 36 | A5 | 931 | C | C2-N3-C4 | -10.88 | 114.46 | 119.90 |
| 36 | A5 | 1119 | C | N3-C4-C5 | 10.88 | 126.25 | 121.90 |
| 36 | A1 | 2198 | A | C8-N9-C4 | 10.88 | 110.15 | 105.80 |
| 36 | A1 | 645 | A | C2-N3-C4 | 10.87 | 116.04 | 110.60 |
| 36 | A5 | 1403 | C | C6-N1-C2 | 10.87 | 124.65 | 120.30 |
| 36 | A5 | 420 | G | C6-N1-C2 | -10.87 | 118.58 | 125.10 |
| 36 | A1 | 3375 | A | C8-N9-C4 | -10.86 | 101.45 | 105.80 |
| 36 | A5 | 41 | G | N1-C6-O6 | 10.86 | 126.42 | 119.90 |
| 36 | A5 | 41 | G | C5-C6-O6 | -10.86 | 122.09 | 128.60 |
| 36 | A1 | 2827 | U | C5-C4-O4 | 10.85 | 132.41 | 125.90 |
| 36 | A1 | 1929 | G | C8-N9-C4 | 10.85 | 110.74 | 106.40 |
| 36 | A5 | 2341 | A | C8-N9-C4 | 10.84 | 110.14 | 105.80 |
| 36 | A1 | 1409 | G | C5-C6-O6 | 10.81 | 135.09 | 128.60 |
| 36 | A1 | 644 | G | C8-N9-C4 | -10.81 | 102.08 | 106.40 |
| 36 | A5 | 2343 | C | N3-C4-C5 | 10.81 | 126.22 | 121.90 |
| 36 | A1 | 3092 | C | C6-N1-C2 | 10.80 | 124.62 | 120.30 |
| 36 | A1 | 1048 | A | N1-C2-N3 | -10.79 | 123.90 | 129.30 |
| 36 | A5 | 2726 | C | N3-C2-O2 | -10.79 | 114.35 | 121.90 |
| 1 | A2 | 144 | U | N3-C2-O2 | -10.79 | 114.65 | 122.20 |
| 36 | A5 | 2634 | U | C5-C6-N1 | -10.78 | 117.31 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 36 | A5 | 922 | U | C2-N1-C1' | -10.76 | 104.79 | 117.70 |
| 36 | A1 | 105 | C | C2-N3-C4 | -10.76 | 114.52 | 119.90 |
| 36 | A1 | 1403 | C | C2-N3-C4 | -10.75 | 114.52 | 119.90 |
| 36 | A5 | 2632 | G | N1-C6-O6 | -10.75 | 113.45 | 119.90 |
| 36 | A1 | 2726 | C | C5-C4-N4 | 10.74 | 127.72 | 120.20 |
| 36 | A1 | 2179 | C | N3-C4-C5 | 10.73 | 126.19 | 121.90 |
| 1 | A2 | 1560 | U | N3-C2-O2 | -10.71 | 114.70 | 122.20 |
| 1 | A2 | 1455 | G | C5-C6-N1 | -10.71 | 106.15 | 111.50 |
| 80 | A6 | 1595 | U | N3-C4-O4 | -10.70 | 111.91 | 119.40 |
| 36 | A5 | 1147 | G | C4-C5-N7 | -10.70 | 106.52 | 110.80 |
| 36 | A1 | 2142 | A | C6-N1-C2 | -10.69 | 112.19 | 118.60 |
| 36 | A5 | 2234 | G | C5-C6-O6 | -10.69 | 122.19 | 128.60 |
| 80 | A6 | 1634 | C | N1-C2-O2 | 10.69 | 125.31 | 118.90 |
| 36 | A1 | 929 | A | N1-C2-N3 | 10.69 | 134.64 | 129.30 |
| 36 | A5 | 2288 | G | C5-C6-N1 | 10.68 | 116.84 | 111.50 |
| 36 | A1 | 340 | C | N3-C4-N4 | -10.68 | 110.53 | 118.00 |
| 36 | A1 | 963 | G | N1-C6-O6 | 10.67 | 126.30 | 119.90 |
| 36 | A5 | 2899 | C | N1-C2-N3 | 10.66 | 126.66 | 119.20 |
| 36 | A5 | 2353 | G | N1-C6-O6 | 10.66 | 126.30 | 119.90 |
| 36 | A5 | 1434 | G | N7-C8-N9 | -10.66 | 107.77 | 113.10 |
| 36 | A1 | 1305 | U | N1-C2-O2 | 10.65 | 130.25 | 122.80 |
| 36 | A5 | 2290 | C | C5-C6-N1 | -10.64 | 115.68 | 121.00 |
| 36 | A1 | 2242 | A | N1-C2-N3 | 10.63 | 134.61 | 129.30 |
| 36 | A1 | 2298 | U | C2-N3-C4 | -10.61 | 120.64 | 127.00 |
| 36 | A5 | 2631 | U | C2-N3-C4 | -10.61 | 120.64 | 127.00 |
| 36 | A5 | 2905 | U | C5-C6-N1 | -10.60 | 117.40 | 122.70 |
| 38 | A4 | 113 | U | C5-C4-O4 | 10.59 | 132.26 | 125.90 |
| 1 | A2 | 553 | G | C5-C6-N1 | -10.57 | 106.21 | 111.50 |
| 38 | A4 | 113 | U | C5-C6-N1 | -10.57 | 117.42 | 122.70 |
| 36 | A5 | 957 | C | N3-C4-C5 | 10.57 | 126.13 | 121.90 |
| 36 | A5 | 2512 | C | C6-N1-C2 | -10.57 | 116.07 | 120.30 |
| 36 | A5 | 1592 | G | N1-C2-N2 | -10.54 | 106.71 | 116.20 |
| 36 | A1 | 1589 | A | C5-C6-N6 | -10.53 | 115.27 | 123.70 |
| 1 | A2 | 577 | G | C6-C5-N7 | -10.53 | 124.08 | 130.40 |
| 36 | A5 | 3122 | A | C8-N9-C4 | -10.53 | 101.59 | 105.80 |
| 36 | A1 | 821 | U | N3-C4-O4 | -10.53 | 112.03 | 119.40 |
| 36 | A1 | 2434 | U | N3-C4-O4 | -10.52 | 112.03 | 119.40 |
| 36 | A1 | 3046 | A | C8-N9-C4 | -10.52 | 101.59 | 105.80 |
| 36 | A5 | 546 | C | C2-N1-C1' | 10.50 | 130.35 | 118.80 |
| 36 | A5 | 2314 | U | C5-C4-O4 | -10.50 | 119.60 | 125.90 |
| 36 | A1 | 3181 | C | C6-N1-C2 | -10.50 | 116.10 | 120.30 |
| 36 | A5 | 1911 | A | C8-N9-C4 | 10.49 | 110.00 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 36 | A1 | 1389 | G | C5-C6-O6 | -10.49 | 122.31 | 128.60 |
| 36 | A1 | 340 | C | N3-C2-O2 | -10.48 | 114.56 | 121.90 |
| 36 | A5 | 1907 | C | C6-N1-C2 | -10.48 | 116.11 | 120.30 |
| 80 | A6 | 1539 | G | N3-C4-C5 | 10.48 | 133.84 | 128.60 |
| 36 | A5 | 2211 | U | C4-C5-C6 | 10.48 | 125.99 | 119.70 |
| 36 | A1 | 30 | G | N1-C6-O6 | -10.47 | 113.62 | 119.90 |
| 36 | A1 | 1492 | G | N3-C4-N9 | 10.47 | 132.28 | 126.00 |
| 36 | A1 | 2868 | U | C5-C6-N1 | -10.47 | 117.47 | 122.70 |
| 36 | A1 | 3344 | A | C5-N7-C8 | -10.46 | 98.67 | 103.90 |
| 36 | A1 | 1119 | C | C2-N3-C4 | -10.44 | 114.68 | 119.90 |
| 36 | A5 | 2314 | U | N3-C4-O4 | 10.44 | 126.71 | 119.40 |
| 36 | A1 | 2846 | U | N1-C2-N3 | 10.44 | 121.16 | 114.90 |
| 80 | A6 | 163 | G | N7-C8-N9 | 10.43 | 118.32 | 113.10 |
| 36 | A5 | 1848 | G | C5-C6-O6 | -10.43 | 122.34 | 128.60 |
| 36 | A1 | 3217 | C | N1-C2-O2 | 10.43 | 125.16 | 118.90 |
| 36 | A1 | 2392 | C | N3-C4-C5 | 10.42 | 126.07 | 121.90 |
| 80 | A6 | 337 | G | C4-C5-N7 | 10.42 | 114.97 | 110.80 |
| 36 | A1 | 1367 | G | N3-C2-N2 | 10.42 | 127.19 | 119.90 |
| 36 | A1 | 2279 | A | N9-C4-C5 | -10.41 | 101.64 | 105.80 |
| 36 | A5 | 3172 | A | C8-N9-C4 | 10.41 | 109.97 | 105.80 |
| 1 | A2 | 639 | U | N1-C2-O2 | 10.40 | 130.08 | 122.80 |
| 36 | A1 | 785 | G | C2-N3-C4 | 10.40 | 117.10 | 111.90 |
| 36 | A5 | 1301 | A | N1-C6-N6 | 10.40 | 124.84 | 118.60 |
| 1 | A2 | 1782 | A | C5-C6-N6 | 10.40 | 132.02 | 123.70 |
| 36 | A1 | 785 | G | N3-C4-C5 | -10.39 | 123.40 | 128.60 |
| 36 | A1 | 931 | C | C5-C6-N1 | -10.39 | 115.80 | 121.00 |
| 68 | De | 27 | ARG | NE-CZ-NH2 | -10.39 | 115.10 | 120.30 |
| 80 | A6 | 308 | C | C2-N1-C1' | -10.39 | 107.37 | 118.80 |
| 36 | A1 | 2983 | C | N3-C2-O2 | -10.38 | 114.64 | 121.90 |
| 80 | A6 | 1329 | A | N1-C6-N6 | 10.37 | 124.82 | 118.60 |
| 36 | A1 | 2392 | C | C2-N3-C4 | -10.36 | 114.72 | 119.90 |
| 36 | A5 | 965 | A | C2-N3-C4 | 10.36 | 115.78 | 110.60 |
| 36 | A5 | 2836 | C | C5-C6-N1 | -10.36 | 115.82 | 121.00 |
| 36 | A1 | 2899 | C | C2-N1-C1' | 10.35 | 130.18 | 118.80 |
| 36 | A5 | 930 | U | N3-C4-C5 | 10.33 | 120.80 | 114.60 |
| 36 | A5 | 2364 | G | N1-C6-O6 | -10.32 | 113.71 | 119.90 |
| 36 | A1 | 1433 | A | C5-C6-N1 | 10.32 | 122.86 | 117.70 |
| 36 | A5 | 2211 | U | C5-C4-O4 | 10.31 | 132.09 | 125.90 |
| 36 | A1 | 847 | A | N1-C6-N6 | 10.30 | 124.78 | 118.60 |
| 36 | A5 | 1797 | A | N7-C8-N9 | -10.30 | 108.65 | 113.80 |
| 36 | A1 | 2879 | C | N3-C4-C5 | -10.29 | 117.78 | 121.90 |
| 36 | A1 | 2361 | A | C8-N9-C4 | -10.29 | 101.68 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 36 | A1 | 1341 | U | C5-C4-O4 | 10.29 | 132.07 | 125.90 |
| 80 | A6 | 543 | C | N3-C2-O2 | -10.29 | 114.70 | 121.90 |
| 36 | A5 | 1303 | A | N1-C2-N3 | -10.29 | 124.16 | 129.30 |
| 36 | A1 | 2156 | C | C6-N1-C2 | 10.28 | 124.41 | 120.30 |
| 36 | A5 | 819 | U | C5-C6-N1 | -10.28 | 117.56 | 122.70 |
| 36 | A1 | 3242 | G | C5-C6-N1 | -10.28 | 106.36 | 111.50 |
| 36 | A5 | 1391 | C | N1-C2-O2 | -10.28 | 112.73 | 118.90 |
| 36 | A1 | 2836 | C | N1-C2-N3 | 10.27 | 126.39 | 119.20 |
| 36 | A5 | 1004 | U | N3-C4-O4 | -10.26 | 112.22 | 119.40 |
| 36 | A5 | 1429 | G | N3-C2-N2 | 10.26 | 127.08 | 119.90 |
| 36 | A5 | 1903 | U | N3-C4-O4 | 10.26 | 126.58 | 119.40 |
| 36 | A1 | 1164 | G | C5-C6-O6 | 10.24 | 134.74 | 128.60 |
| 36 | A5 | 2148 | U | N1-C2-O2 | -10.23 | 115.64 | 122.80 |
| 36 | A1 | 1164 | G | N1-C6-O6 | -10.23 | 113.76 | 119.90 |
| 38 | A8 | 8 | C | C6-N1-C2 | -10.22 | 116.21 | 120.30 |
| 36 | A1 | 2289 | U | N3-C2-O2 | -10.21 | 115.05 | 122.20 |
| 36 | A5 | 1513 | G | C8-N9-C4 | -10.21 | 102.32 | 106.40 |
| 36 | A1 | 979 | U | N1-C2-N3 | 10.20 | 121.02 | 114.90 |
| 36 | A1 | 2314 | U | C5-C4-O4 | -10.20 | 119.78 | 125.90 |
| 36 | A1 | 645 | A | C5-C6-N6 | -10.19 | 115.55 | 123.70 |
| 36 | A5 | 1297 | C | C2-N3-C4 | -10.19 | 114.80 | 119.90 |
| 36 | A5 | 847 | A | C8-N9-C4 | 10.19 | 109.88 | 105.80 |
| 36 | A1 | 2983 | C | C2-N3-C4 | -10.18 | 114.81 | 119.90 |
| 36 | A1 | 979 | U | N3-C2-O2 | -10.18 | 115.08 | 122.20 |
| 36 | A5 | 2257 | C | C6-N1-C2 | -10.18 | 116.23 | 120.30 |
| 36 | A1 | 1119 | C | N3-C4-C5 | 10.16 | 125.96 | 121.90 |
| 36 | A5 | 1056 | U | C6-N1-C2 | -10.14 | 114.91 | 121.00 |
| 36 | A1 | 2278 | C | N3-C4-N4 | -10.14 | 110.90 | 118.00 |
| 36 | A5 | 414 | U | C5-C6-N1 | -10.13 | 117.63 | 122.70 |
| 36 | A1 | 968 | G | C8-N9-C4 | -10.13 | 102.35 | 106.40 |
| 36 | A1 | 369 | A | C2-N3-C4 | 10.12 | 115.66 | 110.60 |
| 36 | A1 | 2369 | G | N3-C4-C5 | -10.12 | 123.54 | 128.60 |
| 36 | A5 | 2343 | C | C2-N3-C4 | -10.12 | 114.84 | 119.90 |
| 36 | A5 | 1481 | A | C8-N9-C4 | -10.12 | 101.75 | 105.80 |
| 36 | A5 | 3096 | C | C4-C5-C6 | 10.11 | 122.46 | 117.40 |
| 36 | A1 | 3143 | C | C6-N1-C2 | 10.10 | 124.34 | 120.30 |
| 36 | A1 | 3306 | U | C2-N3-C4 | -10.10 | 120.94 | 127.00 |
| 36 | A1 | 644 | G | C5-C6-N1 | -10.10 | 106.45 | 111.50 |
| 36 | A1 | 2279 | A | N1-C6-N6 | 10.10 | 124.66 | 118.60 |
| 36 | A5 | 652 | G | N1-C2-N2 | -10.09 | 107.12 | 116.20 |
| 36 | A1 | 2942 | C | N1-C2-O2 | -10.09 | 112.85 | 118.90 |
| 36 | A1 | 639 | G | N1-C6-O6 | 10.09 | 125.95 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 36 | A5 | 2632 | G | C5-C6-O6 | 10.06 | 134.64 | 128.60 |
| 68 | Be | 33 | ARG | NE-CZ-NH1 | 10.06 | 125.33 | 120.30 |
| 36 | A5 | 1124 | U | C4-C5-C6 | -10.06 | 113.66 | 119.70 |
| 36 | A1 | 1480 | G | C5-C6-O6 | -10.05 | 122.57 | 128.60 |
| 36 | A5 | 1208 | U | N3-C2-O2 | -10.05 | 115.16 | 122.20 |
| 80 | A6 | 1572 | G | C5-C6-O6 | -10.05 | 122.57 | 128.60 |
| 36 | A1 | 3344 | A | C8-N9-C4 | -10.04 | 101.78 | 105.80 |
| 80 | A6 | 314 | C | C6-N1-C2 | -10.04 | 116.28 | 120.30 |
| 36 | A5 | 877 | C | N3-C4-C5 | 10.04 | 125.92 | 121.90 |
| 36 | A5 | 1389 | G | N9-C4-C5 | -10.03 | 101.39 | 105.40 |
| 36 | A5 | 1440 | G | N1-C6-O6 | -10.03 | 113.88 | 119.90 |
| 1 | A2 | 1486 | G | C5-N7-C8 | -10.03 | 99.29 | 104.30 |
| 36 | A1 | 2719 | U | C5-C6-N1 | -10.02 | 117.69 | 122.70 |
| 36 | A5 | 3006 | A | C2-N3-C4 | -10.02 | 105.59 | 110.60 |
| 36 | A1 | 1902 | G | N9-C4-C5 | -10.02 | 101.39 | 105.40 |
| 36 | A1 | 2870 | C | C6-N1-C1' | 10.01 | 132.81 | 120.80 |
| 36 | A1 | 1119 | C | C5-C6-N1 | -10.00 | 116.00 | 121.00 |
| 38 | A8 | 25 | G | N1-C6-O6 | -10.00 | 113.90 | 119.90 |
| 36 | A1 | 966 | U | N3-C2-O2 | -9.99 | 115.21 | 122.20 |
| 36 | A5 | 340 | C | C2-N3-C4 | -9.98 | 114.91 | 119.90 |
| 36 | A5 | 1308 | A | C8-N9-C4 | -9.98 | 101.81 | 105.80 |
| 1 | A2 | 507 | U | N3-C2-O2 | -9.97 | 115.22 | 122.20 |
| 36 | A1 | 2292 | U | C2-N3-C4 | -9.97 | 121.02 | 127.00 |
| 38 | A8 | 32 | C | N1-C2-O2 | -9.97 | 112.92 | 118.90 |
| 36 | A1 | 2292 | U | C5-C4-O4 | -9.96 | 119.93 | 125.90 |
| 36 | A1 | 2827 | U | C4-C5-C6 | 9.96 | 125.67 | 119.70 |
| 36 | A1 | 1137 | C | C2-N3-C4 | -9.94 | 114.93 | 119.90 |
| 36 | A1 | 2572 | C | N1-C2-O2 | 9.94 | 124.87 | 118.90 |
| 36 | A5 | 339 | C | N3-C4-N4 | -9.94 | 111.04 | 118.00 |
| 36 | A5 | 3362 | A | C2-N3-C4 | -9.94 | 105.63 | 110.60 |
| 36 | A5 | 2905 | U | C2-N3-C4 | -9.94 | 121.03 | 127.00 |
| 36 | A1 | 958 | C | N3-C4-N4 | -9.93 | 111.05 | 118.00 |
| 80 | A6 | 553 | G | C4-C5-C6 | 9.93 | 124.76 | 118.80 |
| 36 | A1 | 2138 | A | C8-N9-C4 | -9.92 | 101.83 | 105.80 |
| 36 | A1 | 2356 | A | C5-N7-C8 | -9.92 | 98.94 | 103.90 |
| 36 | A1 | 808 | A | N1-C6-N6 | -9.91 | 112.65 | 118.60 |
| 36 | A5 | 2824 | G | N3-C2-N2 | -9.91 | 112.96 | 119.90 |
| 36 | A5 | 2366 | C | C5-C6-N1 | 9.91 | 125.95 | 121.00 |
| 36 | A1 | 743 | C | C6-N1-C2 | 9.91 | 124.26 | 120.30 |
| 36 | A5 | 2952 | G | C5-C6-O6 | -9.91 | 122.66 | 128.60 |
| 36 | A5 | 420 | G | C5-C6-O6 | -9.90 | 122.66 | 128.60 |
| 1 | A2 | 542 | A | N7-C8-N9 | 9.90 | 118.75 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 36 | A1 | 2617 | U | N3-C2-O2 | -9.90 | 115.27 | 122.20 |
| 1 | A2 | 1096 | C | C2-N1-C1' | 9.89 | 129.68 | 118.80 |
| 36 | A1 | 2306 | C | N1-C2-O2 | 9.89 | 124.83 | 118.90 |
| 36 | A1 | 498 | A | N1-C6-N6 | -9.89 | 112.67 | 118.60 |
| 36 | A1 | 2611 | U | C5-C6-N1 | -9.89 | 117.76 | 122.70 |
| 36 | A5 | 1484 | U | C5-C6-N1 | -9.89 | 117.75 | 122.70 |
| 36 | A1 | 1489 | A | N1-C6-N6 | 9.88 | 124.53 | 118.60 |
| 1 | A2 | 1745 | G | C5-C6-O6 | -9.88 | 122.67 | 128.60 |
| 36 | A1 | 960 | U | C6-N1-C2 | 9.87 | 126.92 | 121.00 |
| 80 | A6 | 1634 | C | C2-N1-C1' | 9.87 | 129.66 | 118.80 |
| 36 | A5 | 2808 | A | C8-N9-C4 | 9.86 | 109.75 | 105.80 |
| 80 | A6 | 448 | C | C6-N1-C2 | -9.86 | 116.36 | 120.30 |
| 36 | A5 | 2118 | C | N3-C2-O2 | -9.86 | 115.00 | 121.90 |
| 36 | A1 | 1492 | G | N1-C6-O6 | -9.84 | 113.99 | 119.90 |
| 1 | A2 | 1456 | C | N3-C4-N4 | -9.84 | 111.11 | 118.00 |
| 36 | A1 | 2353 | G | N1-C6-O6 | 9.83 | 125.80 | 119.90 |
| 1 | A2 | 553 | G | C5-C6-O6 | -9.82 | 122.71 | 128.60 |
| 1 | A2 | 1198 | G | C8-N9-C4 | -9.82 | 102.47 | 106.40 |
| 36 | A1 | 2176 | U | N3-C2-O2 | -9.82 | 115.33 | 122.20 |
| 36 | A5 | 1152 | G | N7-C8-N9 | 9.82 | 118.01 | 113.10 |
| 36 | A5 | 1392 | G | C8-N9-C4 | 9.81 | 110.33 | 106.40 |
| 36 | A1 | 2846 | U | N3-C4-O4 | -9.81 | 112.53 | 119.40 |
| 52 | DO | 182[B] | SER | O-C-N | -9.81 | 107.01 | 122.70 |
| 36 | A5 | 1655 | G | N7-C8-N9 | 9.80 | 118.00 | 113.10 |
| 36 | A5 | 1655 | G | C8-N9-C4 | -9.80 | 102.48 | 106.40 |
| 36 | A1 | 1475 | A | C2-N3-C4 | 9.79 | 115.50 | 110.60 |
| 36 | A1 | 940 | G | N1-C6-O6 | -9.79 | 114.03 | 119.90 |
| 36 | A1 | 406 | G | O4'-C1'-N9 | 9.78 | 116.02 | 108.20 |
| 36 | A1 | 50 | U | N1-C2-N3 | 9.78 | 120.77 | 114.90 |
| 36 | A5 | 835 | G | C5-C6-O6 | -9.78 | 122.73 | 128.60 |
| 36 | A1 | 938 | C | C2-N3-C4 | -9.77 | 115.01 | 119.90 |
| 36 | A1 | 2609 | A | N1-C6-N6 | -9.76 | 112.74 | 118.60 |
| 36 | A5 | 2917 | G | C5-C6-O6 | -9.76 | 122.75 | 128.60 |
| 36 | A1 | 2165 | G | C5-C6-O6 | -9.75 | 122.75 | 128.60 |
| 36 | A5 | 947 | G | C5-C6-N1 | 9.75 | 116.38 | 111.50 |
| 36 | A5 | 2134 | G | N1-C6-O6 | -9.75 | 114.05 | 119.90 |
| 36 | A5 | 1064 | A | N1-C6-N6 | 9.75 | 124.45 | 118.60 |
| 36 | A1 | 867 | G | N3-C2-N2 | -9.75 | 113.08 | 119.90 |
| 36 | A5 | 2246 | G | N9-C4-C5 | 9.75 | 109.30 | 105.40 |
| 36 | A1 | 1216 | C | C5-C6-N1 | 9.75 | 125.87 | 121.00 |
| 36 | A5 | 815 | G | N1-C6-O6 | -9.75 | 114.05 | 119.90 |
| 36 | A1 | 3362 | A | C4-C5-N7 | 9.75 | 115.57 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 38 | A4 | 113 | U | N3-C2-O2 | -9.74 | 115.38 | 122.20 |
| 36 | A5 | 1147 | G | C5-N7-C8 | 9.74 | 109.17 | 104.30 |
| 36 | A5 | 3096 | C | C2-N3-C4 | -9.73 | 115.03 | 119.90 |
| 36 | A5 | 1448 | U | C5-C6-N1 | -9.73 | 117.83 | 122.70 |
| 36 | A5 | 2361 | A | N3-C4-C5 | -9.73 | 119.99 | 126.80 |
| 36 | A1 | 350 | C | C6-N1-C2 | -9.73 | 116.41 | 120.30 |
| 80 | A6 | 609 | U | C4-C5-C6 | 9.73 | 125.54 | 119.70 |
| 36 | A5 | 2948 | C | N3-C4-N4 | -9.73 | 111.19 | 118.00 |
| 36 | A5 | 1057 | A | N1-C6-N6 | 9.72 | 124.43 | 118.60 |
| 36 | A1 | 645 | A | N3-C4-C5 | -9.71 | 120.00 | 126.80 |
| 36 | A5 | 645 | A | C6-N1-C2 | -9.71 | 112.77 | 118.60 |
| 36 | A1 | 2679 | A | N1-C6-N6 | 9.71 | 124.43 | 118.60 |
| 36 | A1 | 716 | A | N1-C6-N6 | 9.70 | 124.42 | 118.60 |
| 36 | A1 | 2993 | G | N3-C4-C5 | 9.70 | 133.45 | 128.60 |
| 36 | A1 | 635 | G | C5-C6-O6 | -9.69 | 122.78 | 128.60 |
| 36 | A5 | 2278 | C | C6-N1-C2 | -9.69 | 116.42 | 120.30 |
| 1 | A2 | 553 | G | C6-C5-N7 | -9.69 | 124.59 | 130.40 |
| 36 | A1 | 2350 | C | C2-N3-C4 | -9.68 | 115.06 | 119.90 |
| 36 | A1 | 30 | G | C5-C6-O6 | 9.68 | 134.41 | 128.60 |
| 80 | A6 | 163 | G | C8-N9-C4 | -9.68 | 102.53 | 106.40 |
| 38 | A4 | 81 | U | N3-C2-O2 | -9.67 | 115.43 | 122.20 |
| 36 | A5 | 591 | G | N1-C6-O6 | 9.67 | 125.70 | 119.90 |
| 36 | A5 | 2211 | U | N1-C2-N3 | 9.67 | 120.70 | 114.90 |
| 80 | A6 | 1749 | A | N1-C6-N6 | 9.67 | 124.40 | 118.60 |
| 36 | A1 | 2283 | G | N1-C6-O6 | 9.67 | 125.70 | 119.90 |
| 80 | A6 | 1027 | A | N7-C8-N9 | 9.67 | 118.63 | 113.80 |
| 36 | A5 | 2391 | G | C8-N9-C4 | -9.66 | 102.54 | 106.40 |
| 36 | A5 | 1888 | U | C5-C6-N1 | -9.65 | 117.88 | 122.70 |
| 36 | A5 | 1327 | C | N3-C4-N4 | -9.64 | 111.25 | 118.00 |
| 36 | A1 | 2142 | A | N3-C4-C5 | -9.64 | 120.05 | 126.80 |
| 36 | A1 | 331 | G | N1-C6-O6 | -9.64 | 114.12 | 119.90 |
| 36 | A1 | 2343 | C | N3-C4-C5 | 9.63 | 125.75 | 121.90 |
| 36 | A1 | 2817 | A | C5-C6-N1 | 9.63 | 122.52 | 117.70 |
| 80 | A6 | 99 | C | C2-N3-C4 | -9.63 | 115.08 | 119.90 |
| 36 | A5 | 2757 | U | N1-C2-N3 | 9.63 | 120.68 | 114.90 |
| 36 | A5 | 3060 | C | N3-C4-N4 | 9.63 | 124.74 | 118.00 |
| 36 | A5 | 776 | U | C2-N3-C4 | -9.63 | 121.22 | 127.00 |
| 1 | A2 | 1782 | A | N1-C6-N6 | -9.63 | 112.83 | 118.60 |
| 36 | A5 | 1152 | G | C8-N9-C4 | -9.63 | 102.55 | 106.40 |
| 1 | A2 | 1280 | C | N3-C4-N4 | 9.62 | 124.73 | 118.00 |
| 36 | A5 | 1042 | U | N3-C4-O4 | -9.62 | 112.67 | 119.40 |
| 37 | A7 | 49 | G | N1-C6-O6 | 9.62 | 125.67 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 3181 | C | N1-C2-N3 | 9.61 | 125.93 | 119.20 |
| 36 | A5 | 518 | G | C5-C6-O6 | -9.61 | 122.83 | 128.60 |
| 36 | A1 | 2572 | C | N3-C2-O2 | -9.61 | 115.17 | 121.90 |
| 36 | A1 | 1114 | U | C6-N1-C2 | 9.60 | 126.76 | 121.00 |
| 40 | DB | 10 | ARG | NE-CZ-NH2 | -9.60 | 115.50 | 120.30 |
| 36 | A1 | 1122 | U | C2-N3-C4 | -9.59 | 121.24 | 127.00 |
| 36 | A1 | 1480 | G | N1-C6-O6 | 9.58 | 125.65 | 119.90 |
| 36 | A1 | 3242 | G | C6-C5-N7 | 9.58 | 136.15 | 130.40 |
| 36 | A1 | 1405 | U | N3-C4-C5 | 9.58 | 120.35 | 114.60 |
| 36 | A1 | 952 | A | C5-C6-N6 | -9.58 | 116.04 | 123.70 |
| 38 | A4 | 140 | G | C8-N9-C4 | -9.58 | 102.57 | 106.40 |
| 36 | A5 | 2424 | A | N1-C6-N6 | 9.58 | 124.35 | 118.60 |
| 36 | A5 | 340 | C | C5-C6-N1 | -9.57 | 116.21 | 121.00 |
| 46 | BH | 91 | ARG | NE-CZ-NH2 | 9.57 | 125.09 | 120.30 |
| 36 | A5 | 1127 | G | C5-C6-O6 | -9.57 | 122.86 | 128.60 |
| 36 | A1 | 2356 | A | C4-C5-N7 | 9.57 | 115.48 | 110.70 |
| 36 | A1 | 2944 | U | N3-C4-C5 | 9.57 | 120.34 | 114.60 |
| 37 | A3 | 81 | U | N3-C4-C5 | 9.57 | 120.34 | 114.60 |
| 36 | A1 | 2633 | U | N1-C2-O2 | 9.56 | 129.49 | 122.80 |
| 36 | A5 | 2899 | C | C5-C4-N4 | 9.56 | 126.89 | 120.20 |
| 80 | A6 | 1514 | U | N3-C4-O4 | -9.55 | 112.72 | 119.40 |
| 36 | A5 | 2572 | C | N1-C2-O2 | 9.55 | 124.63 | 118.90 |
| 1 | A2 | 1486 | G | N7-C8-N9 | 9.54 | 117.87 | 113.10 |
| 36 | A1 | 2550 | U | C5-C4-O4 | 9.54 | 131.62 | 125.90 |
| 36 | A1 | 631 | U | N1-C2-N3 | 9.54 | 120.62 | 114.90 |
| 36 | A5 | 1056 | U | N1-C2-N3 | 9.53 | 120.62 | 114.90 |
| 36 | A1 | 2595 | A | C5-N7-C8 | -9.53 | 99.14 | 103.90 |
| 36 | A5 | 905 | U | C5-C4-O4 | -9.53 | 120.18 | 125.90 |
| 36 | A1 | 1339 | C | C2-N3-C4 | -9.52 | 115.14 | 119.90 |
| 36 | A1 | 895 | A | C2-N3-C4 | -9.52 | 105.84 | 110.60 |
| 80 | A6 | 1614 | A | C5-N7-C8 | -9.52 | 99.14 | 103.90 |
| 36 | A5 | 1403 | C | C5-C4-N4 | -9.52 | 113.54 | 120.20 |
| 36 | A5 | 1848 | G | N1-C6-O6 | 9.51 | 125.61 | 119.90 |
| 36 | A1 | 3083 | G | N3-C4-C5 | -9.51 | 123.85 | 128.60 |
| 80 | A6 | 1537 | C | C5-C6-N1 | 9.50 | 125.75 | 121.00 |
| 36 | A1 | 2860 | U | N3-C2-O2 | 9.49 | 128.84 | 122.20 |
| 80 | A6 | 639 | U | N1-C2-O2 | 9.49 | 129.45 | 122.80 |
| 36 | A1 | 3214 | U | C5-C4-O4 | 9.49 | 131.59 | 125.90 |
| 36 | A5 | 1902 | G | C5-C6-O6 | -9.49 | 122.91 | 128.60 |
| 36 | A1 | 637 | C | C2-N1-C1' | -9.48 | 108.37 | 118.80 |
| 36 | A1 | 637 | C | C6-N1-C1' | 9.48 | 132.18 | 120.80 |
| 1 | A2 | 1456 | C | C5-C4-N4 | 9.48 | 126.83 | 120.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 2156 | C | N3-C4-C5 | 9.48 | 125.69 | 121.90 |
| 36 | A5 | 546 | C | N1-C2-O2 | 9.47 | 124.58 | 118.90 |
| 36 | A5 | 1239 | C | C5-C6-N1 | 9.47 | 125.73 | 121.00 |
| 80 | A6 | 553 | G | N3-C2-N2 | -9.46 | 113.28 | 119.90 |
| 36 | A5 | 947 | G | C2-N3-C4 | 9.46 | 116.63 | 111.90 |
| 36 | A1 | 3217 | C | N3-C2-O2 | -9.46 | 115.28 | 121.90 |
| 38 | A4 | 73 | U | N3-C4-C5 | 9.46 | 120.27 | 114.60 |
| 36 | A5 | 1888 | U | C4-C5-C6 | 9.45 | 125.37 | 119.70 |
| 38 | A8 | 113 | U | C5-C6-N1 | 9.45 | 127.42 | 122.70 |
| 36 | A5 | 2705 | A | C5-C6-N1 | 9.45 | 122.42 | 117.70 |
| 80 | A6 | 1481 | C | C6-N1-C2 | -9.45 | 116.52 | 120.30 |
| 80 | A6 | 1560 | U | C5-C4-O4 | 9.44 | 131.57 | 125.90 |
| 36 | A1 | 1117 | G | C8-N9-C4 | 9.44 | 110.18 | 106.40 |
| 36 | A5 | 2202 | C | C5-C4-N4 | -9.44 | 113.59 | 120.20 |
| 36 | A1 | 3344 | A | N1-C6-N6 | 9.44 | 124.26 | 118.60 |
| 1 | A2 | 139 | C | C6-N1-C2 | -9.44 | 116.53 | 120.30 |
| 36 | A1 | 3344 | A | C2-N3-C4 | -9.43 | 105.88 | 110.60 |
| 36 | A5 | 282 | G | C8-N9-C4 | -9.43 | 102.63 | 106.40 |
| 36 | A5 | 3362 | A | N7-C8-N9 | 9.43 | 118.51 | 113.80 |
| 36 | A1 | 80 | G | C6-N1-C2 | -9.42 | 119.45 | 125.10 |
| 36 | A5 | 644 | G | C2-N3-C4 | 9.42 | 116.61 | 111.90 |
| 36 | A5 | 386 | A | N1-C6-N6 | 9.42 | 124.25 | 118.60 |
| 36 | A5 | 708 | G | C4-C5-N7 | 9.42 | 114.57 | 110.80 |
| 36 | A5 | 40 | A | N1-C2-N3 | 9.42 | 134.01 | 129.30 |
| 36 | A5 | 1210 | U | C5-C4-O4 | 9.42 | 131.55 | 125.90 |
| 36 | A5 | 966 | U | N1-C2-O2 | 9.42 | 129.39 | 122.80 |
| 36 | A5 | 2899 | C | C6-N1-C2 | -9.41 | 116.54 | 120.30 |
| 1 | A2 | 453 | U | N3-C2-O2 | -9.40 | 115.62 | 122.20 |
| 36 | A1 | 2726 | C | N3-C4-N4 | -9.40 | 111.42 | 118.00 |
| 36 | A5 | 2364 | G | N9-C4-C5 | 9.40 | 109.16 | 105.40 |
| 36 | A5 | 3376 | A | C8-N9-C4 | -9.39 | 102.04 | 105.80 |
| 1 | A2 | 1282 | U | N3-C2-O2 | -9.39 | 115.63 | 122.20 |
| 36 | A1 | 1169 | A | C4-C5-C6 | 9.38 | 121.69 | 117.00 |
| 36 | A5 | 1449 | A | C2-N3-C4 | -9.38 | 105.91 | 110.60 |
| 36 | A5 | 1858 | A | C8-N9-C4 | -9.38 | 102.05 | 105.80 |
| 36 | A1 | 1173 | U | C5-C6-N1 | -9.37 | 118.01 | 122.70 |
| 80 | A6 | 1280 | C | C6-N1-C2 | -9.38 | 116.55 | 120.30 |
| 1 | A2 | 1654 | G | C5-C6-N1 | 9.37 | 116.19 | 111.50 |
| 36 | A1 | 112 | U | C2-N1-C1' | 9.37 | 128.94 | 117.70 |
| 36 | A1 | 970 | A | C5-N7-C8 | -9.37 | 99.22 | 103.90 |
| 36 | A5 | 811 | U | C5-C6-N1 | -9.37 | 118.02 | 122.70 |
| 36 | A1 | 295 | A | N7-C8-N9 | 9.36 | 118.48 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 1480 | G | N9-C4-C5 | -9.36 | 101.66 | 105.40 |
| 36 | A5 | 2978 | U | N3-C2-O2 | -9.36 | 115.65 | 122.20 |
| 1 | A2 | 1258 | U | N3-C2-O2 | -9.35 | 115.66 | 122.20 |
| 36 | A1 | 1857 | C | N1-C2-O2 | -9.34 | 113.29 | 118.90 |
| 36 | A5 | 3218 | A | C5-N7-C8 | -9.34 | 99.23 | 103.90 |
| 36 | A1 | 2389 | C | C5-C6-N1 | -9.34 | 116.33 | 121.00 |
| 1 | A2 | 1169 | G | C8-N9-C4 | -9.33 | 102.67 | 106.40 |
| 36 | A1 | 24 | G | C5-C6-O6 | -9.33 | 123.00 | 128.60 |
| 36 | A1 | 2827 | U | N3-C4-O4 | -9.33 | 112.87 | 119.40 |
| 68 | Be | 33 | ARG | NE-CZ-NH2 | -9.33 | 115.64 | 120.30 |
| 36 | A5 | 1437 | C | C6-N1-C2 | -9.33 | 116.57 | 120.30 |
| 36 | A5 | 21 | G | C2-N3-C4 | -9.33 | 107.24 | 111.90 |
| 36 | A1 | 2621 | G | N3-C2-N2 | -9.32 | 113.37 | 119.90 |
| 80 | A6 | 415 | C | C6-N1-C2 | 9.32 | 124.03 | 120.30 |
| 36 | A5 | 2340 | U | N3-C4-C5 | 9.32 | 120.19 | 114.60 |
| 36 | A5 | 2830 | G | N9-C4-C5 | 9.31 | 109.12 | 105.40 |
| 36 | A1 | 2719 | U | N1-C2-O2 | -9.31 | 116.28 | 122.80 |
| 36 | A1 | 641 | C | N3-C4-C5 | 9.30 | 125.62 | 121.90 |
| 80 | A6 | 1596 | C | C5-C4-N4 | 9.30 | 126.71 | 120.20 |
| 36 | A5 | 721 | G | N1-C6-O6 | -9.30 | 114.32 | 119.90 |
| 36 | A1 | 2823 | G | C5-C6-O6 | 9.29 | 134.18 | 128.60 |
| 36 | A1 | 3057 | U | C5-C4-O4 | 9.29 | 131.47 | 125.90 |
| 36 | A5 | 1447 | G | C8-N9-C4 | -9.29 | 102.68 | 106.40 |
| 36 | A1 | 1295 | G | N1-C6-O6 | -9.29 | 114.33 | 119.90 |
| 36 | A1 | 718 | G | N3-C4-C5 | 9.28 | 133.24 | 128.60 |
| 80 | A6 | 687 | G | N3-C4-N9 | -9.28 | 120.43 | 126.00 |
| 36 | A5 | 1151 | U | N3-C4-O4 | -9.29 | 112.90 | 119.40 |
| 36 | A1 | 2772 | C | C6-N1-C1' | -9.28 | 109.67 | 120.80 |
| 36 | A1 | 2174 | G | C8-N9-C4 | -9.28 | 102.69 | 106.40 |
| 36 | A5 | 1879 | A | N1-C6-N6 | 9.27 | 124.16 | 118.60 |
| 36 | A5 | 3050 | U | N3-C2-O2 | -9.27 | 115.71 | 122.20 |
| 36 | A1 | 2634 | U | N1-C2-N3 | 9.27 | 120.46 | 114.90 |
| 36 | A5 | 3186 | A | C8-N9-C4 | -9.26 | 102.10 | 105.80 |
| 36 | A5 | 994 | G | C5-C6-N1 | 9.26 | 116.13 | 111.50 |
| 36 | A5 | 1064 | A | N9-C4-C5 | -9.26 | 102.10 | 105.80 |
| 36 | A1 | 410 | U | N1-C2-O2 | -9.25 | 116.32 | 122.80 |
| 36 | A1 | 2320 | A | C2-N3-C4 | -9.25 | 105.97 | 110.60 |
| 36 | A5 | 1849 | C | N1-C2-O2 | 9.25 | 124.45 | 118.90 |
| 36 | A1 | 2302 | G | C5-C6-O6 | 9.24 | 134.15 | 128.60 |
| 36 | A1 | 2763 | U | N1-C2-O2 | -9.24 | 116.33 | 122.80 |
| 36 | A1 | 2302 | G | N1-C6-O6 | -9.23 | 114.36 | 119.90 |
| 36 | A1 | 3057 | U | N3-C2-O2 | -9.23 | 115.74 | 122.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 80 | A6 | 1600 | A | C5-N7-C8 | -9.23 | 99.28 | 103.90 |
| 36 | A1 | 2222 | A | C8-N9-C4 | -9.23 | 102.11 | 105.80 |
| 36 | A5 | 3060 | C | C5-C4-N4 | -9.23 | 113.74 | 120.20 |
| 38 | A8 | 80 | A | C8-N9-C4 | -9.23 | 102.11 | 105.80 |
| 36 | A1 | 645 | A | N3-C4-N9 | 9.23 | 134.78 | 127.40 |
| 36 | A1 | 2393 | G | C8-N9-C4 | 9.23 | 110.09 | 106.40 |
| 36 | A5 | 1449 | A | N1-C6-N6 | 9.23 | 124.14 | 118.60 |
| 36 | A5 | 3309 | G | N3-C4-C5 | -9.23 | 123.99 | 128.60 |
| 36 | A5 | 1371 | G | C5-C6-N1 | 9.22 | 116.11 | 111.50 |
| 36 | A5 | 3214 | U | N3-C4-O4 | -9.22 | 112.95 | 119.40 |
| 36 | A5 | 2246 | G | C4-C5-N7 | -9.22 | 107.11 | 110.80 |
| 36 | A5 | 1156 | C | N3-C4-C5 | 9.22 | 125.59 | 121.90 |
| 36 | A1 | 2378 | C | N3-C4-C5 | -9.20 | 118.22 | 121.90 |
| 36 | A1 | 3242 | G | C2-N3-C4 | -9.20 | 107.30 | 111.90 |
| 36 | A5 | 968 | G | N3-C2-N2 | 9.20 | 126.34 | 119.90 |
| 36 | A5 | 3377 | G | C4-C5-N7 | 9.20 | 114.48 | 110.80 |
| 36 | A1 | 931 | C | N3-C4-N4 | -9.20 | 111.56 | 118.00 |
| 36 | A1 | 2283 | G | N3-C2-N2 | -9.20 | 113.46 | 119.90 |
| 36 | A5 | 3245 | A | C8-N9-C4 | -9.20 | 102.12 | 105.80 |
| 36 | A1 | 3181 | C | N3-C2-O2 | -9.19 | 115.46 | 121.90 |
| 36 | A1 | 154 | U | C5-C6-N1 | -9.19 | 118.10 | 122.70 |
| 36 | A1 | 1480 | G | C8-N9-C4 | 9.19 | 110.08 | 106.40 |
| 36 | A5 | 2550 | U | C5-C4-O4 | 9.19 | 131.41 | 125.90 |
| 36 | A1 | 3181 | C | C5-C4-N4 | 9.18 | 126.63 | 120.20 |
| 36 | A5 | 1101 | G | N3-C2-N2 | 9.17 | 126.32 | 119.90 |
| 40 | DB | 2 | SER | N-CA-C | -9.17 | 86.24 | 111.00 |
| 36 | A1 | 2247 | G | N1-C6-O6 | 9.17 | 125.40 | 119.90 |
| 36 | A5 | 1050 | U | N3-C2-O2 | -9.17 | 115.78 | 122.20 |
| 36 | A5 | 3266 | G | C5-C6-O6 | 9.17 | 134.10 | 128.60 |
| 36 | A5 | 2693 | C | N3-C2-O2 | -9.17 | 115.48 | 121.90 |
| 36 | A1 | 857 | G | C5-C6-N1 | 9.17 | 116.08 | 111.50 |
| 36 | A1 | 3377 | G | C5-C6-N1 | 9.16 | 116.08 | 111.50 |
| 80 | A6 | 1105 | C | N3-C2-O2 | -9.15 | 115.49 | 121.90 |
| 36 | A1 | 2280 | A | C8-N9-C4 | 9.15 | 109.46 | 105.80 |
| 80 | A6 | 163 | G | N1-C6-O6 | 9.15 | 125.39 | 119.90 |
| 36 | A1 | 2356 | A | N9-C4-C5 | -9.14 | 102.14 | 105.80 |
| 36 | A1 | 3057 | U | N3-C4-O4 | -9.14 | 113.00 | 119.40 |
| 36 | A1 | 3278 | C | N1-C2-O2 | 9.14 | 124.39 | 118.90 |
| 36 | A1 | 1514 | G | N1-C6-O6 | -9.14 | 114.42 | 119.90 |
| 36 | A5 | 2142 | A | C6-N1-C2 | -9.14 | 113.12 | 118.60 |
| 36 | A5 | 2354 | C | N1-C2-O2 | -9.14 | 113.42 | 118.90 |
| 36 | A1 | 939 | U | N1-C2-O2 | -9.14 | 116.41 | 122.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | A2 | 558 | U | N3-C2-O2 | -9.13 | 115.81 | 122.20 |
| 36 | A5 | 1911 | A | N9-C4-C5 | -9.13 | 102.15 | 105.80 |
| 36 | A5 | 2365 | C | N3-C4-N4 | -9.12 | 111.61 | 118.00 |
| 36 | A5 | 3308 | C | C4-C5-C6 | 9.12 | 121.96 | 117.40 |
| 36 | A5 | 834 | U | N3-C4-C5 | 9.12 | 120.07 | 114.60 |
| 36 | A5 | 3362 | A | C5-N7-C8 | -9.11 | 99.34 | 103.90 |
| 36 | A5 | 2942 | C | N3-C4-N4 | 9.11 | 124.38 | 118.00 |
| 40 | DB | 4 | ARG | NE-CZ-NH1 | 9.11 | 124.85 | 120.30 |
| 36 | A1 | 959 | C | C6-N1-C2 | 9.10 | 123.94 | 120.30 |
| 36 | A5 | 2176 | U | N3-C2-O2 | -9.10 | 115.83 | 122.20 |
| 1 | A2 | 142 | G | N3-C2-N2 | -9.09 | 113.53 | 119.90 |
| 1 | A2 | 402 | C | C6-N1-C2 | 9.09 | 123.94 | 120.30 |
| 36 | A1 | 907 | G | N3-C4-C5 | -9.09 | 124.05 | 128.60 |
| 36 | A1 | 88 | A | N1-C6-N6 | 9.09 | 124.06 | 118.60 |
| 36 | A1 | 3181 | C | N3-C4-N4 | -9.09 | 111.64 | 118.00 |
| 80 | A6 | 1456 | C | C5-C4-N4 | 9.09 | 126.56 | 120.20 |
| 36 | A1 | 591 | G | N1-C6-O6 | 9.08 | 125.35 | 119.90 |
| 36 | A5 | 1843 | C | C6-N1-C2 | -9.08 | 116.67 | 120.30 |
| 52 | BO | 158[B] | ASP | O-C-N | 9.08 | 137.22 | 122.70 |
| 1 | A2 | 1596 | C | N3-C2-O2 | -9.07 | 115.55 | 121.90 |
| 36 | A1 | 1902 | G | N3-C4-N9 | 9.07 | 131.44 | 126.00 |
| 36 | A5 | 1133 | A | C2-N3-C4 | 9.07 | 115.14 | 110.60 |
| 36 | A1 | 641 | C | C2-N1-C1' | -9.07 | 108.82 | 118.80 |
| 36 | A1 | 818 | C | C6-N1-C2 | -9.06 | 116.67 | 120.30 |
| 36 | A1 | 644 | G | N1-C2-N2 | -9.06 | 108.05 | 116.20 |
| 36 | A5 | 2744 | U | N1-C2-O2 | 9.05 | 129.14 | 122.80 |
| 36 | A1 | 1341 | U | N3-C2-O2 | -9.05 | 115.86 | 122.20 |
| 36 | A1 | 1405 | U | C2-N3-C4 | -9.05 | 121.57 | 127.00 |
| 36 | A5 | 1911 | A | N1-C6-N6 | 9.05 | 124.03 | 118.60 |
| 36 | A1 | 2851 | A | C8-N9-C4 | 9.05 | 109.42 | 105.80 |
| 54 | DQ | 66 | ARG | NE-CZ-NH2 | -9.04 | 115.78 | 120.30 |
| 36 | A5 | 1450 | G | C8-N9-C4 | 9.03 | 110.01 | 106.40 |
| 37 | A3 | 81 | U | C6-N1-C2 | 9.03 | 126.42 | 121.00 |
| 36 | A1 | 2814 | G | C8-N9-C4 | 9.03 | 110.01 | 106.40 |
| 36 | A5 | 1181 | U | C5-C6-N1 | -9.02 | 118.19 | 122.70 |
| 36 | A1 | 2884 | C | N3-C4-C5 | 9.01 | 125.50 | 121.90 |
| 36 | A1 | 2299 | A | C4-C5-C6 | 9.01 | 121.50 | 117.00 |
| 36 | A1 | 655 | C | C5-C6-N1 | -9.00 | 116.50 | 121.00 |
| 36 | A5 | 369 | A | C8-N9-C4 | -9.00 | 102.20 | 105.80 |
| 80 | A6 | 352 | A | C8-N9-C4 | 9.00 | 109.40 | 105.80 |
| 36 | A5 | 1317 | A | C5-C6-N6 | -9.00 | 116.50 | 123.70 |
| 36 | A1 | 1592 | G | N9-C4-C5 | -9.00 | 101.80 | 105.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 38 | A4 | 20 | U | N3-C4-O4 | -8.99 | 113.10 | 119.40 |
| 36 | A1 | 2434 | U | C5-C6-N1 | -8.99 | 118.20 | 122.70 |
| 36 | A5 | 2830 | G | N1-C2-N3 | 8.99 | 129.30 | 123.90 |
| 36 | A1 | 1510 | G | N3-C2-N2 | 8.99 | 126.19 | 119.90 |
| 36 | A5 | 1487 | G | N1-C6-O6 | -8.99 | 114.51 | 119.90 |
| 1 | A2 | 794 | U | N1-C2-O2 | 8.99 | 129.09 | 122.80 |
| 36 | A5 | 2836 | C | C4-C5-C6 | 8.99 | 121.89 | 117.40 |
| 36 | A5 | 631 | U | N1-C2-N3 | 8.98 | 120.29 | 114.90 |
| 36 | A5 | 2320 | A | C5-C6-N6 | 8.98 | 130.88 | 123.70 |
| 38 | A4 | 140 | G | N9-C4-C5 | 8.98 | 108.99 | 105.40 |
| 80 | A6 | 321 | C | N3-C2-O2 | -8.98 | 115.62 | 121.90 |
| 36 | A5 | 2857 | C | N3-C4-C5 | 8.97 | 125.49 | 121.90 |
| 36 | A1 | 112 | U | C5-C6-N1 | 8.97 | 127.19 | 122.70 |
| 36 | A1 | 365 | A | N1-C6-N6 | 8.97 | 123.98 | 118.60 |
| 1 | A2 | 969 | C | C6-N1-C2 | 8.97 | 123.89 | 120.30 |
| 36 | A5 | 3212 | C | C2-N3-C4 | -8.97 | 115.42 | 119.90 |
| 37 | A7 | 101 | G | N1-C6-O6 | 8.97 | 125.28 | 119.90 |
| 37 | A3 | 86 | U | C5-C4-O4 | -8.96 | 120.52 | 125.90 |
| 1 | A2 | 542 | A | C5-N7-C8 | -8.95 | 99.42 | 103.90 |
| 36 | A5 | 2202 | C | N1-C2-O2 | -8.95 | 113.53 | 118.90 |
| 38 | A8 | 113 | U | C2-N1-C1' | 8.95 | 128.44 | 117.70 |
| 36 | A5 | 2327 | U | N3-C4-O4 | -8.95 | 113.13 | 119.40 |
| 36 | A5 | 2372 | A | N7-C8-N9 | 8.95 | 118.28 | 113.80 |
| 36 | A5 | 1116 | G | C4-C5-N7 | -8.95 | 107.22 | 110.80 |
| 36 | A5 | 726 | G | C4-C5-N7 | 8.95 | 114.38 | 110.80 |
| 36 | A5 | 802 | C | C4-C5-C6 | 8.95 | 121.87 | 117.40 |
| 36 | A5 | 2824 | G | C6-N1-C2 | -8.95 | 119.73 | 125.10 |
| 36 | A1 | 2899 | C | N3-C2-O2 | -8.94 | 115.64 | 121.90 |
| 36 | A5 | 2905 | U | N3-C4-O4 | -8.94 | 113.14 | 119.40 |
| 36 | A5 | 2327 | U | C2-N3-C4 | -8.94 | 121.64 | 127.00 |
| 36 | A1 | 2899 | C | C2-N3-C4 | -8.94 | 115.43 | 119.90 |
| 36 | A5 | 2728 | G | N9-C4-C5 | 8.94 | 108.97 | 105.40 |
| 80 | A6 | 1105 | C | N1-C2-O2 | 8.94 | 124.26 | 118.90 |
| 36 | A5 | 802 | C | C5-C6-N1 | -8.94 | 116.53 | 121.00 |
| 36 | A5 | 2833 | A | N1-C6-N6 | -8.94 | 113.24 | 118.60 |
| 1 | A2 | 1596 | C | C6-N1-C2 | -8.93 | 116.73 | 120.30 |
| 4 | CC | 58 | LEU | CA-CB-CG | 8.93 | 135.85 | 115.30 |
| 36 | A5 | 2808 | A | C2-N3-C4 | -8.92 | 106.14 | 110.60 |
| 36 | A5 | 887 | G | C5-C6-N1 | -8.92 | 107.04 | 111.50 |
| 36 | A5 | 1450 | G | C6-C5-N7 | 8.92 | 135.75 | 130.40 |
| 36 | A5 | 2382 | G | C5-C6-O6 | 8.92 | 133.95 | 128.60 |
| 36 | A1 | 2376 | G | C8-N9-C4 | -8.92 | 102.83 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 37 | A3 | 86 | U | C2-N3-C4 | -8.92 | 121.65 | 127.00 |
| 36 | A1 | 1377 | G | C5-C6-N1 | 8.91 | 115.96 | 111.50 |
| 36 | A5 | 1044 | U | N3-C4-O4 | -8.91 | 113.16 | 119.40 |
| 1 | A2 | 1745 | G | N3-C4-N9 | 8.91 | 131.35 | 126.00 |
| 37 | A3 | 101 | G | C8-N9-C4 | 8.91 | 109.96 | 106.40 |
| 80 | A6 | 1503 | A | C5-N7-C8 | -8.91 | 99.45 | 103.90 |
| 80 | A6 | 1745 | G | C6-N1-C2 | -8.91 | 119.76 | 125.10 |
| 36 | A5 | 3382 | U | C2-N1-C1' | 8.91 | 128.39 | 117.70 |
| 36 | A5 | 881 | C | N1-C2-O2 | 8.90 | 124.24 | 118.90 |
| 12 | AK | 88 | PRO | N-CA-CB | 8.90 | 113.98 | 103.30 |
| 36 | A1 | 2983 | C | N1-C2-N3 | 8.89 | 125.43 | 119.20 |
| 36 | A1 | 1404 | G | C8-N9-C4 | 8.89 | 109.96 | 106.40 |
| 80 | A6 | 1572 | G | N1-C6-O6 | 8.89 | 125.23 | 119.90 |
| 36 | A1 | 2808 | A | N1-C6-N6 | 8.88 | 123.93 | 118.60 |
| 36 | A5 | 2719 | U | C2-N1-C1' | -8.88 | 107.04 | 117.70 |
| 80 | A6 | 163 | G | N3-C2-N2 | -8.88 | 113.68 | 119.90 |
| 36 | A5 | 1429 | G | N1-C2-N2 | -8.87 | 108.21 | 116.20 |
| 36 | A5 | 1314 | C | C2-N3-C4 | -8.87 | 115.46 | 119.90 |
| 36 | A5 | 3049 | A | C5-C6-N1 | -8.86 | 113.27 | 117.70 |
| 36 | A5 | 1158 | A | N1-C6-N6 | 8.86 | 123.92 | 118.60 |
| 1 | A2 | 1455 | G | N3-C2-N2 | -8.86 | 113.70 | 119.90 |
| 36 | A1 | 2298 | U | N3-C4-O4 | -8.86 | 113.20 | 119.40 |
| 80 | A6 | 29 | U | C5-C4-O4 | 8.86 | 131.21 | 125.90 |
| 80 | A6 | 1539 | G | N3-C4-N9 | -8.86 | 120.69 | 126.00 |
| 80 | A6 | 1596 | C | N3-C4-N4 | -8.85 | 111.81 | 118.00 |
| 36 | A5 | 420 | G | C5-C6-N1 | 8.85 | 115.92 | 111.50 |
| 36 | A5 | 631 | U | N3-C4-O4 | -8.85 | 113.21 | 119.40 |
| 36 | A5 | 3040 | A | C8-N9-C4 | 8.85 | 109.34 | 105.80 |
| 36 | A5 | 433 | A | C2-N3-C4 | -8.84 | 106.18 | 110.60 |
| 36 | A5 | 3047 | U | C5-C6-N1 | -8.84 | 118.28 | 122.70 |
| 36 | A1 | 1495 | U | C2-N1-C1' | -8.84 | 107.10 | 117.70 |
| 80 | A6 | 1537 | C | C5-C4-N4 | -8.84 | 114.02 | 120.20 |
| 36 | A5 | 2881 | C | C2-N3-C4 | -8.83 | 115.48 | 119.90 |
| 36 | A1 | 3000 | A | C8-N9-C4 | 8.83 | 109.33 | 105.80 |
| 36 | A5 | 1931 | U | C2-N1-C1' | -8.83 | 107.10 | 117.70 |
| 36 | A1 | 644 | G | N9-C4-C5 | 8.83 | 108.93 | 105.40 |
| 36 | A1 | 2280 | A | N9-C4-C5 | -8.82 | 102.27 | 105.80 |
| 36 | A1 | 2142 | A | C2-N3-C4 | 8.81 | 115.01 | 110.60 |
| 36 | A5 | 2647 | A | N9-C4-C5 | 8.81 | 109.33 | 105.80 |
| 37 | A3 | 82 | G | N1-C2-N2 | -8.81 | 108.27 | 116.20 |
| 36 | A5 | 819 | U | C4-C5-C6 | 8.81 | 124.99 | 119.70 |
| 36 | A1 | 2821 | C | C5-C6-N1 | 8.81 | 125.41 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 2393 | G | C8-N9-C4 | 8.81 | 109.92 | 106.40 |
| 36 | A1 | 1832 | C | N3-C2-O2 | -8.81 | 115.73 | 121.90 |
| 38 | A4 | 57 | C | C6-N1-C2 | 8.81 | 123.82 | 120.30 |
| 80 | A6 | 539 | G | N7-C8-N9 | 8.81 | 117.50 | 113.10 |
| 38 | A4 | 39 | G | N3-C2-N2 | 8.80 | 126.06 | 119.90 |
| 36 | A5 | 1113 | G | C2-N3-C4 | -8.80 | 107.50 | 111.90 |
| 36 | A5 | 2757 | U | C4-C5-C6 | 8.80 | 124.98 | 119.70 |
| 36 | A5 | 947 | G | C6-N1-C2 | -8.80 | 119.82 | 125.10 |
| 1 | A2 | 1761 | U | C5-C4-O4 | 8.80 | 131.18 | 125.90 |
| 36 | A1 | 1049 | C | N3-C4-C5 | 8.80 | 125.42 | 121.90 |
| 37 | A3 | 103 | A | C8-N9-C4 | 8.80 | 109.32 | 105.80 |
| 36 | A1 | 1279 | C | C6-N1-C2 | -8.80 | 116.78 | 120.30 |
| 80 | A6 | 1 | U | C2-N1-C1' | 8.80 | 128.26 | 117.70 |
| 36 | A1 | 1911 | A | C5-C6-N6 | -8.79 | 116.67 | 123.70 |
| 36 | A1 | 2870 | C | N3-C4-N4 | -8.79 | 111.84 | 118.00 |
| 36 | A1 | 3143 | C | N1-C2-O2 | -8.79 | 113.62 | 118.90 |
| 80 | A6 | 1456 | C | N3-C2-O2 | -8.79 | 115.74 | 121.90 |
| 36 | A5 | 437 | G | C8-N9-C4 | -8.79 | 102.88 | 106.40 |
| 80 | A6 | 687 | G | N1-C2-N2 | 8.79 | 124.11 | 116.20 |
| 59 | DV | 48 | ARG | NE-CZ-NH1 | 8.79 | 124.69 | 120.30 |
| 36 | A5 | 1311 | G | C2-N3-C4 | 8.78 | 116.29 | 111.90 |
| 1 | A2 | 1749 | A | N1-C6-N6 | 8.78 | 123.87 | 118.60 |
| 36 | A1 | 730 | C | N3-C4-C5 | 8.78 | 125.41 | 121.90 |
| 36 | A5 | 3127 | A | N1-C6-N6 | -8.78 | 113.33 | 118.60 |
| 1 | A2 | 1654 | G | C6-N1-C2 | -8.78 | 119.83 | 125.10 |
| 36 | A1 | 2314 | U | C5-C6-N1 | 8.78 | 127.09 | 122.70 |
| 36 | A5 | 1907 | C | N3-C4-C5 | -8.78 | 118.39 | 121.90 |
| 1 | A2 | 507 | U | N1-C2-O2 | 8.77 | 128.94 | 122.80 |
| 38 | A4 | 25 | G | C4-C5-N7 | -8.77 | 107.29 | 110.80 |
| 80 | A6 | 1600 | A | N1-C2-N3 | 8.77 | 133.69 | 129.30 |
| 80 | A6 | 371 | G | N1-C6-O6 | 8.77 | 125.16 | 119.90 |
| 36 | A1 | 1115 | G | N3-C2-N2 | 8.76 | 126.03 | 119.90 |
| 36 | A1 | 3344 | A | N1-C2-N3 | 8.76 | 133.68 | 129.30 |
| 36 | A5 | 2434 | U | C5-C6-N1 | -8.76 | 118.32 | 122.70 |
| 1 | A2 | 992 | A | N3-C4-C5 | 8.75 | 132.93 | 126.80 |
| 36 | A1 | 2828 | G | N1-C6-O6 | -8.75 | 114.65 | 119.90 |
| 36 | A1 | 1329 | U | N1-C2-N3 | 8.74 | 120.14 | 114.90 |
| 36 | A1 | 2865 | U | N3-C4-C5 | 8.74 | 119.84 | 114.60 |
| 36 | A5 | 1149 | G | C2-N3-C4 | 8.73 | 116.27 | 111.90 |
| 1 | A2 | 1503 | A | C2-N3-C4 | -8.73 | 106.23 | 110.60 |
| 36 | A1 | 1589 | A | N1-C6-N6 | 8.73 | 123.84 | 118.60 |
| 36 | A1 | 159 | A | C8-N9-C4 | 8.73 | 109.29 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 1161 | G | C5-C6-N1 | 8.73 | 115.86 | 111.50 |
| 36 | A5 | 1903 | U | C4-C5-C6 | 8.73 | 124.94 | 119.70 |
| 36 | A5 | 1846 | C | C2-N3-C4 | -8.72 | 115.54 | 119.90 |
| 36 | A5 | 2416 | U | C6-N1-C2 | -8.72 | 115.77 | 121.00 |
| 36 | A1 | 439 | C | N1-C2-O2 | 8.71 | 124.13 | 118.90 |
| 36 | A5 | 3123 | A | C8-N9-C4 | 8.71 | 109.29 | 105.80 |
| 1 | A2 | 453 | U | C2-N1-C1' | 8.71 | 128.16 | 117.70 |
| 36 | A1 | 1007 | U | C6-N1-C2 | 8.71 | 126.23 | 121.00 |
| 36 | A1 | 1138 | U | N3-C2-O2 | -8.71 | 116.10 | 122.20 |
| 1 | A2 | 558 | U | N1-C2-O2 | 8.71 | 128.90 | 122.80 |
| 36 | A1 | 369 | A | C8-N9-C4 | -8.71 | 102.32 | 105.80 |
| 36 | A1 | 2714 | G | C5-N7-C8 | -8.70 | 99.95 | 104.30 |
| 36 | A1 | 1120 | A | N1-C2-N3 | 8.70 | 133.65 | 129.30 |
| 36 | A5 | 834 | U | C4-C5-C6 | -8.70 | 114.48 | 119.70 |
| 80 | A6 | 337 | G | C4-C5-C6 | 8.70 | 124.02 | 118.80 |
| 36 | A5 | 1840 | U | N3-C2-O2 | -8.70 | 116.11 | 122.20 |
| 36 | A1 | 2413 | A | C4-C5-C6 | -8.70 | 112.65 | 117.00 |
| 36 | A5 | 726 | G | C6-C5-N7 | -8.70 | 125.18 | 130.40 |
| 36 | A5 | 1412 | G | C8-N9-C4 | -8.70 | 102.92 | 106.40 |
| 36 | A5 | 2271 | A | N7-C8-N9 | -8.70 | 109.45 | 113.80 |
| 36 | A5 | 2730 | G | N1-C6-O6 | 8.69 | 125.11 | 119.90 |
| 36 | A1 | 49 | A | C5-C6-N1 | -8.69 | 113.36 | 117.70 |
| 36 | A1 | 2977 | G | C5-C6-N1 | 8.69 | 115.84 | 111.50 |
| 38 | A4 | 15 | G | C5-C6-O6 | -8.68 | 123.39 | 128.60 |
| 80 | A6 | 1537 | C | N3-C4-N4 | 8.68 | 124.08 | 118.00 |
| 36 | A5 | 2858 | U | N3-C2-O2 | -8.68 | 116.12 | 122.20 |
| 36 | A5 | 2409 | G | C8-N9-C4 | -8.68 | 102.93 | 106.40 |
| 36 | A5 | 2865 | U | C5-C6-N1 | 8.68 | 127.04 | 122.70 |
| 36 | A1 | 718 | G | C5-N7-C8 | -8.68 | 99.96 | 104.30 |
| 36 | A1 | 960 | U | N3-C4-C5 | 8.67 | 119.80 | 114.60 |
| 36 | A5 | 1134 | G | C5-C6-O6 | -8.67 | 123.40 | 128.60 |
| 36 | A5 | 2292 | U | N3-C2-O2 | -8.67 | 116.13 | 122.20 |
| 36 | A5 | 2832 | C | C5-C6-N1 | -8.67 | 116.66 | 121.00 |
| 36 | A1 | 2653 | C | N3-C4-N4 | -8.67 | 111.93 | 118.00 |
| 36 | A1 | 2679 | A | C6-C5-N7 | -8.67 | 126.23 | 132.30 |
| 40 | BB | 21 | ARG | NE-CZ-NH2 | 8.67 | 124.63 | 120.30 |
| 36 | A5 | 2434 | U | N3-C4-O4 | -8.67 | 113.33 | 119.40 |
| 36 | A5 | 1119 | C | C2-N3-C4 | -8.66 | 115.57 | 119.90 |
| 36 | A5 | 2290 | C | C2-N3-C4 | -8.66 | 115.57 | 119.90 |
| 37 | A7 | 48 | U | C2-N3-C4 | -8.66 | 121.80 | 127.00 |
| 36 | A1 | 2368 | A | N1-C6-N6 | -8.66 | 113.41 | 118.60 |
| 36 | A1 | 3259 | U | N1-C2-O2 | -8.66 | 116.74 | 122.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 2198 | A | N1-C6-N6 | 8.65 | 123.79 | 118.60 |
| 36 | A1 | 2406 | C | C6-N1-C2 | 8.65 | 123.76 | 120.30 |
| 36 | A5 | 2190 | U | C5-C4-O4 | 8.65 | 131.09 | 125.90 |
| 36 | A1 | 959 | C | C5-C6-N1 | -8.65 | 116.68 | 121.00 |
| 38 | A8 | 17 | A | N1-C6-N6 | 8.65 | 123.79 | 118.60 |
| 36 | A5 | 2961 | G | C8-N9-C4 | -8.64 | 102.94 | 106.40 |
| 1 | A2 | 92 | A | C8-N9-C4 | -8.64 | 102.34 | 105.80 |
| 1 | A2 | 1291 | G | N7-C8-N9 | 8.64 | 117.42 | 113.10 |
| 36 | A5 | 3040 | A | N7-C8-N9 | -8.64 | 109.48 | 113.80 |
| 36 | A5 | 796 | U | N3-C2-O2 | -8.64 | 116.15 | 122.20 |
| 36 | A1 | 2728 | G | C5-C6-O6 | -8.63 | 123.42 | 128.60 |
| 36 | A5 | 3143 | C | N1-C2-O2 | -8.64 | 113.72 | 118.90 |
| 54 | DQ | 151 | ARG | NE-CZ-NH1 | -8.64 | 115.98 | 120.30 |
| 36 | A1 | 2777 | G | C2-N3-C4 | -8.63 | 107.58 | 111.90 |
| 36 | A1 | 864 | G | N3-C4-C5 | -8.63 | 124.28 | 128.60 |
| 36 | A1 | 1110 | U | C5-C4-O4 | -8.63 | 120.72 | 125.90 |
| 36 | A5 | 66 | A | C8-N9-C4 | 8.63 | 109.25 | 105.80 |
| 80 | A6 | 558 | U | C2-N1-C1' | 8.62 | 128.05 | 117.70 |
| 36 | A5 | 339 | C | C5-C4-N4 | 8.62 | 126.24 | 120.20 |
| 36 | A1 | 2168 | A | C8-N9-C4 | 8.62 | 109.25 | 105.80 |
| 36 | A1 | 2836 | C | C5-C6-N1 | -8.62 | 116.69 | 121.00 |
| 36 | A5 | 938 | C | C2-N3-C4 | -8.62 | 115.59 | 119.90 |
| 36 | A1 | 2836 | C | N3-C4-N4 | -8.62 | 111.97 | 118.00 |
| 1 | A2 | 17 | C | C6-N1-C2 | -8.62 | 116.85 | 120.30 |
| 36 | A5 | 821 | U | C5-C6-N1 | -8.62 | 118.39 | 122.70 |
| 80 | A6 | 858 | G | C4-C5-N7 | 8.61 | 114.25 | 110.80 |
| 36 | A5 | 2385 | G | N3-C4-C5 | 8.61 | 132.91 | 128.60 |
| 36 | A5 | 3374 | U | N3-C4-C5 | 8.61 | 119.77 | 114.60 |
| 36 | A1 | 1929 | G | N9-C4-C5 | -8.61 | 101.96 | 105.40 |
| 36 | A1 | 2314 | U | C6-N1-C1' | -8.61 | 109.15 | 121.20 |
| 36 | A1 | 2376 | G | N3-C4-C5 | -8.61 | 124.30 | 128.60 |
| 36 | A1 | 3242 | G | C6-N1-C2 | 8.61 | 130.26 | 125.10 |
| 36 | A5 | 1327 | C | N1-C2-O2 | 8.61 | 124.06 | 118.90 |
| 38 | A4 | 53 | A | C2-N3-C4 | 8.61 | 114.90 | 110.60 |
| 36 | A1 | 197 | G | N1-C6-O6 | 8.60 | 125.06 | 119.90 |
| 36 | A5 | 644 | G | C5-C6-N1 | 8.60 | 115.80 | 111.50 |
| 36 | A1 | 407 | A | C8-N9-C4 | -8.60 | 102.36 | 105.80 |
| 36 | A5 | 2728 | G | N3-C2-N2 | -8.60 | 113.88 | 119.90 |
| 37 | A7 | 92 | A | N1-C6-N6 | 8.60 | 123.76 | 118.60 |
| 1 | A2 | 794 | U | N3-C2-O2 | -8.60 | 116.18 | 122.20 |
| 36 | A5 | 2687 | G | N1-C6-O6 | -8.60 | 114.74 | 119.90 |
| 36 | A1 | 2621 | G | N9-C4-C5 | 8.59 | 108.84 | 105.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 2638 | C | N1-C2-O2 | -8.59 | 113.75 | 118.90 |
| 36 | A5 | 2913 | C | C4-C5-C6 | 8.59 | 121.70 | 117.40 |
| 1 | A2 | 7 | G | N1-C6-O6 | -8.59 | 114.75 | 119.90 |
| 36 | A5 | 2391 | G | N1-C6-O6 | -8.59 | 114.75 | 119.90 |
| 36 | A1 | 1911 | A | C4-C5-N7 | 8.59 | 114.99 | 110.70 |
| 36 | A1 | 44 | U | C5-C6-N1 | -8.59 | 118.41 | 122.70 |
| 36 | A5 | 2988 | C | N3-C2-O2 | -8.59 | 115.89 | 121.90 |
| 36 | A1 | 53 | G | C8-N9-C4 | 8.58 | 109.83 | 106.40 |
| 36 | A1 | 2867 | C | N3-C4-N4 | -8.58 | 111.99 | 118.00 |
| 36 | A1 | 2393 | G | N3-C4-N9 | 8.58 | 131.15 | 126.00 |
| 38 | A4 | 96 | A | C2-N3-C4 | -8.58 | 106.31 | 110.60 |
| 36 | A1 | 804 | C | N3-C2-O2 | 8.58 | 127.91 | 121.90 |
| 36 | A1 | 3001 | C | C6-N1-C2 | 8.58 | 123.73 | 120.30 |
| 80 | A6 | 512 | A | N1-C6-N6 | 8.58 | 123.75 | 118.60 |
| 36 | A5 | 2392 | C | C2-N3-C4 | -8.58 | 115.61 | 119.90 |
| 36 | A5 | 2699 | G | C5-C6-O6 | -8.58 | 123.45 | 128.60 |
| 1 | A2 | 1189 | A | C8-N9-C4 | 8.57 | 109.23 | 105.80 |
| 36 | A1 | 2151 | C | N1-C2-O2 | -8.57 | 113.76 | 118.90 |
| 1 | A2 | 992 | A | C5-C6-N1 | -8.57 | 113.42 | 117.70 |
| 36 | A5 | 2758 | A | N1-C2-N3 | -8.57 | 125.02 | 129.30 |
| 36 | A1 | 1060 | U | C5-C6-N1 | -8.56 | 118.42 | 122.70 |
| 36 | A1 | 37 | U | N1-C2-O2 | -8.56 | 116.81 | 122.80 |
| 80 | A6 | 1085 | G | N1-C6-O6 | -8.56 | 114.76 | 119.90 |
| 36 | A5 | 341 | G | C5-C6-O6 | -8.56 | 123.47 | 128.60 |
| 36 | A5 | 345 | G | C5-C6-N1 | 8.55 | 115.78 | 111.50 |
| 36 | A1 | 785 | G | N1-C6-O6 | -8.55 | 114.77 | 119.90 |
| 36 | A1 | 922 | U | N3-C2-O2 | -8.55 | 116.22 | 122.20 |
| 36 | A1 | 3208 | G | N3-C4-N9 | -8.55 | 120.87 | 126.00 |
| 36 | A1 | 709 | A | C5-N7-C8 | 8.54 | 108.17 | 103.90 |
| 36 | A1 | 3217 | C | C2-N1-C1' | 8.54 | 128.20 | 118.80 |
| 36 | A1 | 1904 | C | C6-N1-C2 | -8.54 | 116.88 | 120.30 |
| 36 | A1 | 2823 | G | C4-C5-N7 | -8.54 | 107.38 | 110.80 |
| 36 | A1 | 2899 | C | C6-N1-C1' | -8.54 | 110.55 | 120.80 |
| 36 | A5 | 2634 | U | N1-C2-O2 | -8.54 | 116.82 | 122.80 |
| 36 | A1 | 907 | G | C8-N9-C4 | -8.54 | 102.98 | 106.40 |
| 36 | A1 | 2395 | G | C6-N1-C2 | -8.54 | 119.98 | 125.10 |
| 80 | A6 | 1037 | C | C6-N1-C2 | 8.54 | 123.72 | 120.30 |
| 1 | A2 | 1745 | G | C5-C6-N1 | 8.53 | 115.77 | 111.50 |
| 36 | A1 | 1339 | C | N1-C2-O2 | -8.53 | 113.78 | 118.90 |
| 80 | A6 | 453 | U | C2-N1-C1' | 8.53 | 127.94 | 117.70 |
| 36 | A5 | 726 | G | C5-C6-O6 | -8.53 | 123.48 | 128.60 |
| 36 | A5 | 2988 | C | C4-C5-C6 | 8.53 | 121.67 | 117.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 80 | A6 | 1749 | A | N9-C4-C5 | -8.53 | 102.39 | 105.80 |
| 36 | A5 | 1050 | U | N1-C2-O2 | 8.53 | 128.77 | 122.80 |
| 36 | A5 | 946 | U | N3-C2-O2 | -8.53 | 116.23 | 122.20 |
| 36 | A1 | 2823 | G | N1-C6-O6 | -8.53 | 114.78 | 119.90 |
| 36 | A5 | 3010 | U | N3-C2-O2 | -8.53 | 116.23 | 122.20 |
| 36 | A1 | 883 | A | N1-C2-N3 | -8.52 | 125.04 | 129.30 |
| 80 | A6 | 858 | G | C5-N7-C8 | -8.52 | 100.04 | 104.30 |
| 1 | A2 | 719 | U | C2-N1-C1' | 8.52 | 127.92 | 117.70 |
| 1 | A2 | 1773 | C | N3-C4-N4 | 8.52 | 123.96 | 118.00 |
| 36 | A1 | 2165 | G | C4-C5-N7 | 8.52 | 114.21 | 110.80 |
| 36 | A5 | 326 | U | C5-C4-O4 | -8.52 | 120.79 | 125.90 |
| 36 | A1 | 2282 | U | C2-N3-C4 | -8.51 | 121.89 | 127.00 |
| 36 | A5 | 1409 | G | N1-C6-O6 | -8.51 | 114.79 | 119.90 |
| 36 | A5 | 2301 | U | C2-N3-C4 | -8.51 | 121.89 | 127.00 |
| 38 | A8 | 14 | C | C5-C6-N1 | -8.51 | 116.74 | 121.00 |
| 36 | A1 | 2868 | U | C2-N3-C4 | -8.51 | 121.89 | 127.00 |
| 36 | A1 | 588 | G | N3-C4-C5 | -8.51 | 124.35 | 128.60 |
| 80 | A6 | 1269 | U | N1-C2-N3 | 8.51 | 120.00 | 114.90 |
| 80 | A6 | 314 | C | N3-C2-O2 | -8.50 | 115.95 | 121.90 |
| 36 | A5 | 1143 | A | C5-C6-N1 | -8.50 | 113.45 | 117.70 |
| 1 | A2 | 647 | G | N3-C4-N9 | -8.50 | 120.90 | 126.00 |
| 36 | A1 | 2289 | U | N1-C2-O2 | 8.50 | 128.75 | 122.80 |
| 36 | A5 | 2524 | A | C5-N7-C8 | -8.50 | 99.65 | 103.90 |
| 36 | A5 | 2952 | G | N3-C2-N2 | -8.50 | 113.95 | 119.90 |
| 80 | A6 | 144 | U | C2-N1-C1' | 8.50 | 127.89 | 117.70 |
| 36 | A1 | 931 | C | C2-N3-C4 | -8.49 | 115.66 | 119.90 |
| 1 | A2 | 992 | A | N3-C4-N9 | -8.48 | 120.61 | 127.40 |
| 36 | A5 | 2978 | U | C5-C6-N1 | -8.48 | 118.46 | 122.70 |
| 36 | A1 | 1142 | G | N3-C4-C5 | -8.48 | 124.36 | 128.60 |
| 36 | A1 | 1295 | G | C5-C6-O6 | 8.48 | 133.69 | 128.60 |
| 36 | A1 | 1142 | G | C5-C6-O6 | -8.48 | 123.51 | 128.60 |
| 36 | A5 | 1085 | A | N7-C8-N9 | 8.48 | 118.04 | 113.80 |
| 36 | A5 | 1342 | C | C5-C6-N1 | -8.48 | 116.76 | 121.00 |
| 36 | A1 | 2631 | U | C5-C6-N1 | -8.48 | 118.46 | 122.70 |
| 36 | A5 | 887 | G | C5-C6-O6 | 8.48 | 133.69 | 128.60 |
| 36 | A5 | 2732 | G | N1-C6-O6 | -8.48 | 114.81 | 119.90 |
| 36 | A1 | 2349 | U | C2-N3-C4 | -8.47 | 121.92 | 127.00 |
| 36 | A1 | 592 | A | N9-C4-C5 | -8.47 | 102.41 | 105.80 |
| 36 | A5 | 3377 | G | C5-C6-N1 | 8.47 | 115.74 | 111.50 |
| 36 | A1 | 95 | A | C8-N9-C4 | 8.47 | 109.19 | 105.80 |
| 36 | A1 | 633 | C | C5-C6-N1 | -8.47 | 116.77 | 121.00 |
| 36 | A1 | 2870 | C | C6-N1-C2 | -8.47 | 116.91 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 36 | A5 | 3321 | C | C5-C6-N1 | -8.46 | 116.77 | 121.00 |
| 1 | A2 | 1486 | G | C4-C5-N7 | 8.46 | 114.19 | 110.80 |
| 36 | A5 | 1942 | U | N1-C2-O2 | -8.46 | 116.88 | 122.80 |
| 36 | A1 | 895 | A | C4-C5-N7 | 8.46 | 114.93 | 110.70 |
| 36 | A5 | 343 | U | N3-C2-O2 | -8.46 | 116.28 | 122.20 |
| 36 | A5 | 1047 | A | C2-N3-C4 | 8.46 | 114.83 | 110.60 |
| 36 | A1 | 2892 | A | N1-C6-N6 | -8.46 | 113.53 | 118.60 |
| 36 | A5 | 224 | C | N1-C2-O2 | 8.45 | 123.97 | 118.90 |
| 36 | A1 | 3344 | A | C4-C5-N7 | 8.45 | 114.93 | 110.70 |
| 36 | A5 | 652 | G | N3-C4-C5 | -8.45 | 124.37 | 128.60 |
| 36 | A5 | 2913 | C | C2-N3-C4 | -8.45 | 115.67 | 119.90 |
| 36 | A1 | 1481 | A | C8-N9-C4 | -8.45 | 102.42 | 105.80 |
| 36 | A5 | 2870 | C | C6-N1-C2 | -8.44 | 116.92 | 120.30 |
| 36 | A1 | 3077 | A | C8-N9-C4 | -8.44 | 102.42 | 105.80 |
| 1 | A2 | 1200 | G | C6-C5-N7 | -8.44 | 125.34 | 130.40 |
| 80 | A6 | 1298 | U | C5-C6-N1 | -8.44 | 118.48 | 122.70 |
| 36 | A5 | 2980 | U | N1-C2-N3 | 8.44 | 119.96 | 114.90 |
| 36 | A1 | 3306 | U | C5-C6-N1 | -8.43 | 118.48 | 122.70 |
| 36 | A1 | 106 | A | C8-N9-C4 | 8.43 | 109.17 | 105.80 |
| 37 | A7 | 96 | U | C2-N3-C4 | -8.43 | 121.94 | 127.00 |
| 36 | A5 | 945 | C | N3-C4-C5 | 8.43 | 125.27 | 121.90 |
| 36 | A1 | 1481 | A | N7-C8-N9 | 8.43 | 118.01 | 113.80 |
| 80 | A6 | 1596 | C | C6-N1-C2 | -8.43 | 116.93 | 120.30 |
| 36 | A1 | 2277 | C | N3-C4-C5 | 8.42 | 125.27 | 121.90 |
| 36 | A5 | 3137 | C | N3-C4-C5 | 8.42 | 125.27 | 121.90 |
| 36 | A1 | 1592 | G | N1-C2-N2 | -8.42 | 108.62 | 116.20 |
| 36 | A5 | 1402 | C | N3-C2-O2 | -8.42 | 116.00 | 121.90 |
| 36 | A1 | 63 | A | N1-C2-N3 | -8.42 | 125.09 | 129.30 |
| 1 | A2 | 1387 | G | N1-C6-O6 | 8.42 | 124.95 | 119.90 |
| 36 | A5 | 999 | G | N1-C6-O6 | -8.42 | 114.85 | 119.90 |
| 36 | A5 | 1156 | C | C2-N3-C4 | -8.42 | 115.69 | 119.90 |
| 36 | A5 | 2683 | U | N1-C2-O2 | 8.42 | 128.69 | 122.80 |
| 36 | A1 | 2418 | G | C2-N3-C4 | 8.41 | 116.11 | 111.90 |
| 36 | A5 | 1064 | A | C5-C6-N6 | -8.41 | 116.97 | 123.70 |
| 1 | A2 | 577 | G | N7-C8-N9 | 8.41 | 117.31 | 113.10 |
| 36 | A5 | 2928 | C | C4-C5-C6 | 8.41 | 121.61 | 117.40 |
| 36 | A1 | 2334 | U | C5-C6-N1 | -8.41 | 118.50 | 122.70 |
| 36 | A5 | 2345 | A | N1-C6-N6 | 8.41 | 123.65 | 118.60 |
| 36 | A1 | 2642 | A | C8-N9-C4 | 8.41 | 109.16 | 105.80 |
| 36 | A1 | 2752 | U | N3-C4-O4 | -8.40 | 113.52 | 119.40 |
| 36 | A1 | 3083 | G | C2-N3-C4 | 8.40 | 116.10 | 111.90 |
| 36 | A5 | 1469 | C | N3-C4-C5 | -8.40 | 118.54 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 1336 | U | N1-C2-N3 | 8.40 | 119.94 | 114.90 |
| 36 | A1 | 1403 | C | N3-C4-C5 | 8.40 | 125.26 | 121.90 |
| 80 | A6 | 1535 | U | N1-C2-O2 | 8.40 | 128.68 | 122.80 |
| 36 | A1 | 24 | G | N3-C2-N2 | -8.39 | 114.02 | 119.90 |
| 36 | A1 | 2595 | A | N7-C8-N9 | 8.39 | 118.00 | 113.80 |
| 1 | A2 | 966 | A | C8-N9-C4 | 8.39 | 109.16 | 105.80 |
| 36 | A1 | 2909 | U | N1-C2-O2 | -8.39 | 116.92 | 122.80 |
| 80 | A6 | 17 | C | N3-C2-O2 | -8.39 | 116.02 | 121.90 |
| 36 | A5 | 580 | C | C6-N1-C2 | -8.39 | 116.94 | 120.30 |
| 36 | A5 | 811 | U | C2-N3-C4 | -8.39 | 121.97 | 127.00 |
| 36 | A1 | 2719 | U | C2-N3-C4 | -8.39 | 121.97 | 127.00 |
| 38 | A8 | 55 | U | N1-C2-N3 | 8.39 | 119.93 | 114.90 |
| 36 | A1 | 3222 | U | N3-C2-O2 | -8.39 | 116.33 | 122.20 |
| 36 | A1 | 573 | C | N3-C4-C5 | 8.38 | 125.25 | 121.90 |
| 36 | A1 | 938 | C | N3-C4-C5 | 8.38 | 125.25 | 121.90 |
| 37 | A7 | 48 | U | C5-C4-O4 | -8.38 | 120.87 | 125.90 |
| 36 | A1 | 1119 | C | C6-N1-C2 | 8.38 | 123.65 | 120.30 |
| 80 | A6 | 1614 | A | N1-C6-N6 | 8.38 | 123.63 | 118.60 |
| 36 | A1 | 1382 | G | C8-N9-C4 | 8.38 | 109.75 | 106.40 |
| 80 | A6 | 1 | U | N3-C2-O2 | -8.38 | 116.33 | 122.20 |
| 80 | A6 | 114 | C | N1-C2-O2 | 8.38 | 123.93 | 118.90 |
| 1 | A2 | 1541 | G | C5-C6-O6 | 8.38 | 133.62 | 128.60 |
| 1 | A2 | 1387 | G | C6-C5-N7 | -8.37 | 125.38 | 130.40 |
| 36 | A1 | 2314 | U | C4-C5-C6 | -8.38 | 114.67 | 119.70 |
| 36 | A5 | 2307 | G | N3-C4-C5 | -8.38 | 124.41 | 128.60 |
| 80 | A6 | 1745 | G | C5-C6-O6 | -8.37 | 123.58 | 128.60 |
| 80 | A6 | 102 | U | N1-C2-O2 | -8.36 | 116.94 | 122.80 |
| 36 | A1 | 104 | G | C5-C6-O6 | -8.36 | 123.58 | 128.60 |
| 36 | A5 | 3102 | G | N3-C2-N2 | 8.36 | 125.75 | 119.90 |
| 36 | A1 | 368 | G | N1-C2-N3 | 8.36 | 128.92 | 123.90 |
| 36 | A1 | 2944 | U | N1-C2-O2 | 8.36 | 128.65 | 122.80 |
| 36 | A1 | 2279 | A | C5-C6-N6 | -8.36 | 117.02 | 123.70 |
| 36 | A5 | 817 | A | C8-N9-C4 | -8.36 | 102.46 | 105.80 |
| 37 | A7 | 96 | U | N1-C2-N3 | 8.36 | 119.91 | 114.90 |
| 1 | A2 | 736 | C | C2-N1-C1' | 8.35 | 127.99 | 118.80 |
| 36 | A1 | 1838 | G | C6-C5-N7 | -8.35 | 125.39 | 130.40 |
| 36 | A5 | 511 | G | N1-C6-O6 | -8.35 | 114.89 | 119.90 |
| 36 | A5 | 916 | G | C5-C6-O6 | 8.35 | 133.61 | 128.60 |
| 36 | A1 | 1858 | A | N3-C4-N9 | 8.35 | 134.08 | 127.40 |
| 36 | A5 | 926 | A | C5-C6-N1 | 8.35 | 121.88 | 117.70 |
| 36 | A5 | 2234 | G | N9-C4-C5 | -8.35 | 102.06 | 105.40 |
| 36 | A5 | 2820 | A | C8-N9-C4 | -8.35 | 102.46 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | A2 | 136 | C | C2-N1-C1' | 8.35 | 127.98 | 118.80 |
| 80 | A6 | 359 | A | C4-C5-C6 | -8.35 | 112.83 | 117.00 |
| 36 | A5 | 616 | G | C5-C6-N1 | 8.35 | 115.67 | 111.50 |
| 37 | A7 | 93 | C | C2-N3-C4 | -8.35 | 115.73 | 119.90 |
| 36 | A5 | 3173 | G | C5-C6-O6 | -8.34 | 123.59 | 128.60 |
| 36 | A1 | 3143 | C | C5-C6-N1 | -8.34 | 116.83 | 121.00 |
| 36 | A1 | 347 | G | C5-C6-O6 | -8.34 | 123.60 | 128.60 |
| 36 | A1 | 2356 | A | N1-C6-N6 | 8.33 | 123.60 | 118.60 |
| 36 | A1 | 2763 | U | C5-C6-N1 | -8.33 | 118.53 | 122.70 |
| 36 | A1 | 2393 | G | N9-C4-C5 | -8.33 | 102.07 | 105.40 |
| 36 | A1 | 3180 | A | C8-N9-C4 | -8.33 | 102.47 | 105.80 |
| 36 | A1 | 2237 | C | C6-N1-C2 | 8.33 | 123.63 | 120.30 |
| 36 | A1 | 2409 | G | C5-C6-O6 | 8.33 | 133.60 | 128.60 |
| 36 | A5 | 1487 | G | C5-C6-O6 | 8.33 | 133.60 | 128.60 |
| 36 | A5 | 2320 | A | C2-N3-C4 | -8.33 | 106.44 | 110.60 |
| 36 | A1 | 47 | C | C4-C5-C6 | 8.32 | 121.56 | 117.40 |
| 36 | A1 | 2400 | G | N3-C4-C5 | 8.32 | 132.76 | 128.60 |
| 80 | A6 | 376 | C | N3-C4-C5 | 8.32 | 125.23 | 121.90 |
| 37 | A3 | 28 | C | N3-C4-N4 | 8.32 | 123.82 | 118.00 |
| 36 | A1 | 1191 | U | C5-C6-N1 | -8.32 | 118.54 | 122.70 |
| 36 | A1 | 1507 | G | N3-C2-N2 | -8.31 | 114.08 | 119.90 |
| 36 | A1 | 2283 | G | C5-C6-O6 | -8.31 | 123.61 | 128.60 |
| 36 | A5 | 3050 | U | C5-C4-O4 | 8.31 | 130.89 | 125.90 |
| 73 | Bj | 21 | ARG | NE-CZ-NH2 | -8.31 | 116.14 | 120.30 |
| 36 | A1 | 702 | C | C6-N1-C2 | -8.31 | 116.98 | 120.30 |
| 36 | A1 | 1918 | C | C6-N1-C2 | -8.31 | 116.98 | 120.30 |
| 36 | A1 | 646 | A | C8-N9-C4 | -8.30 | 102.48 | 105.80 |
| 36 | A1 | 1115 | G | N1-C6-O6 | -8.30 | 114.92 | 119.90 |
| 36 | A1 | 2827 | U | N1-C2-N3 | 8.30 | 119.88 | 114.90 |
| 38 | A4 | 21 | C | C6-N1-C2 | 8.30 | 123.62 | 120.30 |
| 36 | A5 | 2683 | U | N3-C2-O2 | -8.30 | 116.39 | 122.20 |
| 36 | A5 | 1898 | G | C2-N3-C4 | 8.30 | 116.05 | 111.90 |
| 36 | A1 | 2836 | C | N3-C4-C5 | -8.29 | 118.58 | 121.90 |
| 36 | A1 | 2958 | A | C5-C6-N1 | 8.29 | 121.85 | 117.70 |
| 36 | A5 | 986 | U | C5-C4-O4 | -8.29 | 120.92 | 125.90 |
| 36 | A5 | 1480 | G | N7-C8-N9 | -8.29 | 108.95 | 113.10 |
| 52 | DO | 197[B] | PHE | C-N-CA | -8.29 | 104.88 | 122.30 |
| 36 | A5 | 715 | A | N1-C6-N6 | -8.29 | 113.62 | 118.60 |
| 38 | A8 | 80 | A | N7-C8-N9 | 8.29 | 117.94 | 113.80 |
| 1 | A2 | 542 | A | C4-N9-C1' | 8.28 | 141.20 | 126.30 |
| 36 | A1 | 106 | A | C2-N3-C4 | -8.28 | 106.46 | 110.60 |
| 36 | A1 | 1890 | U | C5-C6-N1 | -8.28 | 118.56 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 2977 | G | N7-C8-N9 | -8.27 | 108.96 | 113.10 |
| 1 | A2 | 1280 | C | N1-C2-O2 | -8.27 | 113.94 | 118.90 |
| 36 | A1 | 39 | A | C4-C5-C6 | 8.27 | 121.14 | 117.00 |
| 36 | A1 | 957 | C | C6-N1-C2 | 8.27 | 123.61 | 120.30 |
| 36 | A5 | 2360 | C | C4-C5-C6 | 8.27 | 121.53 | 117.40 |
| 1 | A2 | 1131 | A | C8-N9-C4 | 8.27 | 109.11 | 105.80 |
| 36 | A5 | 1392 | G | N7-C8-N9 | -8.27 | 108.97 | 113.10 |
| 36 | A1 | 2814 | G | C5-C6-O6 | -8.26 | 123.64 | 128.60 |
| 37 | A7 | 69 | C | C6-N1-C2 | 8.26 | 123.61 | 120.30 |
| 38 | A4 | 73 | U | N3-C4-O4 | -8.26 | 113.62 | 119.40 |
| 80 | A6 | 272 | U | N3-C2-O2 | -8.26 | 116.42 | 122.20 |
| 36 | A5 | 1604 | G | C8-N9-C1' | -8.26 | 116.26 | 127.00 |
| 80 | A6 | 1614 | A | C4-C5-N7 | 8.26 | 114.83 | 110.70 |
| 36 | A5 | 715 | A | C2-N3-C4 | 8.26 | 114.73 | 110.60 |
| 36 | A1 | 2130 | G | C5-C6-O6 | 8.26 | 133.55 | 128.60 |
| 36 | A1 | 2642 | A | N7-C8-N9 | -8.26 | 109.67 | 113.80 |
| 36 | A5 | 2621 | G | N1-C6-O6 | 8.26 | 124.85 | 119.90 |
| 37 | A7 | 93 | C | C5-C6-N1 | -8.26 | 116.87 | 121.00 |
| 47 | DI | 128 | ARG | NE-CZ-NH2 | -8.25 | 116.17 | 120.30 |
| 1 | A2 | 1782 | A | N1-C2-N3 | 8.25 | 133.42 | 129.30 |
| 47 | BI | 24 | ARG | NE-CZ-NH1 | 8.25 | 124.42 | 120.30 |
| 36 | A1 | 2169 | G | C4-C5-N7 | -8.24 | 107.50 | 110.80 |
| 80 | A6 | 1119 | G | C5-C6-O6 | 8.24 | 133.55 | 128.60 |
| 36 | A1 | 2714 | G | C8-N9-C1' | 8.24 | 137.72 | 127.00 |
| 36 | A1 | 1122 | U | N3-C4-C5 | 8.24 | 119.54 | 114.60 |
| 38 | A8 | 55 | U | C6-N1-C2 | -8.24 | 116.06 | 121.00 |
| 36 | A5 | 2695 | A | C8-N9-C4 | -8.23 | 102.51 | 105.80 |
| 36 | A1 | 3143 | C | N3-C2-O2 | 8.23 | 127.66 | 121.90 |
| 38 | A4 | 125 | U | N1-C2-O2 | 8.23 | 128.56 | 122.80 |
| 36 | A5 | 1494 | U | C6-N1-C2 | 8.23 | 125.94 | 121.00 |
| 36 | A5 | 2371 | G | N3-C2-N2 | 8.23 | 125.66 | 119.90 |
| 36 | A1 | 2426 | U | N3-C4-O4 | -8.23 | 113.64 | 119.40 |
| 36 | A1 | 2808 | A | C6-C5-N7 | -8.23 | 126.54 | 132.30 |
| 1 | A2 | 1119 | G | N1-C6-O6 | -8.23 | 114.96 | 119.90 |
| 80 | A6 | 342 | C | C5-C6-N1 | -8.23 | 116.89 | 121.00 |
| 36 | A1 | 973 | A | C8-N9-C4 | -8.23 | 102.51 | 105.80 |
| 36 | A1 | 3269 | U | N1-C2-N3 | 8.23 | 119.84 | 114.90 |
| 36 | A1 | 2123 | G | C8-N9-C4 | 8.22 | 109.69 | 106.40 |
| 36 | A5 | 2859 | U | N3-C4-O4 | -8.22 | 113.65 | 119.40 |
| 36 | A1 | 369 | A | N1-C6-N6 | -8.22 | 113.67 | 118.60 |
| 1 | A2 | 992 | A | C5-N7-C8 | -8.22 | 99.79 | 103.90 |
| 36 | A5 | 818 | C | N1-C2-O2 | -8.22 | 113.97 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 1178 | G | C8-N9-C4 | -8.22 | 103.11 | 106.40 |
| 1 | A2 | 319 | U | N3-C2-O2 | 8.22 | 127.95 | 122.20 |
| 1 | A2 | 1096 | C | N1-C2-O2 | 8.22 | 123.83 | 118.90 |
| 38 | A4 | 79 | A | C8-N9-C4 | -8.21 | 102.51 | 105.80 |
| 36 | A5 | 15 | C | C5-C6-N1 | 8.21 | 125.11 | 121.00 |
| 36 | A5 | 1586 | G | C5-C6-O6 | -8.21 | 123.67 | 128.60 |
| 36 | A1 | 2293 | C | C5-C4-N4 | -8.21 | 114.45 | 120.20 |
| 36 | A5 | 2735 | U | C5-C6-N1 | 8.21 | 126.81 | 122.70 |
| 36 | A5 | 435 | C | N3-C4-C5 | 8.21 | 125.18 | 121.90 |
| 36 | A1 | 1515 | A | C4-C5-C6 | 8.21 | 121.11 | 117.00 |
| 80 | A6 | 1595 | U | C5-C4-O4 | 8.21 | 130.82 | 125.90 |
| 36 | A5 | 1015 | U | C5-C6-N1 | 8.21 | 126.80 | 122.70 |
| 36 | A5 | 2211 | U | N3-C2-O2 | -8.21 | 116.45 | 122.20 |
| 36 | A1 | 2909 | U | N3-C4-O4 | 8.20 | 125.14 | 119.40 |
| 36 | A5 | 591 | G | N9-C4-C5 | -8.21 | 102.12 | 105.40 |
| 36 | A5 | 922 | U | C6-N1-C1' | 8.21 | 132.69 | 121.20 |
| 36 | A5 | 1404 | G | C8-N9-C4 | 8.20 | 109.68 | 106.40 |
| 36 | A1 | 2169 | G | C6-C5-N7 | 8.20 | 135.32 | 130.40 |
| 36 | A1 | 2816 | G | C5-C6-N1 | 8.20 | 115.60 | 111.50 |
| 36 | A5 | 2202 | C | N3-C2-O2 | 8.20 | 127.64 | 121.90 |
| 36 | A1 | 345 | G | N3-C4-C5 | -8.20 | 124.50 | 128.60 |
| 36 | A1 | 432 | G | C2-N3-C4 | -8.20 | 107.80 | 111.90 |
| 36 | A1 | 2572 | C | C6-N1-C2 | -8.20 | 117.02 | 120.30 |
| 36 | A5 | 1054 | A | C8-N9-C4 | 8.20 | 109.08 | 105.80 |
| 36 | A5 | 968 | G | N9-C4-C5 | -8.20 | 102.12 | 105.40 |
| 36 | A1 | 3318 | G | C4-N9-C1' | 8.20 | 137.16 | 126.50 |
| 36 | A1 | 2618 | G | C5-C6-N1 | 8.20 | 115.60 | 111.50 |
| 36 | A1 | 1133 | A | C8-N9-C4 | 8.19 | 109.08 | 105.80 |
| 36 | A5 | 514 | G | C5-C6-O6 | -8.19 | 123.68 | 128.60 |
| 36 | A1 | 1142 | G | N3-C4-N9 | 8.19 | 130.91 | 126.00 |
| 36 | A1 | 2990 | G | C4-C5-N7 | -8.19 | 107.52 | 110.80 |
| 38 | A4 | 58 | G | N3-C4-N9 | 8.19 | 130.91 | 126.00 |
| 36 | A1 | 2777 | G | N3-C4-C5 | 8.19 | 132.69 | 128.60 |
| 36 | A5 | 2190 | U | N3-C4-O4 | -8.19 | 113.67 | 119.40 |
| 36 | A5 | 343 | U | N1-C2-O2 | 8.19 | 128.53 | 122.80 |
| 36 | A1 | 874 | U | N3-C4-O4 | -8.18 | 113.67 | 119.40 |
| 36 | A5 | 949 | C | C4-C5-C6 | 8.18 | 121.49 | 117.40 |
| 38 | A4 | 103 | G | N1-C6-O6 | -8.18 | 114.99 | 119.90 |
| 56 | DS | 115 | ARG | NE-CZ-NH1 | 8.18 | 124.39 | 120.30 |
| 36 | A1 | 1180 | A | N1-C2-N3 | 8.18 | 133.39 | 129.30 |
| 36 | A1 | 544 | C | C6-N1-C2 | -8.17 | 117.03 | 120.30 |
| 36 | A5 | 2913 | C | N1-C2-N3 | 8.17 | 124.92 | 119.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 38 | A4 | 32 | C | N1-C2-O2 | -8.17 | 114.00 | 118.90 |
| 36 | A5 | 2609 | A | C5-N7-C8 | 8.17 | 107.99 | 103.90 |
| 36 | A1 | 2595 | A | C4-C5-N7 | 8.17 | 114.78 | 110.70 |
| 36 | A5 | 805 | G | C8-N9-C4 | 8.17 | 109.67 | 106.40 |
| 36 | A5 | 280 | U | C2-N3-C4 | -8.17 | 122.10 | 127.00 |
| 36 | A5 | 435 | C | C5-C4-N4 | -8.17 | 114.48 | 120.20 |
| 36 | A5 | 1110 | U | N3-C4-C5 | 8.17 | 119.50 | 114.60 |
| 36 | A5 | 3317 | U | C5-C4-O4 | 8.17 | 130.80 | 125.90 |
| 36 | A1 | 631 | U | C2-N3-C4 | -8.16 | 122.10 | 127.00 |
| 36 | A5 | 926 | A | C5-C6-N6 | -8.16 | 117.17 | 123.70 |
| 36 | A5 | 726 | G | N1-C6-O6 | 8.16 | 124.80 | 119.90 |
| 36 | A5 | 1445 | U | C5-C4-O4 | -8.16 | 121.00 | 125.90 |
| 36 | A5 | 2302 | G | C5-C6-O6 | 8.15 | 133.49 | 128.60 |
| 36 | A5 | 3122 | A | N9-C4-C5 | 8.15 | 109.06 | 105.80 |
| 36 | A5 | 708 | G | C5-N7-C8 | -8.15 | 100.22 | 104.30 |
| 36 | A1 | 2176 | U | N1-C2-O2 | 8.15 | 128.50 | 122.80 |
| 36 | A5 | 2970 | C | C4-C5-C6 | 8.15 | 121.47 | 117.40 |
| 36 | A1 | 2572 | C | C2-N1-C1' | 8.15 | 127.76 | 118.80 |
| 36 | A1 | 2409 | G | N9-C4-C5 | 8.14 | 108.66 | 105.40 |
| 36 | A1 | 2622 | C | C6-N1-C2 | -8.14 | 117.04 | 120.30 |
| 1 | A2 | 1241 | G | C5-N7-C8 | -8.14 | 100.23 | 104.30 |
| 36 | A1 | 883 | A | C2-N3-C4 | 8.14 | 114.67 | 110.60 |
| 36 | A1 | 2278 | C | N3-C4-C5 | 8.14 | 125.16 | 121.90 |
| 80 | A6 | 17 | C | N1-C2-O2 | 8.14 | 123.78 | 118.90 |
| 36 | A5 | 987 | U | N1-C2-N3 | 8.14 | 119.78 | 114.90 |
| 36 | A1 | 2356 | A | N1-C2-N3 | -8.13 | 125.23 | 129.30 |
| 36 | A5 | 1176 | C | C5-C6-N1 | -8.13 | 116.93 | 121.00 |
| 36 | A5 | 2412 | G | C8-N9-C4 | -8.13 | 103.15 | 106.40 |
| 1 | A2 | 308 | C | C5-C6-N1 | -8.13 | 116.94 | 121.00 |
| 36 | A1 | 1434 | G | C4-C5-C6 | 8.13 | 123.68 | 118.80 |
| 36 | A5 | 1085 | A | C5-N7-C8 | -8.13 | 99.83 | 103.90 |
| 36 | A1 | 1617 | G | C8-N9-C4 | 8.13 | 109.65 | 106.40 |
| 1 | A2 | 1129 | U | N3-C4-C5 | 8.13 | 119.48 | 114.60 |
| 36 | A5 | 2838 | A | C5-C6-N6 | -8.13 | 117.20 | 123.70 |
| 36 | A1 | 405 | U | C5-C4-O4 | -8.12 | 121.03 | 125.90 |
| 36 | A1 | 1049 | C | C5-C4-N4 | -8.12 | 114.52 | 120.20 |
| 36 | A1 | 1362 | G | C8-N9-C4 | 8.12 | 109.65 | 106.40 |
| 38 | A4 | 113 | U | C4-C5-C6 | 8.12 | 124.57 | 119.70 |
| 36 | A5 | 2665 | U | N1-C2-N3 | -8.12 | 110.03 | 114.90 |
| 36 | A5 | 2859 | U | C5-C4-O4 | 8.12 | 130.77 | 125.90 |
| 1 | A2 | 1291 | G | N1-C2-N3 | 8.11 | 128.77 | 123.90 |
| 36 | A1 | 3049 | A | C5-C6-N1 | -8.12 | 113.64 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 36 | A5 | 769 | G | C8-N9-C4 | 8.12 | 109.65 | 106.40 |
| 36 | A5 | 842 | G | C5-C6-O6 | -8.11 | 123.73 | 128.60 |
| 36 | A1 | 651 | G | N3-C4-C5 | -8.11 | 124.54 | 128.60 |
| 36 | A1 | 653 | A | C5-C6-N1 | 8.11 | 121.76 | 117.70 |
| 36 | A5 | 2634 | U | N3-C4-C5 | 8.11 | 119.47 | 114.60 |
| 36 | A1 | 847 | A | N9-C4-C5 | -8.11 | 102.56 | 105.80 |
| 36 | A1 | 1132 | C | N3-C4-N4 | -8.11 | 112.33 | 118.00 |
| 36 | A1 | 1947 | G | N3-C2-N2 | -8.11 | 114.23 | 119.90 |
| 36 | A5 | 637 | C | N1-C2-O2 | -8.10 | 114.04 | 118.90 |
| 36 | A1 | 1523 | U | N1-C2-O2 | -8.10 | 117.13 | 122.80 |
| 36 | A5 | 2246 | G | N1-C6-O6 | -8.10 | 115.04 | 119.90 |
| 36 | A5 | 290 | G | C5-C6-O6 | 8.10 | 133.46 | 128.60 |
| 36 | A5 | 817 | A | C2-N3-C4 | 8.10 | 114.65 | 110.60 |
| 36 | A1 | 1123 | U | C5-C6-N1 | -8.10 | 118.65 | 122.70 |
| 36 | A1 | 2165 | G | N1-C6-O6 | 8.09 | 124.76 | 119.90 |
| 36 | A1 | 2288 | G | C8-N9-C4 | -8.09 | 103.16 | 106.40 |
| 36 | A5 | 2175 | U | C5-C6-N1 | -8.09 | 118.65 | 122.70 |
| 36 | A5 | 916 | G | N1-C6-O6 | -8.09 | 115.05 | 119.90 |
| 36 | A1 | 2200 | U | C6-N1-C2 | -8.09 | 116.15 | 121.00 |
| 36 | A5 | 2278 | C | C5-C4-N4 | 8.09 | 125.86 | 120.20 |
| 36 | A5 | 2440 | G | C8-N9-C4 | -8.09 | 103.17 | 106.40 |
| 36 | A5 | 3362 | A | N1-C2-N3 | 8.09 | 133.34 | 129.30 |
| 36 | A1 | 2550 | U | N1-C2-N3 | 8.08 | 119.75 | 114.90 |
| 36 | A1 | 3207 | U | C5-C4-O4 | 8.08 | 130.75 | 125.90 |
| 36 | A5 | 329 | U | C5-C6-N1 | -8.08 | 118.66 | 122.70 |
| 36 | A5 | 1512 | U | N1-C2-N3 | 8.08 | 119.75 | 114.90 |
| 36 | A5 | 2182 | A | N1-C6-N6 | -8.08 | 113.75 | 118.60 |
| 36 | A5 | 3215 | A | N1-C6-N6 | 8.08 | 123.45 | 118.60 |
| 38 | A8 | 38 | U | C5-C6-N1 | -8.08 | 118.66 | 122.70 |
| 36 | A5 | 2290 | C | C4-C5-C6 | 8.08 | 121.44 | 117.40 |
| 1 | A2 | 1773 | C | C5-C6-N1 | 8.08 | 125.04 | 121.00 |
| 36 | A5 | 1390 | A | N9-C4-C5 | 8.07 | 109.03 | 105.80 |
| 36 | A5 | 1516 | C | C2-N3-C4 | -8.07 | 115.86 | 119.90 |
| 36 | A5 | 945 | C | C2-N3-C4 | -8.07 | 115.86 | 119.90 |
| 38 | A8 | 2 | A | C8-N9-C4 | -8.07 | 102.57 | 105.80 |
| 80 | A6 | 418 | G | C6-C5-N7 | -8.07 | 125.56 | 130.40 |
| 36 | A5 | 41 | G | C5-N7-C8 | -8.07 | 100.27 | 104.30 |
| 37 | A7 | 112 | G | N1-C6-O6 | -8.07 | 115.06 | 119.90 |
| 36 | A5 | 1879 | A | C8-N9-C4 | -8.07 | 102.57 | 105.80 |
| 1 | A2 | 1436 | A | N1-C6-N6 | 8.07 | 123.44 | 118.60 |
| 38 | A8 | 113 | U | N3-C4-O4 | 8.06 | 125.04 | 119.40 |
| 36 | A1 | 2735 | U | N3-C4-C5 | 8.05 | 119.43 | 114.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 38 | A4 | 32 | C | C2-N1-C1' | -8.05 | 109.94 | 118.80 |
| 36 | A5 | 1449 | A | C5-N7-C8 | -8.05 | 99.88 | 103.90 |
| 80 | A6 | 1000 | C | C2-N1-C1' | 8.05 | 127.65 | 118.80 |
| 36 | A5 | 359 | U | C2-N3-C4 | -8.05 | 122.17 | 127.00 |
| 36 | A5 | 1193 | A | N1-C2-N3 | 8.05 | 133.32 | 129.30 |
| 36 | A5 | 1858 | A | N3-C4-C5 | -8.05 | 121.17 | 126.80 |
| 1 | A2 | 1200 | G | N1-C2-N2 | 8.04 | 123.44 | 116.20 |
| 36 | A1 | 2318 | U | C2-N3-C4 | -8.04 | 122.17 | 127.00 |
| 36 | A5 | 413 | U | C2-N3-C4 | -8.04 | 122.17 | 127.00 |
| 36 | A5 | 631 | U | C2-N3-C4 | -8.04 | 122.17 | 127.00 |
| 1 | A2 | 1324 | G | N3-C4-N9 | -8.04 | 121.17 | 126.00 |
| 36 | A1 | 2382 | G | N1-C6-O6 | -8.04 | 115.08 | 119.90 |
| 36 | A1 | 2893 | C | N3-C4-C5 | 8.04 | 125.12 | 121.90 |
| 36 | A1 | 2952 | G | C5-N7-C8 | -8.04 | 100.28 | 104.30 |
| 36 | A5 | 3110 | C | C4-C5-C6 | 8.04 | 121.42 | 117.40 |
| 36 | A1 | 2284 | C | C2-N3-C4 | -8.04 | 115.88 | 119.90 |
| 54 | BQ | 178 | ARG | NE-CZ-NH1 | -8.04 | 116.28 | 120.30 |
| 52 | DO | 3[B] | SER | O-C-N | 8.04 | 135.56 | 122.70 |
| 80 | A6 | 100 | A | C8-N9-C4 | 8.04 | 109.02 | 105.80 |
| 36 | A5 | 1879 | A | C6-C5-N7 | -8.04 | 126.67 | 132.30 |
| 44 | DF | 88 | ARG | NE-CZ-NH2 | -8.04 | 116.28 | 120.30 |
| 36 | A1 | 2595 | A | C2-N3-C4 | -8.04 | 106.58 | 110.60 |
| 36 | A1 | 2821 | C | C6-N1-C2 | -8.04 | 117.08 | 120.30 |
| 36 | A1 | 2836 | C | C6-N1-C2 | -8.04 | 117.09 | 120.30 |
| 36 | A1 | 3180 | A | N9-C4-C5 | 8.04 | 109.01 | 105.80 |
| 36 | A5 | 278 | U | C5-C6-N1 | 8.03 | 126.72 | 122.70 |
| 80 | A6 | 1389 | C | C2-N1-C1' | 8.03 | 127.64 | 118.80 |
| 36 | A5 | 945 | C | C6-N1-C2 | 8.03 | 123.51 | 120.30 |
| 36 | A5 | 2278 | C | C2-N3-C4 | -8.03 | 115.89 | 119.90 |
| 36 | A1 | 3119 | U | N3-C4-O4 | -8.03 | 113.78 | 119.40 |
| 36 | A5 | 824 | C | C6-N1-C2 | -8.03 | 117.09 | 120.30 |
| 36 | A1 | 2860 | U | C5-C4-O4 | -8.03 | 121.08 | 125.90 |
| 36 | A5 | 2189 | U | N1-C2-N3 | 8.03 | 119.72 | 114.90 |
| 80 | A6 | 1782 | A | C8-N9-C4 | -8.03 | 102.59 | 105.80 |
| 38 | A8 | 74 | U | C5-C4-O4 | -8.02 | 121.09 | 125.90 |
| 36 | A1 | 1848 | G | C5-C6-O6 | -8.02 | 123.79 | 128.60 |
| 36 | A1 | 2328 | U | N3-C4-O4 | -8.02 | 113.79 | 119.40 |
| 1 | A2 | 1662 | G | N1-C6-O6 | -8.02 | 115.09 | 119.90 |
| 36 | A1 | 817 | A | C6-N1-C2 | -8.02 | 113.79 | 118.60 |
| 36 | A1 | 2329 | C | N1-C2-O2 | -8.02 | 114.09 | 118.90 |
| 80 | A6 | 1735 | U | N3-C4-C5 | 8.02 | 119.41 | 114.60 |
| 36 | A5 | 2572 | C | C2-N1-C1' | 8.02 | 127.62 | 118.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 1395 | G | N3-C2-N2 | 8.02 | 125.51 | 119.90 |
| 36 | A5 | 2630 | C | N3-C4-C5 | 8.02 | 125.11 | 121.90 |
| 1 | A2 | 1490 | C | C6-N1-C2 | -8.01 | 117.09 | 120.30 |
| 36 | A1 | 1397 | C | N1-C2-O2 | -8.01 | 114.09 | 118.90 |
| 36 | A5 | 2281 | A | C8-N9-C4 | 8.01 | 109.00 | 105.80 |
| 36 | A1 | 1483 | G | N1-C6-O6 | -8.01 | 115.09 | 119.90 |
| 80 | A6 | 418 | G | C8-N9-C4 | -8.01 | 103.20 | 106.40 |
| 80 | A6 | 1644 | C | C2-N3-C4 | -8.01 | 115.90 | 119.90 |
| 36 | A5 | 1592 | G | C5-C6-N1 | 8.01 | 115.50 | 111.50 |
| 1 | A2 | 316 | A | C8-N9-C4 | 8.00 | 109.00 | 105.80 |
| 36 | A5 | 857 | G | C5-C6-N1 | 8.00 | 115.50 | 111.50 |
| 36 | A5 | 3309 | G | N3-C4-N9 | 8.00 | 130.80 | 126.00 |
| 37 | A3 | 81 | U | C6-N1-C1' | -8.00 | 110.00 | 121.20 |
| 65 | Db | 39 | PHE | N-CA-CB | 8.00 | 125.00 | 110.60 |
| 1 | A2 | 349 | U | N3-C2-O2 | -8.00 | 116.60 | 122.20 |
| 36 | A1 | 1881 | A | C8-N9-C4 | 8.00 | 109.00 | 105.80 |
| 36 | A1 | 2360 | C | C4-C5-C6 | 8.00 | 121.40 | 117.40 |
| 80 | A6 | 65 | A | N1-C6-N6 | 8.00 | 123.40 | 118.60 |
| 36 | A5 | 3362 | A | C8-N9-C4 | -8.00 | 102.60 | 105.80 |
| 80 | A6 | 858 | G | N7-C8-N9 | 7.99 | 117.10 | 113.10 |
| 36 | A5 | 1481 | A | N7-C8-N9 | 7.99 | 117.80 | 113.80 |
| 36 | A5 | 1441 | G | N1-C6-O6 | -7.99 | 115.11 | 119.90 |
| 36 | A1 | 620 | U | C6-N1-C2 | -7.99 | 116.21 | 121.00 |
| 36 | A1 | 891 | G | C5-C6-O6 | 7.99 | 133.39 | 128.60 |
| 36 | A5 | 1113 | G | C8-N9-C4 | 7.99 | 109.60 | 106.40 |
| 36 | A5 | 2777 | G | C5-C6-O6 | 7.99 | 133.39 | 128.60 |
| 36 | A1 | 3214 | U | N1-C2-N3 | 7.99 | 119.69 | 114.90 |
| 37 | A3 | 82 | G | N1-C2-N3 | 7.99 | 128.69 | 123.90 |
| 36 | A1 | 56 | G | C5-C6-O6 | -7.98 | 123.81 | 128.60 |
| 36 | A5 | 2350 | C | C5-C6-N1 | -7.98 | 117.01 | 121.00 |
| 36 | A1 | 695 | C | N3-C4-N4 | -7.98 | 112.41 | 118.00 |
| 37 | A7 | 81 | U | N3-C4-C5 | 7.98 | 119.39 | 114.60 |
| 36 | A1 | 2395 | G | N3-C4-C5 | -7.98 | 124.61 | 128.60 |
| 36 | A5 | 3215 | A | C2-N3-C4 | -7.98 | 106.61 | 110.60 |
| 36 | A1 | 966 | U | N3-C4-C5 | 7.98 | 119.39 | 114.60 |
| 36 | A5 | 2317 | A | C8-N9-C4 | -7.97 | 102.61 | 105.80 |
| 36 | A5 | 2512 | C | C5-C6-N1 | 7.97 | 124.99 | 121.00 |
| 36 | A5 | 3343 | G | N9-C4-C5 | -7.97 | 102.21 | 105.40 |
| 37 | A7 | 85 | G | N1-C6-O6 | -7.97 | 115.12 | 119.90 |
| 36 | A1 | 281 | G | C8-N9-C4 | -7.97 | 103.21 | 106.40 |
| 36 | A1 | 960 | U | C2-N3-C4 | -7.97 | 122.22 | 127.00 |
| 80 | A6 | 826 | U | C5-C6-N1 | 7.97 | 126.68 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 80 | A6 | 1100 | G | C6-N1-C2 | -7.97 | 120.32 | 125.10 |
| 36 | A5 | 345 | G | N1-C6-O6 | -7.97 | 115.12 | 119.90 |
| 36 | A5 | 1148 | G | C2-N3-C4 | 7.97 | 115.88 | 111.90 |
| 36 | A1 | 24 | G | N1-C6-O6 | 7.97 | 124.68 | 119.90 |
| 36 | A5 | 1297 | C | C5-C6-N1 | -7.97 | 117.02 | 121.00 |
| 36 | A5 | 2366 | C | N3-C4-N4 | 7.96 | 123.58 | 118.00 |
| 36 | A5 | 3343 | G | N3-C4-N9 | 7.96 | 130.78 | 126.00 |
| 36 | A5 | 2288 | G | C2-N3-C4 | 7.96 | 115.88 | 111.90 |
| 36 | A1 | 54 | C | N3-C4-C5 | 7.96 | 125.08 | 121.90 |
| 36 | A1 | 1309 | U | C5-C4-O4 | -7.96 | 121.12 | 125.90 |
| 36 | A1 | 2369 | G | N3-C4-N9 | 7.96 | 130.78 | 126.00 |
| 36 | A5 | 2870 | C | C6-N1-C1' | 7.96 | 130.35 | 120.80 |
| 80 | A6 | 400 | A | N1-C6-N6 | 7.95 | 123.37 | 118.60 |
| 36 | A5 | 784 | A | N1-C6-N6 | 7.95 | 123.37 | 118.60 |
| 36 | A1 | 1003 | A | N1-C6-N6 | 7.95 | 123.37 | 118.60 |
| 36 | A1 | 2138 | A | N9-C4-C5 | 7.95 | 108.98 | 105.80 |
| 80 | A6 | 1749 | A | C4-C5-N7 | 7.95 | 114.67 | 110.70 |
| 36 | A1 | 121 | A | C8-N9-C4 | 7.95 | 108.98 | 105.80 |
| 36 | A1 | 962 | A | N1-C2-N3 | 7.95 | 133.27 | 129.30 |
| 36 | A1 | 2751 | G | C5-C6-O6 | -7.95 | 123.83 | 128.60 |
| 52 | BO | 158[B] | ASP | C-N-CA | -7.95 | 101.84 | 121.70 |
| 36 | A5 | 3377 | G | N9-C4-C5 | -7.94 | 102.22 | 105.40 |
| 36 | A1 | 1556 | C | C6-N1-C2 | -7.94 | 117.12 | 120.30 |
| 36 | A1 | 2885 | C | N3-C4-C5 | 7.94 | 125.08 | 121.90 |
| 36 | A1 | 2952 | G | N9-C4-C5 | -7.94 | 102.22 | 105.40 |
| 36 | A5 | 3151 | U | C6-N1-C2 | 7.94 | 125.76 | 121.00 |
| 1 | A2 | 1611 | A | N7-C8-N9 | 7.94 | 117.77 | 113.80 |
| 36 | A1 | 3278 | C | N3-C2-O2 | -7.94 | 116.34 | 121.90 |
| 36 | A5 | 1317 | A | N1-C6-N6 | 7.94 | 123.36 | 118.60 |
| 36 | A5 | 2757 | U | N3-C4-O4 | 7.94 | 124.96 | 119.40 |
| 36 | A1 | 1907 | C | C2-N3-C4 | 7.94 | 123.87 | 119.90 |
| 36 | A1 | 2356 | A | C5-C6-N6 | -7.94 | 117.35 | 123.70 |
| 36 | A1 | 3277 | U | N3-C2-O2 | -7.94 | 116.64 | 122.20 |
| 36 | A5 | 355 | A | C2-N3-C4 | -7.94 | 106.63 | 110.60 |
| 36 | A5 | 629 | U | N3-C4-C5 | 7.94 | 119.36 | 114.60 |
| 36 | A1 | 2829 | U | N3-C2-O2 | -7.93 | 116.65 | 122.20 |
| 36 | A5 | 3102 | G | N1-C6-O6 | -7.93 | 115.14 | 119.90 |
| 36 | A5 | 1484 | U | C6-N1-C2 | 7.93 | 125.76 | 121.00 |
| 1 | A2 | 145 | A | C8-N9-C4 | -7.93 | 102.63 | 105.80 |
| 36 | A1 | 3375 | A | N7-C8-N9 | 7.93 | 117.76 | 113.80 |
| 36 | A1 | 909 | G | C8-N9-C4 | 7.92 | 109.57 | 106.40 |
| 36 | A1 | 1741 | A | N1-C2-N3 | 7.92 | 133.26 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-------|------|-----------|-------|-------------|----------|
| 1 | A2 | 1432 | U | C6-N1-C2 | 7.92 | 125.75 | 121.00 |
| 1 | A2 | 189 | C | C2-N1-C1' | 7.92 | 127.51 | 118.80 |
| 38 | A4 | 58 | G | C5-C6-O6 | -7.92 | 123.85 | 128.60 |
| 36 | A5 | 277 | G | N1-C6-O6 | -7.92 | 115.15 | 119.90 |
| 80 | A6 | 453 | U | N3-C4-O4 | -7.92 | 113.86 | 119.40 |
| 36 | A5 | 2550 | U | N1-C2-N3 | 7.91 | 119.65 | 114.90 |
| 1 | A2 | 1481 | C | C6-N1-C2 | -7.91 | 117.14 | 120.30 |
| 36 | A1 | 1307 | G | N3-C2-N2 | 7.91 | 125.44 | 119.90 |
| 36 | A1 | 963 | G | C6-C5-N7 | -7.91 | 125.65 | 130.40 |
| 36 | A1 | 2117 | A | N1-C6-N6 | -7.91 | 113.86 | 118.60 |
| 68 | De | 43 | ARG | NE-CZ-NH2 | -7.91 | 116.35 | 120.30 |
| 36 | A5 | 2836 | C | N1-C2-N3 | 7.91 | 124.73 | 119.20 |
| 36 | A5 | 934 | G | C5-C6-O6 | -7.91 | 123.86 | 128.60 |
| 36 | A5 | 2531 | C | C2-N1-C1' | 7.91 | 127.50 | 118.80 |
| 52 | DO | 27[B] | VAL | O-C-N | -7.90 | 110.05 | 122.70 |
| 36 | A1 | 2776 | C | C2-N3-C4 | -7.90 | 115.95 | 119.90 |
| 80 | A6 | 864 | U | N3-C2-O2 | -7.90 | 116.67 | 122.20 |
| 36 | A5 | 960 | U | C5-C6-N1 | -7.90 | 118.75 | 122.70 |
| 36 | A5 | 1940 | G | N3-C2-N2 | 7.90 | 125.43 | 119.90 |
| 36 | A1 | 47 | C | C5-C6-N1 | -7.90 | 117.05 | 121.00 |
| 36 | A5 | 2381 | G | C8-N9-C4 | -7.90 | 103.24 | 106.40 |
| 36 | A5 | 851 | C | C6-N1-C2 | -7.90 | 117.14 | 120.30 |
| 36 | A1 | 2714 | G | C4-C5-C6 | -7.89 | 114.06 | 118.80 |
| 80 | A6 | 1 | U | C6-N1-C2 | -7.89 | 116.26 | 121.00 |
| 36 | A1 | 1919 | G | N1-C6-O6 | -7.89 | 115.16 | 119.90 |
| 36 | A1 | 2380 | U | C2-N3-C4 | -7.89 | 122.26 | 127.00 |
| 36 | A5 | 2618 | G | C5-C6-O6 | -7.89 | 123.86 | 128.60 |
| 36 | A1 | 3302 | U | C6-N1-C2 | 7.89 | 125.73 | 121.00 |
| 80 | A6 | 1535 | U | N3-C2-O2 | -7.89 | 116.68 | 122.20 |
| 36 | A5 | 2913 | C | C5-C6-N1 | -7.89 | 117.06 | 121.00 |
| 36 | A5 | 1939 | G | C5-C6-O6 | 7.89 | 133.33 | 128.60 |
| 36 | A1 | 2281 | A | C8-N9-C4 | 7.88 | 108.95 | 105.80 |
| 36 | A5 | 2919 | A | N1-C6-N6 | -7.88 | 113.87 | 118.60 |
| 36 | A5 | 2993 | G | C5-C6-O6 | -7.88 | 123.87 | 128.60 |
| 1 | A2 | 864 | U | N3-C2-O2 | -7.88 | 116.68 | 122.20 |
| 36 | A1 | 508 | U | C5-C4-O4 | -7.88 | 121.17 | 125.90 |
| 37 | A7 | 26 | C | C4-C5-C6 | 7.88 | 121.34 | 117.40 |
| 36 | A5 | 2130 | G | N3-C2-N2 | 7.88 | 125.41 | 119.90 |
| 36 | A1 | 1048 | A | C6-N1-C2 | 7.87 | 123.32 | 118.60 |
| 36 | A5 | 2865 | U | C5-C4-O4 | -7.87 | 121.18 | 125.90 |
| 36 | A1 | 1138 | U | N1-C2-N3 | 7.87 | 119.62 | 114.90 |
| 80 | A6 | 1489 | U | N3-C2-O2 | -7.87 | 116.69 | 122.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 3146 | G | C5-C6-O6 | 7.87 | 133.32 | 128.60 |
| 36 | A5 | 630 | A | N1-C2-N3 | 7.87 | 133.23 | 129.30 |
| 36 | A5 | 2366 | C | C2-N1-C1' | 7.87 | 127.46 | 118.80 |
| 36 | A1 | 660 | A | N1-C6-N6 | -7.87 | 113.88 | 118.60 |
| 36 | A1 | 718 | G | C4-C5-N7 | 7.87 | 113.95 | 110.80 |
| 36 | A1 | 62 | A | C2-N3-C4 | 7.87 | 114.53 | 110.60 |
| 36 | A1 | 3034 | C | N1-C2-O2 | 7.87 | 123.62 | 118.90 |
| 36 | A5 | 1480 | G | C5-N7-C8 | 7.87 | 108.23 | 104.30 |
| 44 | DF | 88 | ARG | NE-CZ-NH1 | 7.87 | 124.23 | 120.30 |
| 36 | A1 | 344 | A | N1-C6-N6 | -7.86 | 113.88 | 118.60 |
| 36 | A1 | 2870 | C | C2-N1-C1' | -7.86 | 110.15 | 118.80 |
| 80 | A6 | 542 | A | C8-N9-C4 | -7.86 | 102.66 | 105.80 |
| 36 | A1 | 301 | G | N1-C6-O6 | -7.86 | 115.19 | 119.90 |
| 36 | A1 | 1858 | A | C8-N9-C4 | -7.86 | 102.66 | 105.80 |
| 36 | A1 | 2996 | U | N1-C2-O2 | 7.86 | 128.30 | 122.80 |
| 80 | A6 | 337 | G | N3-C4-N9 | 7.86 | 130.71 | 126.00 |
| 36 | A1 | 340 | C | N3-C4-C5 | 7.85 | 125.04 | 121.90 |
| 36 | A1 | 1403 | C | C5-C6-N1 | -7.85 | 117.07 | 121.00 |
| 36 | A1 | 3275 | U | C5-C6-N1 | 7.85 | 126.62 | 122.70 |
| 36 | A5 | 813 | G | C8-N9-C4 | -7.85 | 103.26 | 106.40 |
| 41 | DC | 339 | LEU | CA-CB-CG | 7.85 | 133.35 | 115.30 |
| 80 | A6 | 1456 | C | N3-C4-N4 | -7.85 | 112.51 | 118.00 |
| 36 | A5 | 1140 | G | N1-C6-O6 | -7.85 | 115.19 | 119.90 |
| 36 | A5 | 1793 | C | N3-C4-C5 | -7.85 | 118.76 | 121.90 |
| 36 | A5 | 1834 | U | C2-N1-C1' | -7.85 | 108.28 | 117.70 |
| 36 | A5 | 1845 | G | C5-C6-N1 | 7.85 | 115.42 | 111.50 |
| 36 | A1 | 1796 | G | C8-N9-C4 | -7.85 | 103.26 | 106.40 |
| 1 | A2 | 581 | U | C2-N1-C1' | 7.84 | 127.11 | 117.70 |
| 36 | A1 | 2777 | G | C5-C6-N1 | 7.84 | 115.42 | 111.50 |
| 36 | A5 | 343 | U | N3-C4-O4 | -7.84 | 113.91 | 119.40 |
| 36 | A5 | 2400 | G | C2-N3-C4 | -7.84 | 107.98 | 111.90 |
| 80 | A6 | 1745 | G | N3-C4-N9 | 7.84 | 130.70 | 126.00 |
| 36 | A5 | 2303 | A | N9-C4-C5 | 7.84 | 108.93 | 105.80 |
| 36 | A5 | 3130 | A | N1-C2-N3 | 7.84 | 133.22 | 129.30 |
| 36 | A1 | 434 | U | C4-C5-C6 | -7.83 | 115.00 | 119.70 |
| 36 | A1 | 1341 | U | N1-C2-O2 | 7.83 | 128.28 | 122.80 |
| 36 | A1 | 2814 | G | N7-C8-N9 | -7.83 | 109.18 | 113.10 |
| 36 | A1 | 655 | C | C4-C5-C6 | 7.83 | 121.31 | 117.40 |
| 36 | A5 | 530 | G | N1-C6-O6 | -7.83 | 115.20 | 119.90 |
| 36 | A1 | 1392 | G | N3-C4-N9 | 7.83 | 130.70 | 126.00 |
| 36 | A1 | 1494 | U | C5-C6-N1 | -7.83 | 118.79 | 122.70 |
| 36 | A1 | 2214 | A | N1-C6-N6 | 7.83 | 123.30 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 80 | A6 | 397 | A | C2-N3-C4 | -7.82 | 106.69 | 110.60 |
| 36 | A1 | 545 | U | C2-N1-C1' | 7.82 | 127.09 | 117.70 |
| 80 | A6 | 1185 | U | N1-C2-O2 | 7.82 | 128.28 | 122.80 |
| 36 | A5 | 2288 | G | C6-N1-C2 | -7.82 | 120.41 | 125.10 |
| 36 | A1 | 2719 | U | N1-C2-N3 | 7.82 | 119.59 | 114.90 |
| 36 | A1 | 2400 | G | N3-C4-N9 | -7.81 | 121.31 | 126.00 |
| 1 | A2 | 555 | A | C8-N9-C4 | -7.81 | 102.67 | 105.80 |
| 36 | A1 | 2156 | C | C5-C6-N1 | -7.81 | 117.09 | 121.00 |
| 36 | A5 | 1392 | G | N3-C4-N9 | 7.81 | 130.69 | 126.00 |
| 36 | A5 | 3096 | C | N1-C2-N3 | 7.81 | 124.67 | 119.20 |
| 36 | A1 | 1152 | G | N1-C2-N3 | 7.81 | 128.59 | 123.90 |
| 36 | A1 | 3209 | A | N1-C6-N6 | 7.81 | 123.29 | 118.60 |
| 36 | A5 | 226 | C | C6-N1-C2 | 7.81 | 123.42 | 120.30 |
| 36 | A5 | 2395 | G | C5-N7-C8 | 7.81 | 108.20 | 104.30 |
| 36 | A5 | 2705 | A | C5-C6-N6 | -7.81 | 117.45 | 123.70 |
| 36 | A1 | 644 | G | C4-C5-N7 | -7.80 | 107.68 | 110.80 |
| 36 | A1 | 644 | G | N3-C2-N2 | 7.80 | 125.36 | 119.90 |
| 36 | A5 | 1295 | G | N1-C6-O6 | -7.80 | 115.22 | 119.90 |
| 36 | A5 | 1390 | A | C8-N9-C4 | -7.80 | 102.68 | 105.80 |
| 1 | A2 | 1751 | C | N3-C4-C5 | 7.80 | 125.02 | 121.90 |
| 36 | A1 | 50 | U | C2-N3-C4 | -7.80 | 122.32 | 127.00 |
| 36 | A1 | 659 | G | N3-C2-N2 | 7.80 | 125.36 | 119.90 |
| 36 | A5 | 276 | U | C5-C6-N1 | -7.80 | 118.80 | 122.70 |
| 36 | A5 | 2882 | U | N1-C2-N3 | 7.80 | 119.58 | 114.90 |
| 36 | A5 | 1364 | C | N1-C2-O2 | -7.80 | 114.22 | 118.90 |
| 36 | A5 | 2807 | U | C5-C4-O4 | -7.80 | 121.22 | 125.90 |
| 36 | A5 | 641 | C | N1-C2-O2 | -7.80 | 114.22 | 118.90 |
| 36 | A5 | 708 | G | C5-C6-O6 | -7.79 | 123.92 | 128.60 |
| 1 | A2 | 1560 | U | N3-C4-O4 | -7.79 | 113.94 | 119.40 |
| 36 | A5 | 3206 | C | N3-C2-O2 | -7.79 | 116.44 | 121.90 |
| 36 | A1 | 50 | U | N3-C4-O4 | -7.79 | 113.95 | 119.40 |
| 36 | A1 | 634 | C | N3-C2-O2 | -7.79 | 116.45 | 121.90 |
| 36 | A1 | 635 | G | C5-C6-N1 | 7.79 | 115.39 | 111.50 |
| 80 | A6 | 421 | A | C8-N9-C4 | 7.79 | 108.92 | 105.80 |
| 36 | A1 | 2787 | G | C5-C6-O6 | -7.79 | 123.93 | 128.60 |
| 36 | A5 | 216 | G | N1-C6-O6 | 7.79 | 124.57 | 119.90 |
| 36 | A5 | 2905 | U | N3-C4-C5 | 7.79 | 119.27 | 114.60 |
| 36 | A1 | 2203 | U | N1-C2-N3 | 7.79 | 119.57 | 114.90 |
| 36 | A1 | 1164 | G | N9-C4-C5 | 7.79 | 108.52 | 105.40 |
| 36 | A5 | 1311 | G | C5-C6-N1 | 7.79 | 115.39 | 111.50 |
| 36 | A5 | 1440 | G | C5-C6-O6 | 7.79 | 133.27 | 128.60 |
| 36 | A1 | 53 | G | N9-C4-C5 | -7.79 | 102.29 | 105.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A2 | 1291 | G | C8-N9-C4 | -7.78 | 103.29 | 106.40 |
| 36 | A5 | 2303 | A | C8-N9-C4 | -7.78 | 102.69 | 105.80 |
| 36 | A5 | 3050 | U | N1-C2-O2 | 7.78 | 128.25 | 122.80 |
| 36 | A5 | 3187 | A | C5-N7-C8 | 7.78 | 107.79 | 103.90 |
| 36 | A5 | 1150 | A | C2-N3-C4 | -7.78 | 106.71 | 110.60 |
| 36 | A5 | 2975 | U | N3-C4-C5 | 7.78 | 119.27 | 114.60 |
| 36 | A1 | 1733 | G | N3-C4-C5 | -7.78 | 124.71 | 128.60 |
| 36 | A1 | 2363 | A | N1-C6-N6 | -7.78 | 113.93 | 118.60 |
| 80 | A6 | 306 | U | C5-C6-N1 | -7.78 | 118.81 | 122.70 |
| 36 | A1 | 282 | G | C8-N9-C4 | -7.78 | 103.29 | 106.40 |
| 36 | A1 | 1520 | G | C5-N7-C8 | 7.78 | 108.19 | 104.30 |
| 36 | A1 | 290 | G | C5-C6-N1 | 7.78 | 115.39 | 111.50 |
| 36 | A1 | 2311 | G | C5-C6-O6 | -7.78 | 123.93 | 128.60 |
| 80 | A6 | 364 | G | C5-C6-O6 | -7.78 | 123.93 | 128.60 |
| 80 | A6 | 1514 | U | C5-C6-N1 | -7.78 | 118.81 | 122.70 |
| 36 | A5 | 2134 | G | C5-C6-N1 | 7.78 | 115.39 | 111.50 |
| 36 | A1 | 2130 | G | N3-C4-C5 | -7.78 | 124.71 | 128.60 |
| 80 | A6 | 194 | U | C2-N1-C1' | 7.78 | 127.03 | 117.70 |
| 36 | A5 | 2891 | U | C2-N3-C4 | -7.78 | 122.33 | 127.00 |
| 36 | A1 | 1400 | G | C8-N9-C4 | 7.77 | 109.51 | 106.40 |
| 36 | A5 | 3187 | A | N1-C6-N6 | -7.77 | 113.94 | 118.60 |
| 36 | A1 | 573 | C | C2-N3-C4 | -7.77 | 116.01 | 119.90 |
| 36 | A5 | 1792 | C | N1-C2-O2 | -7.77 | 114.24 | 118.90 |
| 36 | A1 | 651 | G | N3-C4-N9 | 7.77 | 130.66 | 126.00 |
| 36 | A5 | 2550 | U | N3-C4-O4 | -7.77 | 113.96 | 119.40 |
| 80 | A6 | 539 | G | C8-N9-C4 | -7.76 | 103.29 | 106.40 |
| 36 | A5 | 1391 | C | N3-C2-O2 | 7.76 | 127.33 | 121.90 |
| 36 | A1 | 3344 | A | C4-C5-C6 | 7.76 | 120.88 | 117.00 |
| 36 | A1 | 1150 | A | C5-C6-N6 | 7.76 | 129.91 | 123.70 |
| 36 | A5 | 3266 | G | N9-C4-C5 | 7.76 | 108.50 | 105.40 |
| 1 | A2 | 992 | A | C6-N1-C2 | 7.76 | 123.26 | 118.60 |
| 36 | A1 | 368 | G | N1-C2-N2 | -7.76 | 109.22 | 116.20 |
| 36 | A1 | 2714 | G | C4-N9-C1' | -7.76 | 116.41 | 126.50 |
| 36 | A5 | 1480 | G | C8-N9-C4 | 7.76 | 109.50 | 106.40 |
| 36 | A5 | 2246 | G | C5-C6-O6 | 7.76 | 133.26 | 128.60 |
| 36 | A5 | 3185 | U | C2-N3-C4 | -7.76 | 122.34 | 127.00 |
| 36 | A5 | 2899 | C | N3-C4-N4 | -7.76 | 112.57 | 118.00 |
| 36 | A1 | 2632 | G | N3-C2-N2 | 7.76 | 125.33 | 119.90 |
| 36 | A1 | 519 | A | N1-C6-N6 | 7.75 | 123.25 | 118.60 |
| 36 | A5 | 859 | G | C8-N9-C4 | -7.75 | 103.30 | 106.40 |
| 36 | A5 | 990 | U | N1-C2-O2 | 7.75 | 128.23 | 122.80 |
| 36 | A5 | 3377 | G | N3-C4-N9 | 7.75 | 130.65 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 36 | A1 | 1143 | A | C5-N7-C8 | -7.75 | 100.02 | 103.90 |
| 36 | A5 | 2393 | G | N1-C6-O6 | 7.75 | 124.55 | 119.90 |
| 36 | A1 | 664 | U | C2-N3-C4 | -7.75 | 122.35 | 127.00 |
| 38 | A4 | 85 | G | C8-N9-C4 | -7.75 | 103.30 | 106.40 |
| 36 | A1 | 2827 | U | C2-N3-C4 | -7.75 | 122.35 | 127.00 |
| 80 | A6 | 1620 | C | C6-N1-C2 | -7.75 | 117.20 | 120.30 |
| 36 | A1 | 1126 | G | N7-C8-N9 | -7.74 | 109.23 | 113.10 |
| 36 | A1 | 2719 | U | C2-N1-C1' | -7.74 | 108.41 | 117.70 |
| 36 | A5 | 2202 | C | N3-C4-N4 | 7.74 | 123.42 | 118.00 |
| 80 | A6 | 769 | A | C8-N9-C4 | -7.74 | 102.70 | 105.80 |
| 36 | A5 | 1370 | G | N1-C6-O6 | -7.74 | 115.25 | 119.90 |
| 36 | A1 | 2306 | C | N3-C2-O2 | -7.74 | 116.48 | 121.90 |
| 64 | Ba | 42 | ARG | NE-CZ-NH2 | -7.74 | 116.43 | 120.30 |
| 1 | A2 | 142 | G | N3-C4-N9 | -7.74 | 121.36 | 126.00 |
| 36 | A5 | 904 | A | N1-C6-N6 | -7.74 | 113.96 | 118.60 |
| 36 | A5 | 2278 | C | C6-N1-C1' | 7.74 | 130.08 | 120.80 |
| 80 | A6 | 36 | C | C5-C4-N4 | -7.74 | 114.78 | 120.20 |
| 80 | A6 | 1568 | C | C6-N1-C2 | -7.74 | 117.21 | 120.30 |
| 1 | A2 | 704 | C | N1-C2-O2 | 7.73 | 123.54 | 118.90 |
| 36 | A1 | 2653 | C | N3-C2-O2 | -7.73 | 116.49 | 121.90 |
| 80 | A6 | 1634 | C | C6-N1-C1' | -7.73 | 111.52 | 120.80 |
| 36 | A5 | 2960 | C | N3-C4-C5 | 7.73 | 124.99 | 121.90 |
| 36 | A1 | 1492 | G | C4-N9-C1' | 7.73 | 136.55 | 126.50 |
| 47 | DI | 167 | LEU | CA-CB-CG | 7.73 | 133.08 | 115.30 |
| 1 | A2 | 1486 | G | C8-N9-C4 | -7.73 | 103.31 | 106.40 |
| 36 | A5 | 974 | G | N3-C4-C5 | -7.73 | 124.74 | 128.60 |
| 36 | A1 | 1841 | A | C2-N3-C4 | 7.73 | 114.46 | 110.60 |
| 36 | A1 | 891 | G | N1-C6-O6 | -7.72 | 115.27 | 119.90 |
| 36 | A1 | 3112 | G | C5-C6-O6 | -7.72 | 123.97 | 128.60 |
| 36 | A5 | 3308 | C | N1-C2-N3 | 7.72 | 124.60 | 119.20 |
| 80 | A6 | 1549 | C | N3-C4-C5 | -7.72 | 118.81 | 121.90 |
| 36 | A1 | 386 | A | N1-C6-N6 | 7.71 | 123.23 | 118.60 |
| 36 | A1 | 1448 | U | C2-N3-C4 | -7.71 | 122.37 | 127.00 |
| 36 | A5 | 1833 | G | N1-C6-O6 | -7.71 | 115.27 | 119.90 |
| 36 | A5 | 546 | C | C6-N1-C1' | -7.71 | 111.55 | 120.80 |
| 36 | A1 | 664 | U | C4-C5-C6 | 7.71 | 124.32 | 119.70 |
| 36 | A1 | 3208 | G | C8-N9-C1' | 7.71 | 137.02 | 127.00 |
| 36 | A1 | 2249 | G | C3'-C2'-C1' | -7.70 | 95.34 | 101.50 |
| 36 | A5 | 1889 | G | N1-C6-O6 | -7.70 | 115.28 | 119.90 |
| 36 | A5 | 2757 | U | C2-N3-C4 | -7.70 | 122.38 | 127.00 |
| 1 | A2 | 1455 | G | C4-C5-N7 | -7.70 | 107.72 | 110.80 |
| 36 | A1 | 1117 | G | N7-C8-N9 | -7.70 | 109.25 | 113.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 363 | G | N1-C2-N3 | 7.70 | 128.52 | 123.90 |
| 36 | A5 | 376 | G | C5-C6-N1 | 7.70 | 115.35 | 111.50 |
| 36 | A5 | 2315 | G | C8-N9-C4 | 7.70 | 109.48 | 106.40 |
| 36 | A5 | 2584 | G | C4-N9-C1' | 7.70 | 136.50 | 126.50 |
| 80 | A6 | 1473 | U | N3-C2-O2 | -7.69 | 116.81 | 122.20 |
| 36 | A5 | 753 | C | C2-N3-C4 | -7.69 | 116.05 | 119.90 |
| 36 | A1 | 2339 | C | N1-C2-O2 | -7.69 | 114.29 | 118.90 |
| 36 | A1 | 1143 | A | N1-C6-N6 | 7.69 | 123.21 | 118.60 |
| 36 | A1 | 218 | G | C2-N3-C4 | 7.68 | 115.74 | 111.90 |
| 36 | A1 | 2376 | G | C5-C6-N1 | 7.68 | 115.34 | 111.50 |
| 68 | De | 45 | ARG | NE-CZ-NH2 | -7.68 | 116.46 | 120.30 |
| 36 | A1 | 384 | A | C8-N9-C4 | 7.68 | 108.87 | 105.80 |
| 70 | Bg | 51 | LEU | CA-CB-CG | 7.68 | 132.96 | 115.30 |
| 1 | A2 | 334 | G | C2-N3-C4 | -7.68 | 108.06 | 111.90 |
| 36 | A1 | 1156 | C | N3-C4-N4 | -7.68 | 112.63 | 118.00 |
| 36 | A1 | 1846 | C | C5-C6-N1 | -7.68 | 117.16 | 121.00 |
| 36 | A1 | 2811 | A | N1-C6-N6 | -7.68 | 113.99 | 118.60 |
| 49 | DL | 21 | ARG | NE-CZ-NH1 | -7.68 | 116.46 | 120.30 |
| 36 | A1 | 2777 | G | N1-C2-N3 | -7.67 | 119.30 | 123.90 |
| 36 | A5 | 2346 | C | C2-N3-C4 | -7.67 | 116.06 | 119.90 |
| 36 | A5 | 3065 | G | N1-C6-O6 | -7.67 | 115.30 | 119.90 |
| 36 | A5 | 1604 | G | C4-N9-C1' | 7.67 | 136.47 | 126.50 |
| 38 | A8 | 11 | C | N3-C2-O2 | -7.67 | 116.53 | 121.90 |
| 37 | A3 | 96 | U | C5-C6-N1 | -7.67 | 118.86 | 122.70 |
| 38 | A4 | 35 | C | C6-N1-C2 | -7.67 | 117.23 | 120.30 |
| 36 | A5 | 630 | A | C2-N3-C4 | -7.67 | 106.76 | 110.60 |
| 36 | A5 | 519 | A | N1-C6-N6 | 7.67 | 123.20 | 118.60 |
| 36 | A5 | 2703 | A | C8-N9-C4 | -7.67 | 102.73 | 105.80 |
| 36 | A5 | 2887 | A | C5-C6-N1 | -7.67 | 113.87 | 117.70 |
| 36 | A1 | 1507 | G | C6-N1-C2 | -7.67 | 120.50 | 125.10 |
| 37 | A7 | 39 | C | C6-N1-C2 | -7.67 | 117.23 | 120.30 |
| 36 | A1 | 24 | G | C8-N9-C4 | 7.66 | 109.47 | 106.40 |
| 36 | A1 | 874 | U | C4-C5-C6 | -7.66 | 115.10 | 119.70 |
| 36 | A1 | 1305 | U | N3-C2-O2 | -7.66 | 116.83 | 122.20 |
| 80 | A6 | 46 | A | C2-N3-C4 | -7.66 | 106.77 | 110.60 |
| 36 | A1 | 583 | G | N1-C6-O6 | -7.66 | 115.30 | 119.90 |
| 80 | A6 | 1644 | C | C5-C6-N1 | -7.66 | 117.17 | 121.00 |
| 36 | A1 | 1386 | A | C6-N1-C2 | -7.66 | 114.00 | 118.60 |
| 36 | A1 | 1489 | A | C2-N3-C4 | -7.66 | 106.77 | 110.60 |
| 36 | A5 | 594 | U | C6-N1-C2 | -7.66 | 116.40 | 121.00 |
| 1 | A2 | 1305 | U | C5-C4-O4 | 7.66 | 130.49 | 125.90 |
| 36 | A1 | 643 | U | N3-C2-O2 | 7.66 | 127.56 | 122.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 2643 | A | C2-N3-C4 | 7.66 | 114.43 | 110.60 |
| 36 | A1 | 970 | A | C8-N9-C4 | -7.65 | 102.74 | 105.80 |
| 36 | A1 | 1124 | U | N3-C4-C5 | 7.65 | 119.19 | 114.60 |
| 36 | A5 | 3245 | A | C5-C6-N1 | -7.65 | 113.87 | 117.70 |
| 37 | A7 | 11 | A | C8-N9-C4 | 7.65 | 108.86 | 105.80 |
| 36 | A5 | 2634 | U | C6-N1-C2 | 7.65 | 125.59 | 121.00 |
| 36 | A5 | 3330 | A | C5-C6-N1 | 7.65 | 121.52 | 117.70 |
| 1 | A2 | 553 | G | C4-C5-C6 | 7.65 | 123.39 | 118.80 |
| 36 | A5 | 1124 | U | N1-C2-N3 | -7.65 | 110.31 | 114.90 |
| 36 | A5 | 1381 | A | C8-N9-C4 | 7.65 | 108.86 | 105.80 |
| 36 | A1 | 1130 | A | C8-N9-C4 | -7.64 | 102.74 | 105.80 |
| 36 | A1 | 832 | G | N1-C6-O6 | -7.64 | 115.31 | 119.90 |
| 36 | A1 | 2776 | C | N3-C4-C5 | 7.64 | 124.96 | 121.90 |
| 36 | A1 | 39 | A | C5-N7-C8 | 7.64 | 107.72 | 103.90 |
| 36 | A1 | 3382 | U | N3-C2-O2 | -7.64 | 116.85 | 122.20 |
| 36 | A1 | 810 | A | N1-C6-N6 | -7.64 | 114.02 | 118.60 |
| 36 | A1 | 2541 | U | C2-N1-C1' | 7.64 | 126.86 | 117.70 |
| 36 | A5 | 2237 | C | N3-C4-N4 | -7.64 | 112.65 | 118.00 |
| 36 | A5 | 1402 | C | C5-C6-N1 | -7.63 | 117.18 | 121.00 |
| 36 | A5 | 2611 | U | C5-C6-N1 | -7.63 | 118.88 | 122.70 |
| 36 | A1 | 3318 | G | N3-C4-C5 | -7.63 | 124.78 | 128.60 |
| 36 | A1 | 1335 | C | N3-C4-C5 | 7.63 | 124.95 | 121.90 |
| 80 | A6 | 1305 | U | N1-C2-O2 | -7.63 | 117.46 | 122.80 |
| 36 | A5 | 2234 | G | C8-N9-C4 | 7.63 | 109.45 | 106.40 |
| 36 | A1 | 30 | G | C8-N9-C4 | -7.63 | 103.35 | 106.40 |
| 36 | A1 | 1420 | C | N3-C2-O2 | -7.63 | 116.56 | 121.90 |
| 36 | A1 | 2389 | C | C2-N3-C4 | -7.62 | 116.09 | 119.90 |
| 36 | A1 | 678 | G | N3-C2-N2 | -7.62 | 114.56 | 119.90 |
| 36 | A1 | 1110 | U | N3-C4-C5 | 7.62 | 119.17 | 114.60 |
| 36 | A1 | 2343 | C | C2-N3-C4 | -7.62 | 116.09 | 119.90 |
| 12 | CK | 97 | PRO | N-CA-CB | 7.62 | 112.45 | 103.30 |
| 36 | A5 | 665 | A | N1-C6-N6 | 7.62 | 123.17 | 118.60 |
| 36 | A1 | 963 | G | N9-C4-C5 | -7.62 | 102.35 | 105.40 |
| 36 | A1 | 1543 | G | C2-N3-C4 | 7.62 | 115.71 | 111.90 |
| 1 | A2 | 704 | C | C2-N1-C1' | 7.62 | 127.18 | 118.80 |
| 36 | A1 | 417 | A | N1-C6-N6 | 7.62 | 123.17 | 118.60 |
| 36 | A5 | 3055 | U | N3-C2-O2 | -7.62 | 116.87 | 122.20 |
| 80 | A6 | 1280 | C | N1-C2-O2 | -7.62 | 114.33 | 118.90 |
| 36 | A1 | 2415 | C | C6-N1-C2 | 7.61 | 123.34 | 120.30 |
| 36 | A5 | 121 | A | C8-N9-C4 | 7.61 | 108.85 | 105.80 |
| 36 | A1 | 847 | A | C5-C6-N6 | -7.61 | 117.61 | 123.70 |
| 36 | A5 | 877 | C | C4-C5-C6 | -7.61 | 113.59 | 117.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 2433 | U | C6-N1-C2 | 7.61 | 125.57 | 121.00 |
| 38 | A8 | 144 | G | N1-C6-O6 | 7.61 | 124.47 | 119.90 |
| 36 | A1 | 2281 | A | N9-C4-C5 | -7.61 | 102.76 | 105.80 |
| 36 | A5 | 1890 | U | C4-C5-C6 | 7.61 | 124.27 | 119.70 |
| 36 | A1 | 3159 | C | N3-C2-O2 | -7.61 | 116.58 | 121.90 |
| 36 | A5 | 1163 | A | N1-C6-N6 | -7.61 | 114.04 | 118.60 |
| 36 | A1 | 545 | U | N1-C2-O2 | 7.61 | 128.12 | 122.80 |
| 36 | A1 | 890 | C | N3-C4-C5 | 7.60 | 124.94 | 121.90 |
| 36 | A1 | 1313 | G | C5-C6-O6 | -7.60 | 124.04 | 128.60 |
| 80 | A6 | 418 | G | C4-N9-C1' | 7.60 | 136.38 | 126.50 |
| 36 | A5 | 1370 | G | C5-C6-N1 | 7.60 | 115.30 | 111.50 |
| 36 | A5 | 3088 | G | C4-C5-N7 | 7.60 | 113.84 | 110.80 |
| 36 | A1 | 2857 | C | C5-C4-N4 | -7.60 | 114.88 | 120.20 |
| 80 | A6 | 1310 | U | N3-C2-O2 | -7.60 | 116.88 | 122.20 |
| 37 | A7 | 67 | G | N3-C2-N2 | -7.60 | 114.58 | 119.90 |
| 36 | A1 | 54 | C | C5-C4-N4 | 7.59 | 125.52 | 120.20 |
| 80 | A6 | 359 | A | N1-C2-N3 | -7.59 | 125.50 | 129.30 |
| 36 | A5 | 1342 | C | C2-N3-C4 | -7.59 | 116.10 | 119.90 |
| 36 | A1 | 1392 | G | C2-N3-C4 | 7.59 | 115.69 | 111.90 |
| 80 | A6 | 1572 | G | C4-C5-N7 | 7.59 | 113.84 | 110.80 |
| 36 | A1 | 1478 | C | C5-C6-N1 | -7.59 | 117.20 | 121.00 |
| 36 | A5 | 2698 | G | C8-N9-C4 | 7.59 | 109.44 | 106.40 |
| 38 | A8 | 6 | U | C2-N3-C4 | -7.59 | 122.45 | 127.00 |
| 36 | A1 | 1115 | G | N1-C2-N2 | -7.59 | 109.37 | 116.20 |
| 36 | A5 | 419 | G | C5-C6-O6 | -7.59 | 124.05 | 128.60 |
| 36 | A5 | 2289 | U | N1-C2-O2 | 7.59 | 128.11 | 122.80 |
| 36 | A5 | 2372 | A | N9-C4-C5 | 7.59 | 108.83 | 105.80 |
| 36 | A5 | 3006 | A | C5-C6-N1 | -7.59 | 113.91 | 117.70 |
| 36 | A5 | 2138 | A | C8-N9-C4 | -7.59 | 102.77 | 105.80 |
| 36 | A5 | 2693 | C | N3-C4-C5 | 7.59 | 124.94 | 121.90 |
| 36 | A1 | 218 | G | N3-C4-C5 | -7.58 | 124.81 | 128.60 |
| 36 | A1 | 2278 | C | C6-N1-C1' | 7.58 | 129.90 | 120.80 |
| 80 | A6 | 565 | C | N1-C2-O2 | 7.58 | 123.45 | 118.90 |
| 36 | A1 | 61 | A | C8-N9-C4 | 7.58 | 108.83 | 105.80 |
| 36 | A5 | 1014 | U | C2-N1-C1' | 7.58 | 126.79 | 117.70 |
| 36 | A5 | 1390 | A | N1-C6-N6 | -7.58 | 114.05 | 118.60 |
| 36 | A1 | 835 | G | C8-N9-C4 | 7.58 | 109.43 | 106.40 |
| 36 | A1 | 339 | C | N3-C4-N4 | -7.58 | 112.70 | 118.00 |
| 36 | A1 | 2187 | G | C4-C5-N7 | 7.57 | 113.83 | 110.80 |
| 36 | A5 | 2271 | A | C8-N9-C4 | 7.57 | 108.83 | 105.80 |
| 36 | A1 | 83 | U | C5-C4-O4 | -7.57 | 121.36 | 125.90 |
| 36 | A1 | 1467 | A | N9-C4-C5 | 7.57 | 108.83 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 2179 | C | C5-C4-N4 | -7.57 | 114.90 | 120.20 |
| 36 | A1 | 2897 | A | C8-N9-C4 | 7.57 | 108.83 | 105.80 |
| 36 | A5 | 1305 | U | C5-C4-O4 | -7.57 | 121.36 | 125.90 |
| 80 | A6 | 1016 | C | N3-C4-C5 | 7.57 | 124.93 | 121.90 |
| 36 | A1 | 2948 | C | N3-C4-C5 | 7.56 | 124.92 | 121.90 |
| 36 | A5 | 929 | A | C8-N9-C4 | 7.56 | 108.83 | 105.80 |
| 36 | A5 | 1163 | A | C5-N7-C8 | 7.56 | 107.68 | 103.90 |
| 36 | A5 | 3154 | C | N1-C2-O2 | 7.56 | 123.44 | 118.90 |
| 36 | A5 | 3172 | A | N7-C8-N9 | -7.56 | 110.02 | 113.80 |
| 36 | A1 | 1055 | A | C8-N9-C4 | 7.56 | 108.82 | 105.80 |
| 36 | A1 | 106 | A | N9-C4-C5 | -7.56 | 102.78 | 105.80 |
| 80 | A6 | 308 | C | N3-C4-N4 | -7.56 | 112.71 | 118.00 |
| 36 | A5 | 81 | C | N3-C4-C5 | 7.56 | 124.92 | 121.90 |
| 36 | A5 | 2849 | C | N3-C4-C5 | -7.56 | 118.88 | 121.90 |
| 37 | A7 | 49 | G | C5-C6-O6 | -7.56 | 124.06 | 128.60 |
| 36 | A1 | 15 | C | C6-N1-C2 | -7.56 | 117.28 | 120.30 |
| 36 | A1 | 54 | C | C2-N1-C1' | -7.56 | 110.49 | 118.80 |
| 36 | A5 | 1396 | C | N3-C4-C5 | 7.55 | 124.92 | 121.90 |
| 36 | A1 | 2409 | G | C8-N9-C4 | -7.55 | 103.38 | 106.40 |
| 36 | A5 | 641 | C | N3-C4-N4 | -7.55 | 112.71 | 118.00 |
| 36 | A1 | 2246 | G | N9-C4-C5 | 7.55 | 108.42 | 105.40 |
| 36 | A5 | 289 | A | C6-N1-C2 | -7.55 | 114.07 | 118.60 |
| 36 | A5 | 1848 | G | C4-C5-N7 | 7.55 | 113.82 | 110.80 |
| 36 | A1 | 2777 | G | C8-N9-C1' | -7.55 | 117.19 | 127.00 |
| 36 | A5 | 633 | C | N1-C2-O2 | -7.55 | 114.37 | 118.90 |
| 36 | A5 | 3096 | C | C5-C6-N1 | -7.55 | 117.23 | 121.00 |
| 1 | A2 | 1291 | G | C2-N3-C4 | -7.54 | 108.13 | 111.90 |
| 36 | A1 | 2846 | U | C6-N1-C2 | -7.54 | 116.47 | 121.00 |
| 36 | A5 | 1130 | A | C5-C6-N1 | 7.54 | 121.47 | 117.70 |
| 36 | A5 | 3378 | C | N3-C4-C5 | 7.54 | 124.92 | 121.90 |
| 36 | A5 | 324 | A | C8-N9-C4 | -7.54 | 102.78 | 105.80 |
| 36 | A5 | 1176 | C | C2-N3-C4 | -7.54 | 116.13 | 119.90 |
| 36 | A5 | 2838 | A | N1-C6-N6 | 7.54 | 123.13 | 118.60 |
| 36 | A1 | 2714 | G | C4-C5-N7 | 7.54 | 113.82 | 110.80 |
| 36 | A5 | 851 | C | C5-C6-N1 | 7.54 | 124.77 | 121.00 |
| 36 | A5 | 2234 | G | C4-C5-N7 | 7.54 | 113.82 | 110.80 |
| 36 | A1 | 1403 | C | C5-C4-N4 | -7.54 | 114.92 | 120.20 |
| 36 | A5 | 928 | C | C4-C5-C6 | 7.54 | 121.17 | 117.40 |
| 36 | A1 | 88 | A | C8-N9-C4 | 7.54 | 108.82 | 105.80 |
| 80 | A6 | 308 | C | C6-N1-C1' | 7.54 | 129.85 | 120.80 |
| 1 | A2 | 647 | G | N9-C4-C5 | 7.54 | 108.42 | 105.40 |
| 36 | A1 | 3218 | A | C8-N9-C4 | -7.54 | 102.78 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 80 | A6 | 163 | G | C5-C6-O6 | -7.54 | 124.08 | 128.60 |
| 36 | A5 | 400 | G | C5-C6-O6 | -7.54 | 124.08 | 128.60 |
| 59 | DV | 45 | ARG | NE-CZ-NH1 | -7.54 | 116.53 | 120.30 |
| 36 | A1 | 270 | U | N3-C2-O2 | -7.54 | 116.93 | 122.20 |
| 36 | A1 | 1476 | G | C5-C6-O6 | 7.54 | 133.12 | 128.60 |
| 36 | A5 | 1216 | C | N1-C2-O2 | -7.54 | 114.38 | 118.90 |
| 36 | A1 | 582 | G | N9-C4-C5 | 7.53 | 108.41 | 105.40 |
| 36 | A5 | 42 | C | C4-C5-C6 | -7.53 | 113.63 | 117.40 |
| 38 | A8 | 144 | G | N3-C2-N2 | -7.53 | 114.63 | 119.90 |
| 36 | A5 | 2625 | C | C2-N3-C4 | -7.53 | 116.13 | 119.90 |
| 80 | A6 | 65 | A | N3-C4-C5 | 7.53 | 132.07 | 126.80 |
| 36 | A5 | 1910 | A | C8-N9-C4 | 7.53 | 108.81 | 105.80 |
| 1 | A2 | 1280 | C | C6-N1-C2 | -7.53 | 117.29 | 120.30 |
| 36 | A5 | 2381 | G | N9-C4-C5 | 7.53 | 108.41 | 105.40 |
| 80 | A6 | 555 | A | C8-N9-C4 | -7.53 | 102.79 | 105.80 |
| 38 | A8 | 2 | A | N9-C4-C5 | 7.53 | 108.81 | 105.80 |
| 36 | A1 | 1467 | A | N1-C6-N6 | -7.53 | 114.08 | 118.60 |
| 36 | A1 | 1494 | U | C6-N1-C2 | 7.53 | 125.52 | 121.00 |
| 1 | A2 | 1758 | U | N3-C2-O2 | -7.52 | 116.94 | 122.20 |
| 36 | A1 | 1157 | G | N1-C6-O6 | -7.52 | 115.39 | 119.90 |
| 1 | A2 | 323 | A | C8-N9-C4 | -7.52 | 102.79 | 105.80 |
| 1 | A2 | 871 | G | N3-C4-C5 | -7.52 | 124.84 | 128.60 |
| 36 | A1 | 2142 | A | C5-C6-N1 | 7.52 | 121.46 | 117.70 |
| 36 | A1 | 2932 | U | C5-C4-O4 | 7.52 | 130.41 | 125.90 |
| 36 | A5 | 1515 | A | C2-N3-C4 | -7.52 | 106.84 | 110.60 |
| 36 | A5 | 2342 | U | N3-C4-O4 | -7.52 | 114.14 | 119.40 |
| 36 | A5 | 2524 | A | N7-C8-N9 | 7.52 | 117.56 | 113.80 |
| 36 | A1 | 1308 | A | C5-N7-C8 | -7.52 | 100.14 | 103.90 |
| 36 | A1 | 2826 | U | C5-C4-O4 | -7.52 | 121.39 | 125.90 |
| 80 | A6 | 1280 | C | N3-C4-N4 | 7.52 | 123.26 | 118.00 |
| 36 | A1 | 1142 | G | C2-N3-C4 | 7.52 | 115.66 | 111.90 |
| 80 | A6 | 542 | A | C6-C5-N7 | -7.52 | 127.04 | 132.30 |
| 36 | A5 | 1057 | A | C5-C6-N6 | -7.51 | 117.69 | 123.70 |
| 36 | A1 | 2152 | A | N1-C6-N6 | -7.51 | 114.09 | 118.60 |
| 36 | A1 | 662 | U | N3-C4-O4 | -7.51 | 114.14 | 119.40 |
| 36 | A1 | 2756 | C | N1-C2-O2 | -7.51 | 114.39 | 118.90 |
| 36 | A1 | 3058 | U | C2-N1-C1' | 7.51 | 126.71 | 117.70 |
| 80 | A6 | 768 | C | C6-N1-C2 | 7.51 | 123.30 | 120.30 |
| 36 | A5 | 3140 | G | C4-C5-N7 | 7.51 | 113.80 | 110.80 |
| 1 | A2 | 758 | U | N3-C2-O2 | -7.51 | 116.94 | 122.20 |
| 36 | A1 | 2856 | G | C8-N9-C4 | 7.51 | 109.40 | 106.40 |
| 36 | A1 | 2369 | G | C2-N3-C4 | 7.51 | 115.65 | 111.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 2948 | C | N3-C4-N4 | -7.51 | 112.75 | 118.00 |
| 36 | A1 | 880 | G | C5-C6-N1 | 7.50 | 115.25 | 111.50 |
| 38 | A8 | 12 | A | C5-N7-C8 | -7.50 | 100.15 | 103.90 |
| 1 | A2 | 978 | A | C8-N9-C4 | 7.50 | 108.80 | 105.80 |
| 36 | A5 | 2791 | G | C5-C6-O6 | -7.50 | 124.10 | 128.60 |
| 36 | A5 | 426 | G | C8-N9-C4 | 7.50 | 109.40 | 106.40 |
| 36 | A5 | 971 | G | C2-N3-C4 | 7.50 | 115.65 | 111.90 |
| 36 | A5 | 2726 | C | N3-C4-N4 | -7.50 | 112.75 | 118.00 |
| 36 | A1 | 228 | U | N3-C2-O2 | -7.50 | 116.95 | 122.20 |
| 38 | A4 | 20 | U | C5-C4-O4 | 7.50 | 130.40 | 125.90 |
| 80 | A6 | 603 | U | N1-C2-N3 | 7.50 | 119.40 | 114.90 |
| 36 | A5 | 622 | A | N1-C6-N6 | 7.50 | 123.10 | 118.60 |
| 36 | A5 | 971 | G | N7-C8-N9 | -7.50 | 109.35 | 113.10 |
| 36 | A5 | 2718 | U | N1-C2-N3 | 7.50 | 119.40 | 114.90 |
| 36 | A1 | 1052 | U | N3-C4-C5 | 7.50 | 119.10 | 114.60 |
| 36 | A5 | 971 | G | C5-N7-C8 | 7.50 | 108.05 | 104.30 |
| 36 | A5 | 1516 | C | N1-C2-O2 | -7.50 | 114.40 | 118.90 |
| 36 | A1 | 88 | A | N9-C4-C5 | -7.50 | 102.80 | 105.80 |
| 80 | A6 | 1478 | G | C4-N9-C1' | 7.50 | 136.24 | 126.50 |
| 36 | A5 | 1389 | G | N3-C2-N2 | 7.49 | 125.14 | 119.90 |
| 36 | A5 | 1887 | A | N1-C6-N6 | 7.49 | 123.09 | 118.60 |
| 36 | A5 | 2630 | C | C2-N3-C4 | -7.49 | 116.16 | 119.90 |
| 1 | A2 | 594 | A | C2-N3-C4 | 7.49 | 114.34 | 110.60 |
| 38 | A8 | 14 | C | C4-C5-C6 | 7.49 | 121.14 | 117.40 |
| 36 | A1 | 678 | G | N1-C2-N2 | 7.49 | 122.94 | 116.20 |
| 36 | A1 | 2653 | C | C5-C4-N4 | 7.49 | 125.44 | 120.20 |
| 80 | A6 | 144 | U | C6-N1-C2 | -7.49 | 116.51 | 121.00 |
| 36 | A5 | 924 | G | N1-C2-N2 | 7.49 | 122.94 | 116.20 |
| 36 | A5 | 1407 | A | C6-N1-C2 | 7.49 | 123.09 | 118.60 |
| 36 | A5 | 3138 | U | C2-N3-C4 | -7.49 | 122.51 | 127.00 |
| 36 | A5 | 3308 | C | N1-C2-O2 | -7.49 | 114.41 | 118.90 |
| 1 | A2 | 1291 | G | C5-N7-C8 | -7.48 | 100.56 | 104.30 |
| 36 | A1 | 1370 | G | C5-C6-O6 | 7.48 | 133.09 | 128.60 |
| 36 | A5 | 1459 | C | N3-C4-C5 | 7.48 | 124.89 | 121.90 |
| 36 | A5 | 3007 | U | C2-N3-C4 | -7.48 | 122.51 | 127.00 |
| 80 | A6 | 308 | C | N1-C2-N3 | 7.48 | 124.44 | 119.20 |
| 36 | A5 | 150 | A | N1-C6-N6 | 7.48 | 123.09 | 118.60 |
| 1 | A2 | 507 | U | C2-N1-C1' | 7.48 | 126.67 | 117.70 |
| 36 | A1 | 730 | C | C2-N3-C4 | -7.48 | 116.16 | 119.90 |
| 36 | A1 | 2093 | A | C2-N3-C4 | 7.48 | 114.34 | 110.60 |
| 36 | A1 | 1592 | G | N3-C4-N9 | 7.48 | 130.49 | 126.00 |
| 36 | A1 | 1848 | G | N1-C6-O6 | 7.47 | 124.38 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 307 | A | N1-C6-N6 | -7.47 | 114.12 | 118.60 |
| 36 | A1 | 1503 | A | C2-N3-C4 | -7.47 | 106.86 | 110.60 |
| 80 | A6 | 308 | C | C4-C5-C6 | 7.47 | 121.14 | 117.40 |
| 36 | A1 | 686 | G | C4-C5-N7 | -7.47 | 107.81 | 110.80 |
| 36 | A1 | 2276 | G | C2-N3-C4 | 7.47 | 115.63 | 111.90 |
| 36 | A1 | 3279 | A | C8-N9-C4 | -7.47 | 102.81 | 105.80 |
| 36 | A1 | 3312 | U | C2-N3-C4 | -7.47 | 122.52 | 127.00 |
| 36 | A5 | 2366 | C | C5-C4-N4 | -7.47 | 114.97 | 120.20 |
| 36 | A5 | 74 | G | N1-C6-O6 | -7.47 | 115.42 | 119.90 |
| 36 | A5 | 2341 | A | N7-C8-N9 | -7.47 | 110.07 | 113.80 |
| 36 | A1 | 426 | G | C8-N9-C4 | 7.46 | 109.39 | 106.40 |
| 36 | A1 | 2969 | A | C8-N9-C4 | -7.46 | 102.81 | 105.80 |
| 36 | A5 | 1879 | A | N7-C8-N9 | 7.46 | 117.53 | 113.80 |
| 36 | A5 | 3025 | C | N3-C4-N4 | -7.46 | 112.78 | 118.00 |
| 36 | A1 | 2323 | G | C5-C6-O6 | 7.46 | 133.08 | 128.60 |
| 1 | A2 | 1761 | U | C6-N1-C2 | -7.46 | 116.52 | 121.00 |
| 36 | A1 | 93 | C | C6-N1-C2 | -7.46 | 117.31 | 120.30 |
| 36 | A1 | 1279 | C | C5-C6-N1 | 7.46 | 124.73 | 121.00 |
| 80 | A6 | 453 | U | N1-C2-O2 | 7.46 | 128.02 | 122.80 |
| 36 | A1 | 2376 | G | N7-C8-N9 | 7.46 | 116.83 | 113.10 |
| 36 | A5 | 931 | C | N3-C4-C5 | 7.46 | 124.88 | 121.90 |
| 36 | A5 | 1205 | A | C8-N9-C4 | -7.46 | 102.82 | 105.80 |
| 36 | A5 | 3192 | U | C5-C6-N1 | -7.46 | 118.97 | 122.70 |
| 37 | A7 | 41 | G | C8-N9-C4 | 7.46 | 109.38 | 106.40 |
| 36 | A1 | 3209 | A | N9-C4-C5 | -7.46 | 102.82 | 105.80 |
| 36 | A1 | 686 | G | N9-C4-C5 | 7.45 | 108.38 | 105.40 |
| 36 | A1 | 1351 | U | N3-C2-O2 | -7.45 | 116.98 | 122.20 |
| 80 | A6 | 901 | G | C4-C5-N7 | 7.45 | 113.78 | 110.80 |
| 36 | A5 | 3167 | A | C8-N9-C4 | -7.45 | 102.82 | 105.80 |
| 38 | A8 | 2 | A | N1-C6-N6 | -7.45 | 114.13 | 118.60 |
| 36 | A1 | 963 | G | C8-N9-C4 | 7.45 | 109.38 | 106.40 |
| 36 | A1 | 80 | G | N1-C2-N3 | 7.45 | 128.37 | 123.90 |
| 80 | A6 | 610 | G | C8-N9-C1' | -7.45 | 117.32 | 127.00 |
| 36 | A5 | 1586 | G | N3-C4-N9 | 7.45 | 130.47 | 126.00 |
| 36 | A5 | 2621 | G | N3-C2-N2 | -7.45 | 114.69 | 119.90 |
| 1 | A2 | 608 | U | C2-N3-C4 | -7.45 | 122.53 | 127.00 |
| 36 | A1 | 2647 | A | N9-C4-C5 | 7.45 | 108.78 | 105.80 |
| 36 | A5 | 1124 | U | C5-C6-N1 | 7.45 | 126.42 | 122.70 |
| 36 | A5 | 1317 | A | C2-N3-C4 | 7.45 | 114.32 | 110.60 |
| 36 | A5 | 3381 | U | N3-C4-O4 | -7.45 | 114.19 | 119.40 |
| 80 | A6 | 359 | A | C6-N1-C2 | 7.44 | 123.07 | 118.60 |
| 36 | A5 | 645 | A | C5-C6-N6 | -7.44 | 117.75 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 36 | A5 | 2395 | G | N7-C8-N9 | -7.44 | 109.38 | 113.10 |
| 1 | A2 | 1432 | U | C5-C6-N1 | -7.44 | 118.98 | 122.70 |
| 36 | A1 | 1351 | U | N1-C2-O2 | 7.44 | 128.01 | 122.80 |
| 36 | A1 | 1145 | G | N7-C8-N9 | -7.44 | 109.38 | 113.10 |
| 36 | A5 | 2743 | A | C8-N9-C4 | 7.44 | 108.78 | 105.80 |
| 36 | A5 | 1014 | U | C5-C4-O4 | -7.44 | 121.44 | 125.90 |
| 36 | A5 | 436 | A | N1-C6-N6 | 7.44 | 123.06 | 118.60 |
| 36 | A5 | 2311 | G | C8-N9-C4 | 7.44 | 109.37 | 106.40 |
| 1 | A2 | 1075 | C | N1-C2-O2 | -7.43 | 114.44 | 118.90 |
| 36 | A1 | 46 | U | N3-C4-O4 | -7.43 | 114.20 | 119.40 |
| 36 | A1 | 1396 | C | N3-C4-C5 | 7.43 | 124.87 | 121.90 |
| 36 | A5 | 2179 | C | C6-N1-C2 | 7.43 | 123.27 | 120.30 |
| 36 | A5 | 3081 | C | N3-C4-C5 | 7.43 | 124.87 | 121.90 |
| 36 | A1 | 576 | C | C2-N3-C4 | -7.43 | 116.18 | 119.90 |
| 36 | A1 | 646 | A | N1-C2-N3 | 7.43 | 133.02 | 129.30 |
| 36 | A5 | 1144 | U | N1-C2-N3 | 7.43 | 119.36 | 114.90 |
| 36 | A5 | 1372 | C | N1-C2-O2 | -7.43 | 114.44 | 118.90 |
| 36 | A1 | 1130 | A | C2-N3-C4 | 7.43 | 114.31 | 110.60 |
| 36 | A5 | 2908 | G | C8-N9-C4 | -7.43 | 103.43 | 106.40 |
| 36 | A5 | 2991 | A | N1-C6-N6 | -7.43 | 114.14 | 118.60 |
| 36 | A1 | 2600 | C | N1-C2-O2 | 7.42 | 123.35 | 118.90 |
| 36 | A5 | 1506 | A | C8-N9-C4 | -7.42 | 102.83 | 105.80 |
| 36 | A1 | 857 | G | N3-C2-N2 | 7.42 | 125.09 | 119.90 |
| 36 | A1 | 1145 | G | C8-N9-C4 | 7.42 | 109.37 | 106.40 |
| 36 | A5 | 2245 | C | C5-C6-N1 | 7.42 | 124.71 | 121.00 |
| 1 | A2 | 1012 | U | C2-N3-C4 | 7.42 | 131.45 | 127.00 |
| 80 | A6 | 1423 | U | C5-C6-N1 | -7.42 | 118.99 | 122.70 |
| 36 | A5 | 2996 | U | N1-C2-O2 | 7.42 | 127.99 | 122.80 |
| 80 | A6 | 392 | G | N1-C6-O6 | -7.42 | 115.45 | 119.90 |
| 36 | A5 | 1327 | C | N3-C4-C5 | 7.42 | 124.87 | 121.90 |
| 36 | A5 | 1340 | G | C8-N9-C4 | 7.42 | 109.37 | 106.40 |
| 36 | A5 | 2308 | C | N3-C2-O2 | 7.41 | 127.09 | 121.90 |
| 18 | AQ | 40 | GLU | C-N-CD | -7.41 | 104.29 | 120.60 |
| 36 | A1 | 2985 | C | N1-C2-O2 | -7.41 | 114.45 | 118.90 |
| 36 | A5 | 2350 | C | C4-C5-C6 | 7.41 | 121.11 | 117.40 |
| 1 | A2 | 831 | U | C5-C6-N1 | 7.41 | 126.41 | 122.70 |
| 36 | A1 | 1100 | U | C2-N3-C4 | -7.41 | 122.55 | 127.00 |
| 36 | A1 | 2631 | U | C2-N3-C4 | -7.41 | 122.55 | 127.00 |
| 36 | A1 | 1476 | G | N1-C6-O6 | -7.41 | 115.45 | 119.90 |
| 80 | A6 | 60 | U | N1-C2-O2 | 7.41 | 127.99 | 122.80 |
| 80 | A6 | 807 | A | C8-N9-C4 | -7.41 | 102.84 | 105.80 |
| 36 | A5 | 2572 | C | N3-C2-O2 | -7.41 | 116.71 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 36 | A1 | 3207 | U | N1-C2-N3 | 7.41 | 119.34 | 114.90 |
| 36 | A5 | 1085 | A | C2-N3-C4 | -7.41 | 106.90 | 110.60 |
| 36 | A5 | 1484 | U | C2-N3-C4 | -7.41 | 122.56 | 127.00 |
| 36 | A5 | 3151 | U | N1-C2-N3 | -7.41 | 110.46 | 114.90 |
| 37 | A7 | 96 | U | N3-C2-O2 | -7.41 | 117.02 | 122.20 |
| 1 | A2 | 1762 | A | N1-C6-N6 | 7.40 | 123.04 | 118.60 |
| 36 | A5 | 2851 | A | N1-C2-N3 | 7.40 | 133.00 | 129.30 |
| 36 | A1 | 988 | U | C5-C6-N1 | -7.40 | 119.00 | 122.70 |
| 36 | A1 | 2139 | A | C5-N7-C8 | 7.40 | 107.60 | 103.90 |
| 36 | A5 | 2943 | G | N3-C2-N2 | 7.40 | 125.08 | 119.90 |
| 36 | A1 | 942 | U | N3-C4-C5 | 7.40 | 119.04 | 114.60 |
| 36 | A1 | 1180 | A | C2-N3-C4 | -7.40 | 106.90 | 110.60 |
| 80 | A6 | 609 | U | C2-N3-C4 | -7.40 | 122.56 | 127.00 |
| 80 | A6 | 1644 | C | N3-C4-C5 | 7.40 | 124.86 | 121.90 |
| 36 | A5 | 280 | U | C5-C6-N1 | -7.40 | 119.00 | 122.70 |
| 36 | A5 | 2717 | U | C5-C6-N1 | -7.40 | 119.00 | 122.70 |
| 38 | A8 | 144 | G | C5-C6-O6 | -7.40 | 124.16 | 128.60 |
| 80 | A6 | 1643 | U | C5-C6-N1 | -7.40 | 119.00 | 122.70 |
| 36 | A1 | 3208 | G | N9-C4-C5 | 7.40 | 108.36 | 105.40 |
| 36 | A5 | 1117 | G | C5-C6-N1 | 7.40 | 115.20 | 111.50 |
| 36 | A5 | 3102 | G | N1-C2-N2 | -7.40 | 109.54 | 116.20 |
| 38 | A8 | 2 | A | C5-C6-N6 | 7.40 | 129.62 | 123.70 |
| 36 | A1 | 1165 | A | C8-N9-C4 | 7.39 | 108.76 | 105.80 |
| 36 | A5 | 1192 | C | C4-C5-C6 | 7.39 | 121.10 | 117.40 |
| 38 | A8 | 99 | C | C6-N1-C2 | 7.39 | 123.26 | 120.30 |
| 36 | A1 | 1911 | A | C6-C5-N7 | -7.39 | 127.12 | 132.30 |
| 80 | A6 | 622 | A | N9-C4-C5 | 7.39 | 108.76 | 105.80 |
| 36 | A5 | 1604 | G | N3-C4-N9 | 7.39 | 130.44 | 126.00 |
| 36 | A5 | 2370 | G | C6-N1-C2 | -7.39 | 120.67 | 125.10 |
| 36 | A1 | 909 | G | N7-C8-N9 | -7.39 | 109.41 | 113.10 |
| 36 | A1 | 994 | G | N1-C6-O6 | -7.39 | 115.47 | 119.90 |
| 36 | A1 | 3373 | U | C5-C6-N1 | -7.39 | 119.00 | 122.70 |
| 80 | A6 | 1304 | G | C5-C6-O6 | -7.39 | 124.17 | 128.60 |
| 36 | A5 | 2245 | C | N3-C2-O2 | -7.39 | 116.73 | 121.90 |
| 80 | A6 | 815 | G | C4-C5-N7 | 7.39 | 113.75 | 110.80 |
| 36 | A1 | 374 | A | N1-C6-N6 | -7.39 | 114.17 | 118.60 |
| 36 | A1 | 124 | U | N3-C2-O2 | -7.38 | 117.03 | 122.20 |
| 36 | A1 | 966 | U | N1-C2-O2 | 7.38 | 127.97 | 122.80 |
| 36 | A1 | 1118 | C | C4-C5-C6 | 7.38 | 121.09 | 117.40 |
| 36 | A5 | 2142 | A | C2-N3-C4 | 7.38 | 114.29 | 110.60 |
| 36 | A5 | 2639 | G | C5-C6-O6 | -7.38 | 124.17 | 128.60 |
| 1 | A2 | 355 | G | C5-C6-N1 | 7.38 | 115.19 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A2 | 583 | C | C6-N1-C2 | -7.38 | 117.35 | 120.30 |
| 36 | A1 | 333 | G | C5-C6-O6 | 7.38 | 133.03 | 128.60 |
| 36 | A1 | 1082 | U | C2-N1-C1' | 7.38 | 126.55 | 117.70 |
| 36 | A5 | 1437 | C | C5-C6-N1 | 7.38 | 124.69 | 121.00 |
| 38 | A4 | 39 | G | N1-C2-N2 | -7.38 | 109.56 | 116.20 |
| 36 | A5 | 957 | C | C2-N3-C4 | -7.38 | 116.21 | 119.90 |
| 36 | A1 | 1464 | G | C8-N9-C4 | 7.38 | 109.35 | 106.40 |
| 1 | A2 | 1389 | C | N1-C2-O2 | 7.37 | 123.32 | 118.90 |
| 36 | A1 | 1634 | G | C8-N9-C4 | -7.37 | 103.45 | 106.40 |
| 36 | A1 | 2756 | C | C5-C4-N4 | -7.37 | 115.04 | 120.20 |
| 36 | A1 | 2867 | C | N3-C4-C5 | 7.37 | 124.85 | 121.90 |
| 80 | A6 | 1269 | U | N3-C2-O2 | -7.37 | 117.04 | 122.20 |
| 80 | A6 | 1503 | A | N7-C8-N9 | 7.37 | 117.49 | 113.80 |
| 36 | A5 | 2531 | C | N1-C2-O2 | 7.37 | 123.32 | 118.90 |
| 36 | A5 | 2621 | G | C5-C6-N1 | -7.37 | 107.81 | 111.50 |
| 36 | A1 | 98 | G | C8-N9-C4 | 7.37 | 109.35 | 106.40 |
| 36 | A1 | 666 | A | N7-C8-N9 | -7.37 | 110.11 | 113.80 |
| 36 | A1 | 768 | C | C6-N1-C2 | -7.37 | 117.35 | 120.30 |
| 36 | A1 | 1359 | C | C5-C4-N4 | -7.37 | 115.04 | 120.20 |
| 36 | A1 | 2891 | U | C5-C4-O4 | -7.37 | 121.48 | 125.90 |
| 36 | A5 | 65 | A | C8-N9-C4 | -7.37 | 102.85 | 105.80 |
| 36 | A1 | 210 | U | N3-C2-O2 | -7.37 | 117.04 | 122.20 |
| 36 | A5 | 2541 | U | C2-N1-C1' | 7.37 | 126.54 | 117.70 |
| 36 | A5 | 2810 | C | N3-C2-O2 | -7.37 | 116.74 | 121.90 |
| 56 | DS | 40 | ARG | NE-CZ-NH1 | 7.37 | 123.98 | 120.30 |
| 36 | A1 | 3047 | U | C2-N3-C4 | -7.37 | 122.58 | 127.00 |
| 37 | A3 | 53 | U | N1-C2-O2 | -7.37 | 117.64 | 122.80 |
| 36 | A5 | 3369 | G | C5-C6-O6 | -7.37 | 124.18 | 128.60 |
| 36 | A1 | 327 | A | C8-N9-C4 | 7.37 | 108.75 | 105.80 |
| 36 | A1 | 952 | A | N1-C6-N6 | 7.37 | 123.02 | 118.60 |
| 36 | A1 | 2242 | A | C2-N3-C4 | -7.37 | 106.92 | 110.60 |
| 36 | A1 | 2958 | A | N1-C6-N6 | -7.37 | 114.18 | 118.60 |
| 38 | A4 | 38 | U | N3-C2-O2 | -7.37 | 117.04 | 122.20 |
| 36 | A5 | 1855 | U | C2-N3-C4 | -7.37 | 122.58 | 127.00 |
| 36 | A1 | 2772 | C | C3'-C2'-C1' | -7.36 | 95.61 | 101.50 |
| 36 | A5 | 795 | G | N7-C8-N9 | -7.36 | 109.42 | 113.10 |
| 36 | A5 | 2307 | G | N3-C4-N9 | 7.36 | 130.42 | 126.00 |
| 36 | A5 | 2385 | G | C4-N9-C1' | -7.36 | 116.93 | 126.50 |
| 36 | A1 | 644 | G | C2-N3-C4 | -7.36 | 108.22 | 111.90 |
| 36 | A1 | 776 | U | C5-C4-O4 | 7.36 | 130.32 | 125.90 |
| 36 | A1 | 816 | A | N1-C2-N3 | -7.36 | 125.62 | 129.30 |
| 36 | A5 | 98 | G | C5-C6-N1 | 7.36 | 115.18 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 2743 | A | N7-C8-N9 | -7.36 | 110.12 | 113.80 |
| 36 | A1 | 1422 | G | N1-C6-O6 | -7.36 | 115.48 | 119.90 |
| 36 | A1 | 3190 | C | N3-C4-C5 | 7.36 | 124.84 | 121.90 |
| 36 | A1 | 416 | A | N1-C6-N6 | -7.36 | 114.19 | 118.60 |
| 36 | A1 | 643 | U | C4-C5-C6 | -7.36 | 115.29 | 119.70 |
| 36 | A1 | 1492 | G | C5-C6-O6 | 7.36 | 133.01 | 128.60 |
| 80 | A6 | 815 | G | N1-C6-O6 | 7.36 | 124.31 | 119.90 |
| 36 | A1 | 650 | C | C5-C6-N1 | -7.35 | 117.32 | 121.00 |
| 1 | A2 | 1241 | G | N7-C8-N9 | 7.35 | 116.78 | 113.10 |
| 36 | A1 | 1510 | G | N3-C4-N9 | 7.35 | 130.41 | 126.00 |
| 36 | A1 | 3217 | C | C6-N1-C1' | -7.35 | 111.98 | 120.80 |
| 36 | A5 | 2802 | A | C2-N3-C4 | 7.35 | 114.28 | 110.60 |
| 1 | A2 | 142 | G | N3-C4-C5 | 7.35 | 132.28 | 128.60 |
| 36 | A1 | 689 | U | N1-C2-O2 | 7.35 | 127.95 | 122.80 |
| 36 | A1 | 1081 | U | C5-C6-N1 | 7.35 | 126.38 | 122.70 |
| 36 | A1 | 1480 | G | N7-C8-N9 | -7.35 | 109.42 | 113.10 |
| 36 | A5 | 2954 | U | C6-N1-C1' | -7.35 | 110.91 | 121.20 |
| 36 | A1 | 899 | U | N3-C4-O4 | -7.35 | 114.26 | 119.40 |
| 36 | A1 | 2395 | G | C5-C6-N1 | 7.35 | 115.17 | 111.50 |
| 36 | A1 | 1378 | U | C2-N3-C4 | -7.35 | 122.59 | 127.00 |
| 36 | A1 | 2123 | G | N7-C8-N9 | -7.35 | 109.43 | 113.10 |
| 36 | A1 | 1137 | C | C5-C4-N4 | -7.34 | 115.06 | 120.20 |
| 36 | A1 | 3294 | A | C8-N9-C4 | -7.34 | 102.86 | 105.80 |
| 38 | A4 | 125 | U | C2-N1-C1' | 7.34 | 126.51 | 117.70 |
| 36 | A5 | 3290 | G | C8-N9-C4 | -7.34 | 103.46 | 106.40 |
| 36 | A1 | 517 | G | N3-C4-C5 | -7.34 | 124.93 | 128.60 |
| 36 | A1 | 821 | U | C5-C6-N1 | -7.34 | 119.03 | 122.70 |
| 36 | A1 | 1041 | U | C5-C6-N1 | -7.34 | 119.03 | 122.70 |
| 36 | A1 | 716 | A | N9-C4-C5 | -7.34 | 102.86 | 105.80 |
| 36 | A1 | 1665 | C | N3-C4-C5 | 7.34 | 124.84 | 121.90 |
| 36 | A1 | 1848 | G | C6-C5-N7 | -7.34 | 126.00 | 130.40 |
| 36 | A1 | 2124 | G | N1-C6-O6 | 7.34 | 124.30 | 119.90 |
| 36 | A5 | 2288 | G | N3-C4-N9 | 7.34 | 130.41 | 126.00 |
| 1 | A2 | 377 | G | N3-C2-N2 | -7.34 | 114.76 | 119.90 |
| 36 | A5 | 3218 | A | C4-C5-N7 | 7.34 | 114.37 | 110.70 |
| 57 | DT | 130 | ARG | NE-CZ-NH2 | -7.34 | 116.63 | 120.30 |
| 36 | A1 | 652 | G | N1-C2-N2 | -7.34 | 109.60 | 116.20 |
| 36 | A1 | 1496 | C | C5-C6-N1 | 7.34 | 124.67 | 121.00 |
| 36 | A1 | 510 | G | C5-C6-O6 | -7.34 | 124.20 | 128.60 |
| 36 | A5 | 3289 | G | C8-N9-C4 | -7.34 | 103.47 | 106.40 |
| 36 | A1 | 35 | A | C5-N7-C8 | -7.33 | 100.23 | 103.90 |
| 36 | A1 | 874 | U | N3-C4-C5 | 7.33 | 119.00 | 114.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 962 | A | C6-N1-C2 | -7.33 | 114.20 | 118.60 |
| 37 | A7 | 41 | G | N9-C4-C5 | -7.33 | 102.47 | 105.40 |
| 36 | A5 | 2234 | G | N1-C6-O6 | 7.33 | 124.30 | 119.90 |
| 80 | A6 | 240 | U | C2-N1-C1' | 7.33 | 126.50 | 117.70 |
| 36 | A5 | 804 | C | C4-C5-C6 | 7.33 | 121.06 | 117.40 |
| 36 | A5 | 1449 | A | C4-C5-N7 | 7.33 | 114.36 | 110.70 |
| 36 | A1 | 689 | U | N3-C2-O2 | -7.33 | 117.07 | 122.20 |
| 36 | A5 | 931 | C | C5-C6-N1 | -7.33 | 117.34 | 121.00 |
| 36 | A5 | 2410 | U | C4-C5-C6 | -7.33 | 115.30 | 119.70 |
| 36 | A5 | 2701 | U | C5-C4-O4 | -7.33 | 121.50 | 125.90 |
| 36 | A1 | 649 | A | C5-N7-C8 | 7.32 | 107.56 | 103.90 |
| 36 | A1 | 1902 | G | C4-C5-N7 | 7.32 | 113.73 | 110.80 |
| 36 | A1 | 2963 | C | C4-C5-C6 | 7.32 | 121.06 | 117.40 |
| 1 | A2 | 89 | G | C8-N9-C4 | 7.32 | 109.33 | 106.40 |
| 36 | A5 | 2884 | C | C2-N3-C4 | -7.32 | 116.24 | 119.90 |
| 36 | A1 | 959 | C | N1-C2-O2 | -7.32 | 114.51 | 118.90 |
| 36 | A1 | 2247 | G | C5-C6-O6 | -7.32 | 124.21 | 128.60 |
| 38 | A4 | 32 | C | N3-C2-O2 | 7.32 | 127.02 | 121.90 |
| 38 | A4 | 85 | G | N7-C8-N9 | 7.32 | 116.76 | 113.10 |
| 80 | A6 | 421 | A | N1-C6-N6 | 7.32 | 122.99 | 118.60 |
| 36 | A5 | 2320 | A | C5-C6-N1 | -7.32 | 114.04 | 117.70 |
| 36 | A5 | 2736 | A | N1-C6-N6 | -7.32 | 114.21 | 118.60 |
| 36 | A1 | 957 | C | C5-C6-N1 | -7.32 | 117.34 | 121.00 |
| 36 | A1 | 3382 | U | N1-C2-O2 | 7.32 | 127.92 | 122.80 |
| 80 | A6 | 800 | U | C6-N1-C2 | -7.32 | 116.61 | 121.00 |
| 36 | A5 | 834 | U | C6-N1-C2 | 7.31 | 125.39 | 121.00 |
| 36 | A5 | 924 | G | N1-C6-O6 | 7.31 | 124.29 | 119.90 |
| 36 | A1 | 1717 | U | C6-N1-C2 | -7.31 | 116.61 | 121.00 |
| 36 | A1 | 83 | U | N3-C4-C5 | 7.31 | 118.98 | 114.60 |
| 36 | A1 | 1201 | C | C6-N1-C2 | -7.31 | 117.38 | 120.30 |
| 80 | A6 | 794 | U | C2-N1-C1' | 7.31 | 126.47 | 117.70 |
| 36 | A5 | 578 | A | N1-C6-N6 | 7.31 | 122.99 | 118.60 |
| 36 | A5 | 971 | G | C4-C5-N7 | -7.31 | 107.88 | 110.80 |
| 36 | A5 | 1921 | A | N1-C6-N6 | 7.31 | 122.98 | 118.60 |
| 36 | A1 | 2163 | C | N3-C4-N4 | -7.31 | 112.89 | 118.00 |
| 80 | A6 | 542 | A | N7-C8-N9 | 7.31 | 117.45 | 113.80 |
| 80 | A6 | 1542 | G | N9-C4-C5 | 7.31 | 108.32 | 105.40 |
| 36 | A1 | 2130 | G | C4-C5-N7 | -7.31 | 107.88 | 110.80 |
| 36 | A1 | 2632 | G | N1-C6-O6 | -7.30 | 115.52 | 119.90 |
| 36 | A1 | 2967 | A | C8-N9-C4 | 7.30 | 108.72 | 105.80 |
| 36 | A5 | 1133 | A | C5-C6-N1 | 7.30 | 121.35 | 117.70 |
| 36 | A1 | 2977 | G | C8-N9-C4 | 7.30 | 109.32 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 38 | A4 | 28 | C | C5-C6-N1 | -7.30 | 117.35 | 121.00 |
| 80 | A6 | 56 | U | C5-C6-N1 | -7.30 | 119.05 | 122.70 |
| 36 | A5 | 3382 | U | N1-C2-O2 | 7.30 | 127.91 | 122.80 |
| 69 | Df | 18 | ARG | NE-CZ-NH1 | -7.30 | 116.65 | 120.30 |
| 1 | A2 | 1096 | C | C6-N1-C1' | -7.30 | 112.04 | 120.80 |
| 36 | A5 | 1014 | U | C6-N1-C1' | -7.30 | 110.98 | 121.20 |
| 36 | A5 | 1506 | A | N7-C8-N9 | 7.30 | 117.45 | 113.80 |
| 36 | A5 | 2892 | A | C5-C6-N6 | 7.30 | 129.54 | 123.70 |
| 37 | A7 | 104 | A | N1-C6-N6 | 7.30 | 122.98 | 118.60 |
| 36 | A1 | 2798 | C | C4-C5-C6 | 7.29 | 121.05 | 117.40 |
| 36 | A5 | 2620 | G | C5-C6-N1 | 7.29 | 115.15 | 111.50 |
| 36 | A1 | 954 | U | C6-N1-C2 | -7.29 | 116.62 | 121.00 |
| 80 | A6 | 160 | C | N1-C2-O2 | 7.29 | 123.28 | 118.90 |
| 80 | A6 | 1796 | C | C5-C6-N1 | -7.29 | 117.35 | 121.00 |
| 36 | A5 | 800 | G | C8-N9-C4 | 7.29 | 109.32 | 106.40 |
| 36 | A1 | 2857 | C | N3-C4-C5 | 7.29 | 124.82 | 121.90 |
| 36 | A5 | 3122 | A | N7-C8-N9 | 7.29 | 117.44 | 113.80 |
| 36 | A5 | 2611 | U | N3-C2-O2 | -7.29 | 117.10 | 122.20 |
| 36 | A1 | 944 | C | N3-C4-C5 | -7.29 | 118.99 | 121.90 |
| 36 | A5 | 3131 | U | N3-C4-C5 | 7.29 | 118.97 | 114.60 |
| 80 | A6 | 1560 | U | N3-C4-O4 | -7.28 | 114.30 | 119.40 |
| 36 | A1 | 821 | U | C5-C4-O4 | 7.28 | 130.27 | 125.90 |
| 36 | A1 | 2357 | A | N1-C6-N6 | 7.28 | 122.97 | 118.60 |
| 36 | A5 | 2758 | A | C8-N9-C4 | -7.28 | 102.89 | 105.80 |
| 36 | A1 | 1656 | A | C8-N9-C4 | 7.28 | 108.71 | 105.80 |
| 68 | Be | 45 | ARG | NE-CZ-NH1 | 7.28 | 123.94 | 120.30 |
| 36 | A5 | 1189 | C | N1-C2-O2 | -7.28 | 114.53 | 118.90 |
| 36 | A5 | 2836 | C | N3-C4-N4 | -7.28 | 112.90 | 118.00 |
| 36 | A1 | 3046 | A | N7-C8-N9 | 7.28 | 117.44 | 113.80 |
| 37 | A3 | 83 | U | C2-N3-C4 | -7.28 | 122.63 | 127.00 |
| 36 | A5 | 669 | U | N1-C2-N3 | 7.28 | 119.27 | 114.90 |
| 36 | A5 | 2942 | C | C4-C5-C6 | 7.28 | 121.04 | 117.40 |
| 36 | A1 | 28 | C | C6-N1-C2 | 7.28 | 123.21 | 120.30 |
| 36 | A1 | 2376 | G | C6-N1-C2 | -7.28 | 120.73 | 125.10 |
| 36 | A5 | 1426 | C | N3-C4-C5 | 7.28 | 124.81 | 121.90 |
| 36 | A1 | 960 | U | C2-N1-C1' | -7.27 | 108.97 | 117.70 |
| 36 | A1 | 3362 | A | C4-C5-C6 | 7.27 | 120.64 | 117.00 |
| 36 | A1 | 1858 | A | C5-C6-N1 | 7.27 | 121.34 | 117.70 |
| 36 | A1 | 2615 | G | C5-C6-O6 | -7.27 | 124.24 | 128.60 |
| 36 | A5 | 1049 | C | N3-C4-C5 | 7.27 | 124.81 | 121.90 |
| 80 | A6 | 1781 | A | C5-N7-C8 | 7.27 | 107.53 | 103.90 |
| 80 | A6 | 410 | A | N1-C6-N6 | -7.27 | 114.24 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 80 | A6 | 1781 | A | C5-C6-N1 | -7.27 | 114.07 | 117.70 |
| 36 | A5 | 267 | G | C8-N9-C4 | 7.27 | 109.31 | 106.40 |
| 36 | A1 | 345 | G | N3-C4-N9 | 7.26 | 130.36 | 126.00 |
| 80 | A6 | 1542 | G | C8-N9-C4 | -7.26 | 103.49 | 106.40 |
| 36 | A5 | 2815 | G | C8-N9-C4 | 7.26 | 109.31 | 106.40 |
| 36 | A1 | 2902 | A | C8-N9-C4 | 7.26 | 108.70 | 105.80 |
| 36 | A5 | 652 | G | N3-C2-N2 | 7.26 | 124.98 | 119.90 |
| 36 | A5 | 1430 | U | C5-C6-N1 | -7.26 | 119.07 | 122.70 |
| 36 | A1 | 272 | G | N7-C8-N9 | -7.26 | 109.47 | 113.10 |
| 36 | A1 | 885 | U | N3-C4-O4 | -7.26 | 114.32 | 119.40 |
| 80 | A6 | 1600 | A | N7-C8-N9 | 7.26 | 117.43 | 113.80 |
| 80 | A6 | 800 | U | N3-C4-C5 | -7.26 | 110.24 | 114.60 |
| 36 | A5 | 1364 | C | C2-N3-C4 | -7.26 | 116.27 | 119.90 |
| 80 | A6 | 1304 | G | N9-C4-C5 | -7.26 | 102.50 | 105.40 |
| 36 | A1 | 1902 | G | C4-C5-C6 | 7.26 | 123.15 | 118.80 |
| 1 | A2 | 728 | U | C2-N1-C1' | 7.25 | 126.41 | 117.70 |
| 36 | A1 | 786 | A | C2-N3-C4 | 7.25 | 114.23 | 110.60 |
| 36 | A5 | 2848 | G | N3-C2-N2 | -7.25 | 114.82 | 119.90 |
| 36 | A5 | 3255 | U | C5-C4-O4 | -7.25 | 121.55 | 125.90 |
| 36 | A1 | 666 | A | C8-N9-C4 | 7.25 | 108.70 | 105.80 |
| 36 | A5 | 1538 | G | C8-N9-C4 | 7.25 | 109.30 | 106.40 |
| 36 | A5 | 1846 | C | C4-C5-C6 | 7.25 | 121.03 | 117.40 |
| 36 | A5 | 283 | G | C6-C5-N7 | -7.25 | 126.05 | 130.40 |
| 36 | A5 | 580 | C | C4-C5-C6 | 7.25 | 121.03 | 117.40 |
| 80 | A6 | 1073 | G | N1-C6-O6 | -7.25 | 115.55 | 119.90 |
| 36 | A5 | 2699 | G | C2-N3-C4 | 7.25 | 115.52 | 111.90 |
| 36 | A1 | 508 | U | C5-C6-N1 | -7.25 | 119.08 | 122.70 |
| 36 | A5 | 514 | G | C4-C5-N7 | 7.25 | 113.70 | 110.80 |
| 80 | A6 | 1596 | C | N1-C2-N3 | 7.24 | 124.27 | 119.20 |
| 36 | A1 | 521 | A | N1-C6-N6 | 7.24 | 122.94 | 118.60 |
| 36 | A1 | 696 | C | N3-C4-C5 | 7.24 | 124.80 | 121.90 |
| 36 | A1 | 919 | U | N3-C4-C5 | 7.24 | 118.94 | 114.60 |
| 36 | A5 | 2372 | A | P-O3'-C3' | 7.24 | 128.39 | 119.70 |
| 80 | A6 | 1145 | U | N1-C2-O2 | -7.24 | 117.73 | 122.80 |
| 36 | A1 | 1122 | U | C5-C6-N1 | -7.24 | 119.08 | 122.70 |
| 47 | BI | 57 | LEU | CA-CB-CG | 7.24 | 131.94 | 115.30 |
| 10 | CI | 29 | LEU | CA-CB-CG | 7.24 | 131.94 | 115.30 |
| 36 | A5 | 643 | U | N3-C4-C5 | 7.24 | 118.94 | 114.60 |
| 36 | A5 | 1144 | U | C5-C6-N1 | -7.24 | 119.08 | 122.70 |
| 36 | A5 | 2758 | A | N9-C4-C5 | 7.24 | 108.69 | 105.80 |
| 37 | A7 | 11 | A | N7-C8-N9 | -7.24 | 110.18 | 113.80 |
| 36 | A1 | 1741 | A | C6-C5-N7 | -7.23 | 127.24 | 132.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 38 | A4 | 21 | C | N1-C2-O2 | -7.23 | 114.56 | 118.90 |
| 36 | A5 | 1660 | C | C6-N1-C2 | -7.23 | 117.41 | 120.30 |
| 36 | A5 | 1887 | A | C2-N3-C4 | -7.23 | 106.98 | 110.60 |
| 36 | A1 | 112 | U | C6-N1-C1' | -7.23 | 111.08 | 121.20 |
| 36 | A1 | 1327 | C | C4-C5-C6 | -7.23 | 113.78 | 117.40 |
| 36 | A1 | 2857 | C | C2-N3-C4 | -7.23 | 116.28 | 119.90 |
| 80 | A6 | 999 | U | N3-C4-O4 | -7.23 | 114.34 | 119.40 |
| 36 | A5 | 1336 | U | C5-C4-O4 | -7.23 | 121.56 | 125.90 |
| 36 | A5 | 2370 | G | C5-C6-O6 | -7.23 | 124.26 | 128.60 |
| 36 | A5 | 1724 | U | C6-N1-C2 | -7.23 | 116.66 | 121.00 |
| 36 | A1 | 3302 | U | N3-C4-O4 | -7.23 | 114.34 | 119.40 |
| 36 | A1 | 3318 | G | C6-C5-N7 | -7.23 | 126.06 | 130.40 |
| 80 | A6 | 815 | G | C6-C5-N7 | -7.23 | 126.06 | 130.40 |
| 36 | A5 | 1833 | G | N3-C2-N2 | 7.23 | 124.96 | 119.90 |
| 36 | A1 | 2161 | G | C8-N9-C4 | -7.23 | 103.51 | 106.40 |
| 36 | A5 | 1518 | U | N3-C4-O4 | -7.23 | 114.34 | 119.40 |
| 36 | A1 | 1387 | G | C4-C5-N7 | -7.22 | 107.91 | 110.80 |
| 80 | A6 | 1000 | C | C6-N1-C2 | -7.22 | 117.41 | 120.30 |
| 1 | A2 | 1329 | A | N1-C6-N6 | 7.22 | 122.93 | 118.60 |
| 1 | A2 | 1611 | A | C5-N7-C8 | -7.22 | 100.29 | 103.90 |
| 80 | A6 | 1091 | A | N1-C6-N6 | 7.22 | 122.93 | 118.60 |
| 1 | A2 | 1654 | G | C5-C6-O6 | -7.22 | 124.27 | 128.60 |
| 36 | A1 | 695 | C | C5-C6-N1 | -7.22 | 117.39 | 121.00 |
| 36 | A1 | 2169 | G | C5-C6-O6 | 7.22 | 132.93 | 128.60 |
| 80 | A6 | 1787 | C | N1-C2-O2 | -7.22 | 114.57 | 118.90 |
| 36 | A5 | 2662 | G | C8-N9-C4 | -7.22 | 103.51 | 106.40 |
| 36 | A1 | 1496 | C | C2-N1-C1' | 7.22 | 126.74 | 118.80 |
| 36 | A5 | 2383 | C | N1-C2-O2 | -7.22 | 114.57 | 118.90 |
| 80 | A6 | 18 | C | C6-N1-C2 | -7.22 | 117.41 | 120.30 |
| 36 | A1 | 636 | C | C5-C6-N1 | -7.22 | 117.39 | 121.00 |
| 80 | A6 | 1649 | G | C5-C6-O6 | 7.22 | 132.93 | 128.60 |
| 36 | A5 | 2754 | G | N1-C2-N2 | -7.22 | 109.70 | 116.20 |
| 1 | A2 | 1745 | G | C4-C5-N7 | 7.21 | 113.69 | 110.80 |
| 36 | A5 | 810 | A | N1-C6-N6 | -7.21 | 114.27 | 118.60 |
| 36 | A5 | 2964 | G | C8-N9-C4 | 7.21 | 109.28 | 106.40 |
| 37 | A7 | 49 | G | N3-C2-N2 | -7.21 | 114.85 | 119.90 |
| 36 | A1 | 816 | A | C2-N3-C4 | 7.21 | 114.20 | 110.60 |
| 36 | A5 | 594 | U | N3-C2-O2 | -7.21 | 117.15 | 122.20 |
| 36 | A5 | 643 | U | C2-N3-C4 | -7.21 | 122.67 | 127.00 |
| 36 | A5 | 1407 | A | C5-C6-N1 | -7.21 | 114.09 | 117.70 |
| 1 | A2 | 1000 | C | N3-C4-N4 | -7.21 | 112.95 | 118.00 |
| 36 | A1 | 1372 | C | C2-N3-C4 | -7.21 | 116.30 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-------|------|-----------|-------|-------------|----------|
| 36 | A1 | 1116 | G | C8-N9-C4 | -7.21 | 103.52 | 106.40 |
| 36 | A1 | 1376 | C | C4-C5-C6 | 7.21 | 121.00 | 117.40 |
| 36 | A1 | 1442 | U | C5-C4-O4 | -7.21 | 121.58 | 125.90 |
| 36 | A1 | 1510 | G | N1-C2-N2 | -7.21 | 109.71 | 116.20 |
| 36 | A5 | 46 | U | N1-C2-O2 | 7.21 | 127.85 | 122.80 |
| 36 | A5 | 2911 | A | C2-N3-C4 | 7.21 | 114.20 | 110.60 |
| 80 | A6 | 53 | G | N1-C6-O6 | -7.21 | 115.58 | 119.90 |
| 36 | A5 | 2584 | G | C6-C5-N7 | -7.21 | 126.08 | 130.40 |
| 36 | A5 | 639 | G | N1-C6-O6 | 7.21 | 124.22 | 119.90 |
| 36 | A1 | 1304 | A | N9-C4-C5 | 7.20 | 108.68 | 105.80 |
| 36 | A1 | 2179 | C | C6-N1-C2 | 7.20 | 123.18 | 120.30 |
| 80 | A6 | 1793 | G | C4-C5-N7 | -7.20 | 107.92 | 110.80 |
| 36 | A5 | 39 | A | C4-C5-C6 | 7.20 | 120.60 | 117.00 |
| 36 | A5 | 2148 | U | C2-N3-C4 | -7.20 | 122.68 | 127.00 |
| 36 | A5 | 3060 | C | N3-C2-O2 | 7.20 | 126.94 | 121.90 |
| 38 | A4 | 103 | G | N3-C4-C5 | -7.20 | 125.00 | 128.60 |
| 36 | A1 | 1657 | C | N3-C2-O2 | 7.20 | 126.94 | 121.90 |
| 36 | A1 | 153 | U | N3-C4-C5 | -7.20 | 110.28 | 114.60 |
| 36 | A1 | 2768 | U | N1-C2-O2 | 7.20 | 127.84 | 122.80 |
| 80 | A6 | 1634 | C | C5-C6-N1 | 7.20 | 124.60 | 121.00 |
| 36 | A5 | 1858 | A | C2-N3-C4 | 7.20 | 114.20 | 110.60 |
| 36 | A1 | 281 | G | N9-C4-C5 | 7.20 | 108.28 | 105.40 |
| 1 | A2 | 1642 | G | C2-N3-C4 | 7.19 | 115.50 | 111.90 |
| 40 | DB | 266 | ARG | NE-CZ-NH2 | -7.19 | 116.70 | 120.30 |
| 36 | A1 | 2318 | U | N1-C2-N3 | 7.19 | 119.22 | 114.90 |
| 36 | A1 | 2550 | U | N3-C2-O2 | -7.19 | 117.17 | 122.20 |
| 38 | A4 | 16 | G | N7-C8-N9 | -7.19 | 109.50 | 113.10 |
| 80 | A6 | 1190 | C | C6-N1-C2 | 7.19 | 123.18 | 120.30 |
| 36 | A5 | 37 | U | C2-N3-C4 | -7.19 | 122.68 | 127.00 |
| 36 | A5 | 1172 | G | N1-C6-O6 | -7.19 | 115.58 | 119.90 |
| 36 | A5 | 272 | G | C8-N9-C4 | 7.19 | 109.28 | 106.40 |
| 36 | A5 | 1169 | A | C5-C6-N1 | -7.19 | 114.11 | 117.70 |
| 36 | A5 | 1434 | G | C4-C5-C6 | 7.19 | 123.11 | 118.80 |
| 36 | A1 | 340 | C | C2-N3-C4 | -7.19 | 116.31 | 119.90 |
| 36 | A1 | 1017 | C | C6-N1-C2 | -7.19 | 117.42 | 120.30 |
| 80 | A6 | 1031 | U | C6-N1-C2 | 7.19 | 125.31 | 121.00 |
| 52 | DO | 16[B] | LEU | C-N-CA | 7.19 | 137.40 | 122.30 |
| 1 | A2 | 1174 | C | N1-C2-O2 | 7.19 | 123.21 | 118.90 |
| 80 | A6 | 321 | C | N1-C2-O2 | 7.19 | 123.21 | 118.90 |
| 36 | A5 | 2337 | C | C6-N1-C2 | 7.19 | 123.17 | 120.30 |
| 36 | A1 | 1411 | C | N3-C4-N4 | -7.18 | 112.97 | 118.00 |
| 36 | A1 | 2339 | C | N3-C2-O2 | 7.18 | 126.93 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 36 | A5 | 960 | U | N1-C2-O2 | 7.18 | 127.83 | 122.80 |
| 36 | A5 | 1406 | A | C6-N1-C2 | -7.18 | 114.29 | 118.60 |
| 36 | A5 | 2824 | G | N9-C4-C5 | 7.18 | 108.27 | 105.40 |
| 36 | A1 | 279 | U | N3-C2-O2 | -7.18 | 117.17 | 122.20 |
| 80 | A6 | 29 | U | N3-C4-O4 | -7.18 | 114.37 | 119.40 |
| 36 | A5 | 1140 | G | N3-C2-N2 | 7.18 | 124.93 | 119.90 |
| 36 | A1 | 878 | G | C2-N3-C4 | -7.18 | 108.31 | 111.90 |
| 80 | A6 | 542 | A | C4-N9-C1' | 7.18 | 139.22 | 126.30 |
| 36 | A5 | 2244 | A | N1-C6-N6 | -7.18 | 114.29 | 118.60 |
| 36 | A5 | 2870 | C | N3-C4-N4 | -7.18 | 112.97 | 118.00 |
| 36 | A5 | 838 | G | N1-C6-O6 | -7.18 | 115.59 | 119.90 |
| 36 | A5 | 2732 | G | C5-C6-O6 | 7.18 | 132.91 | 128.60 |
| 36 | A1 | 641 | C | N3-C4-N4 | -7.17 | 112.98 | 118.00 |
| 52 | BO | 158[B] | ASP | CA-C-N | -7.17 | 101.42 | 117.20 |
| 80 | A6 | 1106 | U | N1-C2-N3 | 7.17 | 119.20 | 114.90 |
| 36 | A5 | 39 | A | N1-C6-N6 | 7.17 | 122.90 | 118.60 |
| 36 | A1 | 813 | G | C5-C6-N1 | 7.17 | 115.09 | 111.50 |
| 36 | A1 | 672 | A | C5-C6-N6 | -7.17 | 117.96 | 123.70 |
| 36 | A1 | 2389 | C | N3-C4-C5 | 7.17 | 124.77 | 121.90 |
| 38 | A8 | 54 | A | C2-N3-C4 | -7.17 | 107.02 | 110.60 |
| 1 | A2 | 1241 | G | C4-C5-N7 | 7.17 | 113.67 | 110.80 |
| 36 | A1 | 351 | A | C8-N9-C4 | 7.17 | 108.67 | 105.80 |
| 36 | A1 | 2302 | G | N1-C2-N2 | -7.17 | 109.75 | 116.20 |
| 57 | BT | 14 | MET | CG-SD-CE | -7.17 | 88.73 | 100.20 |
| 36 | A5 | 1403 | C | C5-C6-N1 | -7.17 | 117.42 | 121.00 |
| 36 | A5 | 2320 | A | C4-C5-N7 | -7.17 | 107.12 | 110.70 |
| 36 | A1 | 285 | A | N1-C6-N6 | 7.17 | 122.90 | 118.60 |
| 80 | A6 | 376 | C | C6-N1-C2 | 7.17 | 123.17 | 120.30 |
| 36 | A5 | 419 | G | N9-C4-C5 | -7.17 | 102.53 | 105.40 |
| 36 | A5 | 1167 | U | C5-C4-O4 | -7.17 | 121.60 | 125.90 |
| 36 | A5 | 2908 | G | N9-C4-C5 | 7.17 | 108.27 | 105.40 |
| 36 | A5 | 3040 | A | C5-N7-C8 | 7.17 | 107.48 | 103.90 |
| 36 | A1 | 640 | U | N3-C2-O2 | -7.16 | 117.19 | 122.20 |
| 36 | A1 | 2763 | U | C2-N3-C4 | -7.16 | 122.70 | 127.00 |
| 36 | A1 | 3317 | U | N3-C2-O2 | -7.16 | 117.19 | 122.20 |
| 36 | A5 | 969 | C | C2-N3-C4 | -7.16 | 116.32 | 119.90 |
| 36 | A5 | 974 | G | C4-N9-C1' | 7.16 | 135.81 | 126.50 |
| 36 | A1 | 2679 | A | C5-N7-C8 | -7.16 | 100.32 | 103.90 |
| 36 | A1 | 2960 | C | C2-N3-C4 | -7.16 | 116.32 | 119.90 |
| 37 | A3 | 48 | U | C5-C4-O4 | -7.16 | 121.60 | 125.90 |
| 36 | A5 | 2965 | U | C4-C5-C6 | 7.16 | 124.00 | 119.70 |
| 36 | A5 | 3052 | G | N1-C6-O6 | -7.16 | 115.60 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 37 | A7 | 44 | C | N1-C2-O2 | -7.16 | 114.60 | 118.90 |
| 68 | Be | 45 | ARG | NE-CZ-NH2 | -7.16 | 116.72 | 120.30 |
| 36 | A5 | 2305 | G | N9-C4-C5 | -7.16 | 102.54 | 105.40 |
| 36 | A1 | 1405 | U | C6-N1-C2 | 7.16 | 125.29 | 121.00 |
| 80 | A6 | 337 | G | N3-C2-N2 | 7.16 | 124.91 | 119.90 |
| 36 | A1 | 969 | C | C2-N3-C4 | -7.16 | 116.32 | 119.90 |
| 36 | A5 | 629 | U | C2-N3-C4 | -7.16 | 122.71 | 127.00 |
| 36 | A5 | 1206 | G | N9-C4-C5 | 7.16 | 108.26 | 105.40 |
| 36 | A5 | 2979 | U | C6-N1-C2 | 7.16 | 125.29 | 121.00 |
| 36 | A1 | 2726 | C | C2-N3-C4 | -7.15 | 116.32 | 119.90 |
| 36 | A5 | 518 | G | N9-C4-C5 | -7.15 | 102.54 | 105.40 |
| 36 | A1 | 907 | G | N3-C4-N9 | 7.15 | 130.29 | 126.00 |
| 36 | A1 | 1472 | U | C6-N1-C2 | 7.15 | 125.29 | 121.00 |
| 36 | A5 | 1591 | G | N1-C6-O6 | -7.15 | 115.61 | 119.90 |
| 36 | A1 | 50 | U | C5-C4-O4 | 7.15 | 130.19 | 125.90 |
| 36 | A5 | 801 | A | C5-C6-N1 | -7.15 | 114.12 | 117.70 |
| 36 | A5 | 1209 | G | N3-C2-N2 | -7.15 | 114.89 | 119.90 |
| 36 | A5 | 2396 | G | N9-C4-C5 | 7.15 | 108.26 | 105.40 |
| 36 | A5 | 2917 | G | C6-C5-N7 | -7.15 | 126.11 | 130.40 |
| 1 | A2 | 1611 | A | C2-N3-C4 | -7.15 | 107.03 | 110.60 |
| 80 | A6 | 387 | A | N1-C6-N6 | -7.15 | 114.31 | 118.60 |
| 36 | A5 | 563 | U | N1-C2-O2 | 7.15 | 127.80 | 122.80 |
| 36 | A5 | 2942 | C | N3-C4-C5 | -7.15 | 119.04 | 121.90 |
| 36 | A1 | 2952 | G | C6-C5-N7 | -7.15 | 126.11 | 130.40 |
| 36 | A5 | 1158 | A | C5-C6-N6 | -7.15 | 117.98 | 123.70 |
| 36 | A1 | 1507 | G | C5-C6-O6 | -7.15 | 124.31 | 128.60 |
| 36 | A5 | 922 | U | N3-C4-O4 | -7.14 | 114.40 | 119.40 |
| 1 | A2 | 628 | G | C2-N3-C4 | -7.14 | 108.33 | 111.90 |
| 36 | A1 | 921 | A | N1-C6-N6 | 7.14 | 122.89 | 118.60 |
| 36 | A1 | 2647 | A | C6-N1-C2 | -7.14 | 114.31 | 118.60 |
| 36 | A5 | 3379 | C | C5-C6-N1 | -7.14 | 117.43 | 121.00 |
| 36 | A5 | 1458 | U | C2-N3-C4 | -7.14 | 122.72 | 127.00 |
| 36 | A1 | 1164 | G | N1-C2-N3 | 7.14 | 128.18 | 123.90 |
| 36 | A5 | 46 | U | C5-C4-O4 | 7.14 | 130.18 | 125.90 |
| 36 | A5 | 2363 | A | C8-N9-C4 | -7.14 | 102.94 | 105.80 |
| 36 | A1 | 548 | G | N3-C4-N9 | -7.14 | 121.72 | 126.00 |
| 36 | A5 | 3005 | A | N9-C4-C5 | 7.14 | 108.66 | 105.80 |
| 36 | A1 | 2289 | U | C5-C4-O4 | 7.14 | 130.18 | 125.90 |
| 36 | A5 | 1292 | C | C6-N1-C2 | 7.14 | 123.15 | 120.30 |
| 1 | A2 | 992 | A | C2-N3-C4 | -7.13 | 107.03 | 110.60 |
| 36 | A1 | 2899 | C | N3-C4-N4 | 7.13 | 122.99 | 118.00 |
| 80 | A6 | 93 | A | N1-C6-N6 | 7.13 | 122.88 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 2305 | G | N3-C2-N2 | 7.13 | 124.89 | 119.90 |
| 36 | A1 | 2372 | A | C8-N9-C4 | -7.13 | 102.95 | 105.80 |
| 36 | A1 | 2945 | G | C8-N9-C4 | 7.13 | 109.25 | 106.40 |
| 1 | A2 | 783 | G | C4-C5-N7 | 7.13 | 113.65 | 110.80 |
| 80 | A6 | 22 | A | C8-N9-C4 | 7.13 | 108.65 | 105.80 |
| 36 | A1 | 104 | G | C4-C5-N7 | 7.13 | 113.65 | 110.80 |
| 36 | A1 | 2620 | G | C5-C6-N1 | 7.13 | 115.06 | 111.50 |
| 37 | A3 | 81 | U | C2-N3-C4 | -7.13 | 122.72 | 127.00 |
| 80 | A6 | 653 | C | C2-N1-C1' | 7.13 | 126.64 | 118.80 |
| 36 | A5 | 577 | C | C2-N3-C4 | -7.13 | 116.34 | 119.90 |
| 80 | A6 | 371 | G | C6-C5-N7 | -7.13 | 126.12 | 130.40 |
| 36 | A5 | 928 | C | N1-C2-N3 | 7.13 | 124.19 | 119.20 |
| 36 | A5 | 1548 | C | C2-N3-C4 | -7.13 | 116.34 | 119.90 |
| 36 | A5 | 2344 | U | C5-C6-N1 | -7.13 | 119.14 | 122.70 |
| 36 | A1 | 1335 | C | N3-C4-N4 | -7.12 | 113.01 | 118.00 |
| 36 | A1 | 1414 | G | C8-N9-C4 | -7.12 | 103.55 | 106.40 |
| 36 | A5 | 384 | A | C8-N9-C4 | 7.12 | 108.65 | 105.80 |
| 36 | A5 | 2242 | A | N1-C6-N6 | -7.12 | 114.33 | 118.60 |
| 36 | A1 | 2817 | A | N1-C2-N3 | 7.12 | 132.86 | 129.30 |
| 53 | DP | 69 | ARG | NE-CZ-NH2 | -7.12 | 116.74 | 120.30 |
| 36 | A1 | 650 | C | C2-N3-C4 | -7.12 | 116.34 | 119.90 |
| 36 | A1 | 2808 | A | C5-C6-N1 | -7.12 | 114.14 | 117.70 |
| 36 | A5 | 1939 | G | N3-C2-N2 | 7.12 | 124.88 | 119.90 |
| 36 | A1 | 1142 | G | C5-C6-N1 | 7.12 | 115.06 | 111.50 |
| 36 | A5 | 3245 | A | N3-C4-C5 | 7.12 | 131.78 | 126.80 |
| 36 | A1 | 851 | C | C5-C6-N1 | 7.12 | 124.56 | 121.00 |
| 36 | A1 | 2747 | A | N1-C6-N6 | -7.12 | 114.33 | 118.60 |
| 36 | A1 | 2762 | A | C8-N9-C4 | 7.12 | 108.65 | 105.80 |
| 36 | A5 | 3086 | A | N7-C8-N9 | -7.12 | 110.24 | 113.80 |
| 1 | A2 | 1274 | C | C5-C6-N1 | -7.11 | 117.44 | 121.00 |
| 36 | A5 | 1004 | U | N3-C4-C5 | 7.11 | 118.87 | 114.60 |
| 36 | A1 | 1719 | G | N1-C6-O6 | 7.11 | 124.17 | 119.90 |
| 36 | A1 | 369 | A | N9-C4-C5 | 7.11 | 108.64 | 105.80 |
| 36 | A1 | 1719 | G | C6-C5-N7 | -7.11 | 126.13 | 130.40 |
| 36 | A5 | 434 | U | N3-C4-C5 | 7.11 | 118.87 | 114.60 |
| 36 | A5 | 1902 | G | C8-N9-C4 | 7.11 | 109.24 | 106.40 |
| 36 | A5 | 3076 | C | N3-C4-C5 | 7.11 | 124.74 | 121.90 |
| 36 | A1 | 415 | G | C5-C6-O6 | 7.11 | 132.87 | 128.60 |
| 36 | A1 | 821 | U | N3-C2-O2 | -7.11 | 117.22 | 122.20 |
| 36 | A5 | 327 | A | N7-C8-N9 | -7.11 | 110.25 | 113.80 |
| 1 | A2 | 1456 | C | N3-C2-O2 | -7.11 | 116.92 | 121.90 |
| 36 | A5 | 24 | G | N1-C6-O6 | 7.11 | 124.17 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 36 | A5 | 511 | G | C5-C6-O6 | 7.11 | 132.86 | 128.60 |
| 38 | A8 | 42 | G | C8-N9-C4 | 7.11 | 109.24 | 106.40 |
| 36 | A1 | 2323 | G | N1-C6-O6 | -7.11 | 115.64 | 119.90 |
| 36 | A1 | 3269 | U | C5-C4-O4 | 7.11 | 130.16 | 125.90 |
| 38 | A4 | 113 | U | N3-C4-O4 | -7.11 | 114.43 | 119.40 |
| 36 | A1 | 973 | A | N9-C4-C5 | 7.10 | 108.64 | 105.80 |
| 36 | A1 | 1520 | G | N7-C8-N9 | -7.10 | 109.55 | 113.10 |
| 36 | A1 | 718 | G | N3-C4-N9 | -7.10 | 121.74 | 126.00 |
| 36 | A1 | 2710 | C | N3-C4-C5 | 7.10 | 124.74 | 121.90 |
| 48 | DJ | 112 | LEU | CA-CB-CG | 7.10 | 131.64 | 115.30 |
| 36 | A1 | 1342 | C | C2-N3-C4 | -7.10 | 116.35 | 119.90 |
| 36 | A1 | 2177 | G | C5-C6-O6 | -7.10 | 124.34 | 128.60 |
| 1 | A2 | 1121 | C | C4-C5-C6 | 7.10 | 120.95 | 117.40 |
| 1 | A2 | 1324 | G | N3-C2-N2 | -7.10 | 114.93 | 119.90 |
| 36 | A1 | 1741 | A | N1-C6-N6 | 7.10 | 122.86 | 118.60 |
| 36 | A5 | 3086 | A | C5-N7-C8 | 7.10 | 107.45 | 103.90 |
| 36 | A5 | 3110 | C | N1-C2-N3 | 7.10 | 124.17 | 119.20 |
| 1 | A2 | 1749 | A | C2-N3-C4 | -7.10 | 107.05 | 110.60 |
| 37 | A7 | 101 | G | C5-C6-O6 | -7.10 | 124.34 | 128.60 |
| 36 | A1 | 2957 | G | C4-C5-N7 | -7.10 | 107.96 | 110.80 |
| 36 | A1 | 1395 | G | C5-C6-N1 | 7.09 | 115.05 | 111.50 |
| 80 | A6 | 876 | G | C5-N7-C8 | 7.09 | 107.85 | 104.30 |
| 80 | A6 | 1000 | C | N3-C2-O2 | -7.09 | 116.93 | 121.90 |
| 36 | A5 | 2993 | G | C4-C5-N7 | 7.09 | 113.64 | 110.80 |
| 38 | A8 | 139 | U | N3-C4-O4 | -7.09 | 114.43 | 119.40 |
| 36 | A1 | 1878 | G | C5-C6-O6 | -7.09 | 124.34 | 128.60 |
| 36 | A1 | 652 | G | N3-C2-N2 | 7.09 | 124.86 | 119.90 |
| 36 | A1 | 1888 | U | C5-C6-N1 | -7.09 | 119.15 | 122.70 |
| 36 | A5 | 436 | A | C6-C5-N7 | -7.09 | 127.33 | 132.30 |
| 36 | A5 | 2616 | C | C6-N1-C2 | 7.09 | 123.14 | 120.30 |
| 1 | A2 | 1654 | G | N3-C4-C5 | -7.09 | 125.06 | 128.60 |
| 36 | A1 | 302 | U | C2-N3-C4 | -7.09 | 122.75 | 127.00 |
| 36 | A1 | 1125 | U | C2-N3-C4 | -7.09 | 122.75 | 127.00 |
| 36 | A1 | 1507 | G | C5-N7-C8 | 7.09 | 107.84 | 104.30 |
| 36 | A5 | 1328 | C | C4-C5-C6 | 7.09 | 120.94 | 117.40 |
| 36 | A5 | 3006 | A | N1-C2-N3 | 7.09 | 132.84 | 129.30 |
| 36 | A1 | 1175 | C | C2-N3-C4 | -7.09 | 116.36 | 119.90 |
| 80 | A6 | 421 | A | N9-C4-C5 | -7.09 | 102.97 | 105.80 |
| 36 | A5 | 2169 | G | C5-C6-N1 | 7.09 | 115.04 | 111.50 |
| 36 | A5 | 2584 | G | N3-C4-N9 | 7.09 | 130.25 | 126.00 |
| 36 | A1 | 31 | C | N3-C4-C5 | 7.08 | 124.73 | 121.90 |
| 36 | A1 | 920 | A | N1-C2-N3 | 7.08 | 132.84 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 1042 | U | N1-C2-O2 | 7.08 | 127.76 | 122.80 |
| 36 | A1 | 2413 | A | C5-C6-N1 | 7.08 | 121.24 | 117.70 |
| 37 | A3 | 36 | C | N3-C2-O2 | -7.08 | 116.94 | 121.90 |
| 80 | A6 | 1269 | U | C4-C5-C6 | 7.08 | 123.95 | 119.70 |
| 80 | A6 | 1503 | A | C2-N3-C4 | -7.08 | 107.06 | 110.60 |
| 36 | A5 | 622 | A | N9-C4-C5 | -7.08 | 102.97 | 105.80 |
| 36 | A5 | 1340 | G | N1-C2-N2 | -7.08 | 109.82 | 116.20 |
| 36 | A5 | 2881 | C | C5-C6-N1 | -7.08 | 117.46 | 121.00 |
| 36 | A1 | 2389 | C | C6-N1-C2 | 7.08 | 123.13 | 120.30 |
| 36 | A1 | 3092 | C | N3-C4-C5 | 7.08 | 124.73 | 121.90 |
| 36 | A5 | 1085 | A | C8-N9-C4 | -7.08 | 102.97 | 105.80 |
| 36 | A5 | 2127 | U | N1-C2-N3 | 7.08 | 119.15 | 114.90 |
| 36 | A5 | 2631 | U | N3-C4-C5 | 7.08 | 118.85 | 114.60 |
| 56 | DS | 115 | ARG | NE-CZ-NH2 | -7.08 | 116.76 | 120.30 |
| 36 | A1 | 994 | G | C5-C6-N1 | 7.08 | 115.04 | 111.50 |
| 36 | A1 | 2696 | A | N1-C6-N6 | -7.08 | 114.35 | 118.60 |
| 36 | A5 | 1917 | C | N1-C2-O2 | -7.08 | 114.65 | 118.90 |
| 36 | A5 | 2327 | U | C6-N1-C2 | 7.08 | 125.25 | 121.00 |
| 1 | A2 | 577 | G | N9-C4-C5 | -7.08 | 102.57 | 105.40 |
| 36 | A1 | 1166 | G | C5-C6-O6 | -7.08 | 124.35 | 128.60 |
| 36 | A1 | 1307 | G | C5-C6-O6 | 7.08 | 132.85 | 128.60 |
| 36 | A1 | 2198 | A | N9-C4-C5 | -7.08 | 102.97 | 105.80 |
| 36 | A1 | 2373 | A | N1-C6-N6 | 7.08 | 122.85 | 118.60 |
| 80 | A6 | 1796 | C | C5-C4-N4 | 7.08 | 125.15 | 120.20 |
| 1 | A2 | 108 | A | N1-C2-N3 | 7.08 | 132.84 | 129.30 |
| 36 | A1 | 1592 | G | N1-C6-O6 | -7.08 | 115.65 | 119.90 |
| 36 | A1 | 1150 | A | C2-N3-C4 | -7.07 | 107.06 | 110.60 |
| 36 | A1 | 1339 | C | C4-C5-C6 | 7.07 | 120.94 | 117.40 |
| 36 | A5 | 3052 | G | C5-C6-O6 | 7.07 | 132.84 | 128.60 |
| 36 | A5 | 872 | U | N3-C4-C5 | 7.07 | 118.84 | 114.60 |
| 36 | A1 | 711 | A | N1-C6-N6 | -7.07 | 114.36 | 118.60 |
| 36 | A1 | 2727 | A | C2-N3-C4 | 7.07 | 114.14 | 110.60 |
| 36 | A5 | 546 | C | C5-C6-N1 | 7.07 | 124.53 | 121.00 |
| 36 | A5 | 2149 | A | C8-N9-C4 | -7.07 | 102.97 | 105.80 |
| 36 | A1 | 876 | A | N1-C6-N6 | -7.07 | 114.36 | 118.60 |
| 36 | A1 | 1118 | C | C2-N3-C4 | -7.07 | 116.37 | 119.90 |
| 36 | A1 | 742 | G | C8-N9-C4 | 7.07 | 109.23 | 106.40 |
| 36 | A1 | 3362 | A | C5-C6-N6 | -7.07 | 118.05 | 123.70 |
| 36 | A5 | 2988 | C | C5-C6-N1 | -7.07 | 117.47 | 121.00 |
| 36 | A1 | 2145 | A | C2-N3-C4 | 7.06 | 114.13 | 110.60 |
| 36 | A1 | 2595 | A | N1-C6-N6 | 7.06 | 122.84 | 118.60 |
| 80 | A6 | 3 | U | C5-C6-N1 | -7.06 | 119.17 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 1879 | A | C5-N7-C8 | -7.06 | 100.37 | 103.90 |
| 36 | A5 | 3107 | U | N3-C2-O2 | -7.06 | 117.26 | 122.20 |
| 36 | A5 | 3192 | U | N3-C4-O4 | -7.06 | 114.46 | 119.40 |
| 38 | A8 | 101 | U | C6-N1-C2 | -7.06 | 116.76 | 121.00 |
| 36 | A1 | 1589 | A | C6-N1-C2 | -7.06 | 114.37 | 118.60 |
| 36 | A1 | 1447 | G | N9-C4-C5 | 7.06 | 108.22 | 105.40 |
| 36 | A1 | 1528 | G | C8-N9-C4 | -7.06 | 103.58 | 106.40 |
| 36 | A1 | 1870 | C | N3-C4-C5 | 7.06 | 124.72 | 121.90 |
| 36 | A1 | 3052 | G | C5-C6-O6 | 7.06 | 132.83 | 128.60 |
| 41 | BC | 313 | LEU | CA-CB-CG | 7.06 | 131.53 | 115.30 |
| 38 | A8 | 126 | A | C8-N9-C4 | -7.05 | 102.98 | 105.80 |
| 80 | A6 | 1789 | G | C5-N7-C8 | 7.05 | 107.83 | 104.30 |
| 36 | A5 | 641 | C | C6-N1-C1' | 7.05 | 129.26 | 120.80 |
| 36 | A5 | 1592 | G | C5-C6-O6 | 7.05 | 132.83 | 128.60 |
| 36 | A1 | 95 | A | N7-C8-N9 | -7.05 | 110.27 | 113.80 |
| 80 | A6 | 310 | C | N1-C2-O2 | -7.05 | 114.67 | 118.90 |
| 36 | A5 | 437 | G | N7-C8-N9 | 7.05 | 116.63 | 113.10 |
| 36 | A1 | 2139 | A | N1-C6-N6 | -7.05 | 114.37 | 118.60 |
| 36 | A1 | 3208 | G | C4-N9-C1' | -7.05 | 117.33 | 126.50 |
| 37 | A3 | 28 | C | N1-C2-O2 | -7.05 | 114.67 | 118.90 |
| 80 | A6 | 512 | A | C5-C6-N6 | -7.05 | 118.06 | 123.70 |
| 80 | A6 | 1188 | G | C5-C6-O6 | -7.05 | 124.37 | 128.60 |
| 36 | A5 | 834 | U | N3-C4-O4 | -7.05 | 114.47 | 119.40 |
| 1 | A2 | 610 | G | C8-N9-C1' | -7.05 | 117.84 | 127.00 |
| 36 | A5 | 2832 | C | C2-N3-C4 | -7.05 | 116.38 | 119.90 |
| 52 | DO | 4[B] | GLN | O-C-N | 7.05 | 134.49 | 121.10 |
| 36 | A5 | 929 | A | N7-C8-N9 | -7.04 | 110.28 | 113.80 |
| 1 | A2 | 1057 | U | C5-C6-N1 | 7.04 | 126.22 | 122.70 |
| 1 | A2 | 1462 | G | C8-N9-C4 | 7.04 | 109.22 | 106.40 |
| 36 | A1 | 2406 | C | C5-C6-N1 | -7.04 | 117.48 | 121.00 |
| 36 | A1 | 2799 | A | C6-N1-C2 | -7.04 | 114.37 | 118.60 |
| 80 | A6 | 371 | G | C5-C6-O6 | -7.04 | 124.37 | 128.60 |
| 36 | A5 | 1370 | G | N3-C2-N2 | 7.04 | 124.83 | 119.90 |
| 36 | A5 | 2618 | G | C6-N1-C2 | -7.04 | 120.87 | 125.10 |
| 36 | A1 | 700 | C | C6-N1-C2 | 7.04 | 123.12 | 120.30 |
| 80 | A6 | 1606 | C | C6-N1-C2 | 7.04 | 123.12 | 120.30 |
| 80 | A6 | 543 | C | N1-C2-O2 | 7.04 | 123.12 | 118.90 |
| 80 | A6 | 756 | A | N7-C8-N9 | 7.04 | 117.32 | 113.80 |
| 36 | A5 | 1417 | G | N1-C6-O6 | -7.04 | 115.68 | 119.90 |
| 36 | A5 | 2300 | G | N3-C2-N2 | 7.04 | 124.83 | 119.90 |
| 36 | A1 | 1145 | G | N1-C6-O6 | -7.04 | 115.68 | 119.90 |
| 36 | A1 | 1200 | A | N9-C4-C5 | 7.04 | 108.61 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 1389 | G | C5-C6-O6 | -7.04 | 124.38 | 128.60 |
| 36 | A1 | 788 | C | C6-N1-C2 | 7.04 | 123.11 | 120.30 |
| 36 | A1 | 1480 | G | N3-C4-N9 | 7.04 | 130.22 | 126.00 |
| 36 | A1 | 2325 | G | C5-C6-N1 | 7.04 | 115.02 | 111.50 |
| 36 | A5 | 708 | G | N7-C8-N9 | 7.04 | 116.62 | 113.10 |
| 36 | A5 | 2618 | G | N3-C4-N9 | 7.04 | 130.22 | 126.00 |
| 36 | A5 | 2189 | U | C2-N3-C4 | -7.03 | 122.78 | 127.00 |
| 36 | A5 | 2350 | C | C2-N3-C4 | -7.03 | 116.38 | 119.90 |
| 36 | A5 | 2426 | U | N1-C2-O2 | 7.03 | 127.72 | 122.80 |
| 36 | A5 | 3154 | C | N3-C2-O2 | -7.03 | 116.98 | 121.90 |
| 36 | A5 | 2190 | U | N1-C2-N3 | 7.03 | 119.12 | 114.90 |
| 1 | A2 | 1773 | C | C2-N3-C4 | 7.03 | 123.42 | 119.90 |
| 36 | A1 | 22 | G | N9-C4-C5 | 7.03 | 108.21 | 105.40 |
| 36 | A1 | 28 | C | N3-C4-C5 | 7.03 | 124.71 | 121.90 |
| 36 | A1 | 895 | A | N3-C4-C5 | 7.03 | 131.72 | 126.80 |
| 36 | A5 | 1314 | C | C2-N1-C1' | 7.03 | 126.53 | 118.80 |
| 36 | A5 | 1434 | G | C4-C5-N7 | -7.03 | 107.99 | 110.80 |
| 36 | A5 | 2280 | A | C2-N3-C4 | -7.03 | 107.08 | 110.60 |
| 36 | A5 | 3317 | U | C6-N1-C2 | -7.03 | 116.78 | 121.00 |
| 36 | A1 | 357 | A | C6-N1-C2 | -7.03 | 114.38 | 118.60 |
| 80 | A6 | 114 | C | N3-C2-O2 | -7.03 | 116.98 | 121.90 |
| 36 | A1 | 153 | U | C5-C4-O4 | 7.03 | 130.12 | 125.90 |
| 36 | A1 | 1495 | U | C5-C4-O4 | 7.03 | 130.12 | 125.90 |
| 36 | A5 | 2167 | A | C6-N1-C2 | -7.03 | 114.38 | 118.60 |
| 1 | A2 | 1747 | G | C2-N3-C4 | -7.03 | 108.39 | 111.90 |
| 36 | A1 | 2369 | G | C8-N9-C4 | -7.03 | 103.59 | 106.40 |
| 36 | A1 | 3111 | U | N3-C4-O4 | -7.03 | 114.48 | 119.40 |
| 36 | A5 | 1152 | G | N1-C2-N3 | 7.03 | 128.12 | 123.90 |
| 36 | A5 | 2293 | C | N3-C4-C5 | 7.03 | 124.71 | 121.90 |
| 36 | A1 | 1838 | G | C5-C6-O6 | -7.02 | 124.39 | 128.60 |
| 36 | A1 | 3126 | C | C5-C6-N1 | -7.02 | 117.49 | 121.00 |
| 80 | A6 | 1560 | U | N1-C2-N3 | 7.02 | 119.11 | 114.90 |
| 36 | A5 | 1441 | G | N7-C8-N9 | -7.02 | 109.59 | 113.10 |
| 36 | A5 | 2302 | G | N1-C6-O6 | -7.02 | 115.69 | 119.90 |
| 36 | A1 | 2595 | A | C8-N9-C4 | -7.02 | 102.99 | 105.80 |
| 36 | A5 | 2917 | G | C6-N1-C2 | -7.02 | 120.89 | 125.10 |
| 1 | A2 | 159 | U | C6-N1-C2 | 7.02 | 125.21 | 121.00 |
| 36 | A1 | 95 | A | C5-C6-N1 | -7.02 | 114.19 | 117.70 |
| 36 | A1 | 2130 | G | C5-N7-C8 | 7.02 | 107.81 | 104.30 |
| 64 | Da | 12 | ARG | NE-CZ-NH2 | -7.02 | 116.79 | 120.30 |
| 36 | A1 | 81 | C | C2-N3-C4 | -7.02 | 116.39 | 119.90 |
| 36 | A1 | 3129 | A | C8-N9-C4 | 7.02 | 108.61 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 80 | A6 | 11 | A | C2-N3-C4 | 7.02 | 114.11 | 110.60 |
| 36 | A5 | 2693 | C | C2-N3-C4 | -7.02 | 116.39 | 119.90 |
| 36 | A1 | 709 | A | N9-C4-C5 | -7.02 | 102.99 | 105.80 |
| 36 | A1 | 1127 | G | N1-C6-O6 | 7.02 | 124.11 | 119.90 |
| 36 | A1 | 2146 | C | C6-N1-C2 | -7.02 | 117.49 | 120.30 |
| 36 | A5 | 3098 | G | C5-C6-O6 | 7.02 | 132.81 | 128.60 |
| 36 | A1 | 84 | U | C5-C4-O4 | -7.01 | 121.69 | 125.90 |
| 36 | A1 | 889 | U | N3-C2-O2 | -7.01 | 117.29 | 122.20 |
| 36 | A1 | 1893 | A | N1-C2-N3 | 7.01 | 132.81 | 129.30 |
| 36 | A5 | 81 | C | N3-C4-N4 | -7.01 | 113.09 | 118.00 |
| 36 | A5 | 706 | A | C8-N9-C4 | 7.01 | 108.61 | 105.80 |
| 36 | A1 | 814 | U | C5-C6-N1 | -7.01 | 119.19 | 122.70 |
| 36 | A1 | 908 | G | C8-N9-C1' | -7.01 | 117.89 | 127.00 |
| 36 | A5 | 859 | G | N1-C6-O6 | -7.01 | 115.69 | 119.90 |
| 1 | A2 | 321 | C | C6-N1-C2 | -7.01 | 117.50 | 120.30 |
| 36 | A1 | 2274 | U | N1-C2-O2 | 7.01 | 127.70 | 122.80 |
| 36 | A5 | 804 | C | N3-C4-C5 | -7.00 | 119.10 | 121.90 |
| 36 | A5 | 945 | C | C5-C6-N1 | -7.00 | 117.50 | 121.00 |
| 36 | A1 | 1389 | G | C4-C5-N7 | 7.00 | 113.60 | 110.80 |
| 36 | A1 | 1947 | G | N1-C2-N2 | 7.00 | 122.50 | 116.20 |
| 36 | A5 | 591 | G | C4-C5-N7 | 7.00 | 113.60 | 110.80 |
| 36 | A5 | 1110 | U | C4-C5-C6 | -7.00 | 115.50 | 119.70 |
| 1 | A2 | 74 | U | O4'-C1'-N1 | 7.00 | 113.80 | 108.20 |
| 36 | A1 | 895 | A | C5-C6-N1 | -7.00 | 114.20 | 117.70 |
| 36 | A1 | 2814 | G | N1-C6-O6 | 7.00 | 124.10 | 119.90 |
| 80 | A6 | 610 | G | C4-N9-C1' | 7.00 | 135.60 | 126.50 |
| 36 | A5 | 3214 | U | N1-C2-N3 | 7.00 | 119.10 | 114.90 |
| 37 | A3 | 28 | C | C5-C4-N4 | -7.00 | 115.30 | 120.20 |
| 36 | A5 | 418 | A | N1-C6-N6 | 7.00 | 122.80 | 118.60 |
| 36 | A1 | 662 | U | N3-C2-O2 | -7.00 | 117.30 | 122.20 |
| 36 | A1 | 926 | A | C2-N3-C4 | 7.00 | 114.10 | 110.60 |
| 80 | A6 | 297 | U | C2-N1-C1' | 7.00 | 126.10 | 117.70 |
| 36 | A5 | 3182 | G | N1-C6-O6 | -7.00 | 115.70 | 119.90 |
| 36 | A1 | 987 | U | N1-C2-N3 | 7.00 | 119.10 | 114.90 |
| 36 | A1 | 950 | G | C6-N1-C2 | 6.99 | 129.30 | 125.10 |
| 36 | A1 | 2139 | A | C4-C5-N7 | -6.99 | 107.20 | 110.70 |
| 80 | A6 | 424 | C | C6-N1-C2 | 6.99 | 123.10 | 120.30 |
| 36 | A5 | 32 | U | N3-C4-C5 | -6.99 | 110.40 | 114.60 |
| 36 | A5 | 802 | C | C2-N3-C4 | -6.99 | 116.40 | 119.90 |
| 36 | A5 | 1925 | U | C2-N3-C4 | -6.99 | 122.80 | 127.00 |
| 36 | A1 | 361 | A | C2-N3-C4 | 6.99 | 114.09 | 110.60 |
| 36 | A5 | 2943 | G | N1-C6-O6 | -6.99 | 115.70 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 36 | A5 | 930 | U | N3-C4-O4 | -6.99 | 114.51 | 119.40 |
| 36 | A5 | 2169 | G | C6-C5-N7 | 6.99 | 134.59 | 130.40 |
| 36 | A5 | 2932 | U | N1-C2-O2 | 6.99 | 127.69 | 122.80 |
| 36 | A1 | 78 | U | C2-N3-C4 | -6.99 | 122.81 | 127.00 |
| 52 | DO | 104[B] | ILE | O-C-N | 6.99 | 133.88 | 122.70 |
| 36 | A1 | 636 | C | C2-N3-C4 | -6.98 | 116.41 | 119.90 |
| 1 | A2 | 1600 | A | C5-C6-N1 | -6.98 | 114.21 | 117.70 |
| 80 | A6 | 408 | C | C6-N1-C2 | -6.98 | 117.51 | 120.30 |
| 36 | A1 | 363 | G | N3-C2-N2 | -6.98 | 115.01 | 119.90 |
| 36 | A1 | 791 | A | C8-N9-C4 | 6.98 | 108.59 | 105.80 |
| 36 | A1 | 1156 | C | C2-N3-C4 | -6.98 | 116.41 | 119.90 |
| 36 | A5 | 2882 | U | C2-N3-C4 | -6.98 | 122.81 | 127.00 |
| 36 | A1 | 33 | G | N3-C2-N2 | -6.98 | 115.02 | 119.90 |
| 36 | A1 | 54 | C | C6-N1-C2 | 6.98 | 123.09 | 120.30 |
| 36 | A1 | 2364 | G | C5-C6-O6 | -6.98 | 124.41 | 128.60 |
| 80 | A6 | 9 | U | C5-C6-N1 | -6.98 | 119.21 | 122.70 |
| 36 | A1 | 3304 | U | C2-N1-C1' | -6.98 | 109.33 | 117.70 |
| 36 | A5 | 1118 | C | N3-C4-C5 | 6.98 | 124.69 | 121.90 |
| 36 | A5 | 2290 | C | C6-N1-C2 | 6.98 | 123.09 | 120.30 |
| 36 | A5 | 3218 | A | C2-N3-C4 | -6.98 | 107.11 | 110.60 |
| 36 | A5 | 1149 | G | N9-C4-C5 | 6.97 | 108.19 | 105.40 |
| 36 | A1 | 359 | U | C2-N3-C4 | -6.97 | 122.82 | 127.00 |
| 36 | A1 | 958 | C | C5-C4-N4 | 6.97 | 125.08 | 120.20 |
| 36 | A5 | 933 | A | N1-C2-N3 | 6.97 | 132.79 | 129.30 |
| 36 | A5 | 2917 | G | N3-C4-N9 | 6.97 | 130.18 | 126.00 |
| 36 | A5 | 1673 | G | N1-C6-O6 | -6.97 | 115.72 | 119.90 |
| 1 | A2 | 1533 | C | C4-C5-C6 | 6.97 | 120.88 | 117.40 |
| 36 | A1 | 427 | C | C2-N3-C4 | -6.97 | 116.42 | 119.90 |
| 36 | A1 | 2678 | A | N1-C6-N6 | -6.97 | 114.42 | 118.60 |
| 80 | A6 | 605 | A | C8-N9-C4 | 6.97 | 108.59 | 105.80 |
| 38 | A8 | 70 | G | C8-N9-C4 | 6.97 | 109.19 | 106.40 |
| 1 | A2 | 1162 | C | C6-N1-C2 | -6.96 | 117.51 | 120.30 |
| 38 | A4 | 6 | U | C5-C4-O4 | -6.96 | 121.72 | 125.90 |
| 36 | A5 | 2314 | U | C5-C6-N1 | 6.96 | 126.18 | 122.70 |
| 36 | A5 | 369 | A | N7-C8-N9 | 6.96 | 117.28 | 113.80 |
| 36 | A1 | 650 | C | N1-C2-O2 | -6.96 | 114.72 | 118.90 |
| 36 | A1 | 1132 | C | C5-C4-N4 | 6.96 | 125.07 | 120.20 |
| 36 | A1 | 1741 | A | C4-C5-N7 | 6.96 | 114.18 | 110.70 |
| 36 | A1 | 2169 | G | C2-N3-C4 | 6.96 | 115.38 | 111.90 |
| 38 | A8 | 112 | U | C2-N1-C1' | -6.96 | 109.35 | 117.70 |
| 80 | A6 | 1455 | G | N9-C4-C5 | 6.96 | 108.18 | 105.40 |
| 36 | A5 | 3172 | A | C5-N7-C8 | 6.96 | 107.38 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A2 | 61 | A | N7-C8-N9 | 6.96 | 117.28 | 113.80 |
| 36 | A1 | 2757 | U | N1-C2-N3 | 6.96 | 119.08 | 114.90 |
| 80 | A6 | 411 | C | C4-C5-C6 | 6.96 | 120.88 | 117.40 |
| 36 | A5 | 2631 | U | C5-C6-N1 | -6.96 | 119.22 | 122.70 |
| 36 | A5 | 3070 | A | C2-N3-C4 | -6.96 | 107.12 | 110.60 |
| 36 | A5 | 3099 | C | C5-C6-N1 | -6.96 | 117.52 | 121.00 |
| 80 | A6 | 144 | U | N1-C2-O2 | 6.96 | 127.67 | 122.80 |
| 38 | A8 | 139 | U | C5-C6-N1 | -6.96 | 119.22 | 122.70 |
| 36 | A1 | 352 | A | C5-C6-N1 | -6.95 | 114.22 | 117.70 |
| 36 | A1 | 376 | G | C4-C5-N7 | -6.95 | 108.02 | 110.80 |
| 36 | A1 | 1491 | A | N7-C8-N9 | -6.95 | 110.32 | 113.80 |
| 80 | A6 | 647 | G | N3-C4-N9 | -6.95 | 121.83 | 126.00 |
| 36 | A5 | 2644 | C | N1-C2-O2 | -6.95 | 114.73 | 118.90 |
| 36 | A5 | 2689 | A | C6-N1-C2 | -6.95 | 114.43 | 118.60 |
| 36 | A1 | 885 | U | C2-N3-C4 | -6.95 | 122.83 | 127.00 |
| 36 | A1 | 2958 | A | N7-C8-N9 | -6.95 | 110.33 | 113.80 |
| 36 | A5 | 751 | A | C2-N3-C4 | -6.95 | 107.12 | 110.60 |
| 36 | A5 | 2249 | G | C3'-C2'-C1' | -6.95 | 95.94 | 101.50 |
| 36 | A1 | 963 | G | N7-C8-N9 | -6.95 | 109.62 | 113.10 |
| 36 | A1 | 1371 | G | N1-C6-O6 | -6.95 | 115.73 | 119.90 |
| 36 | A5 | 1199 | C | C4-C5-C6 | 6.95 | 120.87 | 117.40 |
| 36 | A1 | 653 | A | C6-N1-C2 | -6.95 | 114.43 | 118.60 |
| 36 | A5 | 2626 | A | C5-C6-N6 | 6.95 | 129.26 | 123.70 |
| 36 | A5 | 3333 | G | C5-C6-O6 | -6.95 | 124.43 | 128.60 |
| 1 | A2 | 981 | U | N3-C2-O2 | -6.95 | 117.34 | 122.20 |
| 1 | A2 | 1782 | A | N7-C8-N9 | 6.95 | 117.27 | 113.80 |
| 36 | A1 | 1429 | G | N1-C2-N2 | -6.95 | 109.95 | 116.20 |
| 1 | A2 | 542 | A | C8-N9-C1' | -6.94 | 115.20 | 127.70 |
| 36 | A1 | 1926 | C | N3-C4-C5 | 6.94 | 124.68 | 121.90 |
| 36 | A5 | 2184 | U | C2-N3-C4 | -6.94 | 122.83 | 127.00 |
| 80 | A6 | 351 | C | C2-N1-C1' | 6.94 | 126.44 | 118.80 |
| 36 | A1 | 2600 | C | N3-C2-O2 | -6.94 | 117.04 | 121.90 |
| 36 | A1 | 3372 | A | C5-C6-N1 | 6.94 | 121.17 | 117.70 |
| 36 | A1 | 407 | A | N7-C8-N9 | 6.94 | 117.27 | 113.80 |
| 36 | A5 | 835 | G | C5-C6-N1 | 6.94 | 114.97 | 111.50 |
| 36 | A5 | 1834 | U | N3-C4-O4 | -6.94 | 114.54 | 119.40 |
| 1 | A2 | 360 | A | N9-C4-C5 | -6.94 | 103.03 | 105.80 |
| 39 | BA | 207 | VAL | CB-CA-C | -6.94 | 98.22 | 111.40 |
| 80 | A6 | 1681 | A | C2-N3-C4 | -6.94 | 107.13 | 110.60 |
| 15 | AN | 22 | ALA | C-N-CD | -6.93 | 105.34 | 120.60 |
| 36 | A1 | 1182 | A | C8-N9-C4 | 6.93 | 108.57 | 105.80 |
| 36 | A1 | 2899 | C | C5-C6-N1 | -6.93 | 117.53 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 80 | A6 | 1793 | G | N1-C6-O6 | -6.93 | 115.74 | 119.90 |
| 1 | A2 | 1548 | G | C2-N3-C4 | 6.93 | 115.36 | 111.90 |
| 36 | A1 | 1858 | A | C6-N1-C2 | -6.93 | 114.44 | 118.60 |
| 36 | A1 | 2977 | G | C6-N1-C2 | -6.93 | 120.94 | 125.10 |
| 80 | A6 | 310 | C | C4-C5-C6 | 6.93 | 120.86 | 117.40 |
| 36 | A5 | 1285 | G | C8-N9-C4 | 6.93 | 109.17 | 106.40 |
| 36 | A5 | 1589 | A | C2-N3-C4 | 6.93 | 114.06 | 110.60 |
| 36 | A5 | 1833 | G | C8-N9-C4 | 6.93 | 109.17 | 106.40 |
| 1 | A2 | 1749 | A | N9-C4-C5 | -6.93 | 103.03 | 105.80 |
| 36 | A5 | 857 | G | N9-C4-C5 | -6.93 | 102.63 | 105.40 |
| 36 | A1 | 371 | G | N9-C4-C5 | -6.93 | 102.63 | 105.40 |
| 36 | A1 | 987 | U | C2-N3-C4 | -6.93 | 122.84 | 127.00 |
| 36 | A1 | 873 | C | C6-N1-C2 | -6.92 | 117.53 | 120.30 |
| 36 | A1 | 1839 | A | C8-N9-C4 | -6.92 | 103.03 | 105.80 |
| 46 | BH | 62 | ARG | NE-CZ-NH1 | 6.92 | 123.76 | 120.30 |
| 80 | A6 | 385 | A | C5-N7-C8 | 6.92 | 107.36 | 103.90 |
| 13 | CL | 103 | ARG | NE-CZ-NH1 | 6.92 | 123.76 | 120.30 |
| 80 | A6 | 65 | A | N9-C4-C5 | -6.92 | 103.03 | 105.80 |
| 36 | A5 | 96 | G | C5-C6-O6 | 6.92 | 132.75 | 128.60 |
| 36 | A1 | 1851 | G | N3-C4-N9 | 6.92 | 130.15 | 126.00 |
| 36 | A1 | 2184 | U | C2-N1-C1' | 6.92 | 126.01 | 117.70 |
| 36 | A5 | 343 | U | C5-C4-O4 | 6.92 | 130.05 | 125.90 |
| 80 | A6 | 339 | C | N1-C2-O2 | -6.92 | 114.75 | 118.90 |
| 80 | A6 | 687 | G | N9-C4-C5 | 6.92 | 108.17 | 105.40 |
| 1 | A2 | 313 | U | N3-C4-O4 | -6.91 | 114.56 | 119.40 |
| 36 | A1 | 903 | U | C2-N3-C4 | -6.91 | 122.85 | 127.00 |
| 36 | A1 | 2393 | G | C5-C6-O6 | -6.91 | 124.45 | 128.60 |
| 36 | A1 | 2631 | U | N3-C4-O4 | -6.91 | 114.56 | 119.40 |
| 37 | A3 | 67 | G | N1-C6-O6 | 6.91 | 124.05 | 119.90 |
| 36 | A5 | 784 | A | C5-C6-N6 | -6.91 | 118.17 | 123.70 |
| 36 | A5 | 2412 | G | N3-C4-C5 | -6.91 | 125.14 | 128.60 |
| 37 | A7 | 74 | C | N1-C2-O2 | -6.91 | 114.75 | 118.90 |
| 52 | DO | 3[B] | SER | CA-C-N | -6.91 | 101.99 | 117.20 |
| 68 | De | 33 | ARG | NE-CZ-NH1 | 6.91 | 123.76 | 120.30 |
| 1 | A2 | 736 | C | C6-N1-C1' | -6.91 | 112.51 | 120.80 |
| 36 | A1 | 2941 | A | C5-C6-N1 | 6.91 | 121.16 | 117.70 |
| 36 | A5 | 3020 | U | N1-C2-O2 | -6.91 | 117.96 | 122.80 |
| 36 | A1 | 57 | A | C2-N3-C4 | -6.91 | 107.14 | 110.60 |
| 36 | A1 | 83 | U | C2-N3-C4 | -6.91 | 122.85 | 127.00 |
| 36 | A1 | 644 | G | N1-C6-O6 | -6.91 | 115.75 | 119.90 |
| 36 | A1 | 2836 | C | N3-C2-O2 | -6.91 | 117.06 | 121.90 |
| 36 | A1 | 3057 | U | N1-C2-N3 | 6.91 | 119.05 | 114.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 24 | G | C6-N1-C2 | -6.91 | 120.95 | 125.10 |
| 36 | A1 | 1460 | A | C5-C6-N1 | 6.91 | 121.15 | 117.70 |
| 36 | A1 | 1515 | A | C6-C5-N7 | -6.91 | 127.46 | 132.30 |
| 38 | A4 | 13 | A | C5-C6-N6 | -6.91 | 118.17 | 123.70 |
| 36 | A5 | 942 | U | C5-C4-O4 | -6.91 | 121.75 | 125.90 |
| 36 | A5 | 1210 | U | N3-C2-O2 | -6.91 | 117.36 | 122.20 |
| 36 | A5 | 3362 | A | C5-C6-N1 | -6.91 | 114.25 | 117.70 |
| 36 | A5 | 3362 | A | C6-C5-N7 | -6.91 | 127.46 | 132.30 |
| 36 | A1 | 967 | A | N7-C8-N9 | -6.91 | 110.35 | 113.80 |
| 36 | A1 | 2252 | A | C8-N9-C4 | -6.91 | 103.04 | 105.80 |
| 37 | A3 | 88 | G | N1-C6-O6 | -6.91 | 115.76 | 119.90 |
| 36 | A1 | 1646 | G | C5-C6-O6 | -6.91 | 124.46 | 128.60 |
| 36 | A1 | 302 | U | N3-C4-C5 | 6.90 | 118.74 | 114.60 |
| 36 | A1 | 917 | A | N1-C6-N6 | -6.90 | 114.46 | 118.60 |
| 36 | A5 | 1609 | C | N3-C4-N4 | 6.90 | 122.83 | 118.00 |
| 73 | Dj | 73 | ARG | NE-CZ-NH2 | -6.90 | 116.85 | 120.30 |
| 36 | A1 | 1130 | A | C5-C6-N6 | -6.90 | 118.18 | 123.70 |
| 36 | A1 | 3179 | U | N3-C2-O2 | -6.90 | 117.37 | 122.20 |
| 36 | A5 | 2732 | G | N3-C2-N2 | 6.90 | 124.73 | 119.90 |
| 36 | A1 | 339 | C | C5-C4-N4 | 6.90 | 125.03 | 120.20 |
| 80 | A6 | 868 | G | C5-C6-O6 | -6.90 | 124.46 | 128.60 |
| 36 | A5 | 3019 | U | C2-N3-C4 | -6.90 | 122.86 | 127.00 |
| 80 | A6 | 29 | U | N3-C2-O2 | -6.90 | 117.37 | 122.20 |
| 36 | A5 | 1883 | A | N1-C6-N6 | -6.90 | 114.46 | 118.60 |
| 36 | A1 | 1741 | A | C5-N7-C8 | -6.89 | 100.45 | 103.90 |
| 36 | A5 | 221 | A | C8-N9-C4 | 6.89 | 108.56 | 105.80 |
| 36 | A1 | 980 | A | C8-N9-C4 | -6.89 | 103.04 | 105.80 |
| 80 | A6 | 987 | G | C5-C6-O6 | -6.89 | 124.46 | 128.60 |
| 48 | DJ | 9 | MET | N-CA-C | -6.89 | 92.39 | 111.00 |
| 80 | A6 | 354 | C | N3-C4-C5 | 6.89 | 124.66 | 121.90 |
| 36 | A5 | 419 | G | N3-C4-N9 | 6.89 | 130.13 | 126.00 |
| 36 | A1 | 1150 | A | C5-C6-N1 | -6.89 | 114.25 | 117.70 |
| 46 | BH | 91 | ARG | NE-CZ-NH1 | -6.89 | 116.86 | 120.30 |
| 1 | A2 | 1206 | U | N3-C4-O4 | 6.89 | 124.22 | 119.40 |
| 38 | A4 | 142 | C | N1-C2-O2 | -6.89 | 114.77 | 118.90 |
| 80 | A6 | 638 | U | N1-C2-O2 | 6.89 | 127.62 | 122.80 |
| 36 | A5 | 1603 | A | C8-N9-C4 | -6.89 | 103.05 | 105.80 |
| 36 | A1 | 1932 | A | C2-N3-C4 | 6.88 | 114.04 | 110.60 |
| 36 | A1 | 2288 | G | N7-C8-N9 | 6.88 | 116.54 | 113.10 |
| 36 | A5 | 1370 | G | N1-C2-N2 | -6.88 | 110.00 | 116.20 |
| 36 | A5 | 2246 | G | C8-N9-C4 | -6.88 | 103.65 | 106.40 |
| 1 | A2 | 305 | C | C6-N1-C2 | -6.88 | 117.55 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A2 | 1361 | U | N1-C2-O2 | 6.88 | 127.62 | 122.80 |
| 80 | A6 | 1124 | A | C8-N9-C4 | 6.88 | 108.55 | 105.80 |
| 80 | A6 | 1631 | A | C2-N3-C4 | -6.88 | 107.16 | 110.60 |
| 36 | A5 | 833 | G | C6-N1-C2 | -6.88 | 120.97 | 125.10 |
| 36 | A5 | 1875 | G | N1-C6-O6 | -6.88 | 115.77 | 119.90 |
| 36 | A1 | 356 | C | C2-N3-C4 | -6.88 | 116.46 | 119.90 |
| 80 | A6 | 1592 | A | N1-C2-N3 | 6.88 | 132.74 | 129.30 |
| 36 | A1 | 317 | A | N1-C2-N3 | -6.88 | 125.86 | 129.30 |
| 36 | A1 | 2641 | U | C5-C6-N1 | -6.88 | 119.26 | 122.70 |
| 36 | A1 | 2669 | G | C2-N3-C4 | -6.88 | 108.46 | 111.90 |
| 80 | A6 | 418 | G | N7-C8-N9 | 6.88 | 116.54 | 113.10 |
| 36 | A5 | 2978 | U | N3-C4-O4 | -6.88 | 114.58 | 119.40 |
| 36 | A1 | 2980 | U | N3-C2-O2 | -6.88 | 117.39 | 122.20 |
| 36 | A5 | 1406 | A | N1-C2-N3 | 6.88 | 132.74 | 129.30 |
| 36 | A1 | 2306 | C | C6-N1-C2 | -6.88 | 117.55 | 120.30 |
| 36 | A1 | 2952 | G | N3-C4-C5 | 6.88 | 132.04 | 128.60 |
| 1 | A2 | 92 | A | N9-C4-C5 | 6.87 | 108.55 | 105.80 |
| 36 | A5 | 864 | G | C6-N1-C2 | -6.87 | 120.98 | 125.10 |
| 36 | A5 | 2207 | A | N1-C6-N6 | 6.87 | 122.72 | 118.60 |
| 36 | A5 | 2695 | A | N7-C8-N9 | 6.87 | 117.24 | 113.80 |
| 36 | A5 | 3308 | C | C6-N1-C2 | -6.87 | 117.55 | 120.30 |
| 36 | A1 | 369 | A | N1-C2-N3 | -6.87 | 125.86 | 129.30 |
| 36 | A1 | 3343 | G | N1-C2-N2 | -6.87 | 110.02 | 116.20 |
| 36 | A5 | 3376 | A | N7-C8-N9 | 6.87 | 117.24 | 113.80 |
| 36 | A1 | 1374 | G | N3-C2-N2 | 6.87 | 124.71 | 119.90 |
| 36 | A5 | 857 | G | C8-N9-C4 | 6.87 | 109.15 | 106.40 |
| 36 | A5 | 1513 | G | N7-C8-N9 | 6.87 | 116.53 | 113.10 |
| 36 | A5 | 1903 | U | N3-C4-C5 | -6.87 | 110.48 | 114.60 |
| 36 | A1 | 1346 | G | C2-N3-C4 | -6.87 | 108.47 | 111.90 |
| 56 | BS | 167 | ARG | NE-CZ-NH1 | 6.87 | 123.73 | 120.30 |
| 36 | A5 | 2705 | A | C2-N3-C4 | 6.87 | 114.03 | 110.60 |
| 36 | A1 | 1409 | G | N9-C4-C5 | 6.87 | 108.15 | 105.40 |
| 36 | A1 | 2921 | U | N3-C4-C5 | 6.87 | 118.72 | 114.60 |
| 36 | A1 | 3268 | A | C2-N3-C4 | -6.87 | 107.17 | 110.60 |
| 38 | A4 | 67 | U | C5-C6-N1 | -6.87 | 119.27 | 122.70 |
| 36 | A5 | 1417 | G | C5-C6-N1 | 6.86 | 114.93 | 111.50 |
| 36 | A5 | 2382 | G | N1-C6-O6 | -6.86 | 115.78 | 119.90 |
| 36 | A1 | 580 | C | C6-N1-C2 | -6.86 | 117.56 | 120.30 |
| 36 | A1 | 2279 | A | C4-C5-N7 | 6.86 | 114.13 | 110.70 |
| 80 | A6 | 18 | C | N1-C2-O2 | -6.86 | 114.78 | 118.90 |
| 80 | A6 | 467 | G | N1-C6-O6 | -6.86 | 115.78 | 119.90 |
| 36 | A5 | 2884 | C | N1-C2-O2 | -6.86 | 114.78 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 36 | A1 | 2306 | C | C5-C4-N4 | 6.86 | 125.00 | 120.20 |
| 80 | A6 | 87 | C | C4-C5-C6 | 6.86 | 120.83 | 117.40 |
| 51 | BN | 105 | ARG | NE-CZ-NH1 | 6.86 | 123.73 | 120.30 |
| 80 | A6 | 638 | U | N3-C2-O2 | -6.86 | 117.40 | 122.20 |
| 1 | A2 | 453 | U | N1-C2-O2 | 6.86 | 127.60 | 122.80 |
| 36 | A5 | 189 | G | N1-C6-O6 | -6.86 | 115.78 | 119.90 |
| 36 | A5 | 3105 | U | N3-C2-O2 | 6.86 | 127.00 | 122.20 |
| 36 | A1 | 281 | G | N7-C8-N9 | 6.86 | 116.53 | 113.10 |
| 80 | A6 | 1782 | A | N7-C8-N9 | 6.86 | 117.23 | 113.80 |
| 36 | A1 | 3230 | G | C6-N1-C2 | -6.85 | 120.99 | 125.10 |
| 36 | A5 | 2729 | U | C5-C6-N1 | 6.85 | 126.13 | 122.70 |
| 36 | A1 | 187 | A | N3-C4-C5 | -6.85 | 122.00 | 126.80 |
| 36 | A1 | 988 | U | N3-C4-O4 | -6.85 | 114.60 | 119.40 |
| 36 | A5 | 2524 | A | C3'-C2'-C1' | -6.85 | 96.02 | 101.50 |
| 36 | A5 | 2987 | A | C5-N7-C8 | 6.85 | 107.33 | 103.90 |
| 36 | A1 | 1191 | U | N1-C2-N3 | 6.85 | 119.01 | 114.90 |
| 36 | A1 | 715 | A | N7-C8-N9 | 6.85 | 117.22 | 113.80 |
| 36 | A1 | 2982 | A | C8-N9-C4 | 6.85 | 108.54 | 105.80 |
| 36 | A5 | 693 | A | N1-C6-N6 | -6.85 | 114.49 | 118.60 |
| 36 | A5 | 2385 | G | C2-N3-C4 | -6.85 | 108.47 | 111.90 |
| 36 | A5 | 3176 | G | N1-C2-N3 | 6.85 | 128.01 | 123.90 |
| 80 | A6 | 9 | U | C2-N3-C4 | -6.85 | 122.89 | 127.00 |
| 36 | A5 | 881 | C | C2-N3-C4 | 6.85 | 123.32 | 119.90 |
| 37 | A7 | 112 | G | C5-C6-O6 | 6.85 | 132.71 | 128.60 |
| 36 | A1 | 517 | G | N9-C4-C5 | 6.85 | 108.14 | 105.40 |
| 36 | A1 | 1515 | A | N1-C6-N6 | 6.84 | 122.71 | 118.60 |
| 36 | A5 | 3149 | G | C2-N3-C4 | -6.84 | 108.48 | 111.90 |
| 36 | A1 | 2823 | G | C5-N7-C8 | 6.84 | 107.72 | 104.30 |
| 1 | A2 | 934 | C | C2-N1-C1' | 6.84 | 126.33 | 118.80 |
| 80 | A6 | 337 | G | N1-C2-N3 | -6.84 | 119.80 | 123.90 |
| 80 | A6 | 351 | C | N3-C4-C5 | -6.84 | 119.16 | 121.90 |
| 36 | A1 | 1076 | C | C6-N1-C2 | 6.84 | 123.04 | 120.30 |
| 36 | A5 | 2237 | C | N1-C2-O2 | 6.84 | 123.00 | 118.90 |
| 36 | A5 | 2359 | C | C6-N1-C2 | 6.84 | 123.04 | 120.30 |
| 36 | A1 | 1136 | A | C5-C6-N1 | 6.84 | 121.12 | 117.70 |
| 80 | A6 | 372 | G | C8-N9-C4 | 6.84 | 109.14 | 106.40 |
| 80 | A6 | 617 | U | C6-N1-C2 | -6.84 | 116.90 | 121.00 |
| 36 | A5 | 815 | G | C4-C5-N7 | -6.84 | 108.06 | 110.80 |
| 36 | A5 | 1297 | C | N1-C2-O2 | -6.84 | 114.80 | 118.90 |
| 36 | A5 | 2362 | C | N3-C4-C5 | 6.84 | 124.64 | 121.90 |
| 36 | A5 | 2401 | A | C2-N3-C4 | 6.84 | 114.02 | 110.60 |
| 36 | A1 | 584 | G | N9-C4-C5 | 6.83 | 108.13 | 105.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 37 | A3 | 22 | A | N1-C6-N6 | 6.83 | 122.70 | 118.60 |
| 80 | A6 | 1030 | A | N9-C4-C5 | 6.83 | 108.53 | 105.80 |
| 80 | A6 | 1796 | C | N3-C4-N4 | -6.83 | 113.22 | 118.00 |
| 36 | A5 | 3056 | U | N1-C2-N3 | 6.83 | 119.00 | 114.90 |
| 1 | A2 | 73 | U | O4'-C1'-N1 | 6.83 | 113.67 | 108.20 |
| 36 | A1 | 2816 | G | C5-C6-O6 | -6.83 | 124.50 | 128.60 |
| 36 | A1 | 3015 | G | C5-C6-N1 | 6.83 | 114.92 | 111.50 |
| 38 | A4 | 25 | G | C5-N7-C8 | 6.83 | 107.72 | 104.30 |
| 80 | A6 | 342 | C | C4-C5-C6 | 6.83 | 120.81 | 117.40 |
| 36 | A1 | 1592 | G | C5-N7-C8 | -6.83 | 100.89 | 104.30 |
| 40 | BB | 7 | GLU | OE1-CD-OE2 | -6.83 | 115.10 | 123.30 |
| 36 | A5 | 2664 | C | N3-C4-C5 | 6.83 | 124.63 | 121.90 |
| 36 | A5 | 3081 | C | C4-C5-C6 | -6.83 | 113.98 | 117.40 |
| 36 | A1 | 750 | G | C5-C6-O6 | 6.83 | 132.70 | 128.60 |
| 36 | A1 | 2280 | A | N1-C6-N6 | 6.83 | 122.70 | 118.60 |
| 80 | A6 | 1246 | C | N3-C2-O2 | -6.83 | 117.12 | 121.90 |
| 36 | A5 | 1868 | G | C8-N9-C4 | 6.83 | 109.13 | 106.40 |
| 1 | A2 | 1146 | G | C8-N9-C4 | -6.83 | 103.67 | 106.40 |
| 36 | A1 | 1169 | A | C6-C5-N7 | -6.83 | 127.52 | 132.30 |
| 36 | A1 | 1695 | U | C5-C6-N1 | -6.83 | 119.29 | 122.70 |
| 36 | A5 | 622 | A | C5-C6-N6 | -6.83 | 118.24 | 123.70 |
| 36 | A5 | 1902 | G | C6-N1-C2 | -6.83 | 121.00 | 125.10 |
| 36 | A5 | 1941 | C | C2-N3-C4 | -6.83 | 116.49 | 119.90 |
| 1 | A2 | 607 | G | N1-C6-O6 | 6.82 | 123.99 | 119.90 |
| 36 | A1 | 3172 | A | C8-N9-C4 | 6.82 | 108.53 | 105.80 |
| 80 | A6 | 453 | U | C6-N1-C2 | -6.82 | 116.91 | 121.00 |
| 80 | A6 | 1472 | C | N3-C4-N4 | -6.82 | 113.22 | 118.00 |
| 1 | A2 | 1319 | A | N1-C6-N6 | 6.82 | 122.69 | 118.60 |
| 36 | A1 | 331 | G | C4-C5-N7 | -6.82 | 108.07 | 110.80 |
| 36 | A1 | 1858 | A | C4-N9-C1' | 6.82 | 138.58 | 126.30 |
| 36 | A5 | 2400 | G | N3-C4-C5 | 6.82 | 132.01 | 128.60 |
| 36 | A5 | 3321 | C | C4-C5-C6 | 6.82 | 120.81 | 117.40 |
| 36 | A5 | 1481 | A | P-O3'-C3' | 6.82 | 127.88 | 119.70 |
| 38 | A8 | 23 | U | N1-C2-N3 | 6.82 | 118.99 | 114.90 |
| 36 | A1 | 639 | G | C6-C5-N7 | -6.82 | 126.31 | 130.40 |
| 36 | A5 | 578 | A | C5-C6-N6 | -6.82 | 118.25 | 123.70 |
| 41 | DC | 90 | PHE | C-N-CA | -6.82 | 107.98 | 122.30 |
| 38 | A4 | 7 | U | C5-C6-N1 | -6.82 | 119.29 | 122.70 |
| 36 | A5 | 1124 | U | N1-C2-O2 | 6.81 | 127.57 | 122.80 |
| 36 | A5 | 1941 | C | N3-C4-C5 | 6.81 | 124.62 | 121.90 |
| 36 | A1 | 851 | C | C2-N1-C1' | 6.81 | 126.30 | 118.80 |
| 36 | A5 | 1138 | U | N3-C4-C5 | 6.81 | 118.69 | 114.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 1940 | G | N1-C6-O6 | -6.81 | 115.81 | 119.90 |
| 36 | A5 | 2389 | C | C2-N3-C4 | -6.81 | 116.49 | 119.90 |
| 36 | A5 | 2821 | C | C6-N1-C2 | -6.81 | 117.58 | 120.30 |
| 1 | A2 | 240 | U | C2-N1-C1' | 6.81 | 125.87 | 117.70 |
| 36 | A1 | 1489 | A | C6-C5-N7 | -6.81 | 127.53 | 132.30 |
| 1 | A2 | 1611 | A | N1-C2-N3 | 6.81 | 132.71 | 129.30 |
| 36 | A1 | 545 | U | N3-C2-O2 | -6.81 | 117.43 | 122.20 |
| 36 | A5 | 327 | A | C8-N9-C4 | 6.81 | 108.52 | 105.80 |
| 36 | A5 | 1369 | A | C8-N9-C4 | 6.81 | 108.52 | 105.80 |
| 36 | A5 | 3101 | G | C5-C6-O6 | 6.81 | 132.69 | 128.60 |
| 36 | A1 | 2678 | A | N9-C4-C5 | 6.81 | 108.52 | 105.80 |
| 36 | A1 | 2865 | U | C5-C4-O4 | -6.81 | 121.82 | 125.90 |
| 36 | A5 | 41 | G | C4-C5-N7 | 6.81 | 113.52 | 110.80 |
| 36 | A5 | 1448 | U | C2-N3-C4 | -6.81 | 122.92 | 127.00 |
| 1 | A2 | 410 | A | C8-N9-C4 | 6.81 | 108.52 | 105.80 |
| 40 | BB | 19 | ARG | NE-CZ-NH2 | -6.81 | 116.90 | 120.30 |
| 1 | A2 | 1195 | C | C6-N1-C2 | -6.80 | 117.58 | 120.30 |
| 38 | A4 | 63 | G | N1-C6-O6 | -6.80 | 115.82 | 119.90 |
| 36 | A5 | 1652 | G | N7-C8-N9 | -6.80 | 109.70 | 113.10 |
| 36 | A5 | 2524 | A | C4-C5-N7 | 6.80 | 114.10 | 110.70 |
| 36 | A1 | 637 | C | N1-C2-N3 | 6.80 | 123.96 | 119.20 |
| 36 | A1 | 864 | G | N1-C6-O6 | -6.80 | 115.82 | 119.90 |
| 36 | A1 | 2111 | G | C5-C6-O6 | 6.80 | 132.68 | 128.60 |
| 36 | A5 | 1556 | C | C6-N1-C2 | -6.80 | 117.58 | 120.30 |
| 36 | A5 | 2341 | A | N9-C4-C5 | -6.80 | 103.08 | 105.80 |
| 1 | A2 | 360 | A | C8-N9-C4 | 6.80 | 108.52 | 105.80 |
| 36 | A5 | 564 | G | C4-C5-N7 | -6.80 | 108.08 | 110.80 |
| 36 | A1 | 1411 | C | N3-C2-O2 | -6.80 | 117.14 | 121.90 |
| 36 | A1 | 2222 | A | N9-C4-C5 | 6.80 | 108.52 | 105.80 |
| 36 | A5 | 3374 | U | N3-C4-O4 | -6.80 | 114.64 | 119.40 |
| 36 | A1 | 347 | G | C8-N9-C4 | 6.80 | 109.12 | 106.40 |
| 36 | A5 | 669 | U | C2-N3-C4 | -6.80 | 122.92 | 127.00 |
| 36 | A1 | 1906 | G | C5-C6-O6 | -6.80 | 124.52 | 128.60 |
| 36 | A1 | 2237 | C | N3-C4-C5 | 6.80 | 124.62 | 121.90 |
| 36 | A5 | 1205 | A | N7-C8-N9 | 6.80 | 117.20 | 113.80 |
| 36 | A5 | 2434 | U | C5-C4-O4 | 6.80 | 129.98 | 125.90 |
| 36 | A1 | 948 | C | C4-C5-C6 | 6.79 | 120.80 | 117.40 |
| 36 | A1 | 1173 | U | C2-N3-C4 | -6.79 | 122.92 | 127.00 |
| 80 | A6 | 1085 | G | C5-C6-O6 | 6.79 | 132.68 | 128.60 |
| 37 | A7 | 11 | A | C5-N7-C8 | 6.79 | 107.30 | 103.90 |
| 1 | A2 | 1006 | C | C6-N1-C2 | -6.79 | 117.58 | 120.30 |
| 36 | A5 | 2619 | G | C5-C6-O6 | -6.79 | 124.52 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 2639 | G | C8-N9-C4 | 6.79 | 109.12 | 106.40 |
| 36 | A5 | 63 | A | N1-C6-N6 | 6.79 | 122.67 | 118.60 |
| 36 | A1 | 394 | G | N3-C2-N2 | 6.79 | 124.65 | 119.90 |
| 36 | A1 | 521 | A | N9-C4-C5 | -6.79 | 103.08 | 105.80 |
| 36 | A1 | 548 | G | N3-C4-C5 | 6.79 | 132.00 | 128.60 |
| 36 | A1 | 2362 | C | N1-C2-O2 | 6.79 | 122.97 | 118.90 |
| 36 | A1 | 2826 | U | C5-C6-N1 | -6.79 | 119.31 | 122.70 |
| 36 | A1 | 2830 | G | N3-C2-N2 | -6.79 | 115.15 | 119.90 |
| 36 | A5 | 2692 | A | N1-C6-N6 | -6.79 | 114.53 | 118.60 |
| 1 | A2 | 1318 | G | N1-C6-O6 | 6.79 | 123.97 | 119.90 |
| 36 | A1 | 1060 | U | C2-N3-C4 | -6.79 | 122.93 | 127.00 |
| 36 | A1 | 1200 | A | N1-C6-N6 | -6.79 | 114.53 | 118.60 |
| 36 | A1 | 1329 | U | N3-C2-O2 | -6.79 | 117.45 | 122.20 |
| 36 | A1 | 2351 | U | N3-C2-O2 | -6.79 | 117.45 | 122.20 |
| 79 | Dp | 17 | ARG | NE-CZ-NH1 | -6.79 | 116.91 | 120.30 |
| 80 | A6 | 622 | A | C4-C5-N7 | -6.79 | 107.31 | 110.70 |
| 1 | A2 | 142 | G | N1-C2-N2 | 6.79 | 122.31 | 116.20 |
| 36 | A1 | 383 | G | C8-N9-C4 | 6.79 | 109.11 | 106.40 |
| 36 | A1 | 1137 | C | N1-C2-N3 | 6.79 | 123.95 | 119.20 |
| 47 | DI | 48 | LEU | CA-CB-CG | 6.79 | 130.91 | 115.30 |
| 38 | A8 | 38 | U | C4-C5-C6 | 6.78 | 123.77 | 119.70 |
| 1 | A2 | 1762 | A | C8-N9-C4 | 6.78 | 108.51 | 105.80 |
| 36 | A1 | 895 | A | N3-C4-N9 | -6.78 | 121.97 | 127.40 |
| 36 | A1 | 2650 | U | C5-C4-O4 | 6.78 | 129.97 | 125.90 |
| 36 | A5 | 1327 | C | N3-C2-O2 | -6.78 | 117.15 | 121.90 |
| 36 | A1 | 304 | G | N1-C2-N2 | 6.78 | 122.30 | 116.20 |
| 36 | A1 | 1300 | G | C8-N9-C4 | 6.78 | 109.11 | 106.40 |
| 36 | A1 | 1432 | C | C6-N1-C2 | -6.78 | 117.59 | 120.30 |
| 80 | A6 | 622 | A | C8-N9-C4 | -6.78 | 103.09 | 105.80 |
| 36 | A5 | 838 | G | C5-C6-O6 | 6.78 | 132.67 | 128.60 |
| 36 | A5 | 1449 | A | C6-C5-N7 | -6.78 | 127.55 | 132.30 |
| 36 | A5 | 2824 | G | C4-C5-N7 | -6.78 | 108.09 | 110.80 |
| 37 | A7 | 49 | G | C8-N9-C4 | 6.78 | 109.11 | 106.40 |
| 36 | A1 | 3137 | C | N1-C2-O2 | -6.78 | 114.83 | 118.90 |
| 36 | A1 | 30 | G | N1-C2-N2 | -6.78 | 110.10 | 116.20 |
| 80 | A6 | 430 | G | C5-C6-O6 | -6.78 | 124.53 | 128.60 |
| 36 | A5 | 2730 | G | C2-N3-C4 | -6.78 | 108.51 | 111.90 |
| 36 | A5 | 2810 | C | C4-C5-C6 | 6.78 | 120.79 | 117.40 |
| 36 | A5 | 3076 | C | C2-N3-C4 | -6.78 | 116.51 | 119.90 |
| 36 | A5 | 48 | A | C8-N9-C4 | -6.78 | 103.09 | 105.80 |
| 36 | A5 | 413 | U | C4-C5-C6 | 6.78 | 123.77 | 119.70 |
| 36 | A5 | 1130 | A | N1-C2-N3 | -6.77 | 125.91 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 1469 | C | C6-N1-C2 | -6.77 | 117.59 | 120.30 |
| 36 | A1 | 2231 | C | C6-N1-C2 | 6.77 | 123.01 | 120.30 |
| 36 | A5 | 652 | G | C6-N1-C2 | -6.77 | 121.04 | 125.10 |
| 36 | A5 | 1685 | C | N3-C2-O2 | -6.77 | 117.16 | 121.90 |
| 36 | A1 | 2831 | G | N3-C2-N2 | -6.77 | 115.16 | 119.90 |
| 36 | A5 | 146 | U | C5-C4-O4 | 6.77 | 129.96 | 125.90 |
| 36 | A5 | 2693 | C | N1-C2-O2 | 6.77 | 122.96 | 118.90 |
| 1 | A2 | 553 | G | N1-C2-N2 | 6.77 | 122.29 | 116.20 |
| 31 | Ad | 36 | LEU | CA-CB-CG | 6.77 | 130.87 | 115.30 |
| 36 | A1 | 2357 | A | C4-C5-C6 | 6.77 | 120.39 | 117.00 |
| 80 | A6 | 297 | U | N3-C4-O4 | 6.77 | 124.14 | 119.40 |
| 80 | A6 | 777 | C | C5-C6-N1 | 6.77 | 124.38 | 121.00 |
| 80 | A6 | 1614 | A | N7-C8-N9 | 6.77 | 117.19 | 113.80 |
| 36 | A5 | 2899 | C | C4-C5-C6 | 6.77 | 120.78 | 117.40 |
| 37 | A7 | 22 | A | N1-C6-N6 | 6.77 | 122.66 | 118.60 |
| 36 | A1 | 2350 | C | N3-C4-C5 | 6.77 | 124.61 | 121.90 |
| 36 | A1 | 2392 | C | C5-C4-N4 | -6.77 | 115.46 | 120.20 |
| 36 | A5 | 2932 | U | N3-C2-O2 | -6.77 | 117.46 | 122.20 |
| 1 | A2 | 1190 | C | C6-N1-C2 | 6.77 | 123.01 | 120.30 |
| 36 | A1 | 1495 | U | C6-N1-C1' | 6.77 | 130.67 | 121.20 |
| 36 | A1 | 2378 | C | N3-C4-N4 | 6.77 | 122.74 | 118.00 |
| 80 | A6 | 163 | G | C8-N9-C1' | 6.77 | 135.80 | 127.00 |
| 36 | A1 | 593 | C | N1-C2-O2 | -6.76 | 114.84 | 118.90 |
| 36 | A1 | 2808 | A | C4-C5-C6 | 6.76 | 120.38 | 117.00 |
| 36 | A1 | 3083 | G | N3-C4-N9 | 6.76 | 130.06 | 126.00 |
| 4 | CC | 235 | LEU | CA-CB-CG | 6.76 | 130.86 | 115.30 |
| 36 | A5 | 644 | G | N3-C4-C5 | -6.76 | 125.22 | 128.60 |
| 36 | A5 | 960 | U | N3-C2-O2 | -6.76 | 117.46 | 122.20 |
| 36 | A5 | 1843 | C | N3-C2-O2 | -6.76 | 117.17 | 121.90 |
| 36 | A1 | 1007 | U | C5-C6-N1 | -6.76 | 119.32 | 122.70 |
| 36 | A1 | 1417 | G | C8-N9-C4 | 6.76 | 109.11 | 106.40 |
| 36 | A1 | 1615 | C | C2-N3-C4 | -6.76 | 116.52 | 119.90 |
| 36 | A1 | 2984 | C | N3-C4-N4 | -6.76 | 113.27 | 118.00 |
| 36 | A1 | 3034 | C | N3-C2-O2 | -6.76 | 117.17 | 121.90 |
| 38 | A4 | 58 | G | N9-C4-C5 | -6.76 | 102.70 | 105.40 |
| 80 | A6 | 677 | G | N3-C4-C5 | 6.76 | 131.98 | 128.60 |
| 80 | A6 | 1008 | G | C5-C6-O6 | -6.76 | 124.54 | 128.60 |
| 36 | A5 | 749 | C | C6-N1-C2 | -6.76 | 117.59 | 120.30 |
| 36 | A5 | 888 | A | C5-C6-N1 | -6.76 | 114.32 | 117.70 |
| 36 | A5 | 2820 | A | C6-N1-C2 | -6.76 | 114.54 | 118.60 |
| 36 | A5 | 3088 | G | N3-C2-N2 | 6.76 | 124.63 | 119.90 |
| 36 | A5 | 3313 | U | C5-C4-O4 | 6.76 | 129.96 | 125.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 1665 | C | C2-N3-C4 | -6.76 | 116.52 | 119.90 |
| 36 | A5 | 205 | C | N3-C2-O2 | -6.76 | 117.17 | 121.90 |
| 36 | A5 | 1116 | G | N9-C4-C5 | 6.76 | 108.10 | 105.40 |
| 36 | A5 | 1421 | G | C2-N3-C4 | -6.76 | 108.52 | 111.90 |
| 36 | A5 | 3375 | A | C2-N3-C4 | 6.76 | 113.98 | 110.60 |
| 36 | A1 | 1405 | U | C5-C6-N1 | -6.76 | 119.32 | 122.70 |
| 36 | A1 | 2611 | U | C2-N3-C4 | -6.76 | 122.94 | 127.00 |
| 80 | A6 | 617 | U | C2-N1-C1' | 6.76 | 125.81 | 117.70 |
| 36 | A1 | 1492 | G | C4-C5-C6 | 6.76 | 122.85 | 118.80 |
| 36 | A1 | 2274 | U | N3-C2-O2 | -6.76 | 117.47 | 122.20 |
| 80 | A6 | 354 | C | C4-C5-C6 | -6.76 | 114.02 | 117.40 |
| 36 | A5 | 2391 | G | N7-C8-N9 | 6.76 | 116.48 | 113.10 |
| 36 | A5 | 2647 | A | N1-C6-N6 | -6.76 | 114.55 | 118.60 |
| 1 | A2 | 539 | G | N7-C8-N9 | 6.75 | 116.48 | 113.10 |
| 36 | A1 | 2415 | C | C5-C6-N1 | -6.75 | 117.62 | 121.00 |
| 36 | A5 | 345 | G | N1-C2-N2 | -6.75 | 110.12 | 116.20 |
| 36 | A5 | 890 | C | N3-C4-C5 | 6.75 | 124.60 | 121.90 |
| 36 | A1 | 3279 | A | N7-C8-N9 | 6.75 | 117.17 | 113.80 |
| 80 | A6 | 95 | G | C8-N9-C4 | -6.75 | 103.70 | 106.40 |
| 80 | A6 | 426 | G | N3-C4-C5 | -6.75 | 125.22 | 128.60 |
| 36 | A5 | 1910 | A | N7-C8-N9 | -6.75 | 110.42 | 113.80 |
| 37 | A7 | 50 | U | C5-C6-N1 | 6.75 | 126.08 | 122.70 |
| 1 | A2 | 1210 | C | N3-C4-C5 | -6.75 | 119.20 | 121.90 |
| 36 | A5 | 908 | G | C4-N9-C1' | 6.75 | 135.27 | 126.50 |
| 36 | A5 | 2908 | G | C5-C6-O6 | 6.75 | 132.65 | 128.60 |
| 36 | A1 | 2286 | U | N1-C2-N3 | 6.75 | 118.95 | 114.90 |
| 80 | A6 | 44 | U | N1-C2-N3 | 6.75 | 118.95 | 114.90 |
| 80 | A6 | 543 | C | C5-C4-N4 | 6.75 | 124.92 | 120.20 |
| 80 | A6 | 624 | G | C8-N9-C4 | 6.75 | 109.10 | 106.40 |
| 80 | A6 | 1280 | C | C4-C5-C6 | 6.75 | 120.77 | 117.40 |
| 36 | A5 | 776 | U | N3-C4-O4 | -6.75 | 114.68 | 119.40 |
| 36 | A5 | 1197 | A | N1-C2-N3 | 6.75 | 132.67 | 129.30 |
| 36 | A5 | 2584 | G | C8-N9-C1' | -6.75 | 118.23 | 127.00 |
| 36 | A1 | 2174 | G | N7-C8-N9 | 6.75 | 116.47 | 113.10 |
| 36 | A5 | 95 | A | C5-C6-N6 | -6.75 | 118.30 | 123.70 |
| 36 | A1 | 96 | G | C2-N3-C4 | -6.74 | 108.53 | 111.90 |
| 36 | A1 | 397 | A | N1-C6-N6 | -6.74 | 114.55 | 118.60 |
| 36 | A1 | 1181 | U | C5-C6-N1 | -6.74 | 119.33 | 122.70 |
| 36 | A1 | 2702 | A | C8-N9-C4 | -6.74 | 103.10 | 105.80 |
| 36 | A5 | 3324 | C | C6-N1-C2 | 6.74 | 123.00 | 120.30 |
| 36 | A5 | 2685 | C | C2-N3-C4 | -6.74 | 116.53 | 119.90 |
| 36 | A1 | 2153 | U | N1-C2-N3 | 6.74 | 118.94 | 114.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 3319 | U | N3-C2-O2 | -6.74 | 117.48 | 122.20 |
| 36 | A5 | 887 | G | C2-N3-C4 | -6.74 | 108.53 | 111.90 |
| 36 | A5 | 2830 | G | C4-C5-N7 | -6.74 | 108.10 | 110.80 |
| 36 | A1 | 1138 | U | C2-N3-C4 | -6.74 | 122.96 | 127.00 |
| 80 | A6 | 382 | C | N3-C4-C5 | 6.74 | 124.59 | 121.90 |
| 36 | A5 | 322 | U | C5-C4-O4 | -6.74 | 121.86 | 125.90 |
| 36 | A5 | 644 | G | C8-N9-C4 | -6.74 | 103.70 | 106.40 |
| 36 | A1 | 1517 | G | C5-N7-C8 | 6.74 | 107.67 | 104.30 |
| 36 | A5 | 1134 | G | C5-C6-N1 | 6.74 | 114.87 | 111.50 |
| 36 | A1 | 374 | A | C5-C6-N6 | 6.74 | 129.09 | 123.70 |
| 36 | A1 | 649 | A | C5-C6-N6 | 6.74 | 129.09 | 123.70 |
| 36 | A1 | 1911 | A | N9-C4-C5 | -6.74 | 103.11 | 105.80 |
| 36 | A5 | 1375 | G | C2-N3-C4 | 6.74 | 115.27 | 111.90 |
| 36 | A5 | 2317 | A | N7-C8-N9 | 6.74 | 117.17 | 113.80 |
| 36 | A5 | 3336 | A | N1-C2-N3 | 6.74 | 132.67 | 129.30 |
| 36 | A5 | 1911 | A | C5-C6-N6 | -6.73 | 118.31 | 123.70 |
| 36 | A1 | 197 | G | C5-C6-O6 | -6.73 | 124.56 | 128.60 |
| 36 | A1 | 1339 | C | C5-C6-N1 | -6.73 | 117.63 | 121.00 |
| 80 | A6 | 1329 | A | N9-C4-C5 | -6.73 | 103.11 | 105.80 |
| 36 | A5 | 2145 | A | N1-C6-N6 | -6.73 | 114.56 | 118.60 |
| 36 | A1 | 1491 | A | C8-N9-C4 | 6.73 | 108.49 | 105.80 |
| 36 | A1 | 1507 | G | C4-C5-C6 | 6.73 | 122.84 | 118.80 |
| 36 | A5 | 1686 | U | C5-C4-O4 | -6.73 | 121.86 | 125.90 |
| 36 | A5 | 2231 | C | C4-C5-C6 | 6.73 | 120.77 | 117.40 |
| 56 | DS | 40 | ARG | CG-CD-NE | 6.73 | 125.94 | 111.80 |
| 1 | A2 | 89 | G | N7-C8-N9 | -6.73 | 109.74 | 113.10 |
| 36 | A1 | 928 | C | C6-N1-C2 | -6.73 | 117.61 | 120.30 |
| 36 | A5 | 1056 | U | N3-C4-O4 | 6.73 | 124.11 | 119.40 |
| 36 | A5 | 1652 | G | C5-N7-C8 | 6.73 | 107.66 | 104.30 |
| 36 | A1 | 1309 | U | N1-C2-O2 | -6.73 | 118.09 | 122.80 |
| 80 | A6 | 1095 | U | C5-C6-N1 | -6.73 | 119.34 | 122.70 |
| 36 | A5 | 587 | U | N3-C4-C5 | 6.73 | 118.64 | 114.60 |
| 36 | A5 | 1044 | U | C5-C6-N1 | -6.73 | 119.34 | 122.70 |
| 36 | A5 | 2920 | U | C2-N3-C4 | -6.73 | 122.96 | 127.00 |
| 36 | A1 | 758 | C | C6-N1-C2 | -6.72 | 117.61 | 120.30 |
| 36 | A1 | 1164 | G | C8-N9-C4 | -6.72 | 103.71 | 106.40 |
| 80 | A6 | 1478 | G | C6-C5-N7 | -6.72 | 126.37 | 130.40 |
| 36 | A5 | 1496 | C | C2-N1-C1' | 6.72 | 126.20 | 118.80 |
| 36 | A1 | 410 | U | N1-C2-N3 | 6.72 | 118.93 | 114.90 |
| 53 | BP | 131 | ARG | NE-CZ-NH1 | -6.72 | 116.94 | 120.30 |
| 36 | A5 | 518 | G | C4-C5-N7 | 6.72 | 113.49 | 110.80 |
| 36 | A5 | 1392 | G | C5-N7-C8 | 6.72 | 107.66 | 104.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 36 | A5 | 1113 | G | N3-C4-C5 | 6.72 | 131.96 | 128.60 |
| 36 | A5 | 3309 | G | C5-C6-O6 | -6.72 | 124.57 | 128.60 |
| 36 | A5 | 3140 | G | C5-C6-O6 | -6.72 | 124.57 | 128.60 |
| 36 | A5 | 3050 | U | N3-C4-O4 | -6.72 | 114.70 | 119.40 |
| 36 | A1 | 251 | G | C4-N9-C1' | 6.71 | 135.23 | 126.50 |
| 36 | A1 | 1169 | A | C5-C6-N1 | -6.71 | 114.34 | 117.70 |
| 44 | BF | 160 | ARG | NE-CZ-NH1 | 6.71 | 123.66 | 120.30 |
| 36 | A5 | 215 | G | C8-N9-C4 | -6.71 | 103.71 | 106.40 |
| 1 | A2 | 838 | G | C8-N9-C4 | 6.71 | 109.08 | 106.40 |
| 36 | A5 | 413 | U | C5-C6-N1 | -6.71 | 119.34 | 122.70 |
| 36 | A5 | 1206 | G | C8-N9-C4 | -6.71 | 103.72 | 106.40 |
| 36 | A5 | 2868 | U | N3-C4-C5 | 6.71 | 118.63 | 114.60 |
| 1 | A2 | 1246 | C | N3-C2-O2 | -6.71 | 117.20 | 121.90 |
| 1 | A2 | 1521 | G | N3-C4-C5 | -6.71 | 125.24 | 128.60 |
| 36 | A1 | 1339 | C | N1-C2-N3 | 6.71 | 123.90 | 119.20 |
| 36 | A1 | 2187 | G | C6-C5-N7 | -6.71 | 126.37 | 130.40 |
| 36 | A1 | 2735 | U | C4-C5-C6 | -6.71 | 115.67 | 119.70 |
| 80 | A6 | 119 | A | C2-N3-C4 | -6.71 | 107.24 | 110.60 |
| 36 | A5 | 2892 | A | N9-C4-C5 | 6.71 | 108.48 | 105.80 |
| 36 | A5 | 3140 | G | N1-C6-O6 | 6.71 | 123.93 | 119.90 |
| 36 | A1 | 196 | G | N9-C4-C5 | -6.71 | 102.72 | 105.40 |
| 36 | A5 | 2767 | U | C5-C4-O4 | 6.71 | 129.93 | 125.90 |
| 36 | A5 | 1042 | U | C5-C4-O4 | 6.71 | 129.93 | 125.90 |
| 36 | A5 | 2407 | C | C5-C4-N4 | -6.71 | 115.50 | 120.20 |
| 36 | A5 | 3266 | G | N1-C6-O6 | -6.71 | 115.87 | 119.90 |
| 36 | A1 | 943 | U | C2-N3-C4 | -6.71 | 122.98 | 127.00 |
| 40 | BB | 323 | MET | CG-SD-CE | -6.71 | 89.47 | 100.20 |
| 36 | A1 | 2909 | U | C5-C4-O4 | -6.71 | 121.88 | 125.90 |
| 36 | A5 | 2422 | C | N1-C2-O2 | 6.71 | 122.92 | 118.90 |
| 36 | A1 | 637 | C | O4'-C1'-N1 | 6.70 | 113.56 | 108.20 |
| 36 | A1 | 1478 | C | C6-N1-C2 | 6.70 | 122.98 | 120.30 |
| 36 | A5 | 2135 | U | C6-N1-C2 | 6.70 | 125.02 | 121.00 |
| 37 | A7 | 25 | G | N1-C6-O6 | 6.70 | 123.92 | 119.90 |
| 1 | A2 | 192 | U | C2-N1-C1' | 6.70 | 125.74 | 117.70 |
| 36 | A1 | 2649 | A | N7-C8-N9 | -6.70 | 110.45 | 113.80 |
| 36 | A5 | 1882 | G | C4-C5-N7 | -6.70 | 108.12 | 110.80 |
| 38 | A8 | 42 | G | C4-N9-C1' | -6.70 | 117.79 | 126.50 |
| 36 | A5 | 3214 | U | N1-C2-O2 | 6.70 | 127.49 | 122.80 |
| 36 | A5 | 614 | C | C6-N1-C2 | 6.70 | 122.98 | 120.30 |
| 36 | A5 | 2929 | C | N1-C2-O2 | -6.70 | 114.88 | 118.90 |
| 36 | A1 | 1452 | A | C8-N9-C4 | 6.70 | 108.48 | 105.80 |
| 36 | A5 | 835 | G | C6-N1-C2 | -6.70 | 121.08 | 125.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 36 | A5 | 1042 | U | N1-C2-O2 | 6.70 | 127.49 | 122.80 |
| 36 | A1 | 2860 | U | N1-C2-N3 | -6.69 | 110.88 | 114.90 |
| 1 | A2 | 266 | A | N9-C4-C5 | -6.69 | 103.12 | 105.80 |
| 1 | A2 | 340 | U | N1-C2-O2 | 6.69 | 127.48 | 122.80 |
| 36 | A1 | 426 | G | N9-C4-C5 | -6.69 | 102.72 | 105.40 |
| 80 | A6 | 110 | U | N3-C4-C5 | 6.69 | 118.61 | 114.60 |
| 36 | A5 | 1057 | A | N9-C4-C5 | -6.69 | 103.12 | 105.80 |
| 38 | A8 | 25 | G | C5-C6-O6 | 6.69 | 132.62 | 128.60 |
| 36 | A1 | 660 | A | C8-N9-C4 | 6.69 | 108.48 | 105.80 |
| 36 | A1 | 1305 | U | N3-C4-O4 | -6.69 | 114.72 | 119.40 |
| 36 | A5 | 376 | G | C2-N3-C4 | 6.69 | 115.25 | 111.90 |
| 50 | DM | 72 | LEU | CA-CB-CG | 6.69 | 130.69 | 115.30 |
| 36 | A5 | 649 | A | C8-N9-C4 | -6.69 | 103.12 | 105.80 |
| 1 | A2 | 736 | C | C5-C6-N1 | 6.69 | 124.34 | 121.00 |
| 36 | A1 | 361 | A | N1-C6-N6 | -6.69 | 114.59 | 118.60 |
| 36 | A1 | 1387 | G | C5-N7-C8 | 6.69 | 107.64 | 104.30 |
| 36 | A1 | 2390 | A | C6-N1-C2 | -6.69 | 114.59 | 118.60 |
| 36 | A1 | 2809 | C | N1-C2-O2 | 6.69 | 122.91 | 118.90 |
| 80 | A6 | 1783 | C | C4-C5-C6 | 6.69 | 120.74 | 117.40 |
| 4 | CC | 111 | VAL | CB-CA-C | -6.69 | 98.69 | 111.40 |
| 36 | A5 | 400 | G | C4-C5-N7 | 6.69 | 113.47 | 110.80 |
| 36 | A1 | 339 | C | N3-C2-O2 | -6.69 | 117.22 | 121.90 |
| 36 | A1 | 2175 | U | C5-C6-N1 | -6.68 | 119.36 | 122.70 |
| 36 | A1 | 3110 | C | C6-N1-C2 | -6.68 | 117.63 | 120.30 |
| 36 | A5 | 620 | U | C5-C6-N1 | 6.68 | 126.04 | 122.70 |
| 36 | A5 | 2411 | U | N3-C4-O4 | -6.68 | 114.72 | 119.40 |
| 36 | A5 | 3138 | U | N1-C2-N3 | 6.68 | 118.91 | 114.90 |
| 39 | DA | 246 | LEU | CA-CB-CG | 6.68 | 130.68 | 115.30 |
| 36 | A1 | 1325 | U | N1-C2-O2 | -6.68 | 118.12 | 122.80 |
| 36 | A1 | 1451 | C | C6-N1-C2 | 6.68 | 122.97 | 120.30 |
| 36 | A1 | 1513 | G | C8-N9-C4 | -6.68 | 103.73 | 106.40 |
| 36 | A1 | 1537 | A | N1-C6-N6 | 6.68 | 122.61 | 118.60 |
| 36 | A1 | 2808 | A | N9-C4-C5 | -6.68 | 103.13 | 105.80 |
| 36 | A5 | 436 | A | N7-C8-N9 | 6.68 | 117.14 | 113.80 |
| 36 | A5 | 1392 | G | N9-C4-C5 | -6.68 | 102.73 | 105.40 |
| 36 | A5 | 1848 | G | C6-C5-N7 | -6.68 | 126.39 | 130.40 |
| 36 | A5 | 3185 | U | C5-C6-N1 | -6.68 | 119.36 | 122.70 |
| 36 | A1 | 2870 | C | C4-C5-C6 | -6.68 | 114.06 | 117.40 |
| 80 | A6 | 232 | U | C2-N1-C1' | 6.68 | 125.72 | 117.70 |
| 36 | A5 | 2279 | A | N1-C2-N3 | 6.68 | 132.64 | 129.30 |
| 1 | A2 | 1679 | G | N3-C4-C5 | -6.68 | 125.26 | 128.60 |
| 52 | BO | 104[B] | ILE | O-C-N | 6.68 | 133.38 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 80 | A6 | 1206 | U | N3-C4-O4 | 6.68 | 124.07 | 119.40 |
| 1 | A2 | 1258 | U | C5-C4-O4 | 6.68 | 129.91 | 125.90 |
| 36 | A5 | 3128 | G | C5-C6-O6 | -6.68 | 124.59 | 128.60 |
| 36 | A1 | 546 | C | C6-N1-C2 | -6.67 | 117.63 | 120.30 |
| 36 | A5 | 1359 | C | C5-C4-N4 | -6.67 | 115.53 | 120.20 |
| 36 | A1 | 421 | G | C5-C6-N1 | 6.67 | 114.83 | 111.50 |
| 36 | A1 | 1382 | G | C5-C6-O6 | -6.67 | 124.60 | 128.60 |
| 36 | A1 | 1402 | C | C2-N3-C4 | -6.67 | 116.56 | 119.90 |
| 36 | A5 | 1389 | G | C6-C5-N7 | -6.67 | 126.40 | 130.40 |
| 36 | A1 | 32 | U | C5-C6-N1 | -6.67 | 119.36 | 122.70 |
| 36 | A1 | 2314 | U | C2-N1-C1' | 6.67 | 125.70 | 117.70 |
| 80 | A6 | 1767 | G | C8-N9-C4 | 6.67 | 109.07 | 106.40 |
| 36 | A1 | 2808 | A | C2-N3-C4 | -6.67 | 107.27 | 110.60 |
| 36 | A5 | 1307 | G | C2-N3-C4 | 6.67 | 115.23 | 111.90 |
| 36 | A1 | 791 | A | C2-N3-C4 | -6.67 | 107.27 | 110.60 |
| 36 | A1 | 1112 | A | N1-C6-N6 | 6.67 | 122.60 | 118.60 |
| 80 | A6 | 1235 | C | C5-C6-N1 | 6.67 | 124.33 | 121.00 |
| 80 | A6 | 1609 | U | N3-C2-O2 | 6.67 | 126.87 | 122.20 |
| 36 | A1 | 664 | U | C5-C4-O4 | -6.67 | 121.90 | 125.90 |
| 36 | A5 | 2403 | G | C5-N7-C8 | 6.67 | 107.63 | 104.30 |
| 80 | A6 | 1778 | G | N1-C6-O6 | -6.66 | 115.90 | 119.90 |
| 36 | A5 | 332 | C | C4-C5-C6 | 6.66 | 120.73 | 117.40 |
| 36 | A5 | 930 | U | C4-C5-C6 | -6.66 | 115.70 | 119.70 |
| 36 | A5 | 1159 | A | C4-C5-N7 | 6.66 | 114.03 | 110.70 |
| 1 | A2 | 131 | C | C6-N1-C2 | -6.66 | 117.64 | 120.30 |
| 36 | A1 | 922 | U | N1-C2-O2 | 6.66 | 127.46 | 122.80 |
| 36 | A5 | 615 | U | C5-C4-O4 | -6.66 | 121.90 | 125.90 |
| 36 | A5 | 3376 | A | N9-C4-C5 | 6.66 | 108.46 | 105.80 |
| 36 | A1 | 935 | U | C5-C6-N1 | -6.66 | 119.37 | 122.70 |
| 36 | A1 | 2977 | G | N1-C6-O6 | -6.66 | 115.91 | 119.90 |
| 36 | A1 | 3362 | A | C4-N9-C1' | 6.66 | 138.28 | 126.30 |
| 80 | A6 | 65 | A | C4-C5-N7 | 6.66 | 114.03 | 110.70 |
| 36 | A5 | 652 | G | N1-C2-N3 | 6.66 | 127.89 | 123.90 |
| 36 | A5 | 2717 | U | N1-C2-N3 | 6.66 | 118.89 | 114.90 |
| 1 | A2 | 566 | C | N1-C2-O2 | 6.66 | 122.89 | 118.90 |
| 36 | A1 | 1807 | G | C8-N9-C4 | -6.66 | 103.74 | 106.40 |
| 36 | A5 | 267 | G | N9-C4-C5 | -6.66 | 102.74 | 105.40 |
| 36 | A1 | 633 | C | C4-C5-C6 | 6.65 | 120.73 | 117.40 |
| 36 | A1 | 2325 | G | C2-N3-C4 | 6.65 | 115.23 | 111.90 |
| 36 | A1 | 2111 | G | N1-C6-O6 | -6.65 | 115.91 | 119.90 |
| 36 | A1 | 2187 | G | C5-C6-O6 | -6.65 | 124.61 | 128.60 |
| 80 | A6 | 355 | G | N1-C6-O6 | -6.65 | 115.91 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 934 | G | C2-N3-C4 | 6.65 | 115.22 | 111.90 |
| 36 | A5 | 1439 | U | C2-N3-C4 | -6.65 | 123.01 | 127.00 |
| 36 | A5 | 1890 | U | C5-C6-N1 | -6.65 | 119.38 | 122.70 |
| 36 | A5 | 2292 | U | C2-N1-C1' | 6.65 | 125.68 | 117.70 |
| 36 | A5 | 2743 | A | C5-N7-C8 | 6.65 | 107.22 | 103.90 |
| 36 | A5 | 3049 | A | C6-N1-C2 | 6.65 | 122.59 | 118.60 |
| 36 | A5 | 355 | A | N1-C2-N3 | 6.65 | 132.62 | 129.30 |
| 36 | A1 | 1056 | U | C6-N1-C2 | -6.65 | 117.01 | 121.00 |
| 36 | A1 | 2550 | U | N3-C4-O4 | -6.65 | 114.75 | 119.40 |
| 36 | A1 | 2799 | A | N1-C2-N3 | 6.65 | 132.62 | 129.30 |
| 36 | A1 | 2993 | G | C5-C6-O6 | 6.65 | 132.59 | 128.60 |
| 36 | A5 | 669 | U | C4-C5-C6 | 6.65 | 123.69 | 119.70 |
| 36 | A5 | 1146 | C | N3-C2-O2 | -6.65 | 117.25 | 121.90 |
| 36 | A5 | 1208 | U | C5-C6-N1 | -6.65 | 119.38 | 122.70 |
| 36 | A5 | 1844 | C | N1-C2-O2 | -6.65 | 114.91 | 118.90 |
| 36 | A5 | 1931 | U | N3-C4-O4 | -6.65 | 114.75 | 119.40 |
| 36 | A5 | 3007 | U | N3-C4-C5 | 6.65 | 118.59 | 114.60 |
| 36 | A1 | 1429 | G | N3-C2-N2 | 6.65 | 124.55 | 119.90 |
| 36 | A1 | 508 | U | C6-N1-C2 | 6.64 | 124.99 | 121.00 |
| 36 | A1 | 2899 | C | N1-C2-N3 | 6.64 | 123.85 | 119.20 |
| 36 | A5 | 361 | A | N1-C6-N6 | -6.64 | 114.61 | 118.60 |
| 36 | A5 | 1409 | G | C5-C6-O6 | 6.64 | 132.59 | 128.60 |
| 36 | A5 | 3216 | G | C6-C5-N7 | -6.64 | 126.41 | 130.40 |
| 10 | AI | 172 | ARG | NE-CZ-NH1 | 6.64 | 123.62 | 120.30 |
| 36 | A1 | 432 | G | C5-C6-N1 | -6.64 | 108.18 | 111.50 |
| 36 | A1 | 546 | C | C2-N1-C1' | 6.64 | 126.11 | 118.80 |
| 36 | A1 | 903 | U | N3-C2-O2 | -6.64 | 117.55 | 122.20 |
| 36 | A1 | 2286 | U | N3-C2-O2 | -6.64 | 117.55 | 122.20 |
| 80 | A6 | 364 | G | C5-C6-N1 | 6.64 | 114.82 | 111.50 |
| 36 | A1 | 2952 | G | C2-N3-C4 | -6.64 | 108.58 | 111.90 |
| 80 | A6 | 825 | U | C6-N1-C2 | 6.64 | 124.98 | 121.00 |
| 36 | A1 | 1050 | U | N1-C2-O2 | 6.64 | 127.45 | 122.80 |
| 38 | A4 | 13 | A | C5-C6-N1 | 6.64 | 121.02 | 117.70 |
| 36 | A1 | 1799 | A | C8-N9-C4 | 6.64 | 108.45 | 105.80 |
| 36 | A1 | 2172 | A | N1-C6-N6 | 6.64 | 122.58 | 118.60 |
| 36 | A5 | 2961 | G | C5-C6-O6 | 6.64 | 132.58 | 128.60 |
| 36 | A1 | 2184 | U | C5-C6-N1 | 6.64 | 126.02 | 122.70 |
| 36 | A1 | 3174 | A | C5-N7-C8 | -6.64 | 100.58 | 103.90 |
| 36 | A5 | 625 | G | N9-C4-C5 | 6.64 | 108.05 | 105.40 |
| 36 | A5 | 3244 | A | C2-N3-C4 | -6.64 | 107.28 | 110.60 |
| 1 | A2 | 1462 | G | N9-C4-C5 | -6.63 | 102.75 | 105.40 |
| 36 | A5 | 2889 | C | N3-C2-O2 | -6.63 | 117.26 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 80 | A6 | 1455 | G | C5-C6-N1 | -6.63 | 108.18 | 111.50 |
| 36 | A5 | 3333 | G | N1-C6-O6 | 6.63 | 123.88 | 119.90 |
| 36 | A1 | 44 | U | N3-C4-C5 | 6.63 | 118.58 | 114.60 |
| 38 | A4 | 96 | A | C8-N9-C4 | 6.63 | 108.45 | 105.80 |
| 1 | A2 | 608 | U | N1-C2-N3 | 6.63 | 118.88 | 114.90 |
| 36 | A1 | 2657 | A | C8-N9-C4 | -6.63 | 103.15 | 105.80 |
| 36 | A1 | 2884 | C | C6-N1-C2 | 6.63 | 122.95 | 120.30 |
| 36 | A5 | 1312 | C | C6-N1-C2 | -6.63 | 117.65 | 120.30 |
| 36 | A5 | 226 | C | N3-C4-C5 | 6.62 | 124.55 | 121.90 |
| 36 | A1 | 112 | U | N1-C2-O2 | 6.62 | 127.44 | 122.80 |
| 80 | A6 | 36 | C | N3-C4-N4 | 6.62 | 122.64 | 118.00 |
| 36 | A5 | 2719 | U | C6-N1-C1' | 6.62 | 130.47 | 121.20 |
| 36 | A5 | 3025 | C | C5-C4-N4 | 6.62 | 124.84 | 120.20 |
| 36 | A5 | 3039 | C | C6-N1-C2 | -6.62 | 117.65 | 120.30 |
| 1 | A2 | 1297 | G | C8-N9-C4 | 6.62 | 109.05 | 106.40 |
| 36 | A1 | 2113 | A | C8-N9-C4 | 6.62 | 108.45 | 105.80 |
| 36 | A1 | 2638 | C | C6-N1-C2 | 6.62 | 122.95 | 120.30 |
| 36 | A5 | 1007 | U | C5-C6-N1 | -6.62 | 119.39 | 122.70 |
| 36 | A5 | 2392 | C | N1-C2-O2 | -6.62 | 114.93 | 118.90 |
| 36 | A1 | 923 | C | N3-C2-O2 | 6.62 | 126.53 | 121.90 |
| 80 | A6 | 380 | U | N3-C2-O2 | -6.62 | 117.57 | 122.20 |
| 80 | A6 | 538 | A | N1-C6-N6 | -6.62 | 114.63 | 118.60 |
| 36 | A1 | 1408 | G | C5-C6-O6 | 6.62 | 132.57 | 128.60 |
| 36 | A1 | 3295 | A | C8-N9-C4 | -6.62 | 103.15 | 105.80 |
| 80 | A6 | 484 | C | C5-C6-N1 | 6.62 | 124.31 | 121.00 |
| 36 | A5 | 600 | G | N7-C8-N9 | 6.62 | 116.41 | 113.10 |
| 36 | A5 | 640 | U | N3-C2-O2 | -6.62 | 117.57 | 122.20 |
| 36 | A5 | 966 | U | C2-N3-C4 | -6.62 | 123.03 | 127.00 |
| 36 | A5 | 1876 | U | C5-C6-N1 | 6.62 | 126.01 | 122.70 |
| 36 | A5 | 925 | A | C4-C5-C6 | 6.62 | 120.31 | 117.00 |
| 36 | A1 | 326 | U | C5-C4-O4 | -6.62 | 121.93 | 125.90 |
| 36 | A1 | 1297 | C | C5-C6-N1 | -6.62 | 117.69 | 121.00 |
| 44 | BF | 216 | VAL | N-CA-C | 6.62 | 128.86 | 111.00 |
| 36 | A5 | 2201 | G | N1-C6-O6 | -6.62 | 115.93 | 119.90 |
| 36 | A1 | 3349 | C | C6-N1-C2 | -6.61 | 117.66 | 120.30 |
| 36 | A5 | 145 | G | N3-C4-N9 | -6.61 | 122.03 | 126.00 |
| 38 | A8 | 24 | G | N1-C6-O6 | -6.61 | 115.93 | 119.90 |
| 36 | A1 | 2198 | A | N7-C8-N9 | -6.61 | 110.50 | 113.80 |
| 80 | A6 | 346 | G | N1-C6-O6 | -6.61 | 115.93 | 119.90 |
| 80 | A6 | 1273 | G | C5-C6-N1 | 6.61 | 114.81 | 111.50 |
| 36 | A1 | 1367 | G | N1-C2-N2 | -6.61 | 110.25 | 116.20 |
| 36 | A5 | 1518 | U | N3-C4-C5 | 6.61 | 118.57 | 114.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 80 | A6 | 1008 | G | N1-C6-O6 | 6.61 | 123.86 | 119.90 |
| 80 | A6 | 1030 | A | N1-C6-N6 | -6.61 | 114.64 | 118.60 |
| 36 | A5 | 986 | U | N3-C4-O4 | 6.61 | 124.03 | 119.40 |
| 36 | A5 | 1754 | G | N1-C6-O6 | -6.61 | 115.94 | 119.90 |
| 36 | A5 | 3303 | G | N3-C2-N2 | 6.61 | 124.53 | 119.90 |
| 47 | DI | 10 | ARG | NE-CZ-NH1 | -6.61 | 117.00 | 120.30 |
| 1 | A2 | 687 | G | N3-C2-N2 | -6.61 | 115.28 | 119.90 |
| 36 | A5 | 3335 | A | C2-N3-C4 | -6.60 | 107.30 | 110.60 |
| 36 | A1 | 970 | A | N7-C8-N9 | 6.60 | 117.10 | 113.80 |
| 36 | A1 | 2752 | U | C5-C4-O4 | 6.60 | 129.86 | 125.90 |
| 36 | A1 | 3000 | A | N7-C8-N9 | -6.60 | 110.50 | 113.80 |
| 36 | A5 | 1049 | C | C4-C5-C6 | -6.60 | 114.10 | 117.40 |
| 80 | A6 | 240 | U | N1-C2-O2 | 6.60 | 127.42 | 122.80 |
| 36 | A5 | 990 | U | N3-C2-O2 | -6.60 | 117.58 | 122.20 |
| 36 | A1 | 35 | A | N7-C8-N9 | 6.60 | 117.10 | 113.80 |
| 36 | A1 | 1152 | G | C2-N3-C4 | -6.60 | 108.60 | 111.90 |
| 36 | A1 | 1507 | G | N1-C6-O6 | 6.60 | 123.86 | 119.90 |
| 36 | A1 | 2552 | C | N3-C2-O2 | -6.60 | 117.28 | 121.90 |
| 36 | A5 | 2357 | A | N1-C6-N6 | 6.60 | 122.56 | 118.60 |
| 36 | A5 | 2954 | U | C2-N1-C1' | 6.60 | 125.62 | 117.70 |
| 36 | A1 | 885 | U | C6-N1-C2 | 6.60 | 124.96 | 121.00 |
| 36 | A1 | 1717 | U | C5-C4-O4 | 6.60 | 129.86 | 125.90 |
| 36 | A5 | 2207 | A | C6-C5-N7 | -6.60 | 127.68 | 132.30 |
| 36 | A5 | 784 | A | C6-C5-N7 | -6.60 | 127.68 | 132.30 |
| 36 | A5 | 792 | G | N1-C2-N3 | 6.60 | 127.86 | 123.90 |
| 36 | A5 | 2851 | A | C8-N9-C4 | 6.60 | 108.44 | 105.80 |
| 36 | A5 | 3122 | A | C4-C5-C6 | 6.60 | 120.30 | 117.00 |
| 36 | A1 | 391 | A | N1-C6-N6 | -6.59 | 114.64 | 118.60 |
| 80 | A6 | 565 | C | C6-N1-C1' | -6.59 | 112.89 | 120.80 |
| 49 | DL | 171 | ARG | NE-CZ-NH1 | -6.59 | 117.00 | 120.30 |
| 36 | A1 | 954 | U | N1-C2-N3 | 6.59 | 118.86 | 114.90 |
| 36 | A5 | 721 | G | C5-C6-N1 | 6.59 | 114.80 | 111.50 |
| 36 | A5 | 2114 | C | C6-N1-C2 | -6.59 | 117.66 | 120.30 |
| 1 | A2 | 783 | G | N9-C4-C5 | -6.59 | 102.76 | 105.40 |
| 36 | A1 | 1903 | U | N1-C2-O2 | 6.59 | 127.42 | 122.80 |
| 36 | A1 | 2400 | G | C2-N3-C4 | -6.59 | 108.60 | 111.90 |
| 80 | A6 | 1200 | G | C8-N9-C1' | 6.59 | 135.57 | 127.00 |
| 36 | A1 | 1846 | C | C4-C5-C6 | 6.59 | 120.69 | 117.40 |
| 36 | A1 | 2115 | G | C5-C6-O6 | -6.59 | 124.65 | 128.60 |
| 36 | A1 | 2293 | C | N3-C4-C5 | 6.59 | 124.54 | 121.90 |
| 36 | A1 | 2958 | A | C8-N9-C4 | 6.59 | 108.44 | 105.80 |
| 80 | A6 | 1 | U | N1-C2-O2 | 6.59 | 127.41 | 122.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 3204 | C | N3-C4-C5 | 6.59 | 124.53 | 121.90 |
| 80 | A6 | 1258 | U | N3-C2-O2 | -6.59 | 117.59 | 122.20 |
| 36 | A5 | 1004 | U | N3-C2-O2 | -6.59 | 117.59 | 122.20 |
| 36 | A5 | 2811 | A | C6-N1-C2 | -6.59 | 114.65 | 118.60 |
| 36 | A5 | 3115 | C | N1-C2-O2 | -6.59 | 114.95 | 118.90 |
| 36 | A5 | 3289 | G | N7-C8-N9 | 6.58 | 116.39 | 113.10 |
| 36 | A1 | 2916 | U | N3-C4-O4 | 6.58 | 124.01 | 119.40 |
| 36 | A5 | 1159 | A | N1-C2-N3 | -6.58 | 126.01 | 129.30 |
| 36 | A5 | 2866 | U | N1-C2-O2 | -6.58 | 118.19 | 122.80 |
| 36 | A1 | 817 | A | C8-N9-C4 | -6.58 | 103.17 | 105.80 |
| 36 | A1 | 2349 | U | C5-C6-N1 | -6.58 | 119.41 | 122.70 |
| 36 | A5 | 828 | A | N3-C4-C5 | -6.58 | 122.19 | 126.80 |
| 36 | A5 | 880 | G | C5-C6-O6 | -6.58 | 124.65 | 128.60 |
| 36 | A5 | 2169 | G | C2-N3-C4 | 6.58 | 115.19 | 111.90 |
| 36 | A5 | 2647 | A | C8-N9-C4 | -6.58 | 103.17 | 105.80 |
| 36 | A1 | 798 | G | N3-C2-N2 | -6.58 | 115.29 | 119.90 |
| 36 | A1 | 1513 | G | C6-N1-C2 | -6.58 | 121.15 | 125.10 |
| 36 | A1 | 2616 | C | C5-C4-N4 | -6.58 | 115.59 | 120.20 |
| 36 | A1 | 3318 | G | C8-N9-C4 | -6.58 | 103.77 | 106.40 |
| 80 | A6 | 711 | U | C5-C6-N1 | 6.58 | 125.99 | 122.70 |
| 80 | A6 | 1389 | C | C6-N1-C1' | -6.58 | 112.91 | 120.80 |
| 37 | A7 | 92 | A | C5-N7-C8 | -6.58 | 100.61 | 103.90 |
| 36 | A1 | 1148 | G | C2-N3-C4 | 6.58 | 115.19 | 111.90 |
| 36 | A1 | 2381 | G | N7-C8-N9 | -6.58 | 109.81 | 113.10 |
| 80 | A6 | 539 | G | C5-N7-C8 | -6.58 | 101.01 | 104.30 |
| 80 | A6 | 1514 | U | N3-C2-O2 | -6.58 | 117.60 | 122.20 |
| 36 | A5 | 2309 | A | N1-C2-N3 | -6.58 | 126.01 | 129.30 |
| 1 | A2 | 557 | G | C4-N9-C1' | 6.58 | 135.05 | 126.50 |
| 39 | BA | 191 | LEU | CA-CB-CG | -6.58 | 100.17 | 115.30 |
| 80 | A6 | 1299 | G | N3-C4-C5 | -6.58 | 125.31 | 128.60 |
| 41 | DC | 138 | ARG | NE-CZ-NH2 | -6.58 | 117.01 | 120.30 |
| 36 | A1 | 2328 | U | C5-C4-O4 | 6.57 | 129.84 | 125.90 |
| 38 | A4 | 55 | U | N3-C2-O2 | -6.57 | 117.60 | 122.20 |
| 36 | A5 | 518 | G | N1-C6-O6 | 6.57 | 123.84 | 119.90 |
| 36 | A5 | 1200 | A | C4-C5-C6 | 6.57 | 120.29 | 117.00 |
| 36 | A5 | 3270 | U | N3-C4-O4 | -6.57 | 114.80 | 119.40 |
| 36 | A5 | 3310 | A | N1-C6-N6 | -6.57 | 114.66 | 118.60 |
| 36 | A5 | 360 | G | C8-N9-C4 | 6.57 | 109.03 | 106.40 |
| 36 | A1 | 1556 | C | N3-C2-O2 | -6.57 | 117.30 | 121.90 |
| 36 | A5 | 1906 | G | N1-C2-N3 | 6.57 | 127.84 | 123.90 |
| 36 | A5 | 3105 | U | N1-C2-O2 | -6.57 | 118.20 | 122.80 |
| 38 | A8 | 59 | A | C2-N3-C4 | 6.57 | 113.89 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 916 | G | C8-N9-C4 | -6.57 | 103.77 | 106.40 |
| 36 | A5 | 1151 | U | N3-C4-C5 | 6.57 | 118.54 | 114.60 |
| 36 | A1 | 500 | C | C4-C5-C6 | 6.57 | 120.68 | 117.40 |
| 36 | A5 | 2675 | C | N1-C2-O2 | -6.57 | 114.96 | 118.90 |
| 36 | A1 | 1472 | U | N3-C2-O2 | 6.57 | 126.80 | 122.20 |
| 36 | A1 | 2860 | U | C4-C5-C6 | -6.57 | 115.76 | 119.70 |
| 36 | A5 | 2257 | C | N3-C2-O2 | -6.57 | 117.30 | 121.90 |
| 38 | A8 | 11 | C | C4-C5-C6 | 6.57 | 120.68 | 117.40 |
| 36 | A1 | 3208 | G | N1-C2-N2 | 6.56 | 122.11 | 116.20 |
| 36 | A1 | 1174 | G | C5-C6-O6 | -6.56 | 124.66 | 128.60 |
| 36 | A1 | 1947 | G | N3-C4-N9 | -6.56 | 122.06 | 126.00 |
| 36 | A1 | 3142 | A | N1-C2-N3 | 6.56 | 132.58 | 129.30 |
| 36 | A5 | 1788 | C | N3-C4-C5 | -6.56 | 119.28 | 121.90 |
| 37 | A7 | 57 | G | C4-C5-N7 | -6.56 | 108.17 | 110.80 |
| 36 | A1 | 3094 | A | C5-C6-N1 | 6.56 | 120.98 | 117.70 |
| 37 | A3 | 36 | C | N1-C2-O2 | 6.56 | 122.84 | 118.90 |
| 80 | A6 | 1781 | A | C4-C5-N7 | -6.56 | 107.42 | 110.70 |
| 36 | A5 | 2347 | U | N3-C4-O4 | -6.56 | 114.81 | 119.40 |
| 36 | A1 | 2649 | A | C5-N7-C8 | 6.56 | 107.18 | 103.90 |
| 36 | A5 | 1151 | U | C4-C5-C6 | -6.56 | 115.77 | 119.70 |
| 36 | A5 | 1342 | C | C4-C5-C6 | 6.56 | 120.68 | 117.40 |
| 36 | A5 | 2301 | U | C5-C6-N1 | -6.56 | 119.42 | 122.70 |
| 36 | A5 | 3153 | U | N1-C2-O2 | 6.56 | 127.39 | 122.80 |
| 36 | A5 | 2385 | G | C8-N9-C4 | 6.56 | 109.02 | 106.40 |
| 36 | A1 | 519 | A | C5-C6-N6 | -6.55 | 118.46 | 123.70 |
| 80 | A6 | 282 | C | C6-N1-C2 | 6.55 | 122.92 | 120.30 |
| 80 | A6 | 901 | G | N1-C6-O6 | 6.55 | 123.83 | 119.90 |
| 36 | A5 | 1138 | U | C2-N3-C4 | -6.55 | 123.07 | 127.00 |
| 36 | A5 | 1365 | G | C8-N9-C1' | -6.55 | 118.48 | 127.00 |
| 36 | A1 | 765 | C | N1-C2-O2 | 6.55 | 122.83 | 118.90 |
| 80 | A6 | 1170 | G | N3-C4-N9 | 6.55 | 129.93 | 126.00 |
| 36 | A1 | 2369 | G | C6-N1-C2 | -6.55 | 121.17 | 125.10 |
| 38 | A4 | 1 | A | C4-C5-N7 | 6.55 | 113.98 | 110.70 |
| 36 | A5 | 2884 | C | N1-C2-N3 | 6.55 | 123.79 | 119.20 |
| 36 | A5 | 3263 | G | N3-C2-N2 | 6.55 | 124.49 | 119.90 |
| 36 | A5 | 3341 | U | C6-N1-C2 | -6.55 | 117.07 | 121.00 |
| 1 | A2 | 647 | G | N3-C2-N2 | -6.55 | 115.31 | 119.90 |
| 36 | A1 | 2967 | A | N7-C8-N9 | -6.55 | 110.53 | 113.80 |
| 80 | A6 | 1414 | U | N1-C2-N3 | 6.55 | 118.83 | 114.90 |
| 36 | A5 | 2957 | G | C8-N9-C4 | 6.55 | 109.02 | 106.40 |
| 36 | A5 | 435 | C | C2-N3-C4 | -6.55 | 116.63 | 119.90 |
| 36 | A5 | 2377 | G | C2-N3-C4 | 6.55 | 115.17 | 111.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 785 | G | C5-C6-N1 | 6.55 | 114.77 | 111.50 |
| 80 | A6 | 1310 | U | N1-C2-O2 | 6.55 | 127.38 | 122.80 |
| 36 | A5 | 648 | C | C6-N1-C2 | -6.55 | 117.68 | 120.30 |
| 36 | A5 | 815 | G | C5-C6-O6 | 6.55 | 132.53 | 128.60 |
| 36 | A1 | 823 | C | C2-N3-C4 | -6.54 | 116.63 | 119.90 |
| 36 | A1 | 1801 | U | C4-C5-C6 | 6.54 | 123.63 | 119.70 |
| 36 | A5 | 2336 | U | N3-C4-O4 | -6.54 | 114.82 | 119.40 |
| 36 | A5 | 3126 | C | N3-C4-C5 | 6.54 | 124.52 | 121.90 |
| 36 | A1 | 628 | A | C8-N9-C4 | 6.54 | 108.42 | 105.80 |
| 36 | A1 | 2870 | C | C5-C4-N4 | 6.54 | 124.78 | 120.20 |
| 80 | A6 | 1106 | U | C4-C5-C6 | 6.54 | 123.63 | 119.70 |
| 36 | A5 | 3186 | A | N9-C4-C5 | 6.54 | 108.42 | 105.80 |
| 36 | A1 | 654 | C | C4-C5-C6 | 6.54 | 120.67 | 117.40 |
| 36 | A1 | 2697 | A | C5-C6-N1 | 6.54 | 120.97 | 117.70 |
| 36 | A1 | 3304 | U | C6-N1-C1' | 6.54 | 130.36 | 121.20 |
| 80 | A6 | 1106 | U | C6-N1-C2 | -6.54 | 117.08 | 121.00 |
| 80 | A6 | 1652 | C | C6-N1-C2 | -6.54 | 117.68 | 120.30 |
| 36 | A1 | 1911 | A | C5-N7-C8 | -6.54 | 100.63 | 103.90 |
| 36 | A5 | 299 | G | C2-N3-C4 | 6.54 | 115.17 | 111.90 |
| 36 | A5 | 424 | G | N3-C2-N2 | 6.54 | 124.48 | 119.90 |
| 37 | A7 | 68 | C | C2-N3-C4 | -6.54 | 116.63 | 119.90 |
| 1 | A2 | 6 | G | N1-C2-N3 | 6.54 | 127.82 | 123.90 |
| 36 | A1 | 63 | A | C2-N3-C4 | 6.54 | 113.87 | 110.60 |
| 36 | A1 | 2198 | A | N1-C2-N3 | 6.54 | 132.57 | 129.30 |
| 36 | A1 | 2388 | U | N1-C2-O2 | -6.54 | 118.22 | 122.80 |
| 36 | A1 | 2958 | A | C5-N7-C8 | 6.54 | 107.17 | 103.90 |
| 36 | A5 | 828 | A | C2-N3-C4 | 6.54 | 113.87 | 110.60 |
| 36 | A5 | 1722 | U | N3-C2-O2 | 6.54 | 126.78 | 122.20 |
| 36 | A5 | 3306 | U | C5-C6-N1 | -6.54 | 119.43 | 122.70 |
| 36 | A1 | 153 | U | C6-N1-C2 | -6.54 | 117.08 | 121.00 |
| 36 | A1 | 281 | G | N3-C2-N2 | -6.54 | 115.33 | 119.90 |
| 80 | A6 | 280 | U | N3-C2-O2 | -6.54 | 117.62 | 122.20 |
| 80 | A6 | 352 | A | N7-C8-N9 | -6.54 | 110.53 | 113.80 |
| 36 | A5 | 386 | A | C6-C5-N7 | -6.54 | 127.73 | 132.30 |
| 36 | A5 | 884 | A | N3-C4-N9 | -6.54 | 122.17 | 127.40 |
| 36 | A5 | 1215 | U | N3-C4-O4 | 6.54 | 123.97 | 119.40 |
| 1 | A2 | 557 | G | C8-N9-C1' | -6.53 | 118.51 | 127.00 |
| 36 | A1 | 785 | G | C4-C5-N7 | -6.53 | 108.19 | 110.80 |
| 80 | A6 | 113 | U | N1-C2-O2 | -6.53 | 118.23 | 122.80 |
| 36 | A5 | 641 | C | C2-N1-C1' | -6.53 | 111.61 | 118.80 |
| 36 | A5 | 2549 | G | C6-C5-N7 | -6.53 | 126.48 | 130.40 |
| 36 | A5 | 2617 | U | N3-C4-O4 | -6.53 | 114.83 | 119.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 47 | DI | 182 | LEU | CA-CB-CG | -6.53 | 100.27 | 115.30 |
| 1 | A2 | 558 | U | C2-N1-C1' | 6.53 | 125.54 | 117.70 |
| 36 | A1 | 1351 | U | C2-N1-C1' | 6.53 | 125.54 | 117.70 |
| 36 | A1 | 3317 | U | C6-N1-C2 | -6.53 | 117.08 | 121.00 |
| 36 | A5 | 859 | G | N9-C4-C5 | 6.53 | 108.01 | 105.40 |
| 36 | A1 | 1114 | U | N3-C4-C5 | 6.53 | 118.52 | 114.60 |
| 80 | A6 | 432 | G | N3-C2-N2 | -6.53 | 115.33 | 119.90 |
| 36 | A5 | 1516 | C | C5-C6-N1 | -6.53 | 117.73 | 121.00 |
| 38 | A8 | 6 | U | C5-C6-N1 | -6.53 | 119.44 | 122.70 |
| 1 | A2 | 355 | G | C6-N1-C2 | -6.53 | 121.18 | 125.10 |
| 36 | A1 | 1433 | A | C6-N1-C2 | -6.53 | 114.68 | 118.60 |
| 80 | A6 | 1110 | G | C4-C5-N7 | -6.53 | 108.19 | 110.80 |
| 36 | A5 | 2211 | U | C5-C6-N1 | -6.53 | 119.44 | 122.70 |
| 1 | A2 | 266 | A | C8-N9-C4 | 6.53 | 108.41 | 105.80 |
| 1 | A2 | 1274 | C | N3-C4-N4 | -6.53 | 113.43 | 118.00 |
| 80 | A6 | 101 | U | C6-N1-C2 | -6.53 | 117.08 | 121.00 |
| 36 | A5 | 675 | C | N3-C4-N4 | 6.53 | 122.57 | 118.00 |
| 36 | A5 | 2626 | A | C4-C5-N7 | -6.53 | 107.44 | 110.70 |
| 1 | A2 | 1282 | U | C5-C4-O4 | 6.53 | 129.82 | 125.90 |
| 36 | A1 | 2787 | G | C2-N3-C4 | 6.53 | 115.16 | 111.90 |
| 68 | Be | 19 | ARG | NE-CZ-NH2 | 6.53 | 123.56 | 120.30 |
| 80 | A6 | 1542 | G | N1-C6-O6 | -6.53 | 115.98 | 119.90 |
| 36 | A5 | 1211 | U | N3-C4-C5 | 6.53 | 118.52 | 114.60 |
| 36 | A5 | 2626 | A | C5-C6-N1 | -6.53 | 114.44 | 117.70 |
| 36 | A5 | 3148 | U | C5-C4-O4 | -6.53 | 121.98 | 125.90 |
| 36 | A1 | 800 | G | C5-C6-N1 | -6.52 | 108.24 | 111.50 |
| 80 | A6 | 999 | U | N3-C2-O2 | -6.52 | 117.63 | 122.20 |
| 36 | A5 | 1901 | A | C4-C5-C6 | 6.52 | 120.26 | 117.00 |
| 36 | A5 | 2147 | A | N1-C6-N6 | 6.52 | 122.51 | 118.60 |
| 36 | A1 | 3268 | A | N1-C6-N6 | 6.52 | 122.51 | 118.60 |
| 36 | A5 | 1448 | U | N1-C2-O2 | -6.52 | 118.23 | 122.80 |
| 36 | A5 | 2699 | G | N1-C6-O6 | 6.52 | 123.81 | 119.90 |
| 36 | A5 | 3306 | U | C6-N1-C2 | 6.52 | 124.91 | 121.00 |
| 37 | A7 | 20 | A | C5-C6-N6 | -6.52 | 118.48 | 123.70 |
| 69 | Df | 49 | ILE | CB-CA-C | -6.52 | 98.56 | 111.60 |
| 36 | A5 | 370 | U | N3-C2-O2 | -6.52 | 117.64 | 122.20 |
| 36 | A1 | 279 | U | N3-C4-O4 | -6.52 | 114.84 | 119.40 |
| 36 | A5 | 1131 | G | C2-N3-C4 | -6.52 | 108.64 | 111.90 |
| 36 | A5 | 2833 | A | C8-N9-C4 | 6.52 | 108.41 | 105.80 |
| 1 | A2 | 1503 | A | N1-C2-N3 | 6.52 | 132.56 | 129.30 |
| 36 | A1 | 623 | U | C2-N1-C1' | -6.52 | 109.88 | 117.70 |
| 36 | A1 | 1515 | A | C2-N3-C4 | -6.52 | 107.34 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 36 | A1 | 2198 | A | C5-C6-N6 | -6.52 | 118.49 | 123.70 |
| 37 | A3 | 97 | A | N1-C6-N6 | -6.52 | 114.69 | 118.60 |
| 36 | A5 | 1215 | U | N1-C2-O2 | -6.52 | 118.24 | 122.80 |
| 36 | A5 | 2800 | G | N9-C4-C5 | 6.52 | 108.01 | 105.40 |
| 38 | A8 | 54 | A | C5-N7-C8 | -6.52 | 100.64 | 103.90 |
| 36 | A1 | 1851 | G | N3-C4-C5 | -6.52 | 125.34 | 128.60 |
| 36 | A1 | 2145 | A | N1-C2-N3 | -6.52 | 126.04 | 129.30 |
| 80 | A6 | 1473 | U | N1-C2-N3 | 6.52 | 118.81 | 114.90 |
| 36 | A5 | 1408 | G | N3-C4-N9 | -6.52 | 122.09 | 126.00 |
| 36 | A1 | 903 | U | C5-C6-N1 | -6.51 | 119.44 | 122.70 |
| 36 | A1 | 1902 | G | C8-N9-C1' | -6.51 | 118.53 | 127.00 |
| 36 | A1 | 2177 | G | C5-C6-N1 | 6.51 | 114.76 | 111.50 |
| 80 | A6 | 1087 | A | C2-N3-C4 | -6.51 | 107.34 | 110.60 |
| 36 | A5 | 290 | G | N3-C2-N2 | 6.51 | 124.46 | 119.90 |
| 36 | A5 | 2303 | A | N3-C4-C5 | -6.51 | 122.24 | 126.80 |
| 36 | A5 | 3190 | C | C6-N1-C2 | -6.51 | 117.69 | 120.30 |
| 36 | A1 | 371 | G | C8-N9-C4 | 6.51 | 109.00 | 106.40 |
| 36 | A5 | 1496 | C | C6-N1-C2 | -6.51 | 117.69 | 120.30 |
| 80 | A6 | 801 | G | N1-C6-O6 | -6.51 | 115.99 | 119.90 |
| 1 | A2 | 1422 | A | C8-N9-C4 | 6.51 | 108.40 | 105.80 |
| 36 | A1 | 573 | C | C5-C6-N1 | -6.51 | 117.75 | 121.00 |
| 80 | A6 | 151 | G | N9-C4-C5 | 6.51 | 108.00 | 105.40 |
| 80 | A6 | 394 | C | C4-C5-C6 | 6.51 | 120.66 | 117.40 |
| 80 | A6 | 448 | C | C6-N1-C1' | 6.51 | 128.61 | 120.80 |
| 80 | A6 | 1510 | U | C5-C4-O4 | 6.51 | 129.81 | 125.90 |
| 36 | A5 | 2984 | C | C2-N3-C4 | -6.51 | 116.64 | 119.90 |
| 36 | A5 | 3174 | A | C4-C5-N7 | 6.51 | 113.95 | 110.70 |
| 35 | Ah | 134 | ASP | OD1-CG-OD2 | -6.51 | 110.94 | 123.30 |
| 80 | A6 | 3 | U | C6-N1-C2 | 6.51 | 124.91 | 121.00 |
| 36 | A1 | 102 | C | C5-C4-N4 | -6.51 | 115.65 | 120.20 |
| 36 | A1 | 1819 | U | C2-N1-C1' | 6.51 | 125.51 | 117.70 |
| 36 | A5 | 420 | G | N3-C4-C5 | -6.51 | 125.35 | 128.60 |
| 36 | A5 | 692 | A | N1-C2-N3 | -6.51 | 126.05 | 129.30 |
| 36 | A1 | 819 | U | N1-C2-O2 | -6.50 | 118.25 | 122.80 |
| 36 | A1 | 2885 | C | C2-N3-C4 | -6.50 | 116.65 | 119.90 |
| 36 | A5 | 2904 | U | C5-C6-N1 | -6.50 | 119.45 | 122.70 |
| 40 | DB | 21 | ARG | NE-CZ-NH1 | 6.50 | 123.55 | 120.30 |
| 36 | A5 | 2849 | C | C5-C6-N1 | 6.50 | 124.25 | 121.00 |
| 36 | A1 | 506 | U | C5-C6-N1 | -6.50 | 119.45 | 122.70 |
| 36 | A1 | 2647 | A | C8-N9-C4 | -6.50 | 103.20 | 105.80 |
| 20 | CS | 18 | LEU | CA-CB-CG | 6.50 | 130.25 | 115.30 |
| 36 | A1 | 1060 | U | C6-N1-C2 | 6.50 | 124.90 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 2948 | C | C5-C6-N1 | -6.50 | 117.75 | 121.00 |
| 37 | A3 | 93 | C | N3-C4-C5 | 6.50 | 124.50 | 121.90 |
| 80 | A6 | 1650 | U | C2-N3-C4 | -6.50 | 123.10 | 127.00 |
| 36 | A5 | 370 | U | C6-N1-C2 | -6.50 | 117.10 | 121.00 |
| 36 | A5 | 2320 | A | N1-C2-N3 | 6.50 | 132.55 | 129.30 |
| 36 | A5 | 3330 | A | N1-C6-N6 | -6.50 | 114.70 | 118.60 |
| 1 | A2 | 132 | U | C2-N1-C1' | -6.50 | 109.91 | 117.70 |
| 36 | A1 | 2679 | A | C4-C5-N7 | 6.50 | 113.95 | 110.70 |
| 49 | BL | 57 | VAL | CB-CA-C | -6.50 | 99.06 | 111.40 |
| 80 | A6 | 1340 | U | N3-C2-O2 | -6.50 | 117.65 | 122.20 |
| 38 | A4 | 81 | U | N1-C2-N3 | 6.50 | 118.80 | 114.90 |
| 36 | A5 | 519 | A | C5-C6-N6 | -6.50 | 118.50 | 123.70 |
| 36 | A1 | 1905 | G | C5-C6-N1 | 6.49 | 114.75 | 111.50 |
| 36 | A1 | 2152 | A | C5-C6-N6 | 6.49 | 128.89 | 123.70 |
| 38 | A4 | 53 | A | C5-C6-N1 | 6.49 | 120.95 | 117.70 |
| 36 | A5 | 783 | A | N1-C6-N6 | 6.49 | 122.50 | 118.60 |
| 36 | A5 | 2314 | U | C2-N1-C1' | 6.49 | 125.49 | 117.70 |
| 36 | A1 | 859 | G | C6-C5-N7 | -6.49 | 126.50 | 130.40 |
| 36 | A1 | 1180 | A | N9-C4-C5 | 6.49 | 108.40 | 105.80 |
| 36 | A1 | 2852 | C | C6-N1-C1' | -6.49 | 113.01 | 120.80 |
| 36 | A5 | 2258 | U | N3-C2-O2 | -6.49 | 117.66 | 122.20 |
| 36 | A1 | 2662 | G | C6-C5-N7 | -6.49 | 126.50 | 130.40 |
| 36 | A1 | 2945 | G | N3-C2-N2 | 6.49 | 124.44 | 119.90 |
| 36 | A5 | 345 | G | N3-C2-N2 | 6.49 | 124.44 | 119.90 |
| 36 | A5 | 429 | U | N3-C4-C5 | 6.49 | 118.49 | 114.60 |
| 36 | A5 | 947 | G | N1-C6-O6 | -6.49 | 116.01 | 119.90 |
| 36 | A5 | 1434 | G | C8-N9-C4 | 6.49 | 109.00 | 106.40 |
| 35 | Ah | 134 | ASP | CB-CG-OD2 | -6.49 | 112.46 | 118.30 |
| 36 | A1 | 3063 | C | N3-C2-O2 | -6.49 | 117.36 | 121.90 |
| 36 | A5 | 1190 | A | C5-C6-N6 | 6.49 | 128.89 | 123.70 |
| 36 | A1 | 184 | U | N3-C2-O2 | -6.49 | 117.66 | 122.20 |
| 38 | A4 | 91 | C | N1-C2-O2 | 6.49 | 122.79 | 118.90 |
| 36 | A5 | 1215 | U | C5-C4-O4 | -6.49 | 122.01 | 125.90 |
| 36 | A5 | 2288 | G | C5-C6-O6 | -6.49 | 124.71 | 128.60 |
| 36 | A5 | 2433 | U | N3-C4-C5 | 6.49 | 118.49 | 114.60 |
| 1 | A2 | 830 | U | N3-C2-O2 | -6.49 | 117.66 | 122.20 |
| 1 | A2 | 1473 | U | N3-C2-O2 | -6.49 | 117.66 | 122.20 |
| 36 | A1 | 1604 | G | C4-N9-C1' | 6.49 | 134.93 | 126.50 |
| 36 | A5 | 3043 | C | N3-C4-C5 | 6.49 | 124.49 | 121.90 |
| 36 | A1 | 644 | G | C4-C5-C6 | 6.48 | 122.69 | 118.80 |
| 80 | A6 | 580 | A | C8-N9-C4 | -6.48 | 103.21 | 105.80 |
| 1 | A2 | 404 | G | C5-C6-O6 | -6.48 | 124.71 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 2909 | U | N3-C2-O2 | 6.48 | 126.74 | 122.20 |
| 80 | A6 | 695 | U | N1-C2-N3 | 6.48 | 118.79 | 114.90 |
| 36 | A5 | 2396 | G | N3-C4-C5 | -6.48 | 125.36 | 128.60 |
| 1 | A2 | 1024 | U | N3-C2-O2 | -6.48 | 117.66 | 122.20 |
| 36 | A1 | 80 | G | C5-C6-N1 | 6.48 | 114.74 | 111.50 |
| 36 | A1 | 1329 | U | C4-C5-C6 | 6.48 | 123.59 | 119.70 |
| 80 | A6 | 1634 | C | C2-N3-C4 | 6.48 | 123.14 | 119.90 |
| 36 | A5 | 963 | G | C5-C6-O6 | -6.48 | 124.71 | 128.60 |
| 1 | A2 | 965 | U | C5-C6-N1 | 6.48 | 125.94 | 122.70 |
| 36 | A5 | 3004 | C | C5-C4-N4 | -6.48 | 115.67 | 120.20 |
| 36 | A1 | 359 | U | C5-C6-N1 | -6.48 | 119.46 | 122.70 |
| 36 | A1 | 715 | A | N1-C6-N6 | 6.48 | 122.49 | 118.60 |
| 36 | A1 | 953 | G | C8-N9-C1' | 6.48 | 135.42 | 127.00 |
| 36 | A1 | 1141 | C | C4-C5-C6 | 6.48 | 120.64 | 117.40 |
| 36 | A1 | 1578 | C | C2-N1-C1' | 6.48 | 125.93 | 118.80 |
| 51 | DN | 68 | ARG | NE-CZ-NH1 | 6.48 | 123.54 | 120.30 |
| 80 | A6 | 1478 | G | C4-C5-C6 | 6.48 | 122.69 | 118.80 |
| 80 | A6 | 1721 | A | C8-N9-C4 | 6.48 | 108.39 | 105.80 |
| 36 | A5 | 1298 | C | N1-C2-O2 | -6.48 | 115.01 | 118.90 |
| 36 | A5 | 1897 | G | C5-C6-O6 | -6.48 | 124.71 | 128.60 |
| 36 | A5 | 2857 | C | C6-N1-C2 | 6.48 | 122.89 | 120.30 |
| 1 | A2 | 1455 | G | N1-C6-O6 | 6.47 | 123.78 | 119.90 |
| 36 | A1 | 1523 | U | N3-C2-O2 | 6.47 | 126.73 | 122.20 |
| 36 | A1 | 1608 | C | N1-C2-O2 | 6.47 | 122.78 | 118.90 |
| 36 | A5 | 1408 | G | N3-C4-C5 | 6.47 | 131.84 | 128.60 |
| 36 | A5 | 2431 | C | N3-C4-C5 | -6.47 | 119.31 | 121.90 |
| 80 | A6 | 815 | G | C5-N7-C8 | -6.47 | 101.06 | 104.30 |
| 80 | A6 | 1298 | U | C2-N3-C4 | -6.47 | 123.12 | 127.00 |
| 36 | A5 | 1392 | G | C8-N9-C1' | -6.47 | 118.59 | 127.00 |
| 36 | A5 | 2320 | A | C5-N7-C8 | 6.47 | 107.14 | 103.90 |
| 36 | A5 | 2518 | C | C5-C6-N1 | -6.47 | 117.76 | 121.00 |
| 36 | A5 | 2719 | U | C5-C6-N1 | -6.47 | 119.46 | 122.70 |
| 67 | Dd | 90 | PHE | CB-CA-C | -6.47 | 97.45 | 110.40 |
| 36 | A1 | 427 | C | N1-C2-O2 | -6.47 | 115.02 | 118.90 |
| 36 | A5 | 1161 | G | N7-C8-N9 | -6.47 | 109.86 | 113.10 |
| 36 | A5 | 1399 | A | C8-N9-C4 | 6.47 | 108.39 | 105.80 |
| 36 | A5 | 1879 | A | C4-C5-N7 | 6.47 | 113.94 | 110.70 |
| 36 | A5 | 2351 | U | N3-C4-O4 | -6.47 | 114.87 | 119.40 |
| 36 | A5 | 2837 | A | C2-N3-C4 | 6.47 | 113.83 | 110.60 |
| 36 | A1 | 579 | G | N3-C2-N2 | 6.47 | 124.43 | 119.90 |
| 36 | A1 | 1717 | U | N3-C4-C5 | -6.47 | 110.72 | 114.60 |
| 36 | A5 | 217 | U | C5-C6-N1 | -6.47 | 119.47 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-------|------|-----------|-------|-------------|----------|
| 36 | A5 | 1284 | C | C6-N1-C2 | -6.47 | 117.71 | 120.30 |
| 1 | A2 | 1085 | G | N3-C2-N2 | 6.47 | 124.43 | 119.90 |
| 36 | A1 | 610 | G | C5-C6-N1 | 6.47 | 114.73 | 111.50 |
| 80 | A6 | 1503 | A | C4-C5-N7 | 6.47 | 113.93 | 110.70 |
| 36 | A5 | 2746 | A | C8-N9-C4 | 6.47 | 108.39 | 105.80 |
| 52 | DO | 27[B] | VAL | C-N-CA | 6.47 | 137.87 | 121.70 |
| 36 | A1 | 686 | G | N1-C6-O6 | -6.46 | 116.02 | 119.90 |
| 36 | A1 | 3060 | C | C5-C4-N4 | -6.46 | 115.68 | 120.20 |
| 36 | A1 | 646 | A | C4-C5-C6 | 6.46 | 120.23 | 117.00 |
| 36 | A1 | 974 | G | N3-C4-C5 | -6.46 | 125.37 | 128.60 |
| 36 | A1 | 1083 | G | N3-C4-C5 | -6.46 | 125.37 | 128.60 |
| 36 | A1 | 1371 | G | C5-C6-O6 | 6.46 | 132.48 | 128.60 |
| 36 | A1 | 1202 | A | N1-C2-N3 | 6.46 | 132.53 | 129.30 |
| 80 | A6 | 941 | A | N1-C6-N6 | -6.46 | 114.72 | 118.60 |
| 36 | A5 | 2998 | U | C5-C6-N1 | -6.46 | 119.47 | 122.70 |
| 37 | A7 | 12 | U | N3-C4-C5 | 6.46 | 118.48 | 114.60 |
| 1 | A2 | 1536 | G | N3-C4-N9 | 6.46 | 129.88 | 126.00 |
| 38 | A4 | 32 | C | C6-N1-C1' | 6.46 | 128.55 | 120.80 |
| 36 | A5 | 284 | A | C2-N3-C4 | 6.46 | 113.83 | 110.60 |
| 36 | A5 | 369 | A | N9-C4-C5 | 6.46 | 108.38 | 105.80 |
| 36 | A5 | 1929 | G | C8-N9-C4 | 6.46 | 108.98 | 106.40 |
| 36 | A5 | 2631 | U | N1-C2-N3 | 6.46 | 118.78 | 114.90 |
| 36 | A5 | 2930 | A | N1-C6-N6 | -6.46 | 114.72 | 118.60 |
| 1 | A2 | 1235 | C | N1-C2-O2 | -6.46 | 115.03 | 118.90 |
| 36 | A1 | 948 | C | C5-C6-N1 | -6.46 | 117.77 | 121.00 |
| 36 | A1 | 1042 | U | N3-C2-O2 | -6.46 | 117.68 | 122.20 |
| 36 | A1 | 1126 | G | C5-N7-C8 | 6.46 | 107.53 | 104.30 |
| 36 | A1 | 1450 | G | N3-C2-N2 | -6.46 | 115.38 | 119.90 |
| 36 | A1 | 2763 | U | N3-C2-O2 | 6.46 | 126.72 | 122.20 |
| 36 | A5 | 2440 | G | N7-C8-N9 | 6.46 | 116.33 | 113.10 |
| 36 | A1 | 324 | A | C4-C5-C6 | 6.46 | 120.23 | 117.00 |
| 36 | A1 | 2276 | G | N9-C4-C5 | 6.46 | 107.98 | 105.40 |
| 36 | A1 | 327 | A | C5-C6-N6 | -6.45 | 118.54 | 123.70 |
| 36 | A1 | 2376 | G | C2-N3-C4 | 6.45 | 115.13 | 111.90 |
| 36 | A1 | 3151 | U | C5-C4-O4 | -6.45 | 122.03 | 125.90 |
| 38 | A4 | 25 | G | C5-C6-O6 | 6.45 | 132.47 | 128.60 |
| 38 | A4 | 96 | A | N9-C4-C5 | -6.45 | 103.22 | 105.80 |
| 36 | A5 | 1749 | A | C8-N9-C4 | 6.45 | 108.38 | 105.80 |
| 36 | A5 | 1894 | U | C2-N3-C4 | -6.45 | 123.13 | 127.00 |
| 37 | A7 | 93 | C | C4-C5-C6 | 6.45 | 120.63 | 117.40 |
| 36 | A1 | 3204 | C | C2-N3-C4 | -6.45 | 116.67 | 119.90 |
| 80 | A6 | 1000 | C | C4-C5-C6 | 6.45 | 120.63 | 117.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 36 | A1 | 588 | G | C5-C6-N1 | 6.45 | 114.73 | 111.50 |
| 36 | A1 | 944 | C | C6-N1-C2 | -6.45 | 117.72 | 120.30 |
| 36 | A1 | 966 | U | C2-N3-C4 | -6.45 | 123.13 | 127.00 |
| 36 | A1 | 2202 | C | C4-C5-C6 | 6.45 | 120.63 | 117.40 |
| 80 | A6 | 139 | C | C6-N1-C2 | -6.45 | 117.72 | 120.30 |
| 37 | A7 | 38 | U | C6-N1-C1' | -6.45 | 112.17 | 121.20 |
| 38 | A4 | 17 | A | C5-C6-N1 | -6.45 | 114.48 | 117.70 |
| 80 | A6 | 565 | C | C2-N1-C1' | 6.45 | 125.89 | 118.80 |
| 80 | A6 | 1035 | G | C8-N9-C4 | 6.45 | 108.98 | 106.40 |
| 36 | A5 | 894 | G | C5-C6-O6 | -6.45 | 124.73 | 128.60 |
| 36 | A5 | 2662 | G | C3'-C2'-C1' | -6.45 | 96.34 | 101.50 |
| 80 | A6 | 687 | G | C8-N9-C1' | 6.45 | 135.38 | 127.00 |
| 1 | A2 | 136 | C | N1-C2-O2 | 6.45 | 122.77 | 118.90 |
| 36 | A1 | 660 | A | C5-C6-N1 | 6.45 | 120.92 | 117.70 |
| 36 | A1 | 1148 | G | C5-C6-N1 | 6.45 | 114.72 | 111.50 |
| 36 | A1 | 1389 | G | N1-C6-O6 | 6.45 | 123.77 | 119.90 |
| 36 | A1 | 2368 | A | N9-C4-C5 | 6.45 | 108.38 | 105.80 |
| 36 | A5 | 343 | U | C5-C6-N1 | -6.45 | 119.48 | 122.70 |
| 1 | A2 | 407 | A | C4-C5-C6 | 6.44 | 120.22 | 117.00 |
| 1 | A2 | 732 | G | N9-C4-C5 | -6.44 | 102.82 | 105.40 |
| 36 | A1 | 802 | C | N3-C2-O2 | -6.44 | 117.39 | 121.90 |
| 36 | A1 | 1727 | G | C8-N9-C4 | -6.44 | 103.82 | 106.40 |
| 36 | A1 | 1934 | G | C8-N9-C4 | -6.44 | 103.82 | 106.40 |
| 36 | A5 | 2993 | G | N9-C4-C5 | -6.44 | 102.82 | 105.40 |
| 1 | A2 | 554 | C | C2-N1-C1' | 6.44 | 125.89 | 118.80 |
| 36 | A1 | 864 | G | N1-C2-N2 | -6.44 | 110.40 | 116.20 |
| 36 | A1 | 1931 | U | C2-N1-C1' | -6.44 | 109.97 | 117.70 |
| 36 | A1 | 2369 | G | N7-C8-N9 | 6.44 | 116.32 | 113.10 |
| 36 | A1 | 3382 | U | C2-N1-C1' | 6.44 | 125.43 | 117.70 |
| 80 | A6 | 1755 | A | C5-N7-C8 | -6.44 | 100.68 | 103.90 |
| 36 | A5 | 971 | G | N1-C2-N2 | 6.44 | 122.00 | 116.20 |
| 36 | A5 | 1451 | C | C5-C6-N1 | -6.44 | 117.78 | 121.00 |
| 36 | A5 | 1607 | U | N1-C2-N3 | 6.44 | 118.77 | 114.90 |
| 36 | A5 | 1843 | C | C2-N1-C1' | 6.44 | 125.89 | 118.80 |
| 36 | A5 | 2124 | G | C8-N9-C4 | 6.44 | 108.98 | 106.40 |
| 36 | A5 | 3306 | U | N3-C4-C5 | 6.44 | 118.47 | 114.60 |
| 1 | A2 | 75 | U | N1-C2-O2 | 6.44 | 127.31 | 122.80 |
| 36 | A1 | 386 | A | C6-C5-N7 | -6.44 | 127.79 | 132.30 |
| 80 | A6 | 805 | U | C6-N1-C2 | -6.44 | 117.14 | 121.00 |
| 36 | A5 | 3175 | U | N3-C4-C5 | -6.44 | 110.74 | 114.60 |
| 36 | A1 | 1107 | C | N3-C4-C5 | 6.44 | 124.48 | 121.90 |
| 36 | A1 | 952 | A | C5-C6-N1 | 6.44 | 120.92 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 1413 | G | N1-C6-O6 | -6.44 | 116.04 | 119.90 |
| 80 | A6 | 1473 | U | C2-N1-C1' | 6.44 | 125.42 | 117.70 |
| 37 | A7 | 1 | G | C4-N9-C1' | 6.44 | 134.87 | 126.50 |
| 36 | A1 | 105 | C | N3-C4-C5 | 6.43 | 124.47 | 121.90 |
| 36 | A5 | 3006 | A | N3-C4-N9 | -6.43 | 122.25 | 127.40 |
| 1 | A2 | 1200 | G | C4-C5-C6 | 6.43 | 122.66 | 118.80 |
| 36 | A1 | 2349 | U | N1-C2-N3 | 6.43 | 118.76 | 114.90 |
| 36 | A5 | 393 | U | N3-C2-O2 | -6.43 | 117.70 | 122.20 |
| 36 | A5 | 1840 | U | C5-C6-N1 | -6.43 | 119.48 | 122.70 |
| 36 | A5 | 2246 | G | N3-C4-C5 | -6.43 | 125.38 | 128.60 |
| 36 | A5 | 2879 | C | N1-C2-O2 | 6.43 | 122.76 | 118.90 |
| 36 | A1 | 2257 | C | N3-C2-O2 | -6.43 | 117.40 | 121.90 |
| 36 | A1 | 1834 | U | C5-C6-N1 | -6.43 | 119.49 | 122.70 |
| 36 | A5 | 667 | C | N3-C4-C5 | 6.43 | 124.47 | 121.90 |
| 36 | A1 | 91 | G | C5-N7-C8 | -6.43 | 101.09 | 104.30 |
| 38 | A4 | 51 | G | N1-C6-O6 | 6.43 | 123.76 | 119.90 |
| 36 | A1 | 922 | U | C5-C6-N1 | 6.43 | 125.91 | 122.70 |
| 80 | A6 | 612 | U | N3-C4-O4 | -6.43 | 114.90 | 119.40 |
| 80 | A6 | 653 | C | N3-C4-N4 | 6.43 | 122.50 | 118.00 |
| 36 | A1 | 205 | C | N3-C4-C5 | 6.42 | 124.47 | 121.90 |
| 36 | A5 | 824 | C | C4-C5-C6 | 6.42 | 120.61 | 117.40 |
| 36 | A5 | 2754 | G | N3-C2-N2 | 6.42 | 124.40 | 119.90 |
| 1 | A2 | 1169 | G | N7-C8-N9 | 6.42 | 116.31 | 113.10 |
| 36 | A5 | 1402 | C | C4-C5-C6 | 6.42 | 120.61 | 117.40 |
| 38 | A4 | 25 | G | N1-C2-N3 | 6.42 | 127.75 | 123.90 |
| 38 | A4 | 38 | U | N1-C2-O2 | 6.42 | 127.30 | 122.80 |
| 36 | A5 | 436 | A | C4-N9-C1' | 6.42 | 137.86 | 126.30 |
| 36 | A5 | 1403 | C | N3-C4-N4 | 6.42 | 122.50 | 118.00 |
| 36 | A1 | 3155 | U | N1-C2-O2 | 6.42 | 127.29 | 122.80 |
| 36 | A5 | 779 | G | C8-N9-C4 | -6.42 | 103.83 | 106.40 |
| 1 | A2 | 610 | G | C4-N9-C1' | 6.42 | 134.84 | 126.50 |
| 80 | A6 | 1571 | C | C4-C5-C6 | 6.42 | 120.61 | 117.40 |
| 36 | A5 | 651 | G | C8-N9-C4 | -6.42 | 103.83 | 106.40 |
| 36 | A5 | 2891 | U | C5-C6-N1 | -6.42 | 119.49 | 122.70 |
| 36 | A1 | 1481 | A | C6-C5-N7 | -6.42 | 127.81 | 132.30 |
| 36 | A1 | 1948 | G | N3-C4-N9 | 6.42 | 129.85 | 126.00 |
| 80 | A6 | 1652 | C | N1-C2-N3 | 6.42 | 123.69 | 119.20 |
| 36 | A5 | 1907 | C | N1-C2-O2 | -6.42 | 115.05 | 118.90 |
| 36 | A5 | 2340 | U | C2-N3-C4 | -6.42 | 123.15 | 127.00 |
| 42 | DD | 152 | ARG | NE-CZ-NH1 | 6.42 | 123.51 | 120.30 |
| 38 | A4 | 16 | G | C8-N9-C4 | 6.42 | 108.97 | 106.40 |
| 36 | A5 | 1064 | A | C4-C5-N7 | 6.42 | 113.91 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 843 | A | C2-N3-C4 | -6.41 | 107.39 | 110.60 |
| 80 | A6 | 317 | C | C2-N3-C4 | -6.41 | 116.69 | 119.90 |
| 13 | CL | 5 | LEU | CA-CB-CG | 6.41 | 130.05 | 115.30 |
| 36 | A5 | 950 | G | N3-C2-N2 | 6.41 | 124.39 | 119.90 |
| 36 | A5 | 1321 | G | C5-C6-N1 | -6.41 | 108.29 | 111.50 |
| 1 | A2 | 1185 | U | C2-N1-C1' | 6.41 | 125.39 | 117.70 |
| 36 | A1 | 2639 | G | N9-C4-C5 | -6.41 | 102.84 | 105.40 |
| 36 | A1 | 2987 | A | N1-C2-N3 | 6.41 | 132.50 | 129.30 |
| 80 | A6 | 1112 | G | C6-N1-C2 | -6.41 | 121.25 | 125.10 |
| 36 | A5 | 2231 | C | N3-C4-C5 | -6.41 | 119.34 | 121.90 |
| 36 | A1 | 2356 | A | C8-N9-C4 | 6.41 | 108.36 | 105.80 |
| 36 | A5 | 679 | U | C5-C6-N1 | -6.41 | 119.50 | 122.70 |
| 36 | A5 | 2302 | G | N1-C2-N2 | -6.41 | 110.43 | 116.20 |
| 37 | A7 | 40 | C | N1-C2-O2 | -6.41 | 115.05 | 118.90 |
| 36 | A5 | 2611 | U | C4-C5-C6 | 6.41 | 123.54 | 119.70 |
| 36 | A1 | 641 | C | C2-N3-C4 | -6.41 | 116.70 | 119.90 |
| 80 | A6 | 1649 | G | N3-C2-N2 | 6.41 | 124.38 | 119.90 |
| 36 | A5 | 2408 | U | N1-C2-N3 | 6.41 | 118.74 | 114.90 |
| 36 | A5 | 3354 | U | N3-C2-O2 | -6.41 | 117.72 | 122.20 |
| 36 | A1 | 1042 | U | N3-C4-C5 | 6.40 | 118.44 | 114.60 |
| 36 | A5 | 584 | G | C5-C6-O6 | 6.40 | 132.44 | 128.60 |
| 1 | A2 | 1000 | C | N1-C2-O2 | 6.40 | 122.74 | 118.90 |
| 36 | A1 | 77 | A | N1-C6-N6 | -6.40 | 114.76 | 118.60 |
| 36 | A1 | 2866 | U | N3-C2-O2 | -6.40 | 117.72 | 122.20 |
| 36 | A5 | 2345 | A | C5-C6-N6 | -6.40 | 118.58 | 123.70 |
| 68 | De | 45 | ARG | NE-CZ-NH1 | 6.40 | 123.50 | 120.30 |
| 80 | A6 | 621 | A | C8-N9-C4 | 6.40 | 108.36 | 105.80 |
| 36 | A5 | 2817 | A | N3-C4-C5 | -6.40 | 122.32 | 126.80 |
| 36 | A1 | 66 | A | C2-N3-C4 | -6.40 | 107.40 | 110.60 |
| 36 | A1 | 408 | A | N1-C6-N6 | -6.40 | 114.76 | 118.60 |
| 36 | A1 | 582 | G | C6-C5-N7 | 6.40 | 134.24 | 130.40 |
| 36 | A1 | 1891 | A | C2-N3-C4 | -6.40 | 107.40 | 110.60 |
| 36 | A1 | 2987 | A | C2-N3-C4 | -6.40 | 107.40 | 110.60 |
| 37 | A3 | 10 | C | C6-N1-C2 | -6.40 | 117.74 | 120.30 |
| 36 | A5 | 1390 | A | C5-C6-N6 | 6.40 | 128.82 | 123.70 |
| 36 | A1 | 2653 | C | N1-C2-N3 | 6.40 | 123.68 | 119.20 |
| 36 | A1 | 2980 | U | N1-C2-N3 | 6.40 | 118.74 | 114.90 |
| 36 | A5 | 2134 | G | N3-C4-C5 | -6.40 | 125.40 | 128.60 |
| 36 | A5 | 3003 | G | C5-C6-N1 | 6.40 | 114.70 | 111.50 |
| 36 | A1 | 87 | U | N1-C2-N3 | 6.39 | 118.74 | 114.90 |
| 36 | A1 | 1166 | G | C4-C5-N7 | 6.39 | 113.36 | 110.80 |
| 80 | A6 | 1484 | G | N3-C4-N9 | 6.39 | 129.84 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 1115 | G | C4-N9-C1' | 6.39 | 134.81 | 126.50 |
| 41 | BC | 95 | ARG | NE-CZ-NH2 | 6.39 | 123.50 | 120.30 |
| 36 | A5 | 1793 | C | C2-N3-C4 | 6.39 | 123.10 | 119.90 |
| 36 | A5 | 2130 | G | N1-C6-O6 | -6.39 | 116.06 | 119.90 |
| 36 | A5 | 2365 | C | C5-C4-N4 | 6.39 | 124.67 | 120.20 |
| 36 | A5 | 3303 | G | N1-C2-N2 | -6.39 | 110.45 | 116.20 |
| 54 | DQ | 176 | ARG | NE-CZ-NH1 | -6.39 | 117.10 | 120.30 |
| 36 | A1 | 641 | C | C6-N1-C1' | 6.39 | 128.47 | 120.80 |
| 37 | A3 | 98 | C | C5-C6-N1 | -6.39 | 117.81 | 121.00 |
| 80 | A6 | 603 | U | N1-C2-O2 | -6.39 | 118.33 | 122.80 |
| 36 | A5 | 65 | A | N7-C8-N9 | 6.39 | 117.00 | 113.80 |
| 36 | A5 | 943 | U | C5-C6-N1 | -6.39 | 119.50 | 122.70 |
| 36 | A5 | 3174 | A | C5-N7-C8 | -6.39 | 100.70 | 103.90 |
| 37 | A7 | 48 | U | N1-C2-O2 | -6.39 | 118.33 | 122.80 |
| 1 | A2 | 136 | C | C6-N1-C1' | -6.39 | 113.13 | 120.80 |
| 36 | A1 | 2193 | U | N1-C2-N3 | 6.39 | 118.73 | 114.90 |
| 80 | A6 | 1111 | G | C5-C6-O6 | -6.39 | 124.77 | 128.60 |
| 36 | A5 | 2677 | G | N3-C2-N2 | -6.39 | 115.43 | 119.90 |
| 37 | A7 | 15 | C | N3-C4-C5 | 6.39 | 124.46 | 121.90 |
| 36 | A1 | 582 | G | N3-C4-N9 | -6.39 | 122.17 | 126.00 |
| 36 | A5 | 645 | A | C5-C6-N1 | 6.39 | 120.89 | 117.70 |
| 36 | A5 | 909 | G | C4-C5-N7 | -6.39 | 108.25 | 110.80 |
| 36 | A1 | 630 | A | N1-C6-N6 | -6.39 | 114.77 | 118.60 |
| 36 | A1 | 2973 | G | C8-N9-C4 | 6.39 | 108.95 | 106.40 |
| 36 | A1 | 3362 | A | C8-N9-C4 | -6.39 | 103.25 | 105.80 |
| 80 | A6 | 541 | A | C8-N9-C4 | -6.39 | 103.25 | 105.80 |
| 36 | A5 | 1211 | U | C4-C5-C6 | -6.39 | 115.87 | 119.70 |
| 36 | A5 | 1518 | U | N1-C2-O2 | 6.39 | 127.27 | 122.80 |
| 36 | A5 | 2389 | C | N3-C4-C5 | 6.39 | 124.45 | 121.90 |
| 36 | A1 | 835 | G | N9-C4-C5 | -6.38 | 102.85 | 105.40 |
| 36 | A1 | 973 | A | N7-C8-N9 | 6.38 | 116.99 | 113.80 |
| 36 | A1 | 1719 | G | N9-C4-C5 | -6.38 | 102.85 | 105.40 |
| 36 | A5 | 2117 | A | N1-C6-N6 | -6.38 | 114.77 | 118.60 |
| 36 | A5 | 2349 | U | N3-C4-C5 | 6.38 | 118.43 | 114.60 |
| 36 | A5 | 2753 | G | N3-C2-N2 | -6.38 | 115.43 | 119.90 |
| 25 | AX | 33 | LEU | CA-CB-CG | -6.38 | 100.62 | 115.30 |
| 36 | A1 | 3072 | C | N1-C2-O2 | 6.38 | 122.73 | 118.90 |
| 36 | A5 | 2416 | U | C5-C6-N1 | 6.38 | 125.89 | 122.70 |
| 36 | A1 | 1060 | U | N3-C4-O4 | -6.38 | 114.93 | 119.40 |
| 36 | A1 | 2870 | C | C5-C6-N1 | 6.38 | 124.19 | 121.00 |
| 36 | A5 | 1851 | G | C4-C5-C6 | 6.38 | 122.63 | 118.80 |
| 54 | BQ | 111 | ARG | NE-CZ-NH1 | -6.38 | 117.11 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 652 | G | N3-C4-N9 | 6.38 | 129.83 | 126.00 |
| 36 | A5 | 891 | G | C5-C6-O6 | 6.38 | 132.43 | 128.60 |
| 38 | A8 | 29 | U | C2-N3-C4 | -6.38 | 123.17 | 127.00 |
| 64 | Da | 28 | HIS | N-CA-C | 6.38 | 128.23 | 111.00 |
| 1 | A2 | 1096 | C | N3-C2-O2 | -6.38 | 117.44 | 121.90 |
| 36 | A1 | 102 | C | N3-C4-N4 | 6.38 | 122.47 | 118.00 |
| 36 | A1 | 2377 | G | C5-C6-O6 | 6.38 | 132.43 | 128.60 |
| 36 | A1 | 2661 | G | C5-C6-O6 | -6.38 | 124.77 | 128.60 |
| 38 | A8 | 19 | C | C4-C5-C6 | 6.38 | 120.59 | 117.40 |
| 36 | A1 | 1589 | A | C5-C6-N1 | 6.38 | 120.89 | 117.70 |
| 36 | A1 | 1846 | C | N1-C2-N3 | 6.38 | 123.66 | 119.20 |
| 36 | A1 | 2921 | U | C2-N3-C4 | -6.38 | 123.17 | 127.00 |
| 80 | A6 | 7 | G | C5-C6-N1 | 6.38 | 114.69 | 111.50 |
| 36 | A5 | 75 | G | C5-C6-O6 | -6.38 | 124.77 | 128.60 |
| 36 | A5 | 2964 | G | N7-C8-N9 | -6.38 | 109.91 | 113.10 |
| 38 | A8 | 28 | C | N3-C4-C5 | 6.38 | 124.45 | 121.90 |
| 36 | A5 | 2363 | A | C2-N3-C4 | 6.38 | 113.79 | 110.60 |
| 1 | A2 | 1758 | U | C6-N1-C2 | -6.37 | 117.17 | 121.00 |
| 36 | A1 | 2187 | G | N1-C6-O6 | 6.37 | 123.72 | 119.90 |
| 80 | A6 | 470 | A | N7-C8-N9 | 6.37 | 116.99 | 113.80 |
| 36 | A5 | 2146 | C | C6-N1-C2 | -6.37 | 117.75 | 120.30 |
| 36 | A5 | 2351 | U | N3-C2-O2 | -6.37 | 117.74 | 122.20 |
| 36 | A5 | 2894 | C | N3-C4-C5 | 6.37 | 124.45 | 121.90 |
| 36 | A1 | 21 | G | N1-C6-O6 | -6.37 | 116.08 | 119.90 |
| 59 | BV | 48 | ARG | NE-CZ-NH1 | 6.37 | 123.48 | 120.30 |
| 25 | CX | 79 | ASN | CB-CA-C | -6.37 | 97.66 | 110.40 |
| 36 | A5 | 2288 | G | N3-C4-C5 | -6.37 | 125.42 | 128.60 |
| 36 | A5 | 2948 | C | C5-C4-N4 | 6.37 | 124.66 | 120.20 |
| 1 | A2 | 144 | U | C6-N1-C2 | -6.37 | 117.18 | 121.00 |
| 36 | A1 | 72 | C | C2-N3-C4 | -6.37 | 116.72 | 119.90 |
| 36 | A1 | 716 | A | C4-C5-N7 | 6.37 | 113.88 | 110.70 |
| 36 | A1 | 1520 | G | C2-N3-C4 | 6.37 | 115.08 | 111.90 |
| 80 | A6 | 101 | U | N3-C2-O2 | -6.37 | 117.74 | 122.20 |
| 80 | A6 | 402 | C | C6-N1-C2 | 6.37 | 122.85 | 120.30 |
| 36 | A5 | 1832 | C | C2-N3-C4 | -6.37 | 116.72 | 119.90 |
| 36 | A5 | 2261 | G | C8-N9-C4 | 6.37 | 108.95 | 106.40 |
| 36 | A1 | 1082 | U | C5-C6-N1 | 6.37 | 125.88 | 122.70 |
| 36 | A1 | 1801 | U | C5-C6-N1 | -6.37 | 119.52 | 122.70 |
| 36 | A1 | 2353 | G | C4-C5-N7 | 6.37 | 113.35 | 110.80 |
| 80 | A6 | 1082 | C | C2-N1-C1' | 6.37 | 125.80 | 118.80 |
| 1 | A2 | 628 | G | N3-C2-N2 | 6.36 | 124.35 | 119.90 |
| 36 | A1 | 702 | C | C2-N3-C4 | -6.36 | 116.72 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-------|------|-----------|-------|-------------|----------|
| 36 | A1 | 2533 | G | N3-C4-N9 | 6.36 | 129.82 | 126.00 |
| 36 | A1 | 2616 | C | C2-N3-C4 | -6.36 | 116.72 | 119.90 |
| 80 | A6 | 1188 | G | N1-C6-O6 | 6.36 | 123.72 | 119.90 |
| 36 | A5 | 1042 | U | C5-C6-N1 | -6.36 | 119.52 | 122.70 |
| 36 | A5 | 1416 | C | N3-C2-O2 | -6.36 | 117.45 | 121.90 |
| 52 | DO | 23[B] | ILE | O-C-N | 6.36 | 132.88 | 122.70 |
| 36 | A1 | 670 | C | C4-C5-C6 | 6.36 | 120.58 | 117.40 |
| 36 | A1 | 2198 | A | C2-N3-C4 | -6.36 | 107.42 | 110.60 |
| 80 | A6 | 1099 | U | C5-C4-O4 | 6.36 | 129.72 | 125.90 |
| 55 | BR | 125 | LYS | CD-CE-NZ | 6.36 | 126.33 | 111.70 |
| 80 | A6 | 539 | G | N3-C4-N9 | -6.36 | 122.18 | 126.00 |
| 80 | A6 | 639 | U | C2-N1-C1' | 6.36 | 125.33 | 117.70 |
| 36 | A5 | 665 | A | C2-N3-C4 | -6.36 | 107.42 | 110.60 |
| 37 | A7 | 92 | A | C4-C5-N7 | 6.36 | 113.88 | 110.70 |
| 1 | A2 | 1611 | A | C8-N9-C4 | -6.36 | 103.26 | 105.80 |
| 1 | A2 | 1745 | G | N9-C4-C5 | -6.36 | 102.86 | 105.40 |
| 36 | A1 | 196 | G | C5-C6-N1 | 6.36 | 114.68 | 111.50 |
| 36 | A1 | 875 | G | N1-C6-O6 | -6.36 | 116.08 | 119.90 |
| 36 | A1 | 1177 | G | N3-C2-N2 | -6.36 | 115.45 | 119.90 |
| 36 | A1 | 1379 | G | C5-C6-O6 | 6.36 | 132.41 | 128.60 |
| 36 | A1 | 2203 | U | N1-C2-O2 | -6.36 | 118.35 | 122.80 |
| 80 | A6 | 795 | U | N3-C2-O2 | -6.36 | 117.75 | 122.20 |
| 80 | A6 | 1113 | A | N1-C2-N3 | 6.36 | 132.48 | 129.30 |
| 36 | A5 | 903 | U | N3-C2-O2 | -6.36 | 117.75 | 122.20 |
| 36 | A5 | 1172 | G | N3-C2-N2 | 6.36 | 124.35 | 119.90 |
| 36 | A1 | 2291 | A | C2-N3-C4 | 6.36 | 113.78 | 110.60 |
| 80 | A6 | 1091 | A | C5-C6-N1 | -6.36 | 114.52 | 117.70 |
| 36 | A5 | 2817 | A | C6-N1-C2 | -6.36 | 114.79 | 118.60 |
| 38 | A8 | 17 | A | C4-C5-N7 | 6.36 | 113.88 | 110.70 |
| 55 | DR | 88 | ARG | NE-CZ-NH1 | -6.36 | 117.12 | 120.30 |
| 36 | A5 | 3189 | G | N1-C2-N3 | 6.35 | 127.71 | 123.90 |
| 36 | A1 | 331 | G | C5-C6-O6 | 6.35 | 132.41 | 128.60 |
| 36 | A1 | 1919 | G | C5-C6-O6 | 6.35 | 132.41 | 128.60 |
| 36 | A1 | 2298 | U | N3-C4-C5 | 6.35 | 118.41 | 114.60 |
| 36 | A1 | 2703 | A | N7-C8-N9 | 6.35 | 116.98 | 113.80 |
| 36 | A5 | 833 | G | N1-C2-N3 | 6.35 | 127.71 | 123.90 |
| 36 | A5 | 940 | G | C8-N9-C4 | -6.35 | 103.86 | 106.40 |
| 36 | A5 | 1147 | G | N7-C8-N9 | -6.35 | 109.92 | 113.10 |
| 36 | A5 | 42 | C | C5-C6-N1 | 6.35 | 124.17 | 121.00 |
| 36 | A1 | 823 | C | C5-C6-N1 | -6.35 | 117.83 | 121.00 |
| 36 | A5 | 1403 | C | C6-N1-C1' | -6.35 | 113.18 | 120.80 |
| 36 | A5 | 3167 | A | N7-C8-N9 | 6.35 | 116.97 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 761 | A | C2-N3-C4 | -6.35 | 107.43 | 110.60 |
| 36 | A1 | 1371 | G | C4-C5-N7 | -6.35 | 108.26 | 110.80 |
| 36 | A1 | 3092 | C | C2-N3-C4 | -6.35 | 116.73 | 119.90 |
| 80 | A6 | 364 | G | C8-N9-C4 | 6.35 | 108.94 | 106.40 |
| 36 | A5 | 787 | G | C2-N3-C4 | -6.35 | 108.73 | 111.90 |
| 36 | A5 | 1200 | A | N1-C2-N3 | 6.35 | 132.47 | 129.30 |
| 38 | A8 | 111 | A | C2-N3-C4 | -6.35 | 107.43 | 110.60 |
| 36 | A5 | 2802 | A | N1-C2-N3 | -6.35 | 126.13 | 129.30 |
| 38 | A4 | 32 | C | N3-C4-C5 | 6.34 | 124.44 | 121.90 |
| 80 | A6 | 1030 | A | C8-N9-C4 | -6.34 | 103.26 | 105.80 |
| 36 | A5 | 938 | C | C6-N1-C2 | 6.34 | 122.84 | 120.30 |
| 36 | A5 | 1690 | C | N1-C2-O2 | -6.34 | 115.09 | 118.90 |
| 36 | A1 | 2409 | G | N1-C6-O6 | -6.34 | 116.09 | 119.90 |
| 41 | DC | 327 | LEU | CA-CB-CG | 6.34 | 129.89 | 115.30 |
| 36 | A1 | 1411 | C | N1-C2-O2 | 6.34 | 122.70 | 118.90 |
| 36 | A5 | 1340 | G | N3-C2-N2 | 6.34 | 124.34 | 119.90 |
| 36 | A5 | 2361 | A | C8-N9-C4 | -6.34 | 103.26 | 105.80 |
| 36 | A5 | 2625 | C | N3-C2-O2 | -6.34 | 117.46 | 121.90 |
| 36 | A5 | 2633 | U | C5-C6-N1 | -6.34 | 119.53 | 122.70 |
| 36 | A1 | 688 | G | N1-C6-O6 | -6.34 | 116.10 | 119.90 |
| 36 | A1 | 295 | A | N9-C4-C5 | 6.34 | 108.33 | 105.80 |
| 80 | A6 | 1520 | U | N1-C2-O2 | -6.34 | 118.36 | 122.80 |
| 36 | A5 | 2305 | G | C4-C5-N7 | 6.34 | 113.33 | 110.80 |
| 36 | A5 | 3309 | G | C4-N9-C1' | 6.34 | 134.74 | 126.50 |
| 36 | A5 | 1149 | G | N1-C2-N3 | -6.33 | 120.10 | 123.90 |
| 36 | A5 | 1496 | C | C5-C6-N1 | 6.33 | 124.17 | 121.00 |
| 80 | A6 | 392 | G | C5-C6-N1 | 6.33 | 114.67 | 111.50 |
| 36 | A1 | 1003 | A | C6-C5-N7 | -6.33 | 127.87 | 132.30 |
| 36 | A1 | 2935 | U | C2-N3-C4 | 6.33 | 130.80 | 127.00 |
| 36 | A5 | 1041 | U | C6-N1-C2 | 6.33 | 124.80 | 121.00 |
| 36 | A5 | 2277 | C | C6-N1-C2 | 6.33 | 122.83 | 120.30 |
| 77 | Dn | 9 | ARG | NE-CZ-NH2 | -6.33 | 117.14 | 120.30 |
| 36 | A1 | 327 | A | N9-C4-C5 | -6.33 | 103.27 | 105.80 |
| 38 | A8 | 29 | U | N1-C2-N3 | 6.33 | 118.70 | 114.90 |
| 1 | A2 | 557 | G | C4-C5-C6 | 6.33 | 122.60 | 118.80 |
| 36 | A1 | 1425 | U | N3-C4-O4 | -6.33 | 114.97 | 119.40 |
| 36 | A1 | 2795 | U | N3-C4-O4 | -6.33 | 114.97 | 119.40 |
| 80 | A6 | 351 | C | C4-C5-C6 | 6.33 | 120.56 | 117.40 |
| 36 | A5 | 1858 | A | N7-C8-N9 | 6.33 | 116.97 | 113.80 |
| 36 | A5 | 2123 | G | C2-N3-C4 | 6.33 | 115.06 | 111.90 |
| 36 | A1 | 953 | G | N3-C4-N9 | -6.33 | 122.20 | 126.00 |
| 80 | A6 | 1627 | U | C5-C4-O4 | 6.33 | 129.69 | 125.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 1869 | C | N3-C4-C5 | 6.32 | 124.43 | 121.90 |
| 36 | A1 | 2608 | G | N3-C2-N2 | 6.32 | 124.33 | 119.90 |
| 80 | A6 | 756 | A | C8-N9-C4 | -6.32 | 103.27 | 105.80 |
| 80 | A6 | 1619 | C | C6-N1-C2 | -6.32 | 117.77 | 120.30 |
| 32 | Ce | 10 | ARG | NE-CZ-NH1 | -6.32 | 117.14 | 120.30 |
| 36 | A5 | 2393 | G | N9-C4-C5 | -6.32 | 102.87 | 105.40 |
| 36 | A1 | 2973 | G | N1-C6-O6 | 6.32 | 123.69 | 119.90 |
| 38 | A4 | 81 | U | C6-N1-C2 | -6.32 | 117.21 | 121.00 |
| 80 | A6 | 355 | G | C5-C6-N1 | 6.32 | 114.66 | 111.50 |
| 36 | A5 | 2375 | G | C5-C6-N1 | 6.32 | 114.66 | 111.50 |
| 1 | A2 | 1246 | C | C5-C4-N4 | 6.32 | 124.62 | 120.20 |
| 36 | A1 | 1474 | A | C2-N3-C4 | -6.32 | 107.44 | 110.60 |
| 36 | A5 | 248 | U | N1-C2-O2 | 6.32 | 127.22 | 122.80 |
| 36 | A5 | 892 | U | N3-C4-C5 | 6.32 | 118.39 | 114.60 |
| 36 | A5 | 1733 | G | N1-C6-O6 | 6.32 | 123.69 | 119.90 |
| 36 | A5 | 1407 | A | C8-N9-C4 | 6.32 | 108.33 | 105.80 |
| 36 | A5 | 2996 | U | C2-N1-C1' | 6.32 | 125.28 | 117.70 |
| 36 | A5 | 625 | G | C5-C6-O6 | 6.32 | 132.39 | 128.60 |
| 36 | A5 | 947 | G | N3-C4-N9 | 6.32 | 129.79 | 126.00 |
| 36 | A5 | 1833 | G | N7-C8-N9 | -6.32 | 109.94 | 113.10 |
| 36 | A5 | 2614 | G | C8-N9-C1' | -6.32 | 118.79 | 127.00 |
| 1 | A2 | 377 | G | C5-C6-O6 | -6.32 | 124.81 | 128.60 |
| 36 | A1 | 335 | G | C8-N9-C4 | -6.32 | 103.87 | 106.40 |
| 36 | A1 | 1294 | A | C8-N9-C4 | -6.32 | 103.27 | 105.80 |
| 36 | A1 | 1518 | U | N1-C2-N3 | 6.32 | 118.69 | 114.90 |
| 36 | A1 | 3001 | C | N3-C4-C5 | 6.32 | 124.43 | 121.90 |
| 36 | A5 | 436 | A | C5-N7-C8 | -6.32 | 100.74 | 103.90 |
| 36 | A5 | 3011 | A | N1-C2-N3 | -6.32 | 126.14 | 129.30 |
| 36 | A5 | 3309 | G | C6-N1-C2 | -6.32 | 121.31 | 125.10 |
| 36 | A1 | 1472 | U | N1-C2-O2 | -6.31 | 118.38 | 122.80 |
| 36 | A1 | 1492 | G | N9-C4-C5 | 6.31 | 107.93 | 105.40 |
| 80 | A6 | 350 | U | N3-C2-O2 | -6.31 | 117.78 | 122.20 |
| 36 | A5 | 510 | G | C5-C6-N1 | 6.31 | 114.66 | 111.50 |
| 36 | A5 | 631 | U | N3-C4-C5 | 6.31 | 118.39 | 114.60 |
| 36 | A5 | 1130 | A | N3-C4-C5 | -6.31 | 122.38 | 126.80 |
| 1 | A2 | 1430 | U | C5-C4-O4 | 6.31 | 129.69 | 125.90 |
| 36 | A1 | 1846 | C | C2-N3-C4 | -6.31 | 116.74 | 119.90 |
| 36 | A1 | 2369 | G | C5-C6-N1 | 6.31 | 114.66 | 111.50 |
| 36 | A5 | 676 | G | C8-N9-C4 | -6.31 | 103.88 | 106.40 |
| 36 | A5 | 1188 | U | C5-C4-O4 | -6.31 | 122.11 | 125.90 |
| 36 | A5 | 1300 | G | C5-C6-O6 | -6.31 | 124.81 | 128.60 |
| 36 | A5 | 1902 | G | N3-C4-N9 | 6.31 | 129.79 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 3245 | A | C5-C6-N6 | -6.31 | 118.65 | 123.70 |
| 36 | A1 | 434 | U | N1-C2-O2 | 6.31 | 127.22 | 122.80 |
| 36 | A5 | 904 | A | C8-N9-C4 | -6.31 | 103.28 | 105.80 |
| 36 | A5 | 2420 | C | C5-C4-N4 | -6.31 | 115.78 | 120.20 |
| 36 | A1 | 2906 | C | N1-C2-N3 | 6.31 | 123.62 | 119.20 |
| 80 | A6 | 65 | A | C5-C6-N1 | -6.31 | 114.55 | 117.70 |
| 36 | A5 | 3187 | A | C4-C5-N7 | -6.31 | 107.55 | 110.70 |
| 36 | A1 | 953 | G | C4-N9-C1' | -6.31 | 118.30 | 126.50 |
| 36 | A1 | 1136 | A | C6-N1-C2 | -6.31 | 114.82 | 118.60 |
| 36 | A1 | 1646 | G | C4-C5-N7 | 6.31 | 113.32 | 110.80 |
| 36 | A5 | 600 | G | C8-N9-C4 | -6.31 | 103.88 | 106.40 |
| 36 | A5 | 1123 | U | C5-C6-N1 | -6.31 | 119.55 | 122.70 |
| 36 | A5 | 3270 | U | C5-C6-N1 | -6.31 | 119.55 | 122.70 |
| 39 | DA | 204 | MET | CG-SD-CE | -6.31 | 90.11 | 100.20 |
| 36 | A5 | 3258 | U | C6-N1-C2 | 6.31 | 124.78 | 121.00 |
| 1 | A2 | 1027 | A | N7-C8-N9 | 6.30 | 116.95 | 113.80 |
| 36 | A1 | 285 | A | C5-C6-N6 | -6.30 | 118.66 | 123.70 |
| 36 | A1 | 658 | G | C4-N9-C1' | 6.30 | 134.69 | 126.50 |
| 36 | A1 | 1153 | A | N1-C6-N6 | 6.30 | 122.38 | 118.60 |
| 64 | Ba | 12 | ARG | NE-CZ-NH2 | -6.30 | 117.15 | 120.30 |
| 80 | A6 | 653 | C | C6-N1-C1' | -6.30 | 113.23 | 120.80 |
| 36 | A5 | 1449 | A | C5-C6-N1 | -6.30 | 114.55 | 117.70 |
| 36 | A5 | 1844 | C | C2-N3-C4 | -6.30 | 116.75 | 119.90 |
| 36 | A5 | 2821 | C | C5-C6-N1 | 6.30 | 124.15 | 121.00 |
| 1 | A2 | 189 | C | N1-C2-O2 | 6.30 | 122.68 | 118.90 |
| 68 | De | 47 | ARG | NE-CZ-NH2 | -6.30 | 117.15 | 120.30 |
| 1 | A2 | 973 | A | C2-N3-C4 | -6.30 | 107.45 | 110.60 |
| 36 | A1 | 509 | U | N1-C2-N3 | 6.30 | 118.68 | 114.90 |
| 36 | A1 | 1000 | C | C6-N1-C1' | -6.30 | 113.24 | 120.80 |
| 36 | A1 | 2851 | A | N7-C8-N9 | -6.30 | 110.65 | 113.80 |
| 62 | BY | 13 | ARG | NE-CZ-NH1 | 6.30 | 123.45 | 120.30 |
| 80 | A6 | 87 | C | N1-C2-O2 | -6.30 | 115.12 | 118.90 |
| 36 | A5 | 112 | U | C5-C4-O4 | -6.30 | 122.12 | 125.90 |
| 36 | A5 | 1306 | G | C6-N1-C2 | -6.30 | 121.32 | 125.10 |
| 36 | A5 | 2303 | A | N1-C6-N6 | -6.30 | 114.82 | 118.60 |
| 37 | A7 | 48 | U | N3-C4-C5 | 6.30 | 118.38 | 114.60 |
| 1 | A2 | 159 | U | C2-N1-C1' | -6.30 | 110.14 | 117.70 |
| 36 | A1 | 228 | U | N1-C2-O2 | 6.30 | 127.21 | 122.80 |
| 36 | A1 | 954 | U | N1-C2-O2 | -6.30 | 118.39 | 122.80 |
| 36 | A1 | 2806 | U | C2-N3-C4 | -6.30 | 123.22 | 127.00 |
| 36 | A5 | 582 | G | C5-C6-O6 | 6.30 | 132.38 | 128.60 |
| 36 | A5 | 2389 | C | C5-C6-N1 | -6.30 | 117.85 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 90 | C | C2-N3-C4 | -6.30 | 116.75 | 119.90 |
| 49 | DL | 27 | ASP | CB-CG-OD2 | 6.30 | 123.97 | 118.30 |
| 36 | A1 | 3328 | G | C8-N9-C4 | -6.30 | 103.88 | 106.40 |
| 38 | A4 | 2 | A | N7-C8-N9 | 6.30 | 116.95 | 113.80 |
| 36 | A5 | 2364 | G | C5-C6-O6 | 6.30 | 132.38 | 128.60 |
| 36 | A5 | 2777 | G | C4-C5-N7 | -6.30 | 108.28 | 110.80 |
| 36 | A5 | 3317 | U | N3-C4-O4 | -6.30 | 114.99 | 119.40 |
| 1 | A2 | 213 | A | C8-N9-C4 | 6.29 | 108.32 | 105.80 |
| 36 | A1 | 1082 | U | C6-N1-C2 | -6.29 | 117.22 | 121.00 |
| 36 | A1 | 2390 | A | N1-C2-N3 | 6.29 | 132.45 | 129.30 |
| 42 | DD | 248 | ARG | NE-CZ-NH2 | -6.29 | 117.15 | 120.30 |
| 36 | A1 | 91 | G | N3-C4-N9 | -6.29 | 122.22 | 126.00 |
| 36 | A1 | 405 | U | C2-N3-C4 | -6.29 | 123.22 | 127.00 |
| 36 | A1 | 1433 | A | C2-N3-C4 | 6.29 | 113.75 | 110.60 |
| 36 | A1 | 1948 | G | C5-C6-O6 | -6.29 | 124.82 | 128.60 |
| 36 | A5 | 276 | U | C2-N3-C4 | -6.29 | 123.22 | 127.00 |
| 36 | A5 | 3360 | C | C6-N1-C2 | -6.29 | 117.78 | 120.30 |
| 36 | A1 | 2805 | G | N3-C2-N2 | 6.29 | 124.31 | 119.90 |
| 36 | A5 | 1115 | G | C8-N9-C4 | -6.29 | 103.88 | 106.40 |
| 36 | A5 | 1314 | C | C6-N1-C1' | -6.29 | 113.25 | 120.80 |
| 36 | A5 | 3330 | A | C2-N3-C4 | 6.29 | 113.75 | 110.60 |
| 38 | A4 | 21 | C | N3-C2-O2 | 6.29 | 126.30 | 121.90 |
| 36 | A5 | 793 | C | N1-C2-O2 | -6.29 | 115.13 | 118.90 |
| 36 | A5 | 2211 | U | N3-C4-C5 | -6.29 | 110.83 | 114.60 |
| 36 | A1 | 907 | G | C2-N3-C4 | 6.29 | 115.04 | 111.90 |
| 80 | A6 | 768 | C | N3-C4-N4 | 6.29 | 122.40 | 118.00 |
| 36 | A5 | 1940 | G | N1-C2-N2 | -6.29 | 110.54 | 116.20 |
| 36 | A5 | 2833 | A | N7-C8-N9 | -6.29 | 110.66 | 113.80 |
| 36 | A1 | 394 | G | N1-C2-N3 | -6.29 | 120.13 | 123.90 |
| 36 | A1 | 1948 | G | N9-C4-C5 | -6.29 | 102.89 | 105.40 |
| 56 | BS | 40 | ARG | CG-CD-NE | 6.29 | 125.00 | 111.80 |
| 36 | A5 | 1506 | A | C5-N7-C8 | -6.29 | 100.76 | 103.90 |
| 38 | A8 | 52 | A | C8-N9-C4 | -6.29 | 103.29 | 105.80 |
| 1 | A2 | 590 | C | C2-N1-C1' | 6.28 | 125.71 | 118.80 |
| 36 | A1 | 1460 | A | C6-N1-C2 | -6.28 | 114.83 | 118.60 |
| 80 | A6 | 687 | G | C6-C5-N7 | 6.28 | 134.17 | 130.40 |
| 80 | A6 | 1469 | A | C8-N9-C4 | 6.28 | 108.31 | 105.80 |
| 80 | A6 | 1793 | G | C5-N7-C8 | 6.28 | 107.44 | 104.30 |
| 36 | A5 | 2289 | U | N3-C4-O4 | -6.28 | 115.00 | 119.40 |
| 1 | A2 | 68 | A | C8-N9-C4 | -6.28 | 103.29 | 105.80 |
| 1 | A2 | 942 | G | N1-C6-O6 | -6.28 | 116.13 | 119.90 |
| 1 | A2 | 627 | C | N3-C4-N4 | 6.28 | 122.40 | 118.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 36 | A1 | 365 | A | C5-C6-N1 | -6.28 | 114.56 | 117.70 |
| 36 | A1 | 938 | C | N1-C2-O2 | -6.28 | 115.13 | 118.90 |
| 36 | A1 | 942 | U | C5-C4-O4 | 6.28 | 129.67 | 125.90 |
| 36 | A1 | 2930 | A | N9-C4-C5 | 6.28 | 108.31 | 105.80 |
| 80 | A6 | 453 | U | N1-C2-N3 | 6.28 | 118.67 | 114.90 |
| 80 | A6 | 565 | C | N3-C2-O2 | -6.28 | 117.50 | 121.90 |
| 80 | A6 | 1438 | G | C8-N9-C4 | 6.28 | 108.91 | 106.40 |
| 36 | A5 | 2616 | C | C5-C4-N4 | -6.28 | 115.80 | 120.20 |
| 36 | A5 | 1168 | U | N3-C4-C5 | 6.28 | 118.37 | 114.60 |
| 36 | A5 | 1408 | G | C2-N3-C4 | -6.28 | 108.76 | 111.90 |
| 36 | A5 | 2952 | G | N1-C6-O6 | 6.28 | 123.67 | 119.90 |
| 36 | A1 | 398 | A | C2-N3-C4 | 6.28 | 113.74 | 110.60 |
| 36 | A1 | 1341 | U | N3-C4-O4 | -6.28 | 115.01 | 119.40 |
| 80 | A6 | 1044 | U | N3-C2-O2 | -6.28 | 117.81 | 122.20 |
| 1 | A2 | 1000 | C | C5-C6-N1 | -6.28 | 117.86 | 121.00 |
| 1 | A2 | 1515 | A | C8-N9-C4 | -6.28 | 103.29 | 105.80 |
| 36 | A1 | 2417 | U | C2-N3-C4 | -6.28 | 123.23 | 127.00 |
| 36 | A5 | 1056 | U | N3-C4-C5 | -6.28 | 110.83 | 114.60 |
| 36 | A1 | 832 | G | C8-N9-C4 | 6.27 | 108.91 | 106.40 |
| 36 | A1 | 2284 | C | N1-C2-O2 | -6.27 | 115.14 | 118.90 |
| 36 | A1 | 2299 | A | C6-N1-C2 | -6.27 | 114.84 | 118.60 |
| 37 | A3 | 86 | U | N1-C2-O2 | -6.27 | 118.41 | 122.80 |
| 80 | A6 | 402 | C | C5-C4-N4 | -6.27 | 115.81 | 120.20 |
| 38 | A8 | 84 | C | C6-N1-C2 | -6.27 | 117.79 | 120.30 |
| 36 | A1 | 808 | A | C5-C6-N6 | 6.27 | 128.72 | 123.70 |
| 36 | A1 | 1007 | U | C5-C4-O4 | -6.27 | 122.14 | 125.90 |
| 36 | A1 | 1393 | A | C6-N1-C2 | -6.27 | 114.84 | 118.60 |
| 38 | A4 | 15 | G | N7-C8-N9 | -6.27 | 109.96 | 113.10 |
| 80 | A6 | 449 | C | N3-C4-N4 | -6.27 | 113.61 | 118.00 |
| 36 | A5 | 2352 | A | N1-C2-N3 | 6.27 | 132.44 | 129.30 |
| 36 | A5 | 3317 | U | C5-C6-N1 | 6.27 | 125.84 | 122.70 |
| 1 | A2 | 1363 | U | N1-C2-O2 | 6.27 | 127.19 | 122.80 |
| 1 | A2 | 1456 | C | C6-N1-C2 | -6.27 | 117.79 | 120.30 |
| 1 | A2 | 1465 | C | N3-C4-C5 | -6.27 | 119.39 | 121.90 |
| 36 | A5 | 586 | C | N3-C4-C5 | 6.27 | 124.41 | 121.90 |
| 36 | A5 | 1383 | G | N1-C6-O6 | -6.27 | 116.14 | 119.90 |
| 36 | A5 | 1511 | U | C5-C6-N1 | -6.27 | 119.56 | 122.70 |
| 1 | A2 | 75 | U | N3-C2-O2 | -6.27 | 117.81 | 122.20 |
| 1 | A2 | 1198 | G | N9-C4-C5 | 6.27 | 107.91 | 105.40 |
| 36 | A1 | 1297 | C | C6-N1-C2 | 6.27 | 122.81 | 120.30 |
| 80 | A6 | 1073 | G | C5-C6-N1 | 6.27 | 114.63 | 111.50 |
| 36 | A5 | 2735 | U | C6-N1-C2 | -6.27 | 117.24 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 3218 | A | N3-C4-C5 | 6.27 | 131.19 | 126.80 |
| 1 | A2 | 340 | U | N3-C2-O2 | -6.27 | 117.81 | 122.20 |
| 1 | A2 | 377 | G | N3-C4-C5 | 6.27 | 131.73 | 128.60 |
| 36 | A1 | 1144 | U | N3-C4-C5 | 6.27 | 118.36 | 114.60 |
| 36 | A1 | 1492 | G | C8-N9-C1' | -6.27 | 118.85 | 127.00 |
| 38 | A4 | 10 | A | N9-C4-C5 | 6.27 | 108.31 | 105.80 |
| 64 | Ba | 46 | ASP | N-CA-C | -6.27 | 94.08 | 111.00 |
| 36 | A5 | 2139 | A | C5-N7-C8 | 6.27 | 107.03 | 103.90 |
| 36 | A1 | 1448 | U | N1-C2-O2 | -6.27 | 118.41 | 122.80 |
| 36 | A1 | 1796 | G | N3-C4-C5 | -6.27 | 125.47 | 128.60 |
| 36 | A5 | 1411 | C | N1-C2-O2 | -6.27 | 115.14 | 118.90 |
| 36 | A1 | 124 | U | N3-C4-O4 | -6.26 | 115.02 | 119.40 |
| 36 | A1 | 1336 | U | C6-N1-C2 | -6.26 | 117.24 | 121.00 |
| 36 | A1 | 3260 | G | C5-C6-O6 | 6.26 | 132.36 | 128.60 |
| 40 | BB | 21 | ARG | NE-CZ-NH1 | -6.26 | 117.17 | 120.30 |
| 80 | A6 | 62 | A | N1-C6-N6 | 6.26 | 122.36 | 118.60 |
| 80 | A6 | 1550 | A | C5-C6-N6 | -6.26 | 118.69 | 123.70 |
| 36 | A5 | 637 | C | C2-N1-C1' | -6.26 | 111.91 | 118.80 |
| 36 | A5 | 2164 | A | C8-N9-C4 | -6.26 | 103.29 | 105.80 |
| 38 | A8 | 38 | U | C5-C4-O4 | 6.26 | 129.66 | 125.90 |
| 1 | A2 | 404 | G | C8-N9-C4 | 6.26 | 108.91 | 106.40 |
| 1 | A2 | 868 | G | N1-C6-O6 | 6.26 | 123.66 | 119.90 |
| 1 | A2 | 942 | G | C8-N9-C4 | -6.26 | 103.89 | 106.40 |
| 36 | A1 | 1003 | A | C5-C6-N6 | -6.26 | 118.69 | 123.70 |
| 36 | A1 | 2382 | G | C5-C6-O6 | 6.26 | 132.36 | 128.60 |
| 80 | A6 | 382 | C | C2-N3-C4 | -6.26 | 116.77 | 119.90 |
| 80 | A6 | 769 | A | N9-C4-C5 | 6.26 | 108.31 | 105.80 |
| 36 | A1 | 847 | A | C6-C5-N7 | -6.26 | 127.92 | 132.30 |
| 36 | A1 | 3143 | C | C2-N1-C1' | -6.26 | 111.91 | 118.80 |
| 38 | A4 | 12 | A | N9-C4-C5 | 6.26 | 108.31 | 105.80 |
| 36 | A5 | 950 | G | C8-N9-C4 | 6.26 | 108.91 | 106.40 |
| 36 | A5 | 1211 | U | N3-C4-O4 | -6.26 | 115.02 | 119.40 |
| 36 | A1 | 2340 | U | N3-C4-O4 | -6.26 | 115.02 | 119.40 |
| 36 | A1 | 2361 | A | C6-N1-C2 | -6.26 | 114.84 | 118.60 |
| 36 | A5 | 314 | U | C5-C4-O4 | 6.26 | 129.66 | 125.90 |
| 36 | A5 | 674 | G | C8-N9-C4 | -6.26 | 103.90 | 106.40 |
| 1 | A2 | 810 | G | C6-C5-N7 | -6.26 | 126.64 | 130.40 |
| 36 | A1 | 281 | G | C6-N1-C2 | -6.26 | 121.34 | 125.10 |
| 36 | A1 | 2308 | C | N1-C2-O2 | -6.26 | 115.14 | 118.90 |
| 36 | A1 | 3219 | G | N3-C4-N9 | 6.26 | 129.75 | 126.00 |
| 38 | A4 | 135 | G | N9-C4-C5 | 6.26 | 107.90 | 105.40 |
| 36 | A1 | 304 | G | C2-N3-C4 | 6.26 | 115.03 | 111.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 347 | G | C4-C5-N7 | 6.26 | 113.30 | 110.80 |
| 36 | A1 | 2249 | G | C5-C6-N1 | 6.26 | 114.63 | 111.50 |
| 41 | BC | 283 | THR | CB-CA-C | -6.26 | 94.70 | 111.60 |
| 36 | A5 | 1297 | C | C4-C5-C6 | 6.26 | 120.53 | 117.40 |
| 36 | A5 | 2808 | A | N1-C2-N3 | 6.26 | 132.43 | 129.30 |
| 37 | A7 | 92 | A | C6-C5-N7 | -6.26 | 127.92 | 132.30 |
| 40 | DB | 10 | ARG | NE-CZ-NH1 | 6.26 | 123.43 | 120.30 |
| 36 | A1 | 498 | A | C5-C6-N6 | 6.25 | 128.70 | 123.70 |
| 36 | A1 | 80 | G | N3-C4-C5 | -6.25 | 125.47 | 128.60 |
| 36 | A1 | 278 | U | C6-N1-C2 | -6.25 | 117.25 | 121.00 |
| 36 | A1 | 421 | G | C4-C5-N7 | 6.25 | 113.30 | 110.80 |
| 36 | A1 | 1204 | A | C5-C6-N1 | -6.25 | 114.57 | 117.70 |
| 36 | A5 | 2429 | G | C8-N9-C4 | -6.25 | 103.90 | 106.40 |
| 36 | A1 | 365 | A | C2-N3-C4 | -6.25 | 107.47 | 110.60 |
| 36 | A1 | 1052 | U | N3-C4-O4 | -6.25 | 115.02 | 119.40 |
| 80 | A6 | 396 | G | C4-C5-N7 | 6.25 | 113.30 | 110.80 |
| 80 | A6 | 400 | A | C5-C6-N6 | -6.25 | 118.70 | 123.70 |
| 36 | A5 | 2516 | U | C2-N3-C4 | -6.25 | 123.25 | 127.00 |
| 36 | A5 | 2886 | U | N3-C2-O2 | -6.25 | 117.82 | 122.20 |
| 80 | A6 | 767 | U | C5-C4-O4 | 6.25 | 129.65 | 125.90 |
| 36 | A5 | 2128 | C | N3-C2-O2 | -6.25 | 117.53 | 121.90 |
| 36 | A1 | 656 | A | C4-C5-C6 | 6.25 | 120.12 | 117.00 |
| 36 | A1 | 808 | A | C4-C5-N7 | -6.25 | 107.58 | 110.70 |
| 36 | A1 | 2877 | G | C4-C5-N7 | -6.25 | 108.30 | 110.80 |
| 36 | A5 | 1389 | G | C5-N7-C8 | -6.25 | 101.18 | 104.30 |
| 36 | A5 | 1688 | U | N1-C2-O2 | 6.25 | 127.17 | 122.80 |
| 37 | A7 | 44 | C | N3-C4-C5 | -6.25 | 119.40 | 121.90 |
| 1 | A2 | 1654 | G | C8-N9-C4 | -6.25 | 103.90 | 106.40 |
| 36 | A1 | 407 | A | C5-N7-C8 | -6.25 | 100.78 | 103.90 |
| 36 | A1 | 979 | U | C5-C4-O4 | 6.25 | 129.65 | 125.90 |
| 36 | A1 | 1173 | U | N3-C4-C5 | 6.25 | 118.35 | 114.60 |
| 36 | A1 | 1337 | A | C5-C6-N1 | 6.25 | 120.82 | 117.70 |
| 80 | A6 | 391 | A | C5-N7-C8 | 6.25 | 107.02 | 103.90 |
| 80 | A6 | 1471 | A | C8-N9-C4 | -6.25 | 103.30 | 105.80 |
| 49 | BL | 85 | LEU | CA-CB-CG | 6.25 | 129.66 | 115.30 |
| 36 | A5 | 644 | G | N1-C6-O6 | -6.25 | 116.15 | 119.90 |
| 36 | A5 | 3052 | G | N7-C8-N9 | -6.25 | 109.98 | 113.10 |
| 1 | A2 | 543 | C | N3-C2-O2 | -6.24 | 117.53 | 121.90 |
| 1 | A2 | 1633 | A | N9-C4-C5 | 6.24 | 108.30 | 105.80 |
| 7 | CF | 92 | ARG | NE-CZ-NH1 | 6.24 | 123.42 | 120.30 |
| 36 | A5 | 2777 | G | N9-C4-C5 | 6.24 | 107.90 | 105.40 |
| 36 | A1 | 417 | A | C8-N9-C4 | 6.24 | 108.30 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 1455 | U | C5-C6-N1 | -6.24 | 119.58 | 122.70 |
| 36 | A1 | 2305 | G | C8-N9-C1' | -6.24 | 118.89 | 127.00 |
| 36 | A5 | 1449 | A | N3-C4-C5 | 6.24 | 131.17 | 126.80 |
| 36 | A1 | 1163 | A | N7-C8-N9 | 6.24 | 116.92 | 113.80 |
| 36 | A1 | 1464 | G | N7-C8-N9 | -6.24 | 109.98 | 113.10 |
| 36 | A1 | 2867 | C | N3-C2-O2 | -6.24 | 117.53 | 121.90 |
| 80 | A6 | 372 | G | C6-C5-N7 | 6.24 | 134.14 | 130.40 |
| 36 | A5 | 2930 | A | C8-N9-C4 | -6.24 | 103.30 | 105.80 |
| 1 | A2 | 1670 | G | C8-N9-C1' | -6.24 | 118.89 | 127.00 |
| 36 | A1 | 1400 | G | N7-C8-N9 | -6.24 | 109.98 | 113.10 |
| 36 | A1 | 2517 | U | C5-C6-N1 | -6.24 | 119.58 | 122.70 |
| 80 | A6 | 1643 | U | C5-C4-O4 | 6.24 | 129.64 | 125.90 |
| 36 | A5 | 146 | U | N3-C4-O4 | -6.24 | 115.03 | 119.40 |
| 36 | A5 | 2754 | G | N1-C6-O6 | -6.24 | 116.16 | 119.90 |
| 1 | A2 | 1766 | A | C8-N9-C4 | 6.24 | 108.30 | 105.80 |
| 36 | A5 | 2728 | G | C8-N9-C4 | -6.24 | 103.91 | 106.40 |
| 1 | A2 | 933 | A | C8-N9-C4 | -6.24 | 103.31 | 105.80 |
| 36 | A1 | 784 | A | N1-C6-N6 | 6.24 | 122.34 | 118.60 |
| 36 | A1 | 797 | U | N3-C4-C5 | 6.24 | 118.34 | 114.60 |
| 38 | A4 | 88 | A | C5-C6-N6 | -6.24 | 118.71 | 123.70 |
| 36 | A5 | 891 | G | C8-N9-C4 | 6.24 | 108.89 | 106.40 |
| 36 | A5 | 1425 | U | N3-C4-O4 | -6.24 | 115.03 | 119.40 |
| 36 | A5 | 1500 | G | C8-N9-C4 | 6.24 | 108.89 | 106.40 |
| 36 | A1 | 331 | G | C6-C5-N7 | 6.23 | 134.14 | 130.40 |
| 36 | A1 | 416 | A | C5-C6-N6 | 6.23 | 128.69 | 123.70 |
| 1 | A2 | 494 | U | N1-C2-O2 | 6.23 | 127.16 | 122.80 |
| 12 | AK | 76 | LEU | CA-CB-CG | 6.23 | 129.63 | 115.30 |
| 36 | A1 | 328 | U | N3-C2-O2 | -6.23 | 117.84 | 122.20 |
| 36 | A1 | 786 | A | C5-N7-C8 | 6.23 | 107.02 | 103.90 |
| 36 | A5 | 670 | C | N3-C4-C5 | 6.23 | 124.39 | 121.90 |
| 36 | A5 | 1009 | A | C8-N9-C4 | -6.23 | 103.31 | 105.80 |
| 1 | A2 | 1595 | U | C5-C4-O4 | -6.23 | 122.16 | 125.90 |
| 36 | A1 | 576 | C | C5-C6-N1 | -6.23 | 117.88 | 121.00 |
| 38 | A4 | 30 | C | N3-C4-N4 | -6.23 | 113.64 | 118.00 |
| 44 | BF | 163 | LEU | CA-CB-CG | -6.23 | 100.97 | 115.30 |
| 36 | A5 | 1911 | A | N7-C8-N9 | -6.23 | 110.69 | 113.80 |
| 36 | A5 | 2133 | U | N3-C4-C5 | 6.23 | 118.34 | 114.60 |
| 36 | A5 | 3216 | G | C6-N1-C2 | -6.23 | 121.36 | 125.10 |
| 36 | A5 | 3298 | C | N1-C2-O2 | -6.23 | 115.16 | 118.90 |
| 36 | A5 | 1115 | G | N3-C4-C5 | -6.23 | 125.49 | 128.60 |
| 36 | A5 | 1753 | G | N3-C4-C5 | -6.23 | 125.49 | 128.60 |
| 1 | A2 | 1329 | A | C5-C6-N6 | -6.23 | 118.72 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 940 | G | C5-C6-O6 | 6.23 | 132.34 | 128.60 |
| 36 | A1 | 1392 | G | N1-C2-N3 | -6.23 | 120.16 | 123.90 |
| 80 | A6 | 1027 | A | C5-N7-C8 | -6.23 | 100.79 | 103.90 |
| 80 | A6 | 1410 | A | N1-C6-N6 | 6.23 | 122.34 | 118.60 |
| 36 | A5 | 437 | G | N3-C2-N2 | -6.23 | 115.54 | 119.90 |
| 36 | A5 | 2716 | U | C6-N1-C2 | -6.23 | 117.26 | 121.00 |
| 36 | A1 | 1515 | A | C5-C6-N1 | -6.23 | 114.59 | 117.70 |
| 36 | A5 | 974 | G | N3-C4-N9 | 6.23 | 129.74 | 126.00 |
| 36 | A1 | 677 | A | N9-C4-C5 | -6.22 | 103.31 | 105.80 |
| 36 | A1 | 2197 | C | C2-N3-C4 | 6.22 | 123.01 | 119.90 |
| 36 | A1 | 2985 | C | N3-C4-C5 | -6.22 | 119.41 | 121.90 |
| 54 | BQ | 99 | THR | N-CA-C | 6.22 | 127.81 | 111.00 |
| 80 | A6 | 66 | U | C5-C6-N1 | -6.22 | 119.59 | 122.70 |
| 36 | A5 | 691 | A | C2-N3-C4 | -6.22 | 107.49 | 110.60 |
| 36 | A5 | 2301 | U | N3-C4-C5 | 6.22 | 118.33 | 114.60 |
| 38 | A8 | 53 | A | C2-N3-C4 | 6.22 | 113.71 | 110.60 |
| 1 | A2 | 1297 | G | N7-C8-N9 | -6.22 | 109.99 | 113.10 |
| 1 | A2 | 1454 | G | C5-C6-O6 | 6.22 | 132.33 | 128.60 |
| 36 | A1 | 935 | U | C4-C5-C6 | 6.22 | 123.43 | 119.70 |
| 36 | A1 | 1051 | U | C5-C4-O4 | 6.22 | 129.63 | 125.90 |
| 36 | A1 | 2762 | A | N7-C8-N9 | -6.22 | 110.69 | 113.80 |
| 36 | A1 | 2960 | C | N3-C4-C5 | 6.22 | 124.39 | 121.90 |
| 36 | A1 | 3119 | U | N3-C2-O2 | -6.22 | 117.84 | 122.20 |
| 36 | A1 | 3190 | C | C2-N3-C4 | -6.22 | 116.79 | 119.90 |
| 80 | A6 | 1030 | A | C5-C6-N6 | 6.22 | 128.68 | 123.70 |
| 80 | A6 | 1257 | U | N3-C2-O2 | -6.22 | 117.84 | 122.20 |
| 36 | A5 | 514 | G | N1-C6-O6 | 6.22 | 123.63 | 119.90 |
| 36 | A5 | 3308 | C | C5-C6-N1 | -6.22 | 117.89 | 121.00 |
| 1 | A2 | 523 | G | N3-C4-C5 | -6.22 | 125.49 | 128.60 |
| 36 | A1 | 702 | C | N1-C2-O2 | -6.22 | 115.17 | 118.90 |
| 36 | A1 | 867 | G | N1-C2-N2 | 6.22 | 121.80 | 116.20 |
| 36 | A1 | 2828 | G | N3-C2-N2 | 6.22 | 124.25 | 119.90 |
| 36 | A5 | 32 | U | N1-C2-O2 | -6.22 | 118.44 | 122.80 |
| 36 | A5 | 150 | A | C5-C6-N6 | -6.22 | 118.72 | 123.70 |
| 36 | A1 | 439 | C | C2-N1-C1' | 6.22 | 125.64 | 118.80 |
| 36 | A1 | 2246 | G | C8-N9-C4 | -6.22 | 103.91 | 106.40 |
| 36 | A1 | 3344 | A | C4-N9-C1' | 6.22 | 137.50 | 126.30 |
| 80 | A6 | 1478 | G | C8-N9-C1' | -6.22 | 118.91 | 127.00 |
| 36 | A5 | 2242 | A | C5-C6-N6 | 6.22 | 128.68 | 123.70 |
| 1 | A2 | 1747 | G | C8-N9-C4 | 6.22 | 108.89 | 106.40 |
| 36 | A1 | 909 | G | C5-C6-N1 | 6.22 | 114.61 | 111.50 |
| 36 | A1 | 1374 | G | C4-C5-N7 | 6.22 | 113.29 | 110.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 36 | A5 | 1148 | G | C5-C6-O6 | -6.22 | 124.87 | 128.60 |
| 36 | A5 | 2572 | C | C6-N1-C2 | -6.22 | 117.81 | 120.30 |
| 36 | A1 | 496 | C | N1-C2-O2 | -6.22 | 115.17 | 118.90 |
| 36 | A1 | 3318 | G | N3-C4-N9 | 6.22 | 129.73 | 126.00 |
| 12 | CK | 83 | PRO | N-CA-CB | 6.22 | 110.76 | 103.30 |
| 36 | A1 | 576 | C | C5-C4-N4 | -6.21 | 115.85 | 120.20 |
| 36 | A1 | 998 | A | C2-N3-C4 | 6.21 | 113.71 | 110.60 |
| 36 | A1 | 1889 | G | C5-C6-N1 | -6.21 | 108.39 | 111.50 |
| 80 | A6 | 396 | G | N3-C2-N2 | 6.21 | 124.25 | 119.90 |
| 36 | A5 | 1300 | G | C4-C5-N7 | 6.21 | 113.29 | 110.80 |
| 36 | A5 | 2198 | A | C2-N3-C4 | -6.21 | 107.49 | 110.60 |
| 36 | A5 | 3000 | A | C8-N9-C4 | 6.21 | 108.29 | 105.80 |
| 36 | A5 | 1468 | A | C8-N9-C4 | -6.21 | 103.31 | 105.80 |
| 36 | A1 | 701 | G | N1-C6-O6 | -6.21 | 116.17 | 119.90 |
| 36 | A5 | 624 | G | C8-N9-C4 | 6.21 | 108.88 | 106.40 |
| 36 | A5 | 656 | A | C8-N9-C4 | 6.21 | 108.28 | 105.80 |
| 1 | A2 | 1218 | G | N1-C6-O6 | 6.21 | 123.63 | 119.90 |
| 36 | A1 | 2246 | G | N3-C2-N2 | -6.21 | 115.55 | 119.90 |
| 80 | A6 | 1396 | U | C6-N1-C2 | -6.21 | 117.27 | 121.00 |
| 36 | A1 | 2276 | G | C8-N9-C4 | -6.21 | 103.92 | 106.40 |
| 36 | A1 | 2361 | A | N9-C4-C5 | 6.21 | 108.28 | 105.80 |
| 38 | A4 | 74 | U | C5-C6-N1 | -6.21 | 119.60 | 122.70 |
| 56 | BS | 58 | ILE | CG1-CB-CG2 | -6.21 | 97.74 | 111.40 |
| 36 | A5 | 359 | U | C5-C4-O4 | -6.21 | 122.17 | 125.90 |
| 36 | A5 | 1161 | G | C2-N3-C4 | 6.21 | 115.00 | 111.90 |
| 36 | A5 | 1888 | U | C2-N3-C4 | -6.21 | 123.28 | 127.00 |
| 36 | A5 | 2117 | A | C6-N1-C2 | -6.21 | 114.87 | 118.60 |
| 36 | A5 | 2645 | G | C6-N1-C2 | -6.21 | 121.38 | 125.10 |
| 1 | A2 | 736 | C | N1-C2-O2 | 6.21 | 122.62 | 118.90 |
| 80 | A6 | 290 | G | C8-N9-C4 | -6.21 | 103.92 | 106.40 |
| 37 | A7 | 25 | G | N3-C2-N2 | -6.21 | 115.56 | 119.90 |
| 36 | A5 | 994 | G | N3-C2-N2 | 6.21 | 124.24 | 119.90 |
| 36 | A5 | 2133 | U | N3-C4-O4 | -6.21 | 115.06 | 119.40 |
| 36 | A1 | 2679 | A | C5-C6-N1 | -6.20 | 114.60 | 117.70 |
| 37 | A3 | 103 | A | N7-C8-N9 | -6.20 | 110.70 | 113.80 |
| 80 | A6 | 447 | U | N1-C2-N3 | 6.20 | 118.62 | 114.90 |
| 36 | A5 | 726 | G | C5-N7-C8 | -6.20 | 101.20 | 104.30 |
| 36 | A1 | 1307 | G | C2-N3-C4 | 6.20 | 115.00 | 111.90 |
| 36 | A1 | 2957 | G | N3-C2-N2 | -6.20 | 115.56 | 119.90 |
| 80 | A6 | 364 | G | C6-N1-C2 | -6.20 | 121.38 | 125.10 |
| 80 | A6 | 987 | G | N3-C2-N2 | -6.20 | 115.56 | 119.90 |
| 36 | A5 | 3014 | U | C5-C4-O4 | -6.20 | 122.18 | 125.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 3175 | U | C6-N1-C2 | -6.20 | 117.28 | 121.00 |
| 53 | DP | 127 | ARG | NE-CZ-NH1 | 6.20 | 123.40 | 120.30 |
| 36 | A1 | 751 | A | N1-C2-N3 | -6.20 | 126.20 | 129.30 |
| 36 | A1 | 1369 | A | N9-C4-C5 | -6.20 | 103.32 | 105.80 |
| 41 | BC | 138 | ARG | NE-CZ-NH2 | -6.20 | 117.20 | 120.30 |
| 80 | A6 | 1200 | G | C4-N9-C1' | -6.20 | 118.44 | 126.50 |
| 80 | A6 | 1600 | A | C4-C5-N7 | 6.20 | 113.80 | 110.70 |
| 36 | A5 | 425 | G | N7-C8-N9 | -6.20 | 110.00 | 113.10 |
| 36 | A5 | 1307 | G | C8-N9-C4 | -6.20 | 103.92 | 106.40 |
| 36 | A5 | 1810 | A | C8-N9-C4 | 6.20 | 108.28 | 105.80 |
| 36 | A5 | 2930 | A | N9-C4-C5 | 6.20 | 108.28 | 105.80 |
| 36 | A1 | 352 | A | C2-N3-C4 | -6.20 | 107.50 | 110.60 |
| 36 | A1 | 3218 | A | N9-C4-C5 | 6.20 | 108.28 | 105.80 |
| 80 | A6 | 1354 | G | C8-N9-C4 | -6.20 | 103.92 | 106.40 |
| 80 | A6 | 1666 | U | C5-C4-O4 | 6.20 | 129.62 | 125.90 |
| 36 | A5 | 326 | U | N3-C4-C5 | 6.20 | 118.32 | 114.60 |
| 36 | A5 | 911 | C | N1-C2-O2 | -6.20 | 115.18 | 118.90 |
| 36 | A5 | 3334 | U | N3-C2-O2 | -6.20 | 117.86 | 122.20 |
| 36 | A1 | 2856 | G | N7-C8-N9 | -6.20 | 110.00 | 113.10 |
| 36 | A5 | 2169 | G | N1-C6-O6 | -6.20 | 116.18 | 119.90 |
| 36 | A5 | 2524 | A | C6-N1-C2 | 6.20 | 122.32 | 118.60 |
| 36 | A5 | 2552 | C | N3-C2-O2 | -6.20 | 117.56 | 121.90 |
| 1 | A2 | 186 | C | C5-C6-N1 | 6.20 | 124.10 | 121.00 |
| 1 | A2 | 189 | C | C6-N1-C1' | -6.20 | 113.36 | 120.80 |
| 1 | A2 | 1436 | A | N9-C4-C5 | -6.20 | 103.32 | 105.80 |
| 1 | A2 | 1560 | U | N1-C2-N3 | 6.20 | 118.62 | 114.90 |
| 36 | A1 | 104 | G | C5-C6-N1 | 6.20 | 114.60 | 111.50 |
| 36 | A1 | 1326 | A | C8-N9-C4 | 6.20 | 108.28 | 105.80 |
| 36 | A1 | 2733 | A | C8-N9-C4 | 6.20 | 108.28 | 105.80 |
| 80 | A6 | 152 | U | C5-C4-O4 | 6.20 | 129.62 | 125.90 |
| 36 | A5 | 511 | G | N3-C2-N2 | 6.20 | 124.24 | 119.90 |
| 36 | A5 | 1389 | G | N3-C4-N9 | 6.20 | 129.72 | 126.00 |
| 36 | A1 | 420 | G | C8-N9-C4 | 6.19 | 108.88 | 106.40 |
| 36 | A1 | 2826 | U | C4-C5-C6 | 6.19 | 123.42 | 119.70 |
| 36 | A5 | 35 | A | C2-N3-C4 | -6.19 | 107.50 | 110.60 |
| 36 | A5 | 494 | G | N3-C4-C5 | -6.19 | 125.50 | 128.60 |
| 36 | A5 | 819 | U | C6-N1-C2 | 6.19 | 124.72 | 121.00 |
| 36 | A5 | 2615 | G | C5-C6-O6 | -6.19 | 124.88 | 128.60 |
| 36 | A1 | 44 | U | C6-N1-C2 | 6.19 | 124.72 | 121.00 |
| 36 | A1 | 576 | C | C6-N1-C2 | 6.19 | 122.78 | 120.30 |
| 36 | A1 | 713 | U | N3-C2-O2 | -6.19 | 117.87 | 122.20 |
| 36 | A1 | 2204 | C | N1-C2-N3 | 6.19 | 123.53 | 119.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 80 | A6 | 1749 | A | C2-N3-C4 | -6.19 | 107.50 | 110.60 |
| 36 | A5 | 294 | U | C5-C4-O4 | -6.19 | 122.19 | 125.90 |
| 36 | A5 | 823 | C | N3-C4-C5 | 6.19 | 124.38 | 121.90 |
| 36 | A5 | 2865 | U | N1-C2-N3 | -6.19 | 111.18 | 114.90 |
| 68 | De | 4 | LEU | C-N-CD | 6.19 | 141.40 | 128.40 |
| 36 | A1 | 1114 | U | N1-C2-O2 | 6.19 | 127.13 | 122.80 |
| 80 | A6 | 1127 | G | C8-N9-C4 | -6.19 | 103.92 | 106.40 |
| 36 | A5 | 1346 | G | N3-C4-C5 | 6.19 | 131.70 | 128.60 |
| 36 | A5 | 1883 | A | N9-C4-C5 | 6.19 | 108.28 | 105.80 |
| 36 | A5 | 3365 | U | N1-C2-N3 | 6.19 | 118.61 | 114.90 |
| 36 | A1 | 2314 | U | N3-C2-O2 | 6.19 | 126.53 | 122.20 |
| 36 | A5 | 83 | U | C5-C4-O4 | -6.19 | 122.19 | 125.90 |
| 36 | A5 | 1035 | G | N3-C4-N9 | 6.19 | 129.71 | 126.00 |
| 36 | A5 | 2846 | U | N1-C2-O2 | -6.19 | 118.47 | 122.80 |
| 36 | A1 | 1387 | G | N7-C8-N9 | -6.19 | 110.01 | 113.10 |
| 36 | A1 | 2182 | A | N1-C6-N6 | -6.19 | 114.89 | 118.60 |
| 36 | A1 | 2618 | G | C6-N1-C2 | -6.19 | 121.39 | 125.10 |
| 36 | A1 | 3301 | U | N3-C2-O2 | -6.19 | 117.87 | 122.20 |
| 80 | A6 | 359 | A | C4-N9-C1' | -6.19 | 115.16 | 126.30 |
| 36 | A5 | 818 | C | N3-C4-C5 | -6.19 | 119.42 | 121.90 |
| 36 | A5 | 2808 | A | N1-C6-N6 | 6.19 | 122.31 | 118.60 |
| 1 | A2 | 874 | C | C5-C6-N1 | 6.19 | 124.09 | 121.00 |
| 24 | AW | 65 | LEU | CA-CB-CG | 6.19 | 129.53 | 115.30 |
| 36 | A1 | 592 | A | C5-C6-N6 | -6.19 | 118.75 | 123.70 |
| 36 | A5 | 436 | A | C8-N9-C1' | -6.19 | 116.56 | 127.70 |
| 36 | A5 | 1430 | U | C6-N1-C2 | 6.19 | 124.71 | 121.00 |
| 36 | A1 | 1415 | U | C5-C4-O4 | 6.18 | 129.61 | 125.90 |
| 41 | BC | 309 | ARG | NE-CZ-NH1 | 6.18 | 123.39 | 120.30 |
| 36 | A5 | 904 | A | N9-C4-C5 | 6.18 | 108.27 | 105.80 |
| 36 | A5 | 1143 | A | C6-N1-C2 | 6.18 | 122.31 | 118.60 |
| 36 | A5 | 1161 | G | C8-N9-C4 | 6.18 | 108.87 | 106.40 |
| 1 | A2 | 767 | U | N3-C4-O4 | -6.18 | 115.07 | 119.40 |
| 1 | A2 | 1628 | U | N3-C2-O2 | -6.18 | 117.87 | 122.20 |
| 36 | A1 | 2422 | C | N1-C2-O2 | 6.18 | 122.61 | 118.90 |
| 36 | A1 | 2786 | G | N3-C4-C5 | -6.18 | 125.51 | 128.60 |
| 36 | A5 | 1119 | C | C5-C4-N4 | -6.18 | 115.87 | 120.20 |
| 52 | DO | 3[B] | SER | C-N-CA | -6.18 | 106.24 | 121.70 |
| 1 | A2 | 1305 | U | N1-C2-N3 | 6.18 | 118.61 | 114.90 |
| 36 | A5 | 3065 | G | C5-C6-O6 | 6.18 | 132.31 | 128.60 |
| 1 | A2 | 1670 | G | C4-N9-C1' | 6.18 | 134.53 | 126.50 |
| 36 | A1 | 857 | G | N1-C6-O6 | -6.18 | 116.19 | 119.90 |
| 36 | A1 | 1382 | G | N9-C4-C5 | -6.18 | 102.93 | 105.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 2197 | C | N1-C2-O2 | 6.18 | 122.61 | 118.90 |
| 36 | A1 | 2533 | G | C4-N9-C1' | 6.18 | 134.53 | 126.50 |
| 36 | A1 | 2611 | U | N3-C4-C5 | 6.18 | 118.31 | 114.60 |
| 36 | A1 | 2952 | G | C8-N9-C4 | 6.18 | 108.87 | 106.40 |
| 68 | Be | 27 | ARG | NE-CZ-NH2 | -6.18 | 117.21 | 120.30 |
| 36 | A5 | 2399 | A | C8-N9-C4 | 6.18 | 108.27 | 105.80 |
| 36 | A1 | 922 | U | C6-N1-C2 | -6.18 | 117.29 | 121.00 |
| 36 | A1 | 776 | U | C2-N3-C4 | -6.18 | 123.30 | 127.00 |
| 36 | A1 | 2798 | C | C5-C4-N4 | 6.18 | 124.52 | 120.20 |
| 38 | A4 | 50 | C | C6-N1-C2 | -6.18 | 117.83 | 120.30 |
| 80 | A6 | 1329 | A | C5-C6-N6 | -6.18 | 118.76 | 123.70 |
| 36 | A5 | 1301 | A | C5-C6-N6 | -6.18 | 118.76 | 123.70 |
| 36 | A1 | 1001 | G | C8-N9-C4 | -6.17 | 103.93 | 106.40 |
| 36 | A1 | 2357 | A | C5-C6-N6 | -6.17 | 118.76 | 123.70 |
| 36 | A1 | 2663 | G | N3-C4-C5 | -6.17 | 125.51 | 128.60 |
| 36 | A5 | 32 | U | C6-N1-C2 | -6.17 | 117.30 | 121.00 |
| 36 | A5 | 722 | G | N9-C4-C5 | 6.17 | 107.87 | 105.40 |
| 36 | A5 | 734 | C | N1-C2-O2 | 6.17 | 122.61 | 118.90 |
| 36 | A5 | 1134 | G | C6-N1-C2 | -6.17 | 121.39 | 125.10 |
| 36 | A1 | 1187 | C | N1-C2-N3 | 6.17 | 123.52 | 119.20 |
| 36 | A1 | 1294 | A | N9-C4-C5 | 6.17 | 108.27 | 105.80 |
| 36 | A5 | 87 | U | N3-C4-O4 | -6.17 | 115.08 | 119.40 |
| 36 | A5 | 1525 | G | C4-N9-C1' | 6.17 | 134.52 | 126.50 |
| 1 | A2 | 734 | A | N1-C6-N6 | 6.17 | 122.30 | 118.60 |
| 36 | A1 | 546 | C | C5-C6-N1 | 6.17 | 124.09 | 121.00 |
| 38 | A4 | 39 | G | N1-C6-O6 | -6.17 | 116.20 | 119.90 |
| 80 | A6 | 603 | U | C2-N3-C4 | -6.17 | 123.30 | 127.00 |
| 36 | A5 | 408 | A | N1-C2-N3 | 6.17 | 132.39 | 129.30 |
| 36 | A5 | 3330 | A | C6-N1-C2 | -6.17 | 114.90 | 118.60 |
| 80 | A6 | 44 | U | N3-C4-O4 | -6.17 | 115.08 | 119.40 |
| 36 | A1 | 1118 | C | C5-C6-N1 | -6.17 | 117.92 | 121.00 |
| 36 | A1 | 2380 | U | N3-C4-C5 | 6.17 | 118.30 | 114.60 |
| 36 | A1 | 2635 | A | C5-N7-C8 | -6.17 | 100.81 | 103.90 |
| 36 | A1 | 3317 | U | C5-C4-O4 | 6.17 | 129.60 | 125.90 |
| 80 | A6 | 956 | C | C5-C6-N1 | -6.17 | 117.92 | 121.00 |
| 80 | A6 | 1480 | G | C8-N9-C4 | -6.17 | 103.93 | 106.40 |
| 80 | A6 | 1595 | U | N1-C2-O2 | 6.17 | 127.12 | 122.80 |
| 36 | A1 | 278 | U | N1-C2-N3 | 6.17 | 118.60 | 114.90 |
| 36 | A5 | 2228 | A | C8-N9-C4 | -6.17 | 103.33 | 105.80 |
| 36 | A5 | 3266 | G | C8-N9-C4 | -6.17 | 103.93 | 106.40 |
| 36 | A1 | 889 | U | N3-C4-O4 | -6.17 | 115.08 | 119.40 |
| 36 | A5 | 1931 | U | C5-C6-N1 | -6.17 | 119.62 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 1227 | C | C5-C6-N1 | 6.16 | 124.08 | 121.00 |
| 80 | A6 | 778 | G | N3-C4-N9 | 6.16 | 129.70 | 126.00 |
| 80 | A6 | 956 | C | C6-N1-C2 | 6.16 | 122.77 | 120.30 |
| 36 | A5 | 386 | A | C4-C5-N7 | 6.16 | 113.78 | 110.70 |
| 36 | A5 | 753 | C | C5-C4-N4 | -6.16 | 115.89 | 120.20 |
| 37 | A7 | 46 | A | C8-N9-C4 | -6.16 | 103.33 | 105.80 |
| 36 | A1 | 1142 | G | C6-N1-C2 | -6.16 | 121.40 | 125.10 |
| 38 | A4 | 85 | G | C6-C5-N7 | -6.16 | 126.70 | 130.40 |
| 80 | A6 | 1433 | G | C8-N9-C4 | -6.16 | 103.94 | 106.40 |
| 36 | A5 | 590 | G | C5-C6-N1 | 6.16 | 114.58 | 111.50 |
| 36 | A5 | 600 | G | C6-C5-N7 | -6.16 | 126.70 | 130.40 |
| 36 | A5 | 949 | C | C5-C6-N1 | -6.16 | 117.92 | 121.00 |
| 36 | A5 | 1064 | A | C8-N9-C4 | 6.16 | 108.26 | 105.80 |
| 1 | A2 | 1258 | U | C4-C5-C6 | 6.16 | 123.39 | 119.70 |
| 36 | A1 | 2302 | G | N3-C2-N2 | 6.16 | 124.21 | 119.90 |
| 80 | A6 | 306 | U | C6-N1-C2 | 6.16 | 124.69 | 121.00 |
| 36 | A5 | 42 | C | C2-N3-C4 | 6.16 | 122.98 | 119.90 |
| 36 | A5 | 999 | G | C2-N3-C4 | 6.16 | 114.98 | 111.90 |
| 36 | A5 | 1007 | U | C2-N3-C4 | -6.16 | 123.30 | 127.00 |
| 36 | A5 | 2381 | G | N1-C6-O6 | -6.16 | 116.20 | 119.90 |
| 36 | A5 | 2858 | U | N1-C2-N3 | 6.16 | 118.59 | 114.90 |
| 1 | A2 | 36 | C | N3-C4-N4 | 6.16 | 122.31 | 118.00 |
| 1 | A2 | 704 | C | C6-N1-C1' | -6.16 | 113.41 | 120.80 |
| 36 | A5 | 2396 | G | C8-N9-C4 | -6.16 | 103.94 | 106.40 |
| 36 | A1 | 61 | A | N9-C4-C5 | -6.16 | 103.34 | 105.80 |
| 36 | A1 | 203 | G | N1-C6-O6 | -6.16 | 116.21 | 119.90 |
| 36 | A1 | 641 | C | N1-C2-O2 | -6.16 | 115.21 | 118.90 |
| 36 | A1 | 1392 | G | C5-C6-N1 | 6.16 | 114.58 | 111.50 |
| 36 | A1 | 2816 | G | N3-C2-N2 | 6.16 | 124.21 | 119.90 |
| 78 | Bo | 74 | CYS | CA-CB-SG | 6.16 | 125.08 | 114.00 |
| 80 | A6 | 1614 | A | C6-C5-N7 | -6.16 | 127.99 | 132.30 |
| 36 | A5 | 351 | A | C5-C6-N6 | -6.16 | 118.78 | 123.70 |
| 36 | A5 | 1381 | A | C2-N3-C4 | -6.16 | 107.52 | 110.60 |
| 36 | A5 | 1591 | G | C5-C6-N1 | 6.16 | 114.58 | 111.50 |
| 36 | A5 | 3272 | C | C6-N1-C2 | 6.16 | 122.76 | 120.30 |
| 36 | A5 | 3358 | U | N3-C2-O2 | -6.16 | 117.89 | 122.20 |
| 36 | A1 | 1336 | U | C5-C4-O4 | 6.15 | 129.59 | 125.90 |
| 36 | A1 | 1916 | U | C6-N1-C2 | 6.15 | 124.69 | 121.00 |
| 36 | A1 | 2973 | G | C5-C6-O6 | -6.15 | 124.91 | 128.60 |
| 1 | A2 | 1490 | C | C2-N1-C1' | 6.15 | 125.57 | 118.80 |
| 36 | A1 | 284 | A | C8-N9-C4 | -6.15 | 103.34 | 105.80 |
| 36 | A1 | 1114 | U | N1-C2-N3 | -6.15 | 111.21 | 114.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 2307 | G | N1-C6-O6 | -6.15 | 116.21 | 119.90 |
| 36 | A5 | 1148 | G | C5-C6-N1 | 6.15 | 114.58 | 111.50 |
| 36 | A5 | 2757 | U | N1-C2-O2 | -6.15 | 118.49 | 122.80 |
| 36 | A5 | 3228 | C | N3-C2-O2 | -6.15 | 117.59 | 121.90 |
| 36 | A5 | 3345 | G | N3-C2-N2 | -6.15 | 115.59 | 119.90 |
| 36 | A1 | 1778 | G | C4-N9-C1' | 6.15 | 134.49 | 126.50 |
| 36 | A1 | 2867 | C | C6-N1-C2 | -6.15 | 117.84 | 120.30 |
| 80 | A6 | 1481 | C | N3-C4-C5 | -6.15 | 119.44 | 121.90 |
| 80 | A6 | 1723 | U | N1-C2-N3 | 6.15 | 118.59 | 114.90 |
| 36 | A5 | 822 | G | N3-C4-N9 | -6.15 | 122.31 | 126.00 |
| 36 | A5 | 917 | A | C8-N9-C4 | -6.15 | 103.34 | 105.80 |
| 36 | A5 | 2824 | G | N3-C4-C5 | -6.15 | 125.53 | 128.60 |
| 36 | A1 | 1546 | A | C4-C5-N7 | -6.15 | 107.63 | 110.70 |
| 36 | A1 | 2704 | A | C5-C6-N6 | 6.15 | 128.62 | 123.70 |
| 36 | A5 | 924 | G | N3-C2-N2 | -6.15 | 115.60 | 119.90 |
| 36 | A1 | 272 | G | C8-N9-C4 | 6.14 | 108.86 | 106.40 |
| 80 | A6 | 947 | U | N1-C2-O2 | -6.14 | 118.50 | 122.80 |
| 80 | A6 | 1631 | A | C8-N9-C4 | 6.14 | 108.26 | 105.80 |
| 36 | A5 | 2207 | A | C5-N7-C8 | -6.14 | 100.83 | 103.90 |
| 36 | A1 | 672 | A | C4-C5-N7 | 6.14 | 113.77 | 110.70 |
| 36 | A1 | 1624 | G | C8-N9-C4 | -6.14 | 103.94 | 106.40 |
| 36 | A1 | 2794 | G | C8-N9-C4 | -6.14 | 103.94 | 106.40 |
| 36 | A5 | 102 | C | N3-C4-N4 | 6.14 | 122.30 | 118.00 |
| 36 | A5 | 2347 | U | N3-C4-C5 | 6.14 | 118.29 | 114.60 |
| 1 | A2 | 1781 | A | C5-C6-N6 | 6.14 | 128.61 | 123.70 |
| 36 | A5 | 1772 | U | N3-C2-O2 | -6.14 | 117.90 | 122.20 |
| 36 | A1 | 1155 | C | C5-C6-N1 | 6.14 | 124.07 | 121.00 |
| 36 | A1 | 3089 | C | N3-C4-C5 | 6.14 | 124.36 | 121.90 |
| 38 | A4 | 2 | A | C8-N9-C4 | -6.14 | 103.34 | 105.80 |
| 80 | A6 | 1122 | G | N3-C4-C5 | 6.14 | 131.67 | 128.60 |
| 80 | A6 | 1730 | A | N1-C6-N6 | 6.14 | 122.28 | 118.60 |
| 36 | A5 | 1303 | A | C2-N3-C4 | 6.14 | 113.67 | 110.60 |
| 36 | A5 | 2728 | G | C6-N1-C2 | -6.14 | 121.42 | 125.10 |
| 36 | A5 | 2928 | C | C6-N1-C2 | -6.14 | 117.84 | 120.30 |
| 36 | A1 | 606 | C | C6-N1-C2 | -6.14 | 117.84 | 120.30 |
| 36 | A5 | 370 | U | N1-C2-N3 | 6.14 | 118.58 | 114.90 |
| 36 | A5 | 1162 | U | C2-N3-C4 | -6.14 | 123.32 | 127.00 |
| 36 | A1 | 30 | G | N3-C2-N2 | 6.14 | 124.19 | 119.90 |
| 80 | A6 | 194 | U | N1-C2-O2 | 6.14 | 127.10 | 122.80 |
| 80 | A6 | 558 | U | C5-C6-N1 | 6.14 | 125.77 | 122.70 |
| 80 | A6 | 1241 | G | C2-N3-C4 | -6.14 | 108.83 | 111.90 |
| 36 | A5 | 2775 | U | C5-C4-O4 | 6.14 | 129.58 | 125.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 36 | A5 | 2978 | U | C2-N3-C4 | -6.14 | 123.32 | 127.00 |
| 21 | CT | 89 | ARG | NE-CZ-NH1 | 6.13 | 123.37 | 120.30 |
| 36 | A5 | 1872 | C | C4-C5-C6 | 6.13 | 120.47 | 117.40 |
| 1 | A2 | 335 | U | N1-C2-O2 | -6.13 | 118.51 | 122.80 |
| 36 | A1 | 574 | U | C2-N3-C4 | -6.13 | 123.32 | 127.00 |
| 80 | A6 | 1347 | U | C5-C6-N1 | -6.13 | 119.63 | 122.70 |
| 36 | A5 | 1165 | A | C8-N9-C4 | 6.13 | 108.25 | 105.80 |
| 36 | A5 | 3098 | G | N1-C6-O6 | -6.13 | 116.22 | 119.90 |
| 52 | DO | 117[A] | ARG | NE-CZ-NH2 | -6.13 | 117.23 | 120.30 |
| 52 | DO | 117[B] | ARG | NE-CZ-NH2 | -6.13 | 117.23 | 120.30 |
| 1 | A2 | 627 | C | C5-C4-N4 | -6.13 | 115.91 | 120.20 |
| 36 | A1 | 340 | C | N1-C2-N3 | 6.13 | 123.49 | 119.20 |
| 36 | A1 | 1163 | A | C5-N7-C8 | -6.13 | 100.83 | 103.90 |
| 36 | A1 | 1343 | A | C2-N3-C4 | -6.13 | 107.53 | 110.60 |
| 68 | Be | 105 | ARG | NE-CZ-NH2 | -6.13 | 117.23 | 120.30 |
| 80 | A6 | 1515 | A | C8-N9-C4 | -6.13 | 103.35 | 105.80 |
| 36 | A5 | 3068 | U | N1-C2-N3 | 6.13 | 118.58 | 114.90 |
| 36 | A5 | 3266 | G | C4-C5-N7 | -6.13 | 108.35 | 110.80 |
| 38 | A8 | 79 | A | N9-C4-C5 | -6.13 | 103.35 | 105.80 |
| 1 | A2 | 781 | U | C2-N1-C1' | 6.13 | 125.06 | 117.70 |
| 36 | A5 | 933 | A | C2-N3-C4 | -6.13 | 107.53 | 110.60 |
| 36 | A5 | 2371 | G | C8-N9-C4 | 6.13 | 108.85 | 106.40 |
| 1 | A2 | 852 | C | C5-C6-N1 | 6.13 | 124.06 | 121.00 |
| 1 | A2 | 865 | A | N1-C6-N6 | -6.13 | 114.92 | 118.60 |
| 1 | A2 | 1746 | A | C8-N9-C4 | 6.13 | 108.25 | 105.80 |
| 36 | A1 | 862 | U | C5-C6-N1 | 6.13 | 125.76 | 122.70 |
| 36 | A1 | 1149 | G | N1-C6-O6 | 6.13 | 123.58 | 119.90 |
| 36 | A1 | 2306 | C | C2-N1-C1' | 6.13 | 125.54 | 118.80 |
| 36 | A5 | 909 | G | C5-N7-C8 | 6.13 | 107.36 | 104.30 |
| 36 | A5 | 2939 | G | N7-C8-N9 | -6.13 | 110.04 | 113.10 |
| 36 | A1 | 1025 | A | C8-N9-C4 | -6.13 | 103.35 | 105.80 |
| 36 | A1 | 1139 | G | N1-C6-O6 | -6.13 | 116.22 | 119.90 |
| 36 | A1 | 2376 | G | N3-C2-N2 | -6.13 | 115.61 | 119.90 |
| 36 | A1 | 2629 | U | C5-C4-O4 | 6.13 | 129.58 | 125.90 |
| 36 | A1 | 3318 | G | C8-N9-C1' | -6.13 | 119.03 | 127.00 |
| 80 | A6 | 1459 | C | N1-C2-O2 | -6.13 | 115.22 | 118.90 |
| 36 | A5 | 2632 | G | N9-C4-C5 | 6.13 | 107.85 | 105.40 |
| 36 | A5 | 3101 | G | N1-C6-O6 | -6.13 | 116.22 | 119.90 |
| 1 | A2 | 932 | U | C5-C4-O4 | 6.12 | 129.57 | 125.90 |
| 36 | A1 | 658 | G | C8-N9-C1' | -6.12 | 119.04 | 127.00 |
| 36 | A5 | 2176 | U | N1-C2-N3 | 6.12 | 118.58 | 114.90 |
| 36 | A1 | 650 | C | C4-C5-C6 | 6.12 | 120.46 | 117.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 1377 | G | C4-C5-C6 | -6.12 | 115.13 | 118.80 |
| 36 | A1 | 2663 | G | C2-N3-C4 | 6.12 | 114.96 | 111.90 |
| 36 | A1 | 3049 | A | N1-C6-N6 | 6.12 | 122.27 | 118.60 |
| 36 | A1 | 3242 | G | C8-N9-C4 | -6.12 | 103.95 | 106.40 |
| 36 | A5 | 33 | G | C6-N1-C2 | -6.12 | 121.43 | 125.10 |
| 36 | A5 | 1114 | U | N3-C4-C5 | 6.12 | 118.27 | 114.60 |
| 36 | A5 | 3150 | A | C2-N3-C4 | -6.12 | 107.54 | 110.60 |
| 1 | A2 | 1099 | U | C5-C6-N1 | 6.12 | 125.76 | 122.70 |
| 36 | A1 | 966 | U | N3-C4-O4 | -6.12 | 115.11 | 119.40 |
| 36 | A1 | 1120 | A | C6-N1-C2 | -6.12 | 114.93 | 118.60 |
| 36 | A1 | 1386 | A | N1-C2-N3 | 6.12 | 132.36 | 129.30 |
| 45 | BG | 158 | ASP | N-CA-C | 6.12 | 127.53 | 111.00 |
| 36 | A5 | 1719 | G | N1-C6-O6 | 6.12 | 123.57 | 119.90 |
| 36 | A1 | 638 | C | N3-C4-C5 | 6.12 | 124.35 | 121.90 |
| 80 | A6 | 1509 | C | N3-C2-O2 | -6.12 | 117.62 | 121.90 |
| 36 | A5 | 2830 | G | C6-N1-C2 | -6.12 | 121.43 | 125.10 |
| 36 | A5 | 3138 | U | C5-C4-O4 | -6.12 | 122.23 | 125.90 |
| 80 | A6 | 15 | U | C5-C4-O4 | -6.12 | 122.23 | 125.90 |
| 36 | A5 | 2359 | C | C5-C6-N1 | -6.12 | 117.94 | 121.00 |
| 36 | A1 | 862 | U | C5-C4-O4 | -6.12 | 122.23 | 125.90 |
| 36 | A5 | 386 | A | N9-C4-C5 | -6.12 | 103.35 | 105.80 |
| 38 | A4 | 113 | U | C2-N3-C4 | -6.12 | 123.33 | 127.00 |
| 80 | A6 | 997 | G | N1-C6-O6 | -6.12 | 116.23 | 119.90 |
| 36 | A5 | 1044 | U | N3-C4-C5 | 6.12 | 118.27 | 114.60 |
| 36 | A1 | 2394 | G | C5-C6-O6 | -6.11 | 124.93 | 128.60 |
| 36 | A5 | 1323 | G | C8-N9-C4 | -6.11 | 103.95 | 106.40 |
| 36 | A1 | 797 | U | C2-N3-C4 | -6.11 | 123.33 | 127.00 |
| 36 | A1 | 1000 | C | C2-N1-C1' | 6.11 | 125.52 | 118.80 |
| 80 | A6 | 341 | A | C8-N9-C4 | -6.11 | 103.36 | 105.80 |
| 36 | A5 | 367 | A | N3-C4-N9 | -6.11 | 122.51 | 127.40 |
| 36 | A5 | 2395 | G | C4-C5-N7 | -6.11 | 108.36 | 110.80 |
| 36 | A1 | 1183 | C | N1-C2-O2 | -6.11 | 115.23 | 118.90 |
| 37 | A3 | 3 | U | C5-C6-N1 | -6.11 | 119.64 | 122.70 |
| 38 | A4 | 21 | C | C5-C6-N1 | -6.11 | 117.94 | 121.00 |
| 80 | A6 | 1299 | G | N3-C4-N9 | 6.11 | 129.67 | 126.00 |
| 36 | A5 | 880 | G | C5-C6-N1 | 6.11 | 114.56 | 111.50 |
| 36 | A5 | 2353 | G | N3-C4-N9 | 6.11 | 129.67 | 126.00 |
| 1 | A2 | 1346 | A | N7-C8-N9 | 6.11 | 116.86 | 113.80 |
| 36 | A5 | 2650 | U | N3-C4-O4 | -6.11 | 115.12 | 119.40 |
| 1 | A2 | 1514 | U | N3-C2-O2 | -6.11 | 117.92 | 122.20 |
| 36 | A1 | 919 | U | C2-N3-C4 | -6.11 | 123.33 | 127.00 |
| 36 | A1 | 2957 | G | N7-C8-N9 | -6.11 | 110.05 | 113.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 3110 | C | C2-N3-C4 | -6.11 | 116.85 | 119.90 |
| 36 | A1 | 1467 | A | C8-N9-C4 | -6.11 | 103.36 | 105.80 |
| 36 | A1 | 2705 | A | C2-N3-C4 | 6.11 | 113.65 | 110.60 |
| 36 | A1 | 2726 | C | C4-C5-C6 | 6.11 | 120.45 | 117.40 |
| 36 | A1 | 3312 | U | C5-C6-N1 | -6.11 | 119.65 | 122.70 |
| 38 | A4 | 25 | G | N9-C4-C5 | 6.11 | 107.84 | 105.40 |
| 36 | A5 | 785 | G | C2-N3-C4 | 6.11 | 114.95 | 111.90 |
| 36 | A5 | 2930 | A | C8-N9-C1' | 6.11 | 138.69 | 127.70 |
| 36 | A5 | 3086 | A | C8-N9-C4 | 6.11 | 108.24 | 105.80 |
| 36 | A1 | 1836 | C | C6-N1-C2 | 6.10 | 122.74 | 120.30 |
| 36 | A1 | 2372 | A | N9-C4-C5 | 6.10 | 108.24 | 105.80 |
| 56 | BS | 51 | VAL | CB-CA-C | -6.10 | 99.80 | 111.40 |
| 36 | A5 | 933 | A | C6-N1-C2 | -6.10 | 114.94 | 118.60 |
| 80 | A6 | 1295 | G | N1-C6-O6 | 6.10 | 123.56 | 119.90 |
| 36 | A5 | 673 | U | C2-N3-C4 | -6.10 | 123.34 | 127.00 |
| 36 | A5 | 1119 | C | N1-C2-O2 | -6.10 | 115.24 | 118.90 |
| 36 | A1 | 2148 | U | C5-C4-O4 | -6.10 | 122.24 | 125.90 |
| 36 | A5 | 2646 | C | N1-C2-O2 | -6.10 | 115.24 | 118.90 |
| 36 | A1 | 702 | C | N1-C2-N3 | 6.10 | 123.47 | 119.20 |
| 36 | A1 | 1505 | C | C2-N3-C4 | -6.10 | 116.85 | 119.90 |
| 36 | A5 | 1124 | U | N3-C4-C5 | 6.10 | 118.26 | 114.60 |
| 36 | A5 | 1206 | G | N3-C4-C5 | -6.10 | 125.55 | 128.60 |
| 38 | A8 | 15 | G | C5-C6-N1 | 6.10 | 114.55 | 111.50 |
| 1 | A2 | 621 | A | C8-N9-C4 | 6.10 | 108.24 | 105.80 |
| 1 | A2 | 1473 | U | C5-C4-O4 | 6.10 | 129.56 | 125.90 |
| 1 | A2 | 1596 | C | C2-N1-C1' | 6.10 | 125.51 | 118.80 |
| 36 | A5 | 216 | G | C6-C5-N7 | -6.10 | 126.74 | 130.40 |
| 36 | A5 | 516 | A | N1-C6-N6 | 6.10 | 122.26 | 118.60 |
| 36 | A1 | 941 | G | C2-N3-C4 | 6.09 | 114.95 | 111.90 |
| 36 | A1 | 2160 | G | C6-C5-N7 | -6.09 | 126.74 | 130.40 |
| 36 | A1 | 2944 | U | C4-C5-C6 | -6.09 | 116.04 | 119.70 |
| 36 | A5 | 1469 | C | C4-C5-C6 | 6.09 | 120.45 | 117.40 |
| 36 | A5 | 2833 | A | C5-C6-N1 | 6.09 | 120.75 | 117.70 |
| 36 | A1 | 617 | G | N1-C2-N3 | 6.09 | 127.56 | 123.90 |
| 40 | DB | 205 | VAL | CB-CA-C | -6.09 | 99.82 | 111.40 |
| 1 | A2 | 266 | A | N1-C6-N6 | 6.09 | 122.25 | 118.60 |
| 1 | A2 | 1749 | A | C8-N9-C4 | 6.09 | 108.24 | 105.80 |
| 36 | A1 | 1103 | A | C2-N3-C4 | 6.09 | 113.65 | 110.60 |
| 80 | A6 | 1121 | C | C6-N1-C2 | 6.09 | 122.74 | 120.30 |
| 80 | A6 | 1244 | A | C8-N9-C4 | -6.09 | 103.36 | 105.80 |
| 80 | A6 | 1482 | C | C6-N1-C2 | 6.09 | 122.74 | 120.30 |
| 80 | A6 | 1662 | G | C5-C6-N1 | 6.09 | 114.55 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 36 | A5 | 1909 | A | N1-C2-N3 | -6.09 | 126.25 | 129.30 |
| 36 | A5 | 2386 | A | C5-C6-N6 | -6.09 | 118.83 | 123.70 |
| 36 | A5 | 2749 | G | N1-C2-N3 | -6.09 | 120.25 | 123.90 |
| 1 | A2 | 192 | U | N3-C2-O2 | -6.09 | 117.94 | 122.20 |
| 80 | A6 | 682 | C | C5-C6-N1 | 6.09 | 124.04 | 121.00 |
| 36 | A5 | 1652 | G | C8-N9-C4 | 6.09 | 108.84 | 106.40 |
| 36 | A5 | 2134 | G | C2-N3-C4 | 6.09 | 114.94 | 111.90 |
| 36 | A5 | 2358 | A | C8-N9-C4 | 6.09 | 108.24 | 105.80 |
| 36 | A5 | 2620 | G | N1-C6-O6 | -6.09 | 116.25 | 119.90 |
| 36 | A1 | 1133 | A | N7-C8-N9 | -6.09 | 110.76 | 113.80 |
| 36 | A5 | 935 | U | C5-C4-O4 | -6.09 | 122.25 | 125.90 |
| 36 | A5 | 2865 | U | C2-N1-C1' | 6.09 | 125.01 | 117.70 |
| 36 | A1 | 1122 | U | N3-C4-O4 | -6.09 | 115.14 | 119.40 |
| 36 | A1 | 2306 | C | N3-C4-N4 | -6.09 | 113.74 | 118.00 |
| 36 | A1 | 2758 | A | C2-N3-C4 | 6.09 | 113.64 | 110.60 |
| 36 | A5 | 1147 | G | C6-C5-N7 | 6.09 | 134.05 | 130.40 |
| 36 | A5 | 2368 | A | N1-C6-N6 | -6.09 | 114.95 | 118.60 |
| 36 | A1 | 302 | U | C5-C6-N1 | -6.08 | 119.66 | 122.70 |
| 36 | A1 | 511 | G | N1-C6-O6 | -6.08 | 116.25 | 119.90 |
| 36 | A1 | 670 | C | C2-N3-C4 | -6.08 | 116.86 | 119.90 |
| 36 | A1 | 1329 | U | C3'-C2'-C1' | 6.08 | 106.37 | 101.50 |
| 80 | A6 | 84 | A | N1-C6-N6 | -6.08 | 114.95 | 118.60 |
| 36 | A5 | 282 | G | N9-C4-C5 | 6.08 | 107.83 | 105.40 |
| 1 | A2 | 61 | A | C8-N9-C4 | -6.08 | 103.37 | 105.80 |
| 36 | A1 | 1472 | U | C5-C6-N1 | -6.08 | 119.66 | 122.70 |
| 80 | A6 | 1792 | G | C6-C5-N7 | -6.08 | 126.75 | 130.40 |
| 36 | A5 | 341 | G | N1-C6-O6 | 6.08 | 123.55 | 119.90 |
| 38 | A8 | 14 | C | C2-N3-C4 | -6.08 | 116.86 | 119.90 |
| 36 | A1 | 371 | G | N3-C2-N2 | 6.08 | 124.16 | 119.90 |
| 36 | A1 | 1145 | G | C5-N7-C8 | 6.08 | 107.34 | 104.30 |
| 36 | A1 | 3242 | G | C4-C5-C6 | -6.08 | 115.15 | 118.80 |
| 36 | A5 | 125 | C | N3-C4-N4 | -6.08 | 113.74 | 118.00 |
| 36 | A1 | 1170 | A | N1-C2-N3 | -6.08 | 126.26 | 129.30 |
| 36 | A1 | 2749 | G | C6-C5-N7 | -6.08 | 126.75 | 130.40 |
| 36 | A5 | 1929 | G | N9-C4-C5 | -6.08 | 102.97 | 105.40 |
| 36 | A5 | 2730 | G | N3-C4-N9 | -6.08 | 122.35 | 126.00 |
| 38 | A8 | 47 | C | N1-C2-O2 | 6.08 | 122.55 | 118.90 |
| 36 | A5 | 2392 | C | N3-C4-C5 | 6.08 | 124.33 | 121.90 |
| 1 | A2 | 1057 | U | C2-N1-C1' | 6.08 | 124.99 | 117.70 |
| 36 | A1 | 1155 | C | C6-N1-C2 | -6.08 | 117.87 | 120.30 |
| 36 | A1 | 1724 | U | N3-C2-O2 | -6.08 | 117.95 | 122.20 |
| 36 | A1 | 2177 | G | N3-C4-N9 | 6.08 | 129.65 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 2393 | G | N1-C6-O6 | 6.08 | 123.55 | 119.90 |
| 36 | A1 | 2434 | U | C4-C5-C6 | 6.08 | 123.34 | 119.70 |
| 36 | A5 | 1666 | G | C5-C6-O6 | 6.08 | 132.25 | 128.60 |
| 36 | A5 | 2128 | C | C2-N3-C4 | -6.08 | 116.86 | 119.90 |
| 36 | A5 | 2791 | G | N1-C6-O6 | 6.08 | 123.55 | 119.90 |
| 36 | A1 | 1494 | U | N3-C4-C5 | 6.07 | 118.24 | 114.60 |
| 36 | A1 | 1719 | G | C5-C6-O6 | -6.07 | 124.96 | 128.60 |
| 36 | A1 | 2770 | G | N7-C8-N9 | 6.07 | 116.14 | 113.10 |
| 37 | A7 | 40 | C | C4-C5-C6 | 6.07 | 120.44 | 117.40 |
| 1 | A2 | 377 | G | N3-C4-N9 | -6.07 | 122.36 | 126.00 |
| 80 | A6 | 337 | G | C5-C6-O6 | -6.07 | 124.96 | 128.60 |
| 80 | A6 | 1304 | G | N3-C4-N9 | 6.07 | 129.64 | 126.00 |
| 36 | A5 | 1136 | A | N1-C2-N3 | -6.07 | 126.26 | 129.30 |
| 36 | A5 | 1192 | C | C2-N3-C4 | -6.07 | 116.86 | 119.90 |
| 51 | BN | 38 | ARG | NE-CZ-NH1 | 6.07 | 123.33 | 120.30 |
| 36 | A5 | 3020 | U | C5-C4-O4 | -6.07 | 122.26 | 125.90 |
| 36 | A5 | 3382 | U | N3-C2-O2 | -6.07 | 117.95 | 122.20 |
| 36 | A1 | 1481 | A | C5-N7-C8 | -6.07 | 100.86 | 103.90 |
| 36 | A5 | 66 | A | N9-C4-C5 | -6.07 | 103.37 | 105.80 |
| 36 | A5 | 2954 | U | C5-C4-O4 | -6.07 | 122.26 | 125.90 |
| 36 | A1 | 509 | U | C2-N3-C4 | -6.07 | 123.36 | 127.00 |
| 36 | A1 | 1145 | G | N3-C2-N2 | 6.07 | 124.15 | 119.90 |
| 80 | A6 | 36 | C | C2-N3-C4 | -6.07 | 116.87 | 119.90 |
| 80 | A6 | 563 | U | C5-C6-N1 | -6.07 | 119.67 | 122.70 |
| 80 | A6 | 1749 | A | C5-N7-C8 | -6.07 | 100.87 | 103.90 |
| 36 | A5 | 976 | U | N3-C2-O2 | -6.07 | 117.95 | 122.20 |
| 36 | A5 | 2764 | C | N3-C4-C5 | 6.07 | 124.33 | 121.90 |
| 36 | A1 | 694 | C | N3-C4-C5 | 6.07 | 124.33 | 121.90 |
| 15 | CN | 114 | ARG | NE-CZ-NH1 | 6.07 | 123.33 | 120.30 |
| 36 | A5 | 1438 | U | C2-N1-C1' | 6.07 | 124.98 | 117.70 |
| 36 | A1 | 2649 | A | N1-C2-N3 | -6.06 | 126.27 | 129.30 |
| 36 | A1 | 3377 | G | N3-C4-N9 | 6.06 | 129.64 | 126.00 |
| 80 | A6 | 387 | A | C2-N3-C4 | 6.06 | 113.63 | 110.60 |
| 36 | A5 | 1902 | G | N7-C8-N9 | -6.06 | 110.07 | 113.10 |
| 36 | A1 | 331 | G | C2-N3-C4 | 6.06 | 114.93 | 111.90 |
| 36 | A1 | 718 | G | C2-N3-C4 | -6.06 | 108.87 | 111.90 |
| 36 | A1 | 1474 | A | N1-C2-N3 | 6.06 | 132.33 | 129.30 |
| 36 | A1 | 1743 | G | C8-N9-C4 | 6.06 | 108.83 | 106.40 |
| 36 | A1 | 2380 | U | N1-C2-N3 | 6.06 | 118.54 | 114.90 |
| 80 | A6 | 1428 | G | C8-N9-C4 | -6.06 | 103.97 | 106.40 |
| 36 | A5 | 80 | G | N1-C6-O6 | -6.06 | 116.26 | 119.90 |
| 36 | A5 | 883 | A | N7-C8-N9 | -6.06 | 110.77 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 36 | A5 | 1808 | G | N1-C6-O6 | 6.06 | 123.54 | 119.90 |
| 36 | A5 | 1042 | U | N3-C2-O2 | -6.06 | 117.96 | 122.20 |
| 36 | A1 | 1092 | C | C6-N1-C2 | -6.06 | 117.88 | 120.30 |
| 36 | A1 | 2349 | U | N3-C4-C5 | 6.06 | 118.23 | 114.60 |
| 46 | BH | 166 | ARG | NE-CZ-NH2 | 6.06 | 123.33 | 120.30 |
| 80 | A6 | 906 | A | C2-N3-C4 | -6.06 | 107.57 | 110.60 |
| 80 | A6 | 1473 | U | C5-C4-O4 | 6.06 | 129.54 | 125.90 |
| 80 | A6 | 1754 | A | N1-C6-N6 | -6.06 | 114.96 | 118.60 |
| 36 | A5 | 1222 | G | P-O3'-C3' | 6.06 | 126.97 | 119.70 |
| 36 | A5 | 2353 | G | C6-C5-N7 | -6.06 | 126.76 | 130.40 |
| 36 | A5 | 3245 | A | N9-C4-C5 | -6.06 | 103.38 | 105.80 |
| 1 | A2 | 397 | A | N1-C6-N6 | -6.06 | 114.97 | 118.60 |
| 1 | A2 | 719 | U | C5-C6-N1 | 6.06 | 125.73 | 122.70 |
| 36 | A1 | 388 | G | C8-N9-C4 | -6.06 | 103.98 | 106.40 |
| 38 | A4 | 10 | A | C6-N1-C2 | -6.06 | 114.97 | 118.60 |
| 36 | A5 | 920 | A | N7-C8-N9 | -6.06 | 110.77 | 113.80 |
| 36 | A5 | 3382 | U | C6-N1-C1' | -6.06 | 112.72 | 121.20 |
| 1 | A2 | 557 | G | N3-C4-N9 | 6.05 | 129.63 | 126.00 |
| 80 | A6 | 799 | A | C8-N9-C4 | -6.05 | 103.38 | 105.80 |
| 80 | A6 | 1473 | U | C6-N1-C2 | -6.05 | 117.37 | 121.00 |
| 36 | A5 | 555 | U | N3-C4-O4 | 6.05 | 123.64 | 119.40 |
| 36 | A5 | 1168 | U | N3-C4-O4 | -6.05 | 115.16 | 119.40 |
| 36 | A5 | 2415 | C | N3-C4-C5 | 6.05 | 124.32 | 121.90 |
| 36 | A5 | 2887 | A | C6-N1-C2 | 6.05 | 122.23 | 118.60 |
| 36 | A5 | 2911 | A | C8-N9-C4 | -6.05 | 103.38 | 105.80 |
| 1 | A2 | 1192 | C | N3-C2-O2 | 6.05 | 126.14 | 121.90 |
| 36 | A1 | 46 | U | N3-C2-O2 | -6.05 | 117.96 | 122.20 |
| 36 | A1 | 677 | A | N1-C6-N6 | 6.05 | 122.23 | 118.60 |
| 36 | A1 | 1379 | G | C2-N3-C4 | -6.05 | 108.87 | 111.90 |
| 38 | A4 | 5 | U | N1-C2-O2 | -6.05 | 118.56 | 122.80 |
| 36 | A5 | 311 | C | N3-C4-C5 | 6.05 | 124.32 | 121.90 |
| 36 | A5 | 2730 | G | C5-N7-C8 | -6.05 | 101.27 | 104.30 |
| 36 | A5 | 2830 | G | N3-C2-N2 | -6.05 | 115.66 | 119.90 |
| 36 | A5 | 3309 | G | C5-C6-N1 | 6.05 | 114.53 | 111.50 |
| 52 | DO | 117[A] | ARG | CG-CD-NE | -6.05 | 99.09 | 111.80 |
| 52 | DO | 117[B] | ARG | CG-CD-NE | -6.05 | 99.09 | 111.80 |
| 36 | A1 | 1175 | C | N3-C4-C5 | 6.05 | 124.32 | 121.90 |
| 36 | A1 | 1820 | U | P-O3'-C3' | 6.05 | 126.96 | 119.70 |
| 80 | A6 | 623 | A | C8-N9-C4 | 6.05 | 108.22 | 105.80 |
| 36 | A5 | 927 | C | N3-C4-C5 | 6.05 | 124.32 | 121.90 |
| 36 | A5 | 1301 | A | N9-C4-C5 | -6.05 | 103.38 | 105.80 |
| 36 | A5 | 1582 | C | C6-N1-C2 | -6.05 | 117.88 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 36 | A5 | 1897 | G | C5-C6-N1 | 6.05 | 114.53 | 111.50 |
| 36 | A5 | 3182 | G | C5-C6-O6 | 6.05 | 132.23 | 128.60 |
| 51 | DN | 96 | ARG | NE-CZ-NH1 | 6.05 | 123.32 | 120.30 |
| 80 | A6 | 1481 | C | C3'-C2'-C1' | -6.05 | 96.66 | 101.50 |
| 36 | A5 | 811 | U | C4-C5-C6 | 6.05 | 123.33 | 119.70 |
| 36 | A5 | 1869 | C | C2-N3-C4 | -6.05 | 116.88 | 119.90 |
| 36 | A1 | 1450 | G | C8-N9-C4 | 6.05 | 108.82 | 106.40 |
| 36 | A1 | 2528 | G | N3-C4-C5 | 6.05 | 131.62 | 128.60 |
| 80 | A6 | 429 | G | C4-C5-N7 | -6.05 | 108.38 | 110.80 |
| 38 | A8 | 42 | G | N7-C8-N9 | -6.05 | 110.08 | 113.10 |
| 36 | A1 | 290 | G | C2-N3-C4 | 6.04 | 114.92 | 111.90 |
| 36 | A5 | 1518 | U | N3-C2-O2 | -6.04 | 117.97 | 122.20 |
| 1 | A2 | 1121 | C | C5-C6-N1 | -6.04 | 117.98 | 121.00 |
| 36 | A1 | 659 | G | N1-C2-N2 | -6.04 | 110.76 | 116.20 |
| 36 | A1 | 1894 | U | N3-C4-C5 | 6.04 | 118.23 | 114.60 |
| 36 | A1 | 2161 | G | N3-C4-C5 | -6.04 | 125.58 | 128.60 |
| 36 | A1 | 2930 | A | C4-C5-N7 | -6.04 | 107.68 | 110.70 |
| 1 | A2 | 349 | U | C4-C5-C6 | 6.04 | 123.33 | 119.70 |
| 1 | A2 | 557 | G | C6-C5-N7 | -6.04 | 126.78 | 130.40 |
| 36 | A1 | 2174 | G | N1-C2-N3 | 6.04 | 127.53 | 123.90 |
| 36 | A1 | 3228 | C | C2-N1-C1' | 6.04 | 125.44 | 118.80 |
| 80 | A6 | 358 | U | N1-C2-O2 | -6.04 | 118.57 | 122.80 |
| 80 | A6 | 640 | U | C5-C6-N1 | -6.04 | 119.68 | 122.70 |
| 80 | A6 | 1164 | G | C8-N9-C4 | 6.04 | 108.82 | 106.40 |
| 36 | A5 | 424 | G | N1-C6-O6 | -6.04 | 116.28 | 119.90 |
| 36 | A5 | 2837 | A | N7-C8-N9 | -6.04 | 110.78 | 113.80 |
| 36 | A1 | 1800 | A | N1-C6-N6 | -6.04 | 114.98 | 118.60 |
| 11 | CJ | 3 | ARG | NE-CZ-NH2 | 6.04 | 123.32 | 120.30 |
| 36 | A5 | 2980 | U | C6-N1-C2 | -6.04 | 117.38 | 121.00 |
| 36 | A5 | 3211 | C | C4-C5-C6 | 6.04 | 120.42 | 117.40 |
| 1 | A2 | 445 | A | C2-N3-C4 | 6.04 | 113.62 | 110.60 |
| 1 | A2 | 719 | U | N1-C2-O2 | 6.04 | 127.03 | 122.80 |
| 36 | A1 | 1347 | U | N3-C2-O2 | -6.04 | 117.97 | 122.20 |
| 36 | A5 | 2993 | G | N3-C4-N9 | 6.04 | 129.62 | 126.00 |
| 1 | A2 | 1246 | C | N3-C4-N4 | -6.04 | 113.78 | 118.00 |
| 36 | A1 | 630 | A | C5-C6-N1 | 6.04 | 120.72 | 117.70 |
| 36 | A1 | 1807 | G | N3-C4-C5 | -6.04 | 125.58 | 128.60 |
| 36 | A1 | 2353 | G | C6-C5-N7 | -6.04 | 126.78 | 130.40 |
| 36 | A1 | 2406 | C | C4-C5-C6 | 6.04 | 120.42 | 117.40 |
| 69 | Bf | 67 | MET | CG-SD-CE | -6.04 | 90.54 | 100.20 |
| 36 | A5 | 1000 | C | C6-N1-C2 | -6.04 | 117.89 | 120.30 |
| 36 | A1 | 3048 | A | N7-C8-N9 | 6.03 | 116.82 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 38 | A4 | 58 | G | C8-N9-C4 | 6.03 | 108.81 | 106.40 |
| 36 | A5 | 813 | G | N9-C4-C5 | 6.03 | 107.81 | 105.40 |
| 36 | A5 | 3003 | G | C4-C5-C6 | -6.03 | 115.18 | 118.80 |
| 36 | A5 | 3148 | U | N3-C4-C5 | 6.03 | 118.22 | 114.60 |
| 80 | A6 | 1572 | G | C6-C5-N7 | -6.03 | 126.78 | 130.40 |
| 36 | A5 | 1368 | U | C6-N1-C2 | 6.03 | 124.62 | 121.00 |
| 1 | A2 | 538 | A | N1-C2-N3 | -6.03 | 126.28 | 129.30 |
| 1 | A2 | 1450 | U | C5-C4-O4 | 6.03 | 129.52 | 125.90 |
| 36 | A1 | 907 | G | N7-C8-N9 | 6.03 | 116.12 | 113.10 |
| 36 | A1 | 1312 | C | N1-C2-O2 | -6.03 | 115.28 | 118.90 |
| 36 | A1 | 1175 | C | C5-C4-N4 | -6.03 | 115.98 | 120.20 |
| 36 | A1 | 1881 | A | N9-C4-C5 | -6.03 | 103.39 | 105.80 |
| 37 | A3 | 98 | C | C4-C5-C6 | 6.03 | 120.41 | 117.40 |
| 64 | Ba | 66 | ALA | N-CA-C | -6.03 | 94.72 | 111.00 |
| 36 | A5 | 1184 | A | C2-N3-C4 | -6.03 | 107.59 | 110.60 |
| 36 | A5 | 3318 | G | N1-C6-O6 | -6.03 | 116.28 | 119.90 |
| 36 | A1 | 2187 | G | N9-C4-C5 | -6.03 | 102.99 | 105.40 |
| 36 | A1 | 2620 | G | C5-C6-O6 | -6.03 | 124.98 | 128.60 |
| 36 | A1 | 2902 | A | C2-N3-C4 | -6.03 | 107.59 | 110.60 |
| 36 | A5 | 1117 | G | C5-C6-O6 | -6.03 | 124.98 | 128.60 |
| 36 | A5 | 1128 | U | C5-C6-N1 | -6.03 | 119.69 | 122.70 |
| 36 | A5 | 2361 | A | C5-N7-C8 | 6.03 | 106.91 | 103.90 |
| 36 | A5 | 3343 | G | N1-C2-N2 | -6.03 | 110.78 | 116.20 |
| 1 | A2 | 144 | U | N1-C2-N3 | 6.03 | 118.52 | 114.90 |
| 36 | A1 | 39 | A | N7-C8-N9 | -6.03 | 110.79 | 113.80 |
| 36 | A1 | 2129 | U | C6-N1-C2 | -6.03 | 117.39 | 121.00 |
| 36 | A1 | 2941 | A | C8-N9-C4 | 6.03 | 108.21 | 105.80 |
| 38 | A4 | 14 | C | C2-N3-C4 | -6.03 | 116.89 | 119.90 |
| 80 | A6 | 1550 | A | N1-C6-N6 | 6.03 | 122.22 | 118.60 |
| 36 | A5 | 2364 | G | N3-C4-C5 | -6.03 | 125.59 | 128.60 |
| 36 | A5 | 2920 | U | N1-C2-N3 | 6.03 | 118.52 | 114.90 |
| 36 | A1 | 639 | G | N9-C4-C5 | -6.02 | 102.99 | 105.40 |
| 36 | A5 | 341 | G | N1-C2-N2 | 6.02 | 121.62 | 116.20 |
| 36 | A1 | 934 | G | C5-C6-N1 | 6.02 | 114.51 | 111.50 |
| 36 | A1 | 3006 | A | N1-C6-N6 | 6.02 | 122.21 | 118.60 |
| 36 | A5 | 226 | C | C5-C4-N4 | -6.02 | 115.98 | 120.20 |
| 36 | A5 | 520 | U | N1-C2-N3 | 6.02 | 118.51 | 114.90 |
| 36 | A5 | 795 | G | C2-N3-C4 | 6.02 | 114.91 | 111.90 |
| 1 | A2 | 1000 | C | C5-C4-N4 | 6.02 | 124.42 | 120.20 |
| 36 | A5 | 884 | A | C4-C5-C6 | -6.02 | 113.99 | 117.00 |
| 36 | A1 | 1335 | C | C2-N3-C4 | -6.02 | 116.89 | 119.90 |
| 36 | A1 | 2284 | C | N1-C2-N3 | 6.02 | 123.41 | 119.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 2844 | C | N1-C2-O2 | 6.02 | 122.51 | 118.90 |
| 1 | A2 | 75 | U | C2-N1-C1' | 6.02 | 124.92 | 117.70 |
| 1 | A2 | 377 | G | N1-C6-O6 | 6.02 | 123.51 | 119.90 |
| 1 | A2 | 389 | G | N3-C4-C5 | -6.02 | 125.59 | 128.60 |
| 1 | A2 | 1387 | G | C5-C6-O6 | -6.02 | 124.99 | 128.60 |
| 36 | A1 | 81 | C | N3-C4-C5 | 6.02 | 124.31 | 121.90 |
| 36 | A1 | 700 | C | N3-C4-C5 | 6.02 | 124.31 | 121.90 |
| 80 | A6 | 879 | G | C5-C6-O6 | 6.02 | 132.21 | 128.60 |
| 36 | A5 | 2108 | C | N3-C4-N4 | -6.02 | 113.79 | 118.00 |
| 36 | A5 | 2976 | A | N7-C8-N9 | -6.02 | 110.79 | 113.80 |
| 36 | A5 | 3095 | U | N3-C4-C5 | 6.02 | 118.21 | 114.60 |
| 1 | A2 | 831 | U | C6-N1-C2 | -6.02 | 117.39 | 121.00 |
| 36 | A1 | 50 | U | N1-C2-O2 | -6.02 | 118.59 | 122.80 |
| 36 | A1 | 1152 | G | C6-N1-C2 | -6.02 | 121.49 | 125.10 |
| 38 | A4 | 96 | A | N1-C6-N6 | 6.02 | 122.21 | 118.60 |
| 80 | A6 | 820 | U | N3-C2-O2 | 6.02 | 126.41 | 122.20 |
| 36 | A5 | 912 | G | N3-C4-N9 | 6.02 | 129.61 | 126.00 |
| 1 | A2 | 404 | G | N9-C4-C5 | -6.01 | 102.99 | 105.40 |
| 36 | A1 | 197 | G | N3-C2-N2 | -6.01 | 115.69 | 119.90 |
| 36 | A1 | 906 | A | C5-C6-N1 | 6.01 | 120.71 | 117.70 |
| 36 | A1 | 2979 | U | N3-C4-O4 | -6.01 | 115.19 | 119.40 |
| 38 | A4 | 51 | G | C5-C6-O6 | -6.01 | 124.99 | 128.60 |
| 80 | A6 | 1111 | G | C4-C5-N7 | 6.01 | 113.20 | 110.80 |
| 36 | A5 | 517 | G | N1-C2-N3 | 6.01 | 127.51 | 123.90 |
| 36 | A5 | 822 | G | N3-C2-N2 | -6.01 | 115.69 | 119.90 |
| 76 | Dm | 97 | ARG | NE-CZ-NH2 | -6.01 | 117.29 | 120.30 |
| 36 | A1 | 968 | G | N7-C8-N9 | 6.01 | 116.11 | 113.10 |
| 36 | A1 | 2417 | U | N1-C2-N3 | 6.01 | 118.51 | 114.90 |
| 36 | A5 | 2939 | G | C5-N7-C8 | 6.01 | 107.31 | 104.30 |
| 36 | A5 | 3140 | G | C5-N7-C8 | -6.01 | 101.29 | 104.30 |
| 36 | A1 | 405 | U | N3-C4-C5 | 6.01 | 118.21 | 114.60 |
| 36 | A1 | 1484 | U | P-O3'-C3' | 6.01 | 126.91 | 119.70 |
| 36 | A1 | 1522 | U | C2-N3-C4 | -6.01 | 123.39 | 127.00 |
| 36 | A1 | 2638 | C | N1-C2-O2 | 6.01 | 122.51 | 118.90 |
| 36 | A1 | 2692 | A | C8-N9-C4 | -6.01 | 103.39 | 105.80 |
| 80 | A6 | 1781 | A | C5-C6-N6 | 6.01 | 128.51 | 123.70 |
| 36 | A1 | 867 | G | N9-C4-C5 | 6.01 | 107.80 | 105.40 |
| 36 | A1 | 1409 | G | C6-C5-N7 | 6.01 | 134.00 | 130.40 |
| 36 | A1 | 1604 | G | C8-N9-C1' | -6.01 | 119.19 | 127.00 |
| 36 | A1 | 933 | A | C8-N9-C4 | -6.01 | 103.40 | 105.80 |
| 36 | A1 | 987 | U | C5-C6-N1 | -6.01 | 119.70 | 122.70 |
| 36 | A1 | 1174 | G | C4-C5-N7 | 6.01 | 113.20 | 110.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 3212 | C | N3-C4-C5 | 6.01 | 124.30 | 121.90 |
| 80 | A6 | 375 | U | N3-C4-C5 | 6.01 | 118.20 | 114.60 |
| 47 | DI | 83 | ASP | CB-CG-OD1 | -6.01 | 112.89 | 118.30 |
| 36 | A1 | 1017 | C | C5-C6-N1 | 6.01 | 124.00 | 121.00 |
| 36 | A1 | 1433 | A | C5-C6-N6 | -6.01 | 118.89 | 123.70 |
| 36 | A1 | 2168 | A | N7-C8-N9 | -6.01 | 110.80 | 113.80 |
| 36 | A1 | 2879 | C | C2-N3-C4 | 6.01 | 122.90 | 119.90 |
| 80 | A6 | 150 | U | N3-C4-O4 | -6.01 | 115.20 | 119.40 |
| 36 | A5 | 1242 | G | C4-N9-C1' | 6.01 | 134.31 | 126.50 |
| 36 | A5 | 1340 | G | N7-C8-N9 | -6.01 | 110.10 | 113.10 |
| 36 | A5 | 2724 | U | C5-C4-O4 | 6.01 | 129.50 | 125.90 |
| 36 | A5 | 2911 | A | N1-C2-N3 | -6.01 | 126.30 | 129.30 |
| 1 | A2 | 1753 | A | C8-N9-C4 | 6.00 | 108.20 | 105.80 |
| 36 | A1 | 290 | G | N1-C6-O6 | -6.00 | 116.30 | 119.90 |
| 36 | A5 | 1858 | A | C4-C5-C6 | 6.00 | 120.00 | 117.00 |
| 1 | A2 | 1157 | A | C8-N9-C4 | -6.00 | 103.40 | 105.80 |
| 36 | A1 | 92 | G | C5-C6-N1 | 6.00 | 114.50 | 111.50 |
| 36 | A1 | 1941 | C | N1-C2-O2 | -6.00 | 115.30 | 118.90 |
| 36 | A1 | 2990 | G | N3-C4-C5 | -6.00 | 125.60 | 128.60 |
| 36 | A5 | 595 | G | N1-C6-O6 | -6.00 | 116.30 | 119.90 |
| 36 | A5 | 1371 | G | C6-N1-C2 | -6.00 | 121.50 | 125.10 |
| 36 | A5 | 3187 | A | N7-C8-N9 | -6.00 | 110.80 | 113.80 |
| 36 | A1 | 2916 | U | C4-C5-C6 | 6.00 | 123.30 | 119.70 |
| 36 | A1 | 3214 | U | C6-N1-C2 | -6.00 | 117.40 | 121.00 |
| 36 | A5 | 392 | G | C5-C6-O6 | -6.00 | 125.00 | 128.60 |
| 36 | A5 | 641 | C | C5-C4-N4 | 6.00 | 124.40 | 120.20 |
| 36 | A5 | 903 | U | C5-C6-N1 | -6.00 | 119.70 | 122.70 |
| 36 | A5 | 2381 | G | C5-C6-O6 | 6.00 | 132.20 | 128.60 |
| 36 | A1 | 1399 | A | C8-N9-C4 | 6.00 | 108.20 | 105.80 |
| 36 | A1 | 3225 | C | C5-C6-N1 | -6.00 | 118.00 | 121.00 |
| 80 | A6 | 631 | G | C8-N9-C4 | -6.00 | 104.00 | 106.40 |
| 36 | A5 | 701 | G | C4-C5-N7 | -6.00 | 108.40 | 110.80 |
| 36 | A5 | 2603 | G | C5-N7-C8 | -6.00 | 101.30 | 104.30 |
| 36 | A5 | 3369 | G | C6-N1-C2 | -6.00 | 121.50 | 125.10 |
| 1 | A2 | 1601 | G | C5-C6-N1 | 6.00 | 114.50 | 111.50 |
| 80 | A6 | 1568 | C | C2-N1-C1' | 6.00 | 125.40 | 118.80 |
| 36 | A5 | 1110 | U | N3-C4-O4 | -6.00 | 115.20 | 119.40 |
| 36 | A5 | 1378 | U | C6-N1-C2 | 6.00 | 124.60 | 121.00 |
| 36 | A5 | 2346 | C | N1-C2-O2 | -6.00 | 115.30 | 118.90 |
| 40 | DB | 232 | ARG | NE-CZ-NH2 | -6.00 | 117.30 | 120.30 |
| 36 | A1 | 440 | A | C8-N9-C4 | -6.00 | 103.40 | 105.80 |
| 80 | A6 | 1594 | G | N3-C4-N9 | 6.00 | 129.60 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-------|------|-----------|-------|-------------|----------|
| 52 | DO | 13[B] | ASP | C-N-CA | 6.00 | 136.69 | 121.70 |
| 36 | A1 | 1374 | G | N1-C2-N2 | -5.99 | 110.81 | 116.20 |
| 38 | A4 | 28 | C | C4-C5-C6 | 5.99 | 120.40 | 117.40 |
| 80 | A6 | 1186 | U | C5-C6-N1 | -5.99 | 119.70 | 122.70 |
| 36 | A5 | 619 | A | N1-C6-N6 | -5.99 | 115.00 | 118.60 |
| 36 | A5 | 994 | G | C8-N9-C4 | 5.99 | 108.80 | 106.40 |
| 38 | A8 | 100 | U | C5-C4-O4 | -5.99 | 122.30 | 125.90 |
| 36 | A1 | 1870 | C | C6-N1-C2 | 5.99 | 122.70 | 120.30 |
| 36 | A1 | 2794 | G | N1-C6-O6 | -5.99 | 116.31 | 119.90 |
| 36 | A5 | 1047 | A | C5-C6-N1 | 5.99 | 120.70 | 117.70 |
| 36 | A5 | 2370 | G | C5-C6-N1 | 5.99 | 114.50 | 111.50 |
| 36 | A5 | 2908 | G | C5-C6-N1 | -5.99 | 108.50 | 111.50 |
| 1 | A2 | 274 | G | C4-N9-C1' | 5.99 | 134.29 | 126.50 |
| 1 | A2 | 1643 | U | C5-C6-N1 | -5.99 | 119.70 | 122.70 |
| 36 | A1 | 919 | U | N3-C4-O4 | -5.99 | 115.21 | 119.40 |
| 36 | A1 | 1362 | G | C5-C6-O6 | -5.99 | 125.00 | 128.60 |
| 36 | A1 | 2514 | U | C5-C6-N1 | -5.99 | 119.70 | 122.70 |
| 36 | A5 | 2116 | G | C6-C5-N7 | -5.99 | 126.81 | 130.40 |
| 36 | A5 | 3028 | G | N3-C4-N9 | 5.99 | 129.59 | 126.00 |
| 36 | A5 | 3343 | G | N3-C2-N2 | 5.99 | 124.09 | 119.90 |
| 36 | A1 | 802 | C | C2-N1-C1' | 5.99 | 125.39 | 118.80 |
| 80 | A6 | 337 | G | C5-C6-N1 | -5.99 | 108.51 | 111.50 |
| 80 | A6 | 1129 | U | N3-C4-C5 | 5.99 | 118.19 | 114.60 |
| 36 | A5 | 2526 | C | N1-C2-O2 | 5.99 | 122.49 | 118.90 |
| 36 | A1 | 384 | A | N9-C4-C5 | -5.99 | 103.41 | 105.80 |
| 59 | BV | 80 | ARG | NE-CZ-NH2 | -5.99 | 117.31 | 120.30 |
| 1 | A2 | 1417 | A | N1-C6-N6 | 5.99 | 122.19 | 118.60 |
| 36 | A1 | 931 | C | C5-C4-N4 | 5.99 | 124.39 | 120.20 |
| 36 | A1 | 1831 | U | N3-C2-O2 | -5.99 | 118.01 | 122.20 |
| 80 | A6 | 1440 | C | N3-C4-N4 | 5.99 | 122.19 | 118.00 |
| 36 | A5 | 283 | G | C4-C5-N7 | 5.99 | 113.19 | 110.80 |
| 36 | A1 | 1369 | A | N3-C4-C5 | 5.98 | 130.99 | 126.80 |
| 37 | A3 | 103 | A | N9-C4-C5 | -5.98 | 103.41 | 105.80 |
| 36 | A5 | 3341 | U | C5-C6-N1 | 5.98 | 125.69 | 122.70 |
| 47 | DI | 57 | LEU | CA-CB-CG | 5.98 | 129.06 | 115.30 |
| 1 | A2 | 554 | C | N1-C2-O2 | 5.98 | 122.49 | 118.90 |
| 36 | A1 | 1425 | U | C5-C4-O4 | 5.98 | 129.49 | 125.90 |
| 36 | A1 | 2193 | U | C5-C6-N1 | -5.98 | 119.71 | 122.70 |
| 36 | A1 | 3046 | A | N9-C4-C5 | 5.98 | 108.19 | 105.80 |
| 36 | A5 | 1808 | G | C8-N9-C4 | 5.98 | 108.79 | 106.40 |
| 36 | A5 | 3298 | C | C4-C5-C6 | 5.98 | 120.39 | 117.40 |
| 38 | A8 | 63 | G | N1-C6-O6 | -5.98 | 116.31 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A2 | 106 | U | C6-N1-C2 | -5.98 | 117.41 | 121.00 |
| 1 | A2 | 829 | A | C8-N9-C4 | -5.98 | 103.41 | 105.80 |
| 36 | A1 | 78 | U | C5-C6-N1 | -5.98 | 119.71 | 122.70 |
| 36 | A1 | 716 | A | C5-C6-N6 | -5.98 | 118.92 | 123.70 |
| 36 | A1 | 2387 | A | N1-C6-N6 | -5.98 | 115.01 | 118.60 |
| 36 | A1 | 2608 | G | N1-C6-O6 | -5.98 | 116.31 | 119.90 |
| 80 | A6 | 1745 | G | N9-C4-C5 | -5.98 | 103.01 | 105.40 |
| 36 | A5 | 351 | A | N1-C6-N6 | 5.98 | 122.19 | 118.60 |
| 36 | A5 | 2426 | U | N3-C4-O4 | -5.98 | 115.21 | 119.40 |
| 36 | A5 | 2617 | U | N3-C4-C5 | 5.98 | 118.19 | 114.60 |
| 50 | DM | 135 | LEU | CA-CB-CG | 5.98 | 129.06 | 115.30 |
| 1 | A2 | 628 | G | C5-C6-O6 | 5.98 | 132.19 | 128.60 |
| 36 | A1 | 2171 | G | C2-N3-C4 | 5.98 | 114.89 | 111.90 |
| 36 | A5 | 892 | U | C2-N3-C4 | -5.98 | 123.41 | 127.00 |
| 1 | A2 | 360 | A | N1-C6-N6 | 5.98 | 122.19 | 118.60 |
| 1 | A2 | 1768 | G | C4-N9-C1' | -5.98 | 118.73 | 126.50 |
| 36 | A5 | 2952 | G | C6-N1-C2 | -5.98 | 121.51 | 125.10 |
| 36 | A1 | 67 | A | C4-C5-C6 | 5.98 | 119.99 | 117.00 |
| 36 | A1 | 1492 | G | N7-C8-N9 | -5.98 | 110.11 | 113.10 |
| 80 | A6 | 416 | A | N1-C6-N6 | 5.98 | 122.19 | 118.60 |
| 80 | A6 | 1090 | C | N1-C2-O2 | -5.98 | 115.31 | 118.90 |
| 36 | A1 | 32 | U | C2-N3-C4 | -5.97 | 123.42 | 127.00 |
| 36 | A1 | 1584 | U | N3-C4-O4 | -5.97 | 115.22 | 119.40 |
| 36 | A1 | 1796 | G | N9-C4-C5 | 5.97 | 107.79 | 105.40 |
| 36 | A1 | 1899 | G | N7-C8-N9 | 5.97 | 116.09 | 113.10 |
| 36 | A1 | 2547 | A | N9-C4-C5 | -5.97 | 103.41 | 105.80 |
| 36 | A5 | 416 | A | N9-C4-C5 | 5.97 | 108.19 | 105.80 |
| 36 | A5 | 1171 | G | N7-C8-N9 | 5.97 | 116.09 | 113.10 |
| 36 | A5 | 2318 | U | N3-C4-O4 | -5.97 | 115.22 | 119.40 |
| 36 | A5 | 2365 | C | C5-C6-N1 | -5.97 | 118.01 | 121.00 |
| 36 | A5 | 2753 | G | N7-C8-N9 | 5.97 | 116.09 | 113.10 |
| 36 | A5 | 3013 | U | N3-C2-O2 | -5.97 | 118.02 | 122.20 |
| 36 | A1 | 923 | C | N1-C2-O2 | -5.97 | 115.32 | 118.90 |
| 36 | A1 | 941 | G | C5-C6-N1 | 5.97 | 114.49 | 111.50 |
| 36 | A1 | 2640 | A | C6-N1-C2 | -5.97 | 115.02 | 118.60 |
| 36 | A1 | 3377 | G | C6-N1-C2 | -5.97 | 121.52 | 125.10 |
| 38 | A4 | 101 | U | N3-C2-O2 | -5.97 | 118.02 | 122.20 |
| 80 | A6 | 622 | A | C4-C5-C6 | 5.97 | 119.99 | 117.00 |
| 80 | A6 | 1120 | U | C2-N3-C4 | -5.97 | 123.42 | 127.00 |
| 80 | A6 | 1519 | U | N3-C2-O2 | -5.97 | 118.02 | 122.20 |
| 36 | A5 | 419 | G | C8-N9-C4 | 5.97 | 108.79 | 106.40 |
| 36 | A5 | 3112 | G | N1-C6-O6 | 5.97 | 123.48 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 802 | C | C4-C5-C6 | 5.97 | 120.39 | 117.40 |
| 36 | A1 | 124 | U | N1-C2-O2 | 5.97 | 126.98 | 122.80 |
| 36 | A1 | 614 | C | C2-N3-C4 | -5.97 | 116.92 | 119.90 |
| 36 | A1 | 3015 | G | N3-C4-C5 | -5.97 | 125.61 | 128.60 |
| 36 | A1 | 3090 | U | N1-C2-O2 | -5.97 | 118.62 | 122.80 |
| 36 | A5 | 2329 | C | N3-C4-N4 | -5.97 | 113.82 | 118.00 |
| 51 | DN | 172 | ARG | NE-CZ-NH2 | 5.97 | 123.28 | 120.30 |
| 1 | A2 | 1000 | C | N3-C2-O2 | -5.97 | 117.72 | 121.90 |
| 1 | A2 | 382 | C | C2-N3-C4 | -5.97 | 116.92 | 119.90 |
| 1 | A2 | 1119 | G | C5-C6-O6 | 5.97 | 132.18 | 128.60 |
| 1 | A2 | 1455 | G | N9-C4-C5 | 5.97 | 107.79 | 105.40 |
| 1 | A2 | 1745 | G | C6-N1-C2 | -5.97 | 121.52 | 125.10 |
| 36 | A1 | 439 | C | C6-N1-C1' | -5.97 | 113.64 | 120.80 |
| 38 | A4 | 10 | A | N1-C6-N6 | -5.97 | 115.02 | 118.60 |
| 36 | A5 | 987 | U | N3-C2-O2 | -5.97 | 118.02 | 122.20 |
| 36 | A5 | 1910 | A | C5-C6-N1 | 5.97 | 120.68 | 117.70 |
| 36 | A5 | 2167 | A | N9-C4-C5 | 5.97 | 108.19 | 105.80 |
| 36 | A5 | 2421 | U | N1-C2-O2 | -5.97 | 118.62 | 122.80 |
| 36 | A5 | 2917 | G | N3-C4-C5 | -5.97 | 125.62 | 128.60 |
| 36 | A5 | 3192 | U | C2-N3-C4 | -5.97 | 123.42 | 127.00 |
| 36 | A5 | 3222 | U | N3-C2-O2 | -5.97 | 118.02 | 122.20 |
| 1 | A2 | 1121 | C | N3-C4-C5 | -5.96 | 119.51 | 121.90 |
| 14 | CM | 62 | LEU | CA-CB-CG | 5.96 | 129.02 | 115.30 |
| 36 | A5 | 679 | U | C5-C4-O4 | 5.96 | 129.48 | 125.90 |
| 36 | A5 | 873 | C | P-O3'-C3' | 5.96 | 126.86 | 119.70 |
| 36 | A5 | 1323 | G | N9-C4-C5 | 5.96 | 107.79 | 105.40 |
| 36 | A5 | 1725 | C | C5-C4-N4 | 5.96 | 124.38 | 120.20 |
| 36 | A5 | 1739 | U | C5-C4-O4 | 5.96 | 129.48 | 125.90 |
| 37 | A7 | 96 | U | C2-N1-C1' | 5.96 | 124.86 | 117.70 |
| 1 | A2 | 1600 | A | C5-N7-C8 | -5.96 | 100.92 | 103.90 |
| 36 | A1 | 1337 | A | C2-N3-C4 | 5.96 | 113.58 | 110.60 |
| 36 | A5 | 594 | U | C5-C6-N1 | 5.96 | 125.68 | 122.70 |
| 36 | A5 | 2411 | U | N3-C4-C5 | 5.96 | 118.18 | 114.60 |
| 36 | A5 | 2799 | A | C2-N3-C4 | -5.96 | 107.62 | 110.60 |
| 1 | A2 | 1521 | G | N3-C4-N9 | 5.96 | 129.58 | 126.00 |
| 36 | A1 | 2794 | G | C5-C6-O6 | 5.96 | 132.18 | 128.60 |
| 36 | A5 | 1305 | U | N3-C4-O4 | 5.96 | 123.57 | 119.40 |
| 36 | A5 | 3216 | G | C4-C5-C6 | 5.96 | 122.38 | 118.80 |
| 50 | DM | 106 | ARG | NE-CZ-NH2 | -5.96 | 117.32 | 120.30 |
| 1 | A2 | 794 | U | C2-N1-C1' | 5.96 | 124.85 | 117.70 |
| 36 | A1 | 417 | A | N9-C4-C5 | -5.96 | 103.42 | 105.80 |
| 36 | A5 | 2166 | A | N1-C6-N6 | 5.96 | 122.18 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 80 | A6 | 554 | C | C2-N3-C4 | -5.96 | 116.92 | 119.90 |
| 36 | A5 | 2323 | G | N1-C6-O6 | -5.96 | 116.33 | 119.90 |
| 36 | A5 | 3351 | U | N3-C2-O2 | -5.96 | 118.03 | 122.20 |
| 36 | A1 | 340 | C | C5-C4-N4 | 5.96 | 124.37 | 120.20 |
| 36 | A1 | 1060 | U | N3-C4-C5 | 5.96 | 118.17 | 114.60 |
| 80 | A6 | 687 | G | C4-N9-C1' | -5.96 | 118.76 | 126.50 |
| 36 | A5 | 3075 | G | C4-C5-N7 | -5.96 | 108.42 | 110.80 |
| 73 | Dj | 21 | ARG | NE-CZ-NH2 | -5.96 | 117.32 | 120.30 |
| 36 | A5 | 2250 | G | N1-C6-O6 | -5.96 | 116.33 | 119.90 |
| 36 | A5 | 3333 | G | N9-C4-C5 | -5.96 | 103.02 | 105.40 |
| 47 | DI | 7 | ARG | NE-CZ-NH1 | -5.96 | 117.32 | 120.30 |
| 36 | A1 | 49 | A | C2-N3-C4 | -5.95 | 107.62 | 110.60 |
| 36 | A1 | 950 | G | N3-C2-N2 | 5.95 | 124.07 | 119.90 |
| 36 | A1 | 1010 | G | C8-N9-C4 | -5.95 | 104.02 | 106.40 |
| 39 | BA | 122 | ASP | CB-CG-OD2 | 5.95 | 123.66 | 118.30 |
| 36 | A5 | 1190 | A | N1-C6-N6 | -5.95 | 115.03 | 118.60 |
| 36 | A5 | 2917 | G | N1-C6-O6 | 5.95 | 123.47 | 119.90 |
| 36 | A5 | 3064 | U | N3-C2-O2 | -5.95 | 118.03 | 122.20 |
| 54 | DQ | 99 | THR | N-CA-C | 5.95 | 127.08 | 111.00 |
| 36 | A1 | 2852 | C | C6-N1-C2 | 5.95 | 122.68 | 120.30 |
| 36 | A5 | 2552 | C | C5-C4-N4 | 5.95 | 124.37 | 120.20 |
| 26 | AY | 44 | LEU | CA-CB-CG | 5.95 | 128.99 | 115.30 |
| 36 | A1 | 200 | C | N1-C2-O2 | 5.95 | 122.47 | 118.90 |
| 36 | A1 | 783 | A | C2-N3-C4 | -5.95 | 107.62 | 110.60 |
| 80 | A6 | 1720 | G | C6-C5-N7 | -5.95 | 126.83 | 130.40 |
| 36 | A5 | 1678 | G | C5-C6-N1 | 5.95 | 114.48 | 111.50 |
| 36 | A5 | 2167 | A | N1-C6-N6 | -5.95 | 115.03 | 118.60 |
| 36 | A5 | 2410 | U | N3-C4-C5 | 5.95 | 118.17 | 114.60 |
| 36 | A5 | 2730 | G | N3-C4-C5 | 5.95 | 131.57 | 128.60 |
| 36 | A5 | 2851 | A | N7-C8-N9 | -5.95 | 110.83 | 113.80 |
| 1 | A2 | 781 | U | N1-C2-O2 | 5.95 | 126.96 | 122.80 |
| 36 | A1 | 413 | U | C5-C4-O4 | -5.95 | 122.33 | 125.90 |
| 36 | A1 | 651 | G | C5-N7-C8 | 5.95 | 107.28 | 104.30 |
| 36 | A1 | 1332 | A | N9-C4-C5 | -5.95 | 103.42 | 105.80 |
| 36 | A1 | 2948 | C | C2-N3-C4 | -5.95 | 116.93 | 119.90 |
| 36 | A1 | 3001 | C | C5-C6-N1 | -5.95 | 118.03 | 121.00 |
| 36 | A1 | 3130 | A | C8-N9-C4 | -5.95 | 103.42 | 105.80 |
| 36 | A5 | 655 | C | C6-N1-C2 | -5.95 | 117.92 | 120.30 |
| 36 | A5 | 2349 | U | C4-C5-C6 | -5.95 | 116.13 | 119.70 |
| 36 | A5 | 2792 | A | C8-N9-C4 | -5.95 | 103.42 | 105.80 |
| 36 | A5 | 337 | G | N1-C6-O6 | -5.95 | 116.33 | 119.90 |
| 36 | A5 | 1548 | C | N1-C2-O2 | -5.95 | 115.33 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A2 | 542 | A | C6-C5-N7 | -5.95 | 128.14 | 132.30 |
| 36 | A1 | 173 | G | C4-N9-C1' | 5.95 | 134.23 | 126.50 |
| 37 | A3 | 91 | G | C2-N3-C4 | -5.95 | 108.93 | 111.90 |
| 80 | A6 | 1792 | G | C4-C5-N7 | 5.95 | 113.18 | 110.80 |
| 36 | A5 | 359 | U | C6-N1-C2 | 5.95 | 124.57 | 121.00 |
| 36 | A5 | 1753 | G | C2-N3-C4 | 5.95 | 114.87 | 111.90 |
| 36 | A5 | 2416 | U | N3-C2-O2 | -5.95 | 118.04 | 122.20 |
| 36 | A5 | 3395 | G | N3-C4-C5 | 5.95 | 131.57 | 128.60 |
| 80 | A6 | 553 | G | N1-C2-N3 | 5.94 | 127.47 | 123.90 |
| 80 | A6 | 1662 | G | N1-C6-O6 | -5.94 | 116.33 | 119.90 |
| 36 | A5 | 3240 | C | N3-C4-N4 | -5.94 | 113.84 | 118.00 |
| 1 | A2 | 1796 | C | C4-C5-C6 | 5.94 | 120.37 | 117.40 |
| 36 | A5 | 971 | G | N1-C2-N3 | -5.94 | 120.33 | 123.90 |
| 36 | A5 | 974 | G | C8-N9-C1' | -5.94 | 119.28 | 127.00 |
| 36 | A5 | 1035 | G | C4-N9-C1' | 5.94 | 134.22 | 126.50 |
| 36 | A5 | 1772 | U | C5-C4-O4 | 5.94 | 129.47 | 125.90 |
| 36 | A5 | 2758 | A | N3-C4-C5 | -5.94 | 122.64 | 126.80 |
| 1 | A2 | 1582 | U | C6-N1-C2 | 5.94 | 124.56 | 121.00 |
| 80 | A6 | 59 | C | N1-C2-O2 | 5.94 | 122.47 | 118.90 |
| 80 | A6 | 1003 | A | C8-N9-C4 | 5.94 | 108.18 | 105.80 |
| 36 | A5 | 39 | A | N3-C4-N9 | 5.94 | 132.15 | 127.40 |
| 36 | A5 | 546 | C | N3-C2-O2 | -5.94 | 117.74 | 121.90 |
| 36 | A5 | 708 | G | C8-N9-C4 | -5.94 | 104.02 | 106.40 |
| 36 | A5 | 968 | G | C4-C5-N7 | 5.94 | 113.18 | 110.80 |
| 36 | A1 | 1144 | U | C2-N3-C4 | -5.94 | 123.44 | 127.00 |
| 36 | A1 | 2888 | U | C2-N3-C4 | -5.94 | 123.44 | 127.00 |
| 36 | A5 | 83 | U | C2-N1-C1' | 5.94 | 124.83 | 117.70 |
| 36 | A5 | 182 | U | C5-C6-N1 | 5.94 | 125.67 | 122.70 |
| 36 | A5 | 2130 | G | N1-C2-N2 | -5.94 | 110.86 | 116.20 |
| 36 | A1 | 960 | U | C5-C6-N1 | -5.94 | 119.73 | 122.70 |
| 36 | A1 | 1152 | G | C4-C5-N7 | 5.94 | 113.17 | 110.80 |
| 36 | A1 | 1202 | A | C5-C6-N1 | -5.94 | 114.73 | 117.70 |
| 36 | A1 | 2680 | A | N1-C2-N3 | 5.94 | 132.27 | 129.30 |
| 37 | A3 | 103 | A | N1-C6-N6 | 5.94 | 122.16 | 118.60 |
| 80 | A6 | 87 | C | C6-N1-C2 | -5.94 | 117.92 | 120.30 |
| 80 | A6 | 1638 | G | N1-C6-O6 | -5.94 | 116.34 | 119.90 |
| 36 | A5 | 386 | A | C5-C6-N6 | -5.94 | 118.95 | 123.70 |
| 36 | A5 | 2421 | U | N1-C2-N3 | 5.94 | 118.46 | 114.90 |
| 36 | A5 | 2607 | G | N1-C6-O6 | -5.94 | 116.34 | 119.90 |
| 37 | A7 | 25 | G | C5-C6-O6 | -5.94 | 125.04 | 128.60 |
| 1 | A2 | 279 | G | C8-N9-C4 | -5.94 | 104.03 | 106.40 |
| 36 | A1 | 1164 | G | N1-C2-N2 | -5.94 | 110.86 | 116.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 1928 | G | N3-C4-N9 | -5.94 | 122.44 | 126.00 |
| 36 | A5 | 1181 | U | C6-N1-C2 | 5.94 | 124.56 | 121.00 |
| 36 | A5 | 2424 | A | C5-C6-N6 | -5.94 | 118.95 | 123.70 |
| 1 | A2 | 1097 | U | C2-N1-C1' | 5.93 | 124.82 | 117.70 |
| 36 | A1 | 3361 | G | N3-C4-N9 | 5.93 | 129.56 | 126.00 |
| 36 | A5 | 1699 | A | N1-C6-N6 | 5.93 | 122.16 | 118.60 |
| 36 | A5 | 2184 | U | N3-C2-O2 | -5.93 | 118.05 | 122.20 |
| 36 | A1 | 78 | U | N1-C2-N3 | 5.93 | 118.46 | 114.90 |
| 36 | A1 | 637 | C | C5-C4-N4 | 5.93 | 124.35 | 120.20 |
| 36 | A1 | 1717 | U | N3-C2-O2 | -5.93 | 118.05 | 122.20 |
| 41 | BC | 212 | ASP | CB-CG-OD1 | 5.93 | 123.64 | 118.30 |
| 36 | A5 | 216 | G | C5-C6-O6 | -5.93 | 125.04 | 128.60 |
| 36 | A5 | 416 | A | C8-N9-C4 | -5.93 | 103.43 | 105.80 |
| 36 | A5 | 749 | C | N3-C4-C5 | -5.93 | 119.53 | 121.90 |
| 36 | A5 | 1456 | A | C8-N9-C4 | 5.93 | 108.17 | 105.80 |
| 36 | A5 | 2405 | C | N3-C2-O2 | -5.93 | 117.75 | 121.90 |
| 36 | A5 | 2518 | C | C2-N3-C4 | -5.93 | 116.93 | 119.90 |
| 36 | A5 | 3269 | U | N3-C2-O2 | -5.93 | 118.05 | 122.20 |
| 36 | A5 | 1175 | C | N3-C4-C5 | 5.93 | 124.27 | 121.90 |
| 1 | A2 | 393 | C | N3-C4-C5 | 5.93 | 124.27 | 121.90 |
| 36 | A1 | 2328 | U | N3-C2-O2 | -5.93 | 118.05 | 122.20 |
| 41 | BC | 189 | ALA | C-N-CA | -5.93 | 109.85 | 122.30 |
| 80 | A6 | 1149 | G | N1-C2-N2 | -5.93 | 110.86 | 116.20 |
| 36 | A5 | 283 | G | N1-C6-O6 | 5.93 | 123.46 | 119.90 |
| 36 | A5 | 1307 | G | P-O3'-C3' | 5.93 | 126.82 | 119.70 |
| 36 | A5 | 2988 | C | N1-C2-N3 | 5.93 | 123.35 | 119.20 |
| 37 | A7 | 92 | A | N9-C4-C5 | -5.93 | 103.43 | 105.80 |
| 1 | A2 | 1537 | C | C5-C6-N1 | 5.93 | 123.96 | 121.00 |
| 36 | A1 | 1472 | U | C2-N3-C4 | -5.93 | 123.44 | 127.00 |
| 36 | A1 | 1489 | A | C5-C6-N6 | -5.93 | 118.96 | 123.70 |
| 80 | A6 | 1085 | G | N3-C2-N2 | 5.93 | 124.05 | 119.90 |
| 36 | A5 | 667 | C | C2-N1-C1' | -5.93 | 112.28 | 118.80 |
| 36 | A5 | 2639 | G | C6-C5-N7 | -5.93 | 126.84 | 130.40 |
| 36 | A5 | 2849 | C | C6-N1-C2 | -5.93 | 117.93 | 120.30 |
| 1 | A2 | 703 | G | C8-N9-C4 | -5.93 | 104.03 | 106.40 |
| 80 | A6 | 49 | C | C5-C4-N4 | -5.93 | 116.05 | 120.20 |
| 80 | A6 | 272 | U | N1-C2-O2 | 5.93 | 126.95 | 122.80 |
| 38 | A8 | 12 | A | N7-C8-N9 | 5.93 | 116.76 | 113.80 |
| 38 | A8 | 33 | A | C8-N9-C4 | 5.93 | 108.17 | 105.80 |
| 36 | A1 | 2768 | U | N3-C2-O2 | -5.92 | 118.05 | 122.20 |
| 80 | A6 | 826 | U | C6-N1-C2 | -5.92 | 117.44 | 121.00 |
| 80 | A6 | 1428 | G | C5-C6-O6 | 5.92 | 132.16 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 36 | A5 | 1122 | U | N3-C2-O2 | -5.92 | 118.05 | 122.20 |
| 36 | A5 | 1369 | A | N1-C6-N6 | 5.92 | 122.16 | 118.60 |
| 36 | A5 | 2687 | G | C5-C6-N1 | 5.92 | 114.46 | 111.50 |
| 36 | A5 | 2965 | U | N1-C2-O2 | -5.92 | 118.65 | 122.80 |
| 36 | A5 | 3120 | C | N3-C4-C5 | -5.92 | 119.53 | 121.90 |
| 36 | A5 | 3215 | A | C8-N9-C4 | 5.92 | 108.17 | 105.80 |
| 44 | DF | 191 | VAL | C-N-CA | -5.92 | 109.86 | 122.30 |
| 1 | A2 | 538 | A | C4-C5-C6 | -5.92 | 114.04 | 117.00 |
| 1 | A2 | 1188 | G | C5-C6-O6 | -5.92 | 125.05 | 128.60 |
| 36 | A1 | 794 | U | N3-C2-O2 | -5.92 | 118.06 | 122.20 |
| 36 | A1 | 1881 | A | C5-C6-N6 | -5.92 | 118.96 | 123.70 |
| 36 | A1 | 3175 | U | C5-C6-N1 | -5.92 | 119.74 | 122.70 |
| 38 | A4 | 94 | C | C6-N1-C2 | 5.92 | 122.67 | 120.30 |
| 36 | A5 | 2709 | C | N3-C4-C5 | 5.92 | 124.27 | 121.90 |
| 38 | A8 | 99 | C | N3-C4-C5 | 5.92 | 124.27 | 121.90 |
| 38 | A4 | 145 | U | C5-C6-N1 | -5.92 | 119.74 | 122.70 |
| 36 | A5 | 1438 | U | N3-C2-O2 | -5.92 | 118.06 | 122.20 |
| 36 | A5 | 1866 | C | N3-C2-O2 | 5.92 | 126.04 | 121.90 |
| 36 | A1 | 301 | G | C6-C5-N7 | 5.92 | 133.95 | 130.40 |
| 36 | A1 | 635 | G | C4-C5-N7 | 5.92 | 113.17 | 110.80 |
| 36 | A1 | 860 | G | N3-C2-N2 | -5.92 | 115.76 | 119.90 |
| 36 | A1 | 885 | U | C4-C5-C6 | 5.92 | 123.25 | 119.70 |
| 36 | A1 | 1434 | G | N3-C4-C5 | -5.92 | 125.64 | 128.60 |
| 36 | A1 | 2942 | C | N3-C2-O2 | 5.92 | 126.04 | 121.90 |
| 36 | A5 | 965 | A | N3-C4-C5 | -5.92 | 122.66 | 126.80 |
| 36 | A5 | 2692 | A | C5-C6-N6 | 5.92 | 128.43 | 123.70 |
| 36 | A5 | 2943 | G | N1-C2-N2 | -5.92 | 110.87 | 116.20 |
| 37 | A7 | 12 | U | C5-C4-O4 | -5.92 | 122.35 | 125.90 |
| 38 | A8 | 24 | G | N3-C2-N2 | 5.92 | 124.04 | 119.90 |
| 40 | DB | 114 | VAL | CB-CA-C | -5.92 | 100.15 | 111.40 |
| 36 | A1 | 392 | G | C8-N9-C4 | 5.92 | 108.77 | 106.40 |
| 36 | A1 | 899 | U | N3-C2-O2 | -5.92 | 118.06 | 122.20 |
| 36 | A1 | 1443 | G | C4-C5-N7 | 5.92 | 113.17 | 110.80 |
| 36 | A1 | 1733 | G | N3-C4-N9 | 5.92 | 129.55 | 126.00 |
| 36 | A1 | 3047 | U | N1-C2-N3 | 5.92 | 118.45 | 114.90 |
| 37 | A3 | 91 | G | N1-C2-N3 | 5.92 | 127.45 | 123.90 |
| 36 | A5 | 1882 | G | N9-C4-C5 | 5.92 | 107.77 | 105.40 |
| 36 | A5 | 3326 | G | N1-C6-O6 | -5.92 | 116.35 | 119.90 |
| 36 | A1 | 1327 | C | C5-C6-N1 | 5.92 | 123.96 | 121.00 |
| 80 | A6 | 555 | A | C3'-C2'-C1' | -5.92 | 96.77 | 101.50 |
| 36 | A5 | 590 | G | C5-C6-O6 | -5.92 | 125.05 | 128.60 |
| 36 | A5 | 2347 | U | C2-N3-C4 | -5.92 | 123.45 | 127.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A2 | 151 | G | N1-C6-O6 | -5.91 | 116.35 | 119.90 |
| 36 | A1 | 1929 | G | N3-C4-C5 | 5.91 | 131.56 | 128.60 |
| 36 | A1 | 2383 | C | N1-C2-O2 | -5.91 | 115.35 | 118.90 |
| 40 | BB | 10 | ARG | CB-CA-C | -5.91 | 98.57 | 110.40 |
| 80 | A6 | 144 | U | N1-C2-N3 | 5.91 | 118.45 | 114.90 |
| 80 | A6 | 422 | G | C8-N9-C4 | -5.91 | 104.03 | 106.40 |
| 36 | A5 | 1178 | G | C5-N7-C8 | -5.91 | 101.34 | 104.30 |
| 42 | DD | 248 | ARG | NE-CZ-NH1 | 5.91 | 123.26 | 120.30 |
| 1 | A2 | 13 | C | N3-C4-C5 | 5.91 | 124.27 | 121.90 |
| 36 | A1 | 970 | A | N3-C4-N9 | -5.91 | 122.67 | 127.40 |
| 36 | A1 | 2816 | G | C4-C5-N7 | 5.91 | 113.17 | 110.80 |
| 36 | A1 | 3090 | U | C5-C6-N1 | -5.91 | 119.74 | 122.70 |
| 36 | A5 | 847 | A | N7-C8-N9 | -5.91 | 110.84 | 113.80 |
| 36 | A5 | 3075 | G | C5-C6-N1 | -5.91 | 108.54 | 111.50 |
| 36 | A1 | 667 | C | N3-C4-N4 | -5.91 | 113.86 | 118.00 |
| 36 | A1 | 2798 | C | N3-C4-C5 | -5.91 | 119.54 | 121.90 |
| 80 | A6 | 1640 | C | C2-N3-C4 | -5.91 | 116.94 | 119.90 |
| 36 | A5 | 201 | A | C2-N3-C4 | -5.91 | 107.64 | 110.60 |
| 36 | A5 | 365 | A | C5-C6-N6 | -5.91 | 118.97 | 123.70 |
| 36 | A5 | 2931 | C | C2-N3-C4 | -5.91 | 116.94 | 119.90 |
| 36 | A5 | 3055 | U | N1-C2-O2 | 5.91 | 126.94 | 122.80 |
| 36 | A1 | 2286 | U | C4-C5-C6 | 5.91 | 123.25 | 119.70 |
| 80 | A6 | 356 | G | C5-N7-C8 | 5.91 | 107.25 | 104.30 |
| 80 | A6 | 542 | A | C4-C5-C6 | 5.91 | 119.95 | 117.00 |
| 80 | A6 | 991 | G | C5-C6-O6 | -5.91 | 125.05 | 128.60 |
| 36 | A5 | 587 | U | C5-C6-N1 | -5.91 | 119.75 | 122.70 |
| 36 | A5 | 2114 | C | N1-C2-N3 | 5.91 | 123.34 | 119.20 |
| 41 | DC | 84 | ARG | NE-CZ-NH2 | -5.91 | 117.35 | 120.30 |
| 1 | A2 | 1274 | C | C4-C5-C6 | 5.91 | 120.35 | 117.40 |
| 36 | A1 | 388 | G | N9-C4-C5 | 5.91 | 107.76 | 105.40 |
| 80 | A6 | 471 | A | N1-C6-N6 | -5.91 | 115.06 | 118.60 |
| 80 | A6 | 901 | G | C5-N7-C8 | -5.91 | 101.35 | 104.30 |
| 80 | A6 | 1458 | G | C6-C5-N7 | -5.91 | 126.86 | 130.40 |
| 80 | A6 | 1472 | C | C2-N3-C4 | -5.91 | 116.95 | 119.90 |
| 36 | A5 | 894 | G | N3-C4-N9 | 5.91 | 129.54 | 126.00 |
| 36 | A5 | 3277 | U | C6-N1-C2 | -5.91 | 117.46 | 121.00 |
| 36 | A1 | 329 | U | N1-C2-O2 | -5.90 | 118.67 | 122.80 |
| 36 | A1 | 340 | C | C6-N1-C2 | -5.90 | 117.94 | 120.30 |
| 36 | A1 | 2957 | G | C5-N7-C8 | 5.90 | 107.25 | 104.30 |
| 80 | A6 | 945 | U | N1-C2-O2 | 5.90 | 126.93 | 122.80 |
| 1 | A2 | 1387 | G | C4-C5-N7 | 5.90 | 113.16 | 110.80 |
| 36 | A1 | 52 | A | N1-C6-N6 | 5.90 | 122.14 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 939 | U | N1-C2-N3 | 5.90 | 118.44 | 114.90 |
| 36 | A1 | 2210 | G | N1-C6-O6 | -5.90 | 116.36 | 119.90 |
| 49 | BL | 141 | ALA | N-CA-C | -5.90 | 95.06 | 111.00 |
| 80 | A6 | 976 | G | N3-C2-N2 | 5.90 | 124.03 | 119.90 |
| 80 | A6 | 1766 | A | C5-C6-N1 | -5.90 | 114.75 | 117.70 |
| 1 | A2 | 192 | U | N1-C2-O2 | 5.90 | 126.93 | 122.80 |
| 36 | A1 | 1838 | G | N9-C4-C5 | -5.90 | 103.04 | 105.40 |
| 36 | A5 | 2410 | U | N3-C4-O4 | -5.90 | 115.27 | 119.40 |
| 36 | A1 | 1191 | U | C4-C5-C6 | 5.90 | 123.24 | 119.70 |
| 36 | A1 | 2631 | U | N3-C4-C5 | 5.90 | 118.14 | 114.60 |
| 80 | A6 | 65 | A | C5-N7-C8 | -5.90 | 100.95 | 103.90 |
| 36 | A5 | 1189 | C | C6-N1-C2 | 5.90 | 122.66 | 120.30 |
| 36 | A5 | 2409 | G | N7-C8-N9 | 5.90 | 116.05 | 113.10 |
| 36 | A1 | 1073 | U | N1-C2-O2 | -5.90 | 118.67 | 122.80 |
| 36 | A1 | 2289 | U | C4-C5-C6 | 5.90 | 123.24 | 119.70 |
| 36 | A1 | 2595 | A | C6-C5-N7 | -5.90 | 128.17 | 132.30 |
| 80 | A6 | 280 | U | N1-C2-O2 | 5.90 | 126.93 | 122.80 |
| 36 | A5 | 2148 | U | N3-C2-O2 | 5.90 | 126.33 | 122.20 |
| 36 | A5 | 2320 | A | N1-C6-N6 | -5.90 | 115.06 | 118.60 |
| 36 | A5 | 2366 | C | C6-N1-C1' | -5.90 | 113.72 | 120.80 |
| 36 | A5 | 2617 | U | C6-N1-C2 | 5.90 | 124.54 | 121.00 |
| 36 | A5 | 3075 | G | C4-C5-C6 | 5.90 | 122.34 | 118.80 |
| 36 | A1 | 23 | A | N1-C6-N6 | 5.90 | 122.14 | 118.60 |
| 36 | A1 | 98 | G | C2-N3-C4 | -5.90 | 108.95 | 111.90 |
| 36 | A1 | 1137 | C | N3-C4-C5 | 5.90 | 124.26 | 121.90 |
| 36 | A1 | 1489 | A | N1-C2-N3 | 5.90 | 132.25 | 129.30 |
| 36 | A1 | 1514 | G | C8-N9-C4 | -5.90 | 104.04 | 106.40 |
| 36 | A1 | 2825 | C | C2-N3-C4 | 5.90 | 122.85 | 119.90 |
| 80 | A6 | 1476 | C | C6-N1-C2 | -5.90 | 117.94 | 120.30 |
| 36 | A5 | 2426 | U | N3-C2-O2 | -5.90 | 118.07 | 122.20 |
| 1 | A2 | 1503 | A | C5-N7-C8 | -5.89 | 100.95 | 103.90 |
| 36 | A1 | 1174 | G | N9-C4-C5 | -5.89 | 103.04 | 105.40 |
| 36 | A1 | 1269 | U | N1-C2-O2 | 5.89 | 126.93 | 122.80 |
| 36 | A1 | 1329 | U | C2-N3-C4 | -5.89 | 123.46 | 127.00 |
| 36 | A1 | 1386 | A | C5-C6-N1 | 5.89 | 120.65 | 117.70 |
| 36 | A1 | 1444 | G | C4-C5-N7 | 5.89 | 113.16 | 110.80 |
| 36 | A1 | 1556 | C | C2-N1-C1' | 5.89 | 125.28 | 118.80 |
| 36 | A1 | 3215 | A | C8-N9-C4 | 5.89 | 108.16 | 105.80 |
| 52 | BO | 3[B] | SER | O-C-N | 5.89 | 132.13 | 122.70 |
| 36 | A1 | 347 | G | N9-C4-C5 | -5.89 | 103.04 | 105.40 |
| 36 | A1 | 2816 | G | C8-N9-C4 | 5.89 | 108.76 | 106.40 |
| 36 | A1 | 3045 | G | C2-N3-C4 | 5.89 | 114.85 | 111.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 80 | A6 | 640 | U | N3-C2-O2 | -5.89 | 118.08 | 122.20 |
| 36 | A5 | 426 | G | N7-C8-N9 | -5.89 | 110.15 | 113.10 |
| 36 | A5 | 874 | U | C5-C6-N1 | -5.89 | 119.75 | 122.70 |
| 36 | A5 | 2188 | A | N7-C8-N9 | -5.89 | 110.85 | 113.80 |
| 36 | A5 | 2915 | U | N3-C2-O2 | -5.89 | 118.08 | 122.20 |
| 36 | A5 | 2992 | U | N3-C2-O2 | -5.89 | 118.08 | 122.20 |
| 59 | DV | 33 | ASN | CB-CA-C | -5.89 | 98.62 | 110.40 |
| 36 | A1 | 2142 | A | N3-C4-N9 | 5.89 | 132.11 | 127.40 |
| 38 | A4 | 10 | A | C5-C6-N1 | 5.89 | 120.65 | 117.70 |
| 36 | A5 | 1586 | G | N3-C4-C5 | -5.89 | 125.66 | 128.60 |
| 36 | A5 | 2292 | U | C2-N3-C4 | -5.89 | 123.47 | 127.00 |
| 36 | A5 | 3088 | G | C5-N7-C8 | -5.89 | 101.36 | 104.30 |
| 36 | A1 | 361 | A | C5-C6-N1 | 5.89 | 120.64 | 117.70 |
| 36 | A1 | 2293 | C | C2-N3-C4 | -5.89 | 116.95 | 119.90 |
| 36 | A5 | 345 | G | C6-N1-C2 | -5.89 | 121.57 | 125.10 |
| 36 | A5 | 509 | U | N1-C2-N3 | 5.89 | 118.43 | 114.90 |
| 36 | A5 | 1311 | G | N1-C2-N3 | -5.89 | 120.37 | 123.90 |
| 1 | A2 | 308 | C | C2-N3-C4 | -5.89 | 116.96 | 119.90 |
| 1 | A2 | 1314 | U | N3-C2-O2 | -5.89 | 118.08 | 122.20 |
| 36 | A5 | 1206 | G | C4-C5-N7 | -5.89 | 108.44 | 110.80 |
| 36 | A1 | 351 | A | N7-C8-N9 | -5.89 | 110.86 | 113.80 |
| 36 | A1 | 922 | U | C5-C4-O4 | 5.89 | 129.43 | 125.90 |
| 36 | A1 | 1802 | C | C5-C4-N4 | -5.89 | 116.08 | 120.20 |
| 80 | A6 | 184 | C | C6-N1-C2 | 5.89 | 122.65 | 120.30 |
| 80 | A6 | 465 | G | C8-N9-C4 | 5.89 | 108.75 | 106.40 |
| 1 | A2 | 416 | A | C8-N9-C4 | 5.88 | 108.15 | 105.80 |
| 36 | A1 | 2203 | U | C6-N1-C2 | -5.88 | 117.47 | 121.00 |
| 36 | A1 | 2933 | A | C4-C5-N7 | 5.88 | 113.64 | 110.70 |
| 38 | A4 | 36 | G | N1-C6-O6 | -5.88 | 116.37 | 119.90 |
| 36 | A5 | 874 | U | N3-C4-O4 | -5.88 | 115.28 | 119.40 |
| 36 | A5 | 1481 | A | N3-C4-C5 | -5.88 | 122.68 | 126.80 |
| 36 | A5 | 1834 | U | C6-N1-C2 | 5.88 | 124.53 | 121.00 |
| 36 | A5 | 1892 | G | N3-C2-N2 | -5.88 | 115.78 | 119.90 |
| 36 | A5 | 2118 | C | N1-C2-O2 | 5.88 | 122.43 | 118.90 |
| 36 | A5 | 2271 | A | N1-C6-N6 | -5.88 | 115.07 | 118.60 |
| 36 | A5 | 2843 | U | C2-N1-C1' | 5.88 | 124.76 | 117.70 |
| 38 | A8 | 55 | U | N3-C4-C5 | -5.88 | 111.07 | 114.60 |
| 36 | A1 | 1198 | C | C6-N1-C2 | -5.88 | 117.95 | 120.30 |
| 36 | A1 | 1928 | G | N3-C4-C5 | 5.88 | 131.54 | 128.60 |
| 38 | A4 | 1 | A | C5-C6-N6 | -5.88 | 118.99 | 123.70 |
| 36 | A5 | 2113 | A | C8-N9-C4 | 5.88 | 108.15 | 105.80 |
| 36 | A1 | 1056 | U | C5-C6-N1 | 5.88 | 125.64 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 80 | A6 | 5 | U | N3-C4-C5 | -5.88 | 111.07 | 114.60 |
| 80 | A6 | 999 | U | N1-C2-O2 | 5.88 | 126.92 | 122.80 |
| 36 | A5 | 993 | G | C8-N9-C4 | -5.88 | 104.05 | 106.40 |
| 36 | A5 | 1317 | A | N3-C4-N9 | 5.88 | 132.10 | 127.40 |
| 36 | A5 | 2549 | G | C4-N9-C1' | 5.88 | 134.15 | 126.50 |
| 36 | A1 | 3058 | U | C6-N1-C1' | -5.88 | 112.97 | 121.20 |
| 36 | A5 | 591 | G | N3-C4-N9 | 5.88 | 129.53 | 126.00 |
| 36 | A5 | 3226 | A | N1-C2-N3 | -5.88 | 126.36 | 129.30 |
| 1 | A2 | 997 | G | N9-C4-C5 | -5.88 | 103.05 | 105.40 |
| 36 | A1 | 157 | A | C6-N1-C2 | -5.88 | 115.07 | 118.60 |
| 36 | A1 | 359 | U | N3-C4-C5 | 5.88 | 118.13 | 114.60 |
| 36 | A1 | 617 | G | C6-N1-C2 | -5.88 | 121.57 | 125.10 |
| 36 | A1 | 825 | U | N3-C4-O4 | -5.88 | 115.29 | 119.40 |
| 36 | A1 | 1124 | U | N1-C2-O2 | 5.88 | 126.92 | 122.80 |
| 36 | A1 | 1269 | U | C2-N1-C1' | 5.88 | 124.75 | 117.70 |
| 36 | A1 | 2325 | G | C8-N9-C4 | -5.88 | 104.05 | 106.40 |
| 80 | A6 | 13 | C | C5-C6-N1 | -5.88 | 118.06 | 121.00 |
| 80 | A6 | 1641 | C | N1-C2-O2 | -5.88 | 115.37 | 118.90 |
| 31 | Cd | 36 | LEU | CA-CB-CG | 5.88 | 128.82 | 115.30 |
| 36 | A5 | 908 | G | C8-N9-C1' | -5.88 | 119.36 | 127.00 |
| 36 | A5 | 2745 | G | C5-C6-O6 | -5.88 | 125.07 | 128.60 |
| 36 | A5 | 2893 | C | C4-C5-C6 | 5.88 | 120.34 | 117.40 |
| 36 | A1 | 663 | C | C5-C4-N4 | -5.88 | 116.09 | 120.20 |
| 36 | A1 | 875 | G | C6-C5-N7 | 5.88 | 133.93 | 130.40 |
| 36 | A1 | 953 | G | N3-C4-C5 | 5.88 | 131.54 | 128.60 |
| 36 | A1 | 3077 | A | N9-C4-C5 | 5.88 | 108.15 | 105.80 |
| 38 | A4 | 6 | U | C2-N3-C4 | -5.88 | 123.47 | 127.00 |
| 80 | A6 | 1739 | C | N1-C2-O2 | -5.88 | 115.38 | 118.90 |
| 36 | A5 | 861 | C | N1-C2-O2 | -5.88 | 115.37 | 118.90 |
| 36 | A5 | 2961 | G | N7-C8-N9 | 5.88 | 116.04 | 113.10 |
| 1 | A2 | 1776 | A | N9-C4-C5 | 5.88 | 108.15 | 105.80 |
| 36 | A1 | 905 | U | C5-C6-N1 | -5.88 | 119.76 | 122.70 |
| 36 | A1 | 98 | G | N1-C2-N2 | -5.87 | 110.91 | 116.20 |
| 36 | A1 | 214 | G | C5-N7-C8 | 5.87 | 107.24 | 104.30 |
| 36 | A1 | 975 | C | N1-C2-O2 | -5.87 | 115.38 | 118.90 |
| 80 | A6 | 114 | C | C2-N1-C1' | 5.87 | 125.26 | 118.80 |
| 80 | A6 | 1654 | G | N1-C2-N3 | 5.87 | 127.42 | 123.90 |
| 36 | A5 | 1043 | C | C5-C6-N1 | -5.87 | 118.06 | 121.00 |
| 36 | A5 | 2910 | A | N1-C6-N6 | -5.87 | 115.08 | 118.60 |
| 1 | A2 | 1479 | A | N1-C6-N6 | 5.87 | 122.12 | 118.60 |
| 36 | A1 | 142 | C | N3-C4-N4 | 5.87 | 122.11 | 118.00 |
| 80 | A6 | 385 | A | C4-C5-N7 | -5.87 | 107.76 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A2 | 1798 | U | C2-N1-C1' | 5.87 | 124.74 | 117.70 |
| 49 | DL | 46 | ILE | CG1-CB-CG2 | -5.87 | 98.49 | 111.40 |
| 36 | A1 | 696 | C | N1-C2-O2 | 5.87 | 122.42 | 118.90 |
| 36 | A1 | 1434 | G | C5-N7-C8 | 5.87 | 107.23 | 104.30 |
| 36 | A1 | 1719 | G | C4-C5-N7 | 5.87 | 113.15 | 110.80 |
| 36 | A1 | 2370 | G | C5-C6-O6 | -5.87 | 125.08 | 128.60 |
| 36 | A5 | 1838 | G | N7-C8-N9 | -5.87 | 110.17 | 113.10 |
| 36 | A5 | 1907 | C | C5-C6-N1 | 5.87 | 123.94 | 121.00 |
| 36 | A5 | 3112 | G | C5-C6-O6 | -5.87 | 125.08 | 128.60 |
| 1 | A2 | 1542 | G | C5-C6-O6 | 5.87 | 132.12 | 128.60 |
| 36 | A1 | 504 | A | N7-C8-N9 | -5.87 | 110.87 | 113.80 |
| 36 | A1 | 901 | G | N1-C6-O6 | 5.87 | 123.42 | 119.90 |
| 36 | A1 | 2623 | G | N1-C2-N2 | -5.87 | 110.92 | 116.20 |
| 36 | A1 | 251 | G | C8-N9-C1' | -5.87 | 119.38 | 127.00 |
| 36 | A1 | 776 | U | N3-C2-O2 | -5.87 | 118.09 | 122.20 |
| 36 | A1 | 1298 | C | C6-N1-C2 | -5.87 | 117.95 | 120.30 |
| 36 | A1 | 1300 | G | N7-C8-N9 | -5.87 | 110.17 | 113.10 |
| 36 | A1 | 2131 | A | N1-C6-N6 | 5.87 | 122.12 | 118.60 |
| 36 | A1 | 2775 | U | C5-C6-N1 | -5.87 | 119.77 | 122.70 |
| 79 | Bp | 71 | VAL | CB-CA-C | -5.87 | 100.26 | 111.40 |
| 36 | A5 | 593 | C | C2-N1-C1' | 5.87 | 125.25 | 118.80 |
| 36 | A5 | 2641 | U | N1-C2-O2 | -5.87 | 118.69 | 122.80 |
| 36 | A5 | 2744 | U | C5-C6-N1 | -5.87 | 119.77 | 122.70 |
| 36 | A1 | 1778 | G | C6-C5-N7 | -5.86 | 126.88 | 130.40 |
| 36 | A1 | 2669 | G | N1-C2-N3 | 5.86 | 127.42 | 123.90 |
| 80 | A6 | 298 | C | C6-N1-C2 | -5.86 | 117.95 | 120.30 |
| 36 | A5 | 1495 | U | N3-C4-C5 | -5.86 | 111.08 | 114.60 |
| 36 | A5 | 2145 | A | C5-C6-N1 | 5.86 | 120.63 | 117.70 |
| 36 | A5 | 3216 | G | N1-C2-N3 | 5.86 | 127.42 | 123.90 |
| 1 | A2 | 1745 | G | C6-C5-N7 | -5.86 | 126.88 | 130.40 |
| 80 | A6 | 1037 | C | C2-N1-C1' | -5.86 | 112.35 | 118.80 |
| 36 | A5 | 2346 | C | C5-C4-N4 | -5.86 | 116.10 | 120.20 |
| 1 | A2 | 628 | G | N1-C2-N2 | -5.86 | 110.92 | 116.20 |
| 36 | A1 | 80 | G | N1-C6-O6 | -5.86 | 116.38 | 119.90 |
| 36 | A1 | 1791 | C | C2-N3-C4 | -5.86 | 116.97 | 119.90 |
| 36 | A1 | 2819 | A | C6-N1-C2 | -5.86 | 115.08 | 118.60 |
| 36 | A1 | 3259 | U | C2-N3-C4 | -5.86 | 123.48 | 127.00 |
| 36 | A5 | 2248 | C | C5-C6-N1 | -5.86 | 118.07 | 121.00 |
| 36 | A5 | 2792 | A | C2-N3-C4 | 5.86 | 113.53 | 110.60 |
| 36 | A5 | 3340 | G | N1-C6-O6 | -5.86 | 116.38 | 119.90 |
| 36 | A1 | 86 | G | C5-N7-C8 | 5.86 | 107.23 | 104.30 |
| 36 | A1 | 148 | G | N1-C6-O6 | 5.86 | 123.42 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 80 | A6 | 815 | G | N7-C8-N9 | 5.86 | 116.03 | 113.10 |
| 36 | A5 | 2338 | C | N3-C4-C5 | -5.86 | 119.56 | 121.90 |
| 36 | A1 | 639 | G | C5-C6-O6 | -5.86 | 125.09 | 128.60 |
| 36 | A1 | 1388 | U | C2-N3-C4 | -5.86 | 123.49 | 127.00 |
| 36 | A1 | 2541 | U | C6-N1-C1' | -5.86 | 113.00 | 121.20 |
| 80 | A6 | 1130 | G | C6-N1-C2 | -5.86 | 121.59 | 125.10 |
| 80 | A6 | 1594 | G | C8-N9-C4 | 5.86 | 108.74 | 106.40 |
| 36 | A5 | 2314 | U | C6-N1-C1' | -5.86 | 113.00 | 121.20 |
| 36 | A5 | 2531 | C | C6-N1-C1' | -5.86 | 113.77 | 120.80 |
| 36 | A5 | 3296 | A | C8-N9-C4 | 5.86 | 108.14 | 105.80 |
| 36 | A1 | 343 | U | C5-C6-N1 | -5.86 | 119.77 | 122.70 |
| 36 | A1 | 1431 | G | C8-N9-C4 | 5.86 | 108.74 | 106.40 |
| 36 | A1 | 2877 | G | C5-C6-O6 | 5.86 | 132.11 | 128.60 |
| 80 | A6 | 1320 | U | C2-N1-C1' | 5.86 | 124.73 | 117.70 |
| 80 | A6 | 1490 | C | C6-N1-C2 | -5.86 | 117.96 | 120.30 |
| 36 | A5 | 1911 | A | C2-N3-C4 | -5.86 | 107.67 | 110.60 |
| 36 | A5 | 2711 | C | C4-C5-C6 | 5.86 | 120.33 | 117.40 |
| 36 | A1 | 857 | G | C4-C5-N7 | 5.85 | 113.14 | 110.80 |
| 80 | A6 | 1304 | G | C4-C5-N7 | 5.85 | 113.14 | 110.80 |
| 36 | A5 | 795 | G | C5-N7-C8 | 5.85 | 107.23 | 104.30 |
| 1 | A2 | 611 | U | N1-C2-O2 | -5.85 | 118.70 | 122.80 |
| 36 | A5 | 376 | G | N1-C6-O6 | -5.85 | 116.39 | 119.90 |
| 36 | A5 | 1429 | G | C2-N3-C4 | -5.85 | 108.97 | 111.90 |
| 36 | A5 | 1437 | C | C2-N1-C1' | 5.85 | 125.24 | 118.80 |
| 36 | A5 | 1495 | U | C2-N1-C1' | 5.85 | 124.72 | 117.70 |
| 36 | A5 | 3113 | A | C5-C6-N1 | 5.85 | 120.63 | 117.70 |
| 36 | A1 | 2418 | G | C5-C6-N1 | 5.85 | 114.42 | 111.50 |
| 36 | A5 | 1136 | A | C2-N3-C4 | 5.85 | 113.53 | 110.60 |
| 36 | A1 | 2369 | G | C5-C6-O6 | -5.85 | 125.09 | 128.60 |
| 36 | A1 | 2611 | U | N3-C4-O4 | -5.85 | 115.31 | 119.40 |
| 80 | A6 | 389 | G | N3-C4-N9 | 5.85 | 129.51 | 126.00 |
| 4 | CC | 113 | LEU | CA-CB-CG | 5.85 | 128.75 | 115.30 |
| 36 | A5 | 2643 | A | N1-C2-N3 | -5.85 | 126.38 | 129.30 |
| 36 | A1 | 926 | A | N1-C2-N3 | -5.85 | 126.38 | 129.30 |
| 36 | A1 | 1510 | G | C6-C5-N7 | -5.85 | 126.89 | 130.40 |
| 77 | Bn | 9 | ARG | NE-CZ-NH1 | 5.85 | 123.22 | 120.30 |
| 1 | A2 | 21 | U | N3-C2-O2 | -5.84 | 118.11 | 122.20 |
| 1 | A2 | 810 | G | N1-C6-O6 | 5.84 | 123.41 | 119.90 |
| 1 | A2 | 1536 | G | C4-N9-C1' | 5.84 | 134.10 | 126.50 |
| 36 | A1 | 1610 | G | N1-C6-O6 | 5.84 | 123.41 | 119.90 |
| 36 | A1 | 2127 | U | N1-C2-O2 | -5.84 | 118.71 | 122.80 |
| 36 | A1 | 2193 | U | C2-N3-C4 | -5.84 | 123.49 | 127.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 2547 | A | C8-N9-C1' | -5.84 | 117.18 | 127.70 |
| 38 | A4 | 120 | C | N1-C2-O2 | -5.84 | 115.39 | 118.90 |
| 80 | A6 | 757 | A | C8-N9-C4 | 5.84 | 108.14 | 105.80 |
| 36 | A5 | 2141 | U | N3-C2-O2 | -5.84 | 118.11 | 122.20 |
| 36 | A5 | 2361 | A | N3-C4-N9 | 5.84 | 132.07 | 127.40 |
| 36 | A5 | 3019 | U | N3-C4-C5 | 5.84 | 118.11 | 114.60 |
| 36 | A1 | 363 | G | C6-N1-C2 | -5.84 | 121.59 | 125.10 |
| 36 | A1 | 2298 | U | C6-N1-C2 | 5.84 | 124.51 | 121.00 |
| 36 | A1 | 2602 | G | C5-N7-C8 | 5.84 | 107.22 | 104.30 |
| 38 | A4 | 125 | U | C6-N1-C1' | -5.84 | 113.02 | 121.20 |
| 36 | A5 | 1490 | A | C2-N3-C4 | -5.84 | 107.68 | 110.60 |
| 36 | A5 | 3241 | G | C4-C5-N7 | 5.84 | 113.14 | 110.80 |
| 1 | A2 | 1340 | U | C5-C4-O4 | 5.84 | 129.41 | 125.90 |
| 36 | A1 | 959 | C | N3-C2-O2 | 5.84 | 125.99 | 121.90 |
| 36 | A1 | 1387 | G | C5-C6-O6 | 5.84 | 132.10 | 128.60 |
| 36 | A1 | 1907 | C | N3-C4-C5 | -5.84 | 119.56 | 121.90 |
| 36 | A1 | 2522 | G | C4-N9-C1' | 5.84 | 134.09 | 126.50 |
| 36 | A1 | 2626 | A | C5-C6-N1 | -5.84 | 114.78 | 117.70 |
| 36 | A1 | 2756 | C | N3-C4-N4 | 5.84 | 122.09 | 118.00 |
| 80 | A6 | 376 | C | C2-N3-C4 | -5.84 | 116.98 | 119.90 |
| 80 | A6 | 1340 | U | N1-C2-O2 | 5.84 | 126.89 | 122.80 |
| 36 | A5 | 994 | G | C6-N1-C2 | -5.84 | 121.59 | 125.10 |
| 36 | A5 | 1477 | A | N1-C2-N3 | 5.84 | 132.22 | 129.30 |
| 36 | A5 | 1902 | G | C5-C6-N1 | 5.84 | 114.42 | 111.50 |
| 36 | A5 | 1939 | G | N1-C2-N2 | -5.84 | 110.94 | 116.20 |
| 36 | A5 | 2381 | G | C2-N3-C4 | 5.84 | 114.82 | 111.90 |
| 38 | A4 | 57 | C | C5-C6-N1 | -5.84 | 118.08 | 121.00 |
| 38 | A4 | 73 | U | C4-C5-C6 | -5.84 | 116.20 | 119.70 |
| 56 | BS | 117 | ARG | NE-CZ-NH1 | -5.84 | 117.38 | 120.30 |
| 36 | A5 | 1086 | C | N1-C2-O2 | 5.84 | 122.40 | 118.90 |
| 36 | A5 | 1181 | U | C2-N3-C4 | -5.84 | 123.50 | 127.00 |
| 36 | A5 | 1917 | C | C2-N3-C4 | -5.84 | 116.98 | 119.90 |
| 36 | A5 | 2838 | A | C6-N1-C2 | -5.84 | 115.10 | 118.60 |
| 36 | A5 | 3224 | G | N1-C6-O6 | -5.84 | 116.40 | 119.90 |
| 36 | A5 | 3373 | U | C5-C6-N1 | -5.84 | 119.78 | 122.70 |
| 80 | A6 | 96 | G | C8-N9-C4 | -5.84 | 104.06 | 106.40 |
| 80 | A6 | 359 | A | N3-C4-C5 | 5.84 | 130.89 | 126.80 |
| 36 | A5 | 741 | U | C2-N3-C4 | 5.84 | 130.50 | 127.00 |
| 36 | A5 | 2976 | A | C8-N9-C4 | 5.84 | 108.14 | 105.80 |
| 36 | A5 | 3100 | U | N1-C2-O2 | 5.84 | 126.89 | 122.80 |
| 36 | A1 | 2200 | U | N3-C4-C5 | -5.84 | 111.10 | 114.60 |
| 36 | A1 | 3316 | A | C5-N7-C8 | -5.84 | 100.98 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 2305 | G | N1-C2-N2 | -5.84 | 110.95 | 116.20 |
| 36 | A5 | 2846 | U | C5-C6-N1 | -5.84 | 119.78 | 122.70 |
| 36 | A5 | 3212 | C | C5-C6-N1 | -5.84 | 118.08 | 121.00 |
| 80 | A6 | 240 | U | N3-C2-O2 | -5.83 | 118.12 | 122.20 |
| 80 | A6 | 355 | G | C5-N7-C8 | 5.83 | 107.22 | 104.30 |
| 80 | A6 | 1540 | G | N1-C6-O6 | -5.83 | 116.40 | 119.90 |
| 80 | A6 | 1658 | G | C5-C6-O6 | 5.83 | 132.10 | 128.60 |
| 36 | A1 | 3092 | C | C5-C6-N1 | -5.83 | 118.08 | 121.00 |
| 51 | BN | 105 | ARG | NE-CZ-NH2 | -5.83 | 117.38 | 120.30 |
| 64 | Ba | 115 | LYS | C-N-CA | -5.83 | 110.05 | 122.30 |
| 36 | A5 | 680 | G | N3-C2-N2 | 5.83 | 123.98 | 119.90 |
| 36 | A5 | 1485 | G | N3-C4-C5 | -5.83 | 125.68 | 128.60 |
| 1 | A2 | 542 | A | C4-C5-N7 | 5.83 | 113.61 | 110.70 |
| 44 | BF | 110 | ARG | NE-CZ-NH2 | -5.83 | 117.39 | 120.30 |
| 80 | A6 | 1014 | G | N1-C2-N2 | -5.83 | 110.95 | 116.20 |
| 36 | A5 | 272 | G | C2-N3-C4 | -5.83 | 108.98 | 111.90 |
| 36 | A5 | 966 | U | C2-N1-C1' | 5.83 | 124.70 | 117.70 |
| 36 | A5 | 1133 | A | N1-C2-N3 | -5.83 | 126.39 | 129.30 |
| 36 | A5 | 1247 | U | C5-C6-N1 | 5.83 | 125.62 | 122.70 |
| 36 | A5 | 3267 | A | N1-C2-N3 | 5.83 | 132.22 | 129.30 |
| 1 | A2 | 1291 | G | N3-C2-N2 | -5.83 | 115.82 | 119.90 |
| 36 | A1 | 1144 | U | N3-C4-O4 | -5.83 | 115.32 | 119.40 |
| 36 | A1 | 1586 | G | N1-C2-N2 | -5.83 | 110.95 | 116.20 |
| 38 | A4 | 25 | G | N1-C6-O6 | -5.83 | 116.40 | 119.90 |
| 36 | A5 | 795 | G | N1-C2-N3 | -5.83 | 120.40 | 123.90 |
| 36 | A5 | 815 | G | N9-C4-C5 | 5.83 | 107.73 | 105.40 |
| 37 | A7 | 5 | G | C8-N9-C4 | 5.83 | 108.73 | 106.40 |
| 36 | A1 | 66 | A | C8-N9-C4 | 5.83 | 108.13 | 105.80 |
| 36 | A1 | 100 | A | C2-N3-C4 | -5.83 | 107.69 | 110.60 |
| 36 | A1 | 1615 | C | C5-C6-N1 | -5.83 | 118.09 | 121.00 |
| 36 | A1 | 1849 | C | N3-C2-O2 | 5.83 | 125.98 | 121.90 |
| 36 | A1 | 2737 | C | N1-C2-O2 | -5.83 | 115.40 | 118.90 |
| 36 | A1 | 3227 | A | C2-N3-C4 | -5.83 | 107.69 | 110.60 |
| 37 | A3 | 83 | U | N3-C4-C5 | 5.83 | 118.10 | 114.60 |
| 80 | A6 | 858 | G | C4-N9-C1' | 5.83 | 134.08 | 126.50 |
| 36 | A5 | 153 | U | C5-C4-O4 | 5.83 | 129.40 | 125.90 |
| 36 | A5 | 968 | G | C8-N9-C4 | 5.83 | 108.73 | 106.40 |
| 36 | A5 | 1669 | C | C6-N1-C2 | 5.83 | 122.63 | 120.30 |
| 36 | A5 | 3130 | A | C6-N1-C2 | -5.83 | 115.10 | 118.60 |
| 36 | A1 | 3077 | A | C4-C5-C6 | 5.83 | 119.91 | 117.00 |
| 36 | A5 | 432 | G | C2-N3-C4 | -5.83 | 108.99 | 111.90 |
| 36 | A1 | 1190 | A | C2-N3-C4 | 5.83 | 113.51 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 2640 | A | N1-C6-N6 | -5.83 | 115.11 | 118.60 |
| 36 | A5 | 96 | G | N1-C2-N3 | 5.83 | 127.40 | 123.90 |
| 36 | A5 | 1607 | U | C2-N3-C4 | -5.83 | 123.50 | 127.00 |
| 36 | A5 | 2920 | U | C4-C5-C6 | 5.83 | 123.19 | 119.70 |
| 36 | A5 | 3095 | U | C2-N3-C4 | -5.83 | 123.50 | 127.00 |
| 37 | A7 | 106 | U | C5-C6-N1 | -5.83 | 119.79 | 122.70 |
| 36 | A1 | 743 | C | N3-C4-C5 | 5.82 | 124.23 | 121.90 |
| 36 | A1 | 2647 | A | C2-N3-C4 | 5.82 | 113.51 | 110.60 |
| 36 | A1 | 2990 | G | N9-C4-C5 | 5.82 | 107.73 | 105.40 |
| 36 | A1 | 3111 | U | N1-C2-O2 | 5.82 | 126.88 | 122.80 |
| 80 | A6 | 1458 | G | C4-N9-C1' | 5.82 | 134.07 | 126.50 |
| 36 | A5 | 2584 | G | C4-C5-N7 | 5.82 | 113.13 | 110.80 |
| 36 | A5 | 2817 | A | C2-N3-C4 | 5.82 | 113.51 | 110.60 |
| 38 | A8 | 16 | G | N1-C2-N3 | 5.82 | 127.39 | 123.90 |
| 36 | A1 | 46 | U | C5-C4-O4 | 5.82 | 129.39 | 125.90 |
| 36 | A1 | 929 | A | C6-N1-C2 | -5.82 | 115.11 | 118.60 |
| 36 | A1 | 1175 | C | C5-C6-N1 | -5.82 | 118.09 | 121.00 |
| 36 | A1 | 3192 | U | C5-C6-N1 | -5.82 | 119.79 | 122.70 |
| 38 | A4 | 10 | A | C8-N9-C4 | -5.82 | 103.47 | 105.80 |
| 80 | A6 | 560 | U | N3-C4-O4 | 5.82 | 123.47 | 119.40 |
| 36 | A5 | 1116 | G | C5-C6-O6 | 5.82 | 132.09 | 128.60 |
| 1 | A2 | 294 | C | C6-N1-C2 | 5.82 | 122.63 | 120.30 |
| 1 | A2 | 1291 | G | N3-C4-N9 | -5.82 | 122.51 | 126.00 |
| 36 | A1 | 1589 | A | N9-C4-C5 | -5.82 | 103.47 | 105.80 |
| 36 | A1 | 2299 | A | N1-C2-N3 | 5.82 | 132.21 | 129.30 |
| 38 | A4 | 79 | A | N7-C8-N9 | 5.82 | 116.71 | 113.80 |
| 80 | A6 | 419 | G | N1-C6-O6 | -5.82 | 116.41 | 119.90 |
| 36 | A5 | 2516 | U | C5-C4-O4 | -5.82 | 122.41 | 125.90 |
| 40 | DB | 19 | ARG | NE-CZ-NH2 | -5.82 | 117.39 | 120.30 |
| 36 | A1 | 159 | A | N9-C4-C5 | -5.82 | 103.47 | 105.80 |
| 36 | A5 | 2846 | U | C2-N3-C4 | -5.82 | 123.51 | 127.00 |
| 36 | A1 | 1950 | U | C5-C6-N1 | 5.82 | 125.61 | 122.70 |
| 36 | A1 | 2130 | G | N1-C2-N2 | -5.82 | 110.97 | 116.20 |
| 36 | A1 | 3140 | G | C8-N9-C1' | -5.82 | 119.44 | 127.00 |
| 36 | A1 | 3312 | U | N1-C2-N3 | 5.82 | 118.39 | 114.90 |
| 44 | BF | 215 | GLY | N-CA-C | -5.82 | 98.56 | 113.10 |
| 56 | BS | 115 | ARG | NE-CZ-NH1 | 5.82 | 123.21 | 120.30 |
| 80 | A6 | 1788 | G | C4-C5-N7 | -5.82 | 108.47 | 110.80 |
| 36 | A5 | 798 | G | C5-C6-N1 | 5.82 | 114.41 | 111.50 |
| 36 | A5 | 2370 | G | N1-C2-N3 | 5.82 | 127.39 | 123.90 |
| 1 | A2 | 1666 | U | C6-N1-C2 | -5.82 | 117.51 | 121.00 |
| 36 | A1 | 388 | G | N3-C2-N2 | -5.82 | 115.83 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 859 | G | N1-C6-O6 | 5.82 | 123.39 | 119.90 |
| 36 | A1 | 973 | A | N1-C2-N3 | 5.82 | 132.21 | 129.30 |
| 36 | A1 | 2960 | C | N1-C2-O2 | -5.82 | 115.41 | 118.90 |
| 36 | A1 | 3278 | C | C2-N1-C1' | 5.82 | 125.20 | 118.80 |
| 80 | A6 | 341 | A | N9-C4-C5 | 5.82 | 108.13 | 105.80 |
| 80 | A6 | 1037 | C | C5-C6-N1 | -5.82 | 118.09 | 121.00 |
| 36 | A5 | 689 | U | N3-C4-O4 | -5.82 | 115.33 | 119.40 |
| 36 | A5 | 916 | G | N3-C4-N9 | -5.82 | 122.51 | 126.00 |
| 36 | A5 | 1045 | C | N1-C2-N3 | 5.82 | 123.27 | 119.20 |
| 36 | A5 | 1127 | G | C5-C6-N1 | 5.82 | 114.41 | 111.50 |
| 36 | A5 | 2971 | A | C2-N3-C4 | 5.82 | 113.51 | 110.60 |
| 36 | A5 | 3099 | C | C4-C5-C6 | 5.82 | 120.31 | 117.40 |
| 36 | A1 | 1948 | G | N1-C6-O6 | 5.81 | 123.39 | 119.90 |
| 80 | A6 | 1509 | C | N1-C2-O2 | 5.81 | 122.39 | 118.90 |
| 36 | A5 | 404 | G | N3-C2-N2 | -5.81 | 115.83 | 119.90 |
| 36 | A5 | 2920 | U | N1-C2-O2 | -5.81 | 118.73 | 122.80 |
| 1 | A2 | 344 | A | N1-C6-N6 | -5.81 | 115.11 | 118.60 |
| 36 | A1 | 1137 | C | N1-C2-O2 | -5.81 | 115.41 | 118.90 |
| 36 | A1 | 1523 | U | C5-C4-O4 | -5.81 | 122.41 | 125.90 |
| 36 | A1 | 1947 | G | N3-C4-C5 | 5.81 | 131.51 | 128.60 |
| 36 | A1 | 2385 | G | N3-C4-C5 | 5.81 | 131.51 | 128.60 |
| 36 | A1 | 2816 | G | N9-C4-C5 | -5.81 | 103.08 | 105.40 |
| 36 | A1 | 2980 | U | C6-N1-C2 | -5.81 | 117.51 | 121.00 |
| 36 | A5 | 432 | G | C4-C5-N7 | 5.81 | 113.12 | 110.80 |
| 36 | A5 | 2335 | G | N1-C6-O6 | -5.81 | 116.41 | 119.90 |
| 36 | A5 | 2510 | U | C2-N1-C1' | -5.81 | 110.73 | 117.70 |
| 36 | A5 | 3152 | U | C6-N1-C2 | 5.81 | 124.49 | 121.00 |
| 36 | A1 | 857 | G | C4-C5-C6 | -5.81 | 115.31 | 118.80 |
| 36 | A1 | 1151 | U | C6-N1-C2 | -5.81 | 117.51 | 121.00 |
| 36 | A1 | 1232 | C | C6-N1-C2 | -5.81 | 117.98 | 120.30 |
| 1 | A2 | 92 | A | N1-C6-N6 | -5.81 | 115.11 | 118.60 |
| 1 | A2 | 581 | U | C6-N1-C1' | -5.81 | 113.07 | 121.20 |
| 36 | A1 | 804 | C | C2-N3-C4 | -5.81 | 117.00 | 119.90 |
| 36 | A1 | 908 | G | C4-N9-C1' | 5.81 | 134.05 | 126.50 |
| 67 | Bd | 64 | VAL | CB-CA-C | -5.81 | 100.36 | 111.40 |
| 80 | A6 | 647 | G | N3-C2-N2 | -5.81 | 115.83 | 119.90 |
| 36 | A5 | 1158 | A | C4-C5-N7 | 5.81 | 113.61 | 110.70 |
| 36 | A5 | 1415 | U | C5-C6-N1 | -5.81 | 119.80 | 122.70 |
| 36 | A5 | 1494 | U | N3-C2-O2 | 5.81 | 126.27 | 122.20 |
| 1 | A2 | 1633 | A | N3-C4-C5 | -5.81 | 122.73 | 126.80 |
| 36 | A1 | 649 | A | N1-C6-N6 | -5.81 | 115.12 | 118.60 |
| 36 | A1 | 796 | U | C5-C4-O4 | -5.81 | 122.42 | 125.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 36 | A1 | 901 | G | C8-N9-C4 | 5.81 | 108.72 | 106.40 |
| 36 | A1 | 1396 | C | C6-N1-C2 | 5.81 | 122.62 | 120.30 |
| 36 | A1 | 2965 | U | N3-C4-C5 | 5.81 | 118.08 | 114.60 |
| 80 | A6 | 102 | U | N1-C2-N3 | 5.81 | 118.38 | 114.90 |
| 80 | A6 | 767 | U | N1-C2-N3 | 5.81 | 118.39 | 114.90 |
| 80 | A6 | 1755 | A | C4-C5-N7 | 5.81 | 113.60 | 110.70 |
| 36 | A5 | 1210 | U | N3-C4-O4 | -5.81 | 115.33 | 119.40 |
| 1 | A2 | 934 | C | C6-N1-C1' | -5.81 | 113.83 | 120.80 |
| 36 | A1 | 3049 | A | C4-C5-C6 | 5.81 | 119.90 | 117.00 |
| 49 | BL | 63 | VAL | CB-CA-C | -5.81 | 100.37 | 111.40 |
| 80 | A6 | 858 | G | C6-C5-N7 | -5.81 | 126.92 | 130.40 |
| 36 | A5 | 35 | A | C8-N9-C4 | 5.81 | 108.12 | 105.80 |
| 36 | A5 | 590 | G | C5-N7-C8 | -5.81 | 101.40 | 104.30 |
| 36 | A5 | 1438 | U | C6-N1-C2 | -5.81 | 117.52 | 121.00 |
| 36 | A1 | 864 | G | C6-N1-C2 | -5.80 | 121.62 | 125.10 |
| 36 | A1 | 2281 | A | C2-N3-C4 | -5.80 | 107.70 | 110.60 |
| 36 | A1 | 2417 | U | N1-C2-O2 | -5.80 | 118.74 | 122.80 |
| 36 | A1 | 3201 | C | C6-N1-C2 | -5.80 | 117.98 | 120.30 |
| 80 | A6 | 1075 | C | N3-C2-O2 | 5.80 | 125.96 | 121.90 |
| 36 | A5 | 1129 | A | C2-N3-C4 | 5.80 | 113.50 | 110.60 |
| 36 | A5 | 2327 | U | N3-C4-C5 | 5.80 | 118.08 | 114.60 |
| 36 | A5 | 2692 | A | C5-N7-C8 | 5.80 | 106.80 | 103.90 |
| 1 | A2 | 1324 | G | C8-N9-C1' | 5.80 | 134.54 | 127.00 |
| 36 | A5 | 1889 | G | N3-C4-C5 | -5.80 | 125.70 | 128.60 |
| 1 | A2 | 732 | G | C4-C5-N7 | 5.80 | 113.12 | 110.80 |
| 36 | A1 | 304 | G | N9-C4-C5 | 5.80 | 107.72 | 105.40 |
| 36 | A1 | 376 | G | N9-C4-C5 | 5.80 | 107.72 | 105.40 |
| 36 | A1 | 835 | G | O4'-C1'-N9 | 5.80 | 112.84 | 108.20 |
| 36 | A5 | 25 | U | N1-C2-O2 | -5.80 | 118.74 | 122.80 |
| 36 | A5 | 332 | C | C5-C6-N1 | -5.80 | 118.10 | 121.00 |
| 36 | A5 | 801 | A | C6-N1-C2 | 5.80 | 122.08 | 118.60 |
| 36 | A5 | 979 | U | N1-C2-O2 | 5.80 | 126.86 | 122.80 |
| 49 | DL | 76 | THR | N-CA-CB | 5.80 | 121.32 | 110.30 |
| 36 | A1 | 730 | C | C5-C6-N1 | -5.80 | 118.10 | 121.00 |
| 36 | A1 | 851 | C | N3-C4-N4 | 5.80 | 122.06 | 118.00 |
| 36 | A1 | 2961 | G | C8-N9-C4 | -5.80 | 104.08 | 106.40 |
| 80 | A6 | 5 | U | C4-C5-C6 | 5.80 | 123.18 | 119.70 |
| 80 | A6 | 151 | G | N3-C2-N2 | -5.80 | 115.84 | 119.90 |
| 36 | A5 | 2147 | A | C5-C6-N6 | -5.80 | 119.06 | 123.70 |
| 36 | A1 | 24 | G | N1-C2-N3 | 5.80 | 127.38 | 123.90 |
| 36 | A1 | 892 | U | N3-C4-C5 | 5.80 | 118.08 | 114.60 |
| 73 | Bj | 65 | ARG | NE-CZ-NH1 | 5.80 | 123.20 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 80 | A6 | 43 | A | N1-C6-N6 | -5.80 | 115.12 | 118.60 |
| 36 | A5 | 3388 | C | N3-C2-O2 | -5.80 | 117.84 | 121.90 |
| 1 | A2 | 1241 | G | C8-N9-C4 | -5.80 | 104.08 | 106.40 |
| 1 | A2 | 1324 | G | N9-C4-C5 | 5.80 | 107.72 | 105.40 |
| 36 | A1 | 786 | A | C4-C5-N7 | -5.80 | 107.80 | 110.70 |
| 36 | A1 | 994 | G | N7-C8-N9 | -5.80 | 110.20 | 113.10 |
| 36 | A1 | 1081 | U | N1-C2-N3 | -5.80 | 111.42 | 114.90 |
| 36 | A1 | 2939 | G | N3-C2-N2 | -5.80 | 115.84 | 119.90 |
| 36 | A1 | 3377 | G | C5-C6-O6 | -5.80 | 125.12 | 128.60 |
| 36 | A5 | 706 | A | C5-C6-N6 | -5.80 | 119.06 | 123.70 |
| 36 | A5 | 798 | G | C5-C6-O6 | -5.80 | 125.12 | 128.60 |
| 36 | A5 | 1297 | C | C5-C4-N4 | -5.80 | 116.14 | 120.20 |
| 1 | A2 | 811 | A | C8-N9-C4 | -5.79 | 103.48 | 105.80 |
| 80 | A6 | 470 | A | C5-N7-C8 | -5.79 | 101.00 | 103.90 |
| 80 | A6 | 557 | G | N1-C6-O6 | -5.79 | 116.42 | 119.90 |
| 80 | A6 | 1145 | U | N3-C4-O4 | 5.79 | 123.46 | 119.40 |
| 36 | A5 | 1060 | U | C2-N3-C4 | -5.79 | 123.52 | 127.00 |
| 36 | A5 | 2770 | G | C2-N3-C4 | 5.79 | 114.80 | 111.90 |
| 36 | A1 | 1340 | G | C5-C6-N1 | 5.79 | 114.40 | 111.50 |
| 36 | A1 | 1929 | G | C5-C6-O6 | -5.79 | 125.12 | 128.60 |
| 38 | A4 | 81 | U | C6-N1-C1' | 5.79 | 129.31 | 121.20 |
| 63 | BZ | 135 | ARG | NE-CZ-NH2 | 5.79 | 123.20 | 120.30 |
| 80 | A6 | 272 | U | C2-N1-C1' | 5.79 | 124.65 | 117.70 |
| 80 | A6 | 553 | G | C6-N1-C2 | -5.79 | 121.62 | 125.10 |
| 80 | A6 | 768 | C | C5-C4-N4 | -5.79 | 116.14 | 120.20 |
| 80 | A6 | 1414 | U | N3-C2-O2 | -5.79 | 118.14 | 122.20 |
| 36 | A5 | 523 | A | C5-C6-N6 | 5.79 | 128.34 | 123.70 |
| 36 | A5 | 2207 | A | N7-C8-N9 | 5.79 | 116.70 | 113.80 |
| 36 | A5 | 2306 | C | C2-N1-C1' | 5.79 | 125.17 | 118.80 |
| 36 | A5 | 2835 | U | N1-C2-N3 | 5.79 | 118.38 | 114.90 |
| 1 | A2 | 460 | A | N1-C6-N6 | -5.79 | 115.12 | 118.60 |
| 1 | A2 | 1416 | G | C8-N9-C4 | -5.79 | 104.08 | 106.40 |
| 36 | A1 | 582 | G | C8-N9-C4 | -5.79 | 104.08 | 106.40 |
| 36 | A1 | 2188 | A | C8-N9-C4 | 5.79 | 108.12 | 105.80 |
| 36 | A1 | 2298 | U | N1-C2-N3 | 5.79 | 118.38 | 114.90 |
| 36 | A1 | 2299 | A | C5-N7-C8 | 5.79 | 106.80 | 103.90 |
| 80 | A6 | 1510 | U | N3-C4-C5 | -5.79 | 111.12 | 114.60 |
| 36 | A5 | 159 | A | C8-N9-C4 | 5.79 | 108.12 | 105.80 |
| 36 | A5 | 1512 | U | C5-C6-N1 | -5.79 | 119.80 | 122.70 |
| 36 | A5 | 3102 | G | C5-C6-O6 | 5.79 | 132.07 | 128.60 |
| 36 | A5 | 3285 | C | C2-N1-C1' | 5.79 | 125.17 | 118.80 |
| 36 | A1 | 1407 | A | C5-N7-C8 | 5.79 | 106.80 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 1607 | U | P-O3'-C3' | 5.79 | 126.65 | 119.70 |
| 36 | A5 | 3218 | A | N7-C8-N9 | 5.79 | 116.69 | 113.80 |
| 1 | A2 | 1198 | G | N7-C8-N9 | 5.79 | 116.00 | 113.10 |
| 36 | A1 | 23 | A | C5-C6-N6 | -5.79 | 119.07 | 123.70 |
| 36 | A1 | 2177 | G | N3-C4-C5 | -5.79 | 125.70 | 128.60 |
| 36 | A1 | 2434 | U | N3-C2-O2 | -5.79 | 118.15 | 122.20 |
| 36 | A1 | 2763 | U | C4-C5-C6 | 5.79 | 123.17 | 119.70 |
| 13 | CL | 120 | GLY | N-CA-C | -5.79 | 98.63 | 113.10 |
| 36 | A5 | 1322 | U | N3-C4-C5 | 5.79 | 118.07 | 114.60 |
| 36 | A5 | 2899 | C | C5-C6-N1 | -5.79 | 118.11 | 121.00 |
| 1 | A2 | 1131 | A | N7-C8-N9 | -5.79 | 110.91 | 113.80 |
| 36 | A1 | 1420 | C | C6-N1-C2 | -5.79 | 117.98 | 120.30 |
| 38 | A8 | 7 | U | C5-C6-N1 | -5.79 | 119.81 | 122.70 |
| 56 | DS | 155 | ARG | CG-CD-NE | 5.79 | 123.95 | 111.80 |
| 1 | A2 | 1129 | U | N3-C4-O4 | -5.79 | 115.35 | 119.40 |
| 36 | A1 | 299 | G | N3-C2-N2 | 5.79 | 123.95 | 119.90 |
| 36 | A1 | 922 | U | C2-N1-C1' | 5.79 | 124.64 | 117.70 |
| 36 | A1 | 1303 | A | C4-C5-C6 | -5.79 | 114.11 | 117.00 |
| 36 | A1 | 1327 | C | N3-C4-C5 | 5.79 | 124.22 | 121.90 |
| 80 | A6 | 1122 | G | C4-N9-C1' | -5.79 | 118.98 | 126.50 |
| 80 | A6 | 1521 | G | C2-N3-C4 | 5.79 | 114.79 | 111.90 |
| 36 | A5 | 1044 | U | C2-N3-C4 | -5.79 | 123.53 | 127.00 |
| 36 | A5 | 1159 | A | N3-C4-C5 | 5.79 | 130.85 | 126.80 |
| 36 | A5 | 1369 | A | N9-C4-C5 | -5.79 | 103.49 | 105.80 |
| 36 | A5 | 2926 | A | C2-N3-C4 | 5.79 | 113.49 | 110.60 |
| 36 | A5 | 3000 | A | C5-C6-N6 | -5.79 | 119.07 | 123.70 |
| 36 | A5 | 3141 | A | C4-C5-C6 | 5.79 | 119.89 | 117.00 |
| 36 | A5 | 3375 | A | N1-C2-N3 | -5.79 | 126.41 | 129.30 |
| 36 | A1 | 269 | G | C2-N3-C4 | 5.78 | 114.79 | 111.90 |
| 36 | A1 | 2607 | G | N1-C6-O6 | -5.78 | 116.43 | 119.90 |
| 36 | A5 | 1116 | G | N3-C4-C5 | -5.78 | 125.71 | 128.60 |
| 36 | A5 | 2706 | G | C2-N3-C4 | 5.78 | 114.79 | 111.90 |
| 36 | A1 | 341 | G | C5-C6-O6 | -5.78 | 125.13 | 128.60 |
| 36 | A5 | 2549 | G | N1-C6-O6 | 5.78 | 123.37 | 119.90 |
| 1 | A2 | 1602 | C | C6-N1-C2 | 5.78 | 122.61 | 120.30 |
| 36 | A1 | 356 | C | N3-C4-C5 | 5.78 | 124.21 | 121.90 |
| 36 | A1 | 598 | A | N1-C6-N6 | 5.78 | 122.07 | 118.60 |
| 36 | A1 | 814 | U | C2-N3-C4 | -5.78 | 123.53 | 127.00 |
| 36 | A1 | 2148 | U | C2-N3-C4 | -5.78 | 123.53 | 127.00 |
| 41 | BC | 139 | GLY | N-CA-C | -5.78 | 98.65 | 113.10 |
| 80 | A6 | 613 | G | N3-C2-N2 | 5.78 | 123.95 | 119.90 |
| 36 | A5 | 289 | A | C5-C6-N1 | 5.78 | 120.59 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 524 | U | N1-C2-O2 | -5.78 | 118.75 | 122.80 |
| 36 | A5 | 2412 | G | N9-C4-C5 | 5.78 | 107.71 | 105.40 |
| 36 | A5 | 2665 | U | C2-N3-C4 | 5.78 | 130.47 | 127.00 |
| 36 | A1 | 2408 | U | C5-C4-O4 | -5.78 | 122.43 | 125.90 |
| 80 | A6 | 1120 | U | C5-C6-N1 | -5.78 | 119.81 | 122.70 |
| 36 | A5 | 427 | C | C2-N3-C4 | -5.78 | 117.01 | 119.90 |
| 36 | A1 | 2165 | G | C5-N7-C8 | -5.78 | 101.41 | 104.30 |
| 36 | A5 | 666 | A | C8-N9-C4 | 5.78 | 108.11 | 105.80 |
| 1 | A2 | 339 | C | N1-C2-O2 | -5.78 | 115.43 | 118.90 |
| 36 | A1 | 499 | G | C5-C6-O6 | 5.78 | 132.06 | 128.60 |
| 36 | A1 | 968 | G | N3-C4-C5 | -5.78 | 125.71 | 128.60 |
| 80 | A6 | 153 | G | N3-C4-N9 | -5.78 | 122.53 | 126.00 |
| 80 | A6 | 418 | G | C8-N9-C1' | -5.78 | 119.49 | 127.00 |
| 80 | A6 | 622 | A | N1-C6-N6 | -5.78 | 115.14 | 118.60 |
| 36 | A5 | 365 | A | N1-C6-N6 | 5.78 | 122.06 | 118.60 |
| 36 | A5 | 526 | C | C5-C4-N4 | -5.78 | 116.16 | 120.20 |
| 36 | A1 | 3270 | U | N3-C4-C5 | 5.77 | 118.06 | 114.60 |
| 1 | A2 | 1370 | U | N3-C2-O2 | -5.77 | 118.16 | 122.20 |
| 36 | A1 | 212 | G | N3-C4-N9 | 5.77 | 129.46 | 126.00 |
| 36 | A1 | 1747 | G | C4-C5-N7 | 5.77 | 113.11 | 110.80 |
| 36 | A1 | 2227 | C | N1-C2-O2 | -5.77 | 115.44 | 118.90 |
| 36 | A1 | 2361 | A | C2-N3-C4 | 5.77 | 113.49 | 110.60 |
| 36 | A5 | 1193 | A | C2-N3-C4 | -5.77 | 107.71 | 110.60 |
| 36 | A5 | 1206 | G | C2-N3-C4 | 5.77 | 114.79 | 111.90 |
| 1 | A2 | 570 | A | N3-C4-C5 | -5.77 | 122.76 | 126.80 |
| 36 | A1 | 1591 | G | N1-C6-O6 | -5.77 | 116.44 | 119.90 |
| 80 | A6 | 1749 | A | C5-C6-N6 | -5.77 | 119.08 | 123.70 |
| 36 | A5 | 411 | U | N1-C2-N3 | 5.77 | 118.36 | 114.90 |
| 36 | A5 | 1904 | C | N1-C2-O2 | 5.77 | 122.36 | 118.90 |
| 36 | A5 | 2774 | C | N1-C2-O2 | -5.77 | 115.44 | 118.90 |
| 36 | A1 | 505 | G | N9-C4-C5 | 5.77 | 107.71 | 105.40 |
| 36 | A1 | 968 | G | C6-C5-N7 | -5.77 | 126.94 | 130.40 |
| 36 | A1 | 1192 | C | N1-C2-O2 | 5.77 | 122.36 | 118.90 |
| 36 | A1 | 1458 | U | C6-N1-C2 | 5.77 | 124.46 | 121.00 |
| 36 | A1 | 1665 | C | C5-C4-N4 | -5.77 | 116.16 | 120.20 |
| 36 | A1 | 2343 | C | C6-N1-C2 | 5.77 | 122.61 | 120.30 |
| 36 | A1 | 2728 | G | C2-N3-C4 | 5.77 | 114.78 | 111.90 |
| 1 | A2 | 1339 | C | C6-N1-C2 | -5.77 | 117.99 | 120.30 |
| 36 | A1 | 44 | U | N3-C4-O4 | -5.77 | 115.36 | 119.40 |
| 36 | A1 | 420 | G | N1-C2-N2 | -5.77 | 111.01 | 116.20 |
| 36 | A1 | 658 | G | C5-C6-N1 | -5.77 | 108.62 | 111.50 |
| 36 | A1 | 947 | G | N3-C2-N2 | 5.77 | 123.94 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 36 | A1 | 2805 | G | N3-C4-N9 | 5.77 | 129.46 | 126.00 |
| 36 | A1 | 2989 | U | C2-N3-C4 | -5.77 | 123.54 | 127.00 |
| 80 | A6 | 1241 | G | N3-C4-C5 | 5.77 | 131.48 | 128.60 |
| 36 | A5 | 1208 | U | N1-C2-N3 | 5.77 | 118.36 | 114.90 |
| 36 | A5 | 3088 | G | N7-C8-N9 | 5.77 | 115.98 | 113.10 |
| 1 | A2 | 1614 | A | C4-C5-C6 | 5.77 | 119.88 | 117.00 |
| 36 | A1 | 1379 | G | N1-C2-N2 | -5.77 | 111.01 | 116.20 |
| 36 | A1 | 2279 | A | C8-N9-C4 | 5.77 | 108.11 | 105.80 |
| 36 | A5 | 3076 | C | N3-C2-O2 | -5.77 | 117.86 | 121.90 |
| 38 | A8 | 104 | A | N1-C6-N6 | 5.77 | 122.06 | 118.60 |
| 1 | A2 | 1112 | G | C6-N1-C2 | -5.76 | 121.64 | 125.10 |
| 36 | A1 | 2525 | G | C3'-C2'-C1' | -5.76 | 96.89 | 101.50 |
| 36 | A1 | 2653 | C | C2-N3-C4 | -5.76 | 117.02 | 119.90 |
| 80 | A6 | 1028 | C | C5-C6-N1 | -5.76 | 118.12 | 121.00 |
| 36 | A5 | 1116 | G | C4-C5-C6 | 5.76 | 122.26 | 118.80 |
| 36 | A5 | 1524 | A | N1-C2-N3 | 5.76 | 132.18 | 129.30 |
| 36 | A5 | 2329 | C | C5-C4-N4 | 5.76 | 124.23 | 120.20 |
| 36 | A5 | 3131 | U | C5-C4-O4 | -5.76 | 122.44 | 125.90 |
| 1 | A2 | 144 | U | N1-C2-O2 | 5.76 | 126.83 | 122.80 |
| 36 | A5 | 2320 | A | N3-C4-N9 | -5.76 | 122.79 | 127.40 |
| 1 | A2 | 1027 | A | C8-N9-C4 | -5.76 | 103.50 | 105.80 |
| 36 | A1 | 1432 | C | N1-C2-N3 | 5.76 | 123.23 | 119.20 |
| 36 | A1 | 1447 | G | N3-C4-N9 | -5.76 | 122.54 | 126.00 |
| 36 | A1 | 1905 | G | C5-C6-O6 | -5.76 | 125.14 | 128.60 |
| 36 | A1 | 2623 | G | N9-C4-C5 | -5.76 | 103.10 | 105.40 |
| 36 | A1 | 3092 | C | C2-N1-C1' | -5.76 | 112.46 | 118.80 |
| 52 | DO | 197[B] | PHE | O-C-N | 5.76 | 133.00 | 123.20 |
| 80 | A6 | 1772 | C | N1-C2-O2 | -5.76 | 115.44 | 118.90 |
| 36 | A5 | 706 | A | N1-C2-N3 | -5.76 | 126.42 | 129.30 |
| 36 | A5 | 1126 | G | C2-N3-C4 | -5.76 | 109.02 | 111.90 |
| 36 | A5 | 1724 | U | C2-N1-C1' | 5.76 | 124.61 | 117.70 |
| 36 | A5 | 2129 | U | N3-C4-C5 | 5.76 | 118.06 | 114.60 |
| 36 | A5 | 2342 | U | N3-C2-O2 | -5.76 | 118.17 | 122.20 |
| 1 | A2 | 377 | G | N1-C2-N2 | 5.76 | 121.38 | 116.20 |
| 1 | A2 | 1274 | C | C5-C4-N4 | 5.76 | 124.23 | 120.20 |
| 80 | A6 | 1324 | G | N3-C2-N2 | -5.76 | 115.87 | 119.90 |
| 36 | A5 | 1888 | U | N1-C2-N3 | 5.76 | 118.36 | 114.90 |
| 36 | A5 | 3316 | A | N1-C6-N6 | 5.76 | 122.06 | 118.60 |
| 36 | A1 | 2357 | A | C6-N1-C2 | -5.76 | 115.15 | 118.60 |
| 36 | A1 | 2752 | U | N3-C2-O2 | -5.76 | 118.17 | 122.20 |
| 36 | A5 | 1846 | C | N3-C2-O2 | -5.76 | 117.87 | 121.90 |
| 36 | A5 | 2305 | G | C6-C5-N7 | -5.76 | 126.95 | 130.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 2337 | C | C2-N3-C4 | -5.76 | 117.02 | 119.90 |
| 1 | A2 | 169 | A | C8-N9-C4 | 5.75 | 108.10 | 105.80 |
| 36 | A5 | 2335 | G | N9-C4-C5 | 5.75 | 107.70 | 105.40 |
| 36 | A5 | 3298 | C | C2-N3-C4 | -5.75 | 117.02 | 119.90 |
| 1 | A2 | 971 | A | C5-C6-N1 | -5.75 | 114.82 | 117.70 |
| 36 | A1 | 1747 | G | C5-N7-C8 | -5.75 | 101.42 | 104.30 |
| 36 | A1 | 3046 | A | C2-N3-C4 | 5.75 | 113.48 | 110.60 |
| 80 | A6 | 1681 | A | N1-C6-N6 | 5.75 | 122.05 | 118.60 |
| 36 | A5 | 518 | G | C8-N9-C4 | 5.75 | 108.70 | 106.40 |
| 36 | A5 | 1931 | U | C6-N1-C1' | 5.75 | 129.25 | 121.20 |
| 1 | A2 | 158 | U | N3-C2-O2 | -5.75 | 118.17 | 122.20 |
| 1 | A2 | 864 | U | N1-C2-N3 | 5.75 | 118.35 | 114.90 |
| 80 | A6 | 1124 | A | N9-C4-C5 | -5.75 | 103.50 | 105.80 |
| 36 | A1 | 702 | C | C5-C4-N4 | -5.75 | 116.17 | 120.20 |
| 36 | A5 | 2747 | A | N9-C4-C5 | 5.75 | 108.10 | 105.80 |
| 1 | A2 | 639 | U | N3-C4-O4 | -5.75 | 115.38 | 119.40 |
| 36 | A1 | 368 | G | C2-N3-C4 | -5.75 | 109.03 | 111.90 |
| 36 | A1 | 984 | G | N1-C2-N2 | -5.75 | 111.03 | 116.20 |
| 36 | A1 | 1167 | U | C2-N3-C4 | -5.75 | 123.55 | 127.00 |
| 53 | BP | 24 | VAL | CB-CA-C | -5.75 | 100.48 | 111.40 |
| 80 | A6 | 99 | C | C2-N1-C1' | 5.75 | 125.12 | 118.80 |
| 80 | A6 | 1164 | G | C5-C6-N1 | 5.75 | 114.37 | 111.50 |
| 36 | A5 | 591 | G | C8-N9-C4 | 5.75 | 108.70 | 106.40 |
| 36 | A5 | 1143 | A | C5-N7-C8 | -5.75 | 101.03 | 103.90 |
| 36 | A5 | 2192 | C | C4-C5-C6 | 5.75 | 120.27 | 117.40 |
| 36 | A5 | 3212 | C | N1-C2-O2 | -5.75 | 115.45 | 118.90 |
| 38 | A8 | 31 | G | N7-C8-N9 | -5.75 | 110.23 | 113.10 |
| 36 | A1 | 817 | A | N1-C2-N3 | 5.75 | 132.17 | 129.30 |
| 36 | A1 | 1904 | C | N3-C2-O2 | 5.75 | 125.92 | 121.90 |
| 36 | A1 | 2571 | U | N1-C2-O2 | 5.75 | 126.82 | 122.80 |
| 36 | A1 | 3204 | C | C5-C6-N1 | -5.75 | 118.13 | 121.00 |
| 36 | A1 | 3218 | A | N3-C4-N9 | -5.75 | 122.80 | 127.40 |
| 80 | A6 | 677 | G | C4-N9-C1' | -5.75 | 119.03 | 126.50 |
| 36 | A5 | 911 | C | C2-N3-C4 | -5.75 | 117.03 | 119.90 |
| 36 | A5 | 1512 | U | C4-C5-C6 | 5.75 | 123.15 | 119.70 |
| 36 | A5 | 1553 | U | N3-C2-O2 | 5.75 | 126.22 | 122.20 |
| 36 | A1 | 1669 | C | N1-C2-O2 | -5.75 | 115.45 | 118.90 |
| 36 | A5 | 613 | G | N1-C6-O6 | -5.75 | 116.45 | 119.90 |
| 36 | A5 | 1128 | U | N1-C2-N3 | 5.75 | 118.35 | 114.90 |
| 38 | A8 | 17 | A | C5-C6-N6 | -5.75 | 119.10 | 123.70 |
| 1 | A2 | 1169 | G | N3-C4-C5 | -5.74 | 125.73 | 128.60 |
| 36 | A1 | 1377 | G | C2-N3-C4 | 5.74 | 114.77 | 111.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 80 | A6 | 1091 | A | C5-N7-C8 | -5.74 | 101.03 | 103.90 |
| 36 | A5 | 3301 | U | C6-N1-C2 | 5.74 | 124.45 | 121.00 |
| 36 | A1 | 187 | A | N3-C4-N9 | 5.74 | 131.99 | 127.40 |
| 36 | A1 | 2117 | A | C5-C6-N6 | 5.74 | 128.29 | 123.70 |
| 38 | A4 | 135 | G | C8-N9-C4 | -5.74 | 104.10 | 106.40 |
| 36 | A5 | 363 | G | N9-C4-C5 | 5.74 | 107.70 | 105.40 |
| 36 | A5 | 382 | U | N1-C2-N3 | 5.74 | 118.34 | 114.90 |
| 36 | A5 | 3123 | A | N9-C4-C5 | -5.74 | 103.50 | 105.80 |
| 1 | A2 | 527 | A | C8-N9-C4 | -5.74 | 103.50 | 105.80 |
| 36 | A1 | 804 | C | C2-N1-C1' | -5.74 | 112.49 | 118.80 |
| 36 | A1 | 1391 | C | C5-C6-N1 | -5.74 | 118.13 | 121.00 |
| 80 | A6 | 944 | A | N7-C8-N9 | 5.74 | 116.67 | 113.80 |
| 36 | A5 | 88 | A | C5-C6-N1 | -5.74 | 114.83 | 117.70 |
| 36 | A1 | 87 | U | C2-N3-C4 | -5.74 | 123.56 | 127.00 |
| 36 | A1 | 1143 | A | C4-C5-N7 | 5.74 | 113.57 | 110.70 |
| 36 | A1 | 1314 | C | C2-N3-C4 | -5.74 | 117.03 | 119.90 |
| 80 | A6 | 524 | U | N3-C2-O2 | -5.74 | 118.18 | 122.20 |
| 80 | A6 | 901 | G | C6-C5-N7 | -5.74 | 126.96 | 130.40 |
| 36 | A5 | 201 | A | C5-C6-N1 | -5.74 | 114.83 | 117.70 |
| 36 | A5 | 216 | G | C4-C5-N7 | 5.74 | 113.10 | 110.80 |
| 36 | A5 | 672 | A | N1-C6-N6 | 5.74 | 122.04 | 118.60 |
| 36 | A5 | 3047 | U | C2-N3-C4 | -5.74 | 123.56 | 127.00 |
| 36 | A5 | 3339 | A | C5-C6-N6 | -5.74 | 119.11 | 123.70 |
| 1 | A2 | 1354 | G | N3-C4-C5 | -5.74 | 125.73 | 128.60 |
| 36 | A1 | 1130 | A | N1-C6-N6 | 5.74 | 122.04 | 118.60 |
| 80 | A6 | 988 | A | C8-N9-C4 | -5.74 | 103.50 | 105.80 |
| 36 | A1 | 1778 | G | N7-C8-N9 | 5.74 | 115.97 | 113.10 |
| 36 | A1 | 2815 | G | N1-C2-N2 | -5.74 | 111.04 | 116.20 |
| 36 | A5 | 3241 | G | C5-C6-O6 | -5.74 | 125.16 | 128.60 |
| 40 | DB | 266 | ARG | NE-CZ-NH1 | 5.74 | 123.17 | 120.30 |
| 75 | DI | 45 | ARG | NE-CZ-NH2 | -5.74 | 117.43 | 120.30 |
| 80 | A6 | 448 | C | N1-C2-O2 | -5.73 | 115.46 | 118.90 |
| 36 | A5 | 1113 | G | N7-C8-N9 | -5.73 | 110.23 | 113.10 |
| 38 | A8 | 106 | C | N3-C4-C5 | 5.73 | 124.19 | 121.90 |
| 78 | Bo | 87 | ARG | NE-CZ-NH1 | -5.73 | 117.43 | 120.30 |
| 47 | DI | 139 | ARG | NE-CZ-NH1 | 5.73 | 123.17 | 120.30 |
| 80 | A6 | 798 | C | N3-C4-C5 | 5.73 | 124.19 | 121.90 |
| 36 | A5 | 2148 | U | C5-C4-O4 | -5.73 | 122.46 | 125.90 |
| 80 | A6 | 1489 | U | N3-C4-O4 | -5.73 | 115.39 | 119.40 |
| 36 | A5 | 666 | A | C2-N3-C4 | -5.73 | 107.73 | 110.60 |
| 36 | A5 | 1035 | G | C8-N9-C1' | -5.73 | 119.55 | 127.00 |
| 36 | A5 | 1242 | G | N3-C4-N9 | 5.73 | 129.44 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 2906 | C | N3-C4-C5 | -5.73 | 119.61 | 121.90 |
| 37 | A7 | 47 | C | C2-N3-C4 | -5.73 | 117.04 | 119.90 |
| 1 | A2 | 1776 | A | N1-C6-N6 | -5.73 | 115.16 | 118.60 |
| 36 | A1 | 689 | U | C2-N1-C1' | 5.73 | 124.57 | 117.70 |
| 36 | A1 | 1101 | G | C2-N3-C4 | -5.73 | 109.04 | 111.90 |
| 38 | A4 | 102 | U | C2-N3-C4 | -5.73 | 123.56 | 127.00 |
| 36 | A5 | 1443 | G | C5-C6-N1 | -5.73 | 108.64 | 111.50 |
| 36 | A5 | 1445 | U | C2-N3-C4 | -5.73 | 123.56 | 127.00 |
| 36 | A5 | 1832 | C | C5-C4-N4 | -5.73 | 116.19 | 120.20 |
| 36 | A5 | 2422 | C | N3-C2-O2 | -5.73 | 117.89 | 121.90 |
| 36 | A5 | 2658 | G | N7-C8-N9 | -5.73 | 110.24 | 113.10 |
| 36 | A1 | 435 | C | C2-N1-C1' | -5.73 | 112.50 | 118.80 |
| 80 | A6 | 96 | G | N9-C4-C5 | 5.73 | 107.69 | 105.40 |
| 36 | A5 | 224 | C | N3-C2-O2 | -5.73 | 117.89 | 121.90 |
| 36 | A5 | 1045 | C | N1-C2-O2 | -5.73 | 115.46 | 118.90 |
| 36 | A5 | 2736 | A | C5-C6-N6 | 5.73 | 128.28 | 123.70 |
| 40 | DB | 21 | ARG | NE-CZ-NH2 | -5.73 | 117.44 | 120.30 |
| 1 | A2 | 1421 | A | C8-N9-C4 | 5.72 | 108.09 | 105.80 |
| 27 | AZ | 95 | HIS | N-CA-C | 5.72 | 126.46 | 111.00 |
| 36 | A1 | 670 | C | C5-C6-N1 | -5.72 | 118.14 | 121.00 |
| 36 | A1 | 2728 | G | C5-C6-N1 | 5.72 | 114.36 | 111.50 |
| 80 | A6 | 396 | G | N9-C4-C5 | -5.72 | 103.11 | 105.40 |
| 36 | A5 | 920 | A | C8-N9-C4 | 5.72 | 108.09 | 105.80 |
| 36 | A5 | 2142 | A | N3-C4-N9 | 5.72 | 131.98 | 127.40 |
| 36 | A5 | 3197 | G | N3-C4-N9 | -5.72 | 122.56 | 126.00 |
| 36 | A1 | 120 | G | C8-N9-C4 | 5.72 | 108.69 | 106.40 |
| 36 | A1 | 591 | G | C6-C5-N7 | -5.72 | 126.97 | 130.40 |
| 36 | A1 | 2348 | A | N1-C2-N3 | 5.72 | 132.16 | 129.30 |
| 80 | A6 | 571 | G | N3-C4-N9 | -5.72 | 122.57 | 126.00 |
| 36 | A5 | 1856 | C | C6-N1-C2 | -5.72 | 118.01 | 120.30 |
| 36 | A1 | 2748 | A | N1-C2-N3 | 5.72 | 132.16 | 129.30 |
| 36 | A1 | 3054 | U | C5-C6-N1 | -5.72 | 119.84 | 122.70 |
| 36 | A5 | 1512 | U | C2-N3-C4 | -5.72 | 123.57 | 127.00 |
| 36 | A5 | 2827 | U | N3-C2-O2 | -5.72 | 118.19 | 122.20 |
| 38 | A8 | 28 | C | C4-C5-C6 | -5.72 | 114.54 | 117.40 |
| 36 | A1 | 311 | C | C6-N1-C2 | 5.72 | 122.59 | 120.30 |
| 36 | A1 | 434 | U | N3-C4-C5 | 5.72 | 118.03 | 114.60 |
| 36 | A1 | 658 | G | C4-C5-N7 | -5.72 | 108.51 | 110.80 |
| 36 | A1 | 1100 | U | C5-C6-N1 | -5.72 | 119.84 | 122.70 |
| 36 | A5 | 2108 | C | N3-C4-C5 | 5.72 | 124.19 | 121.90 |
| 1 | A2 | 142 | G | N1-C6-O6 | 5.72 | 123.33 | 119.90 |
| 36 | A5 | 1159 | A | C6-N1-C2 | 5.72 | 122.03 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 36 | A5 | 2361 | A | C5-C6-N1 | 5.72 | 120.56 | 117.70 |
| 36 | A5 | 2978 | U | N1-C2-N3 | 5.72 | 118.33 | 114.90 |
| 54 | DQ | 50 | LYS | CD-CE-NZ | 5.72 | 124.85 | 111.70 |
| 36 | A1 | 2817 | A | N3-C4-C5 | -5.72 | 122.80 | 126.80 |
| 80 | A6 | 137 | U | C2-N1-C1' | 5.72 | 124.56 | 117.70 |
| 80 | A6 | 1274 | C | N3-C4-N4 | -5.72 | 114.00 | 118.00 |
| 80 | A6 | 1781 | A | C4-C5-C6 | 5.72 | 119.86 | 117.00 |
| 36 | A5 | 2619 | G | C5-C6-N1 | 5.72 | 114.36 | 111.50 |
| 36 | A1 | 811 | U | N1-C2-N3 | 5.71 | 118.33 | 114.90 |
| 36 | A1 | 994 | G | C8-N9-C4 | 5.71 | 108.69 | 106.40 |
| 36 | A1 | 1160 | C | C5-C4-N4 | 5.71 | 124.20 | 120.20 |
| 36 | A1 | 2142 | A | C8-N9-C4 | -5.71 | 103.51 | 105.80 |
| 36 | A1 | 2533 | G | C8-N9-C1' | -5.71 | 119.57 | 127.00 |
| 80 | A6 | 922 | G | C5-C6-N1 | 5.71 | 114.36 | 111.50 |
| 80 | A6 | 1136 | U | C5-C4-O4 | -5.71 | 122.47 | 125.90 |
| 36 | A5 | 760 | G | C5-C6-O6 | -5.71 | 125.17 | 128.60 |
| 36 | A5 | 884 | A | N1-C6-N6 | -5.71 | 115.17 | 118.60 |
| 36 | A5 | 1371 | G | N7-C8-N9 | -5.71 | 110.24 | 113.10 |
| 36 | A5 | 2392 | C | C5-C6-N1 | -5.71 | 118.14 | 121.00 |
| 36 | A5 | 3259 | U | C5-C6-N1 | 5.71 | 125.56 | 122.70 |
| 36 | A1 | 755 | A | C2-N3-C4 | -5.71 | 107.74 | 110.60 |
| 36 | A1 | 773 | G | N1-C6-O6 | -5.71 | 116.47 | 119.90 |
| 36 | A1 | 959 | C | C2-N3-C4 | -5.71 | 117.04 | 119.90 |
| 36 | A1 | 1333 | C | C6-N1-C2 | -5.71 | 118.02 | 120.30 |
| 36 | A1 | 1582 | C | C6-N1-C1' | 5.71 | 127.66 | 120.80 |
| 36 | A1 | 1586 | G | N3-C2-N2 | 5.71 | 123.90 | 119.90 |
| 36 | A1 | 3149 | G | N3-C2-N2 | -5.71 | 115.90 | 119.90 |
| 37 | A3 | 82 | G | C2-N3-C4 | -5.71 | 109.04 | 111.90 |
| 80 | A6 | 1 | U | C5-C6-N1 | 5.71 | 125.56 | 122.70 |
| 80 | A6 | 163 | G | N1-C2-N3 | 5.71 | 127.33 | 123.90 |
| 36 | A5 | 670 | C | C2-N3-C4 | -5.71 | 117.04 | 119.90 |
| 36 | A5 | 1159 | A | C5-N7-C8 | -5.71 | 101.04 | 103.90 |
| 38 | A8 | 23 | U | C4-C5-C6 | 5.71 | 123.13 | 119.70 |
| 47 | DI | 21 | ARG | NE-CZ-NH1 | 5.71 | 123.16 | 120.30 |
| 36 | A1 | 2906 | C | C2-N3-C4 | -5.71 | 117.05 | 119.90 |
| 36 | A1 | 3269 | U | N1-C2-O2 | 5.71 | 126.80 | 122.80 |
| 36 | A5 | 3365 | U | C6-N1-C2 | -5.71 | 117.57 | 121.00 |
| 36 | A1 | 280 | U | C5-C4-O4 | -5.71 | 122.47 | 125.90 |
| 80 | A6 | 136 | C | C2-N1-C1' | 5.71 | 125.08 | 118.80 |
| 80 | A6 | 541 | A | C3'-C2'-C1' | -5.71 | 96.93 | 101.50 |
| 36 | A5 | 270 | U | N3-C2-O2 | -5.71 | 118.20 | 122.20 |
| 36 | A5 | 1364 | C | C5-C6-N1 | -5.71 | 118.14 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 2730 | G | N3-C2-N2 | -5.71 | 115.90 | 119.90 |
| 36 | A5 | 2804 | A | C8-N9-C4 | 5.71 | 108.08 | 105.80 |
| 36 | A5 | 2979 | U | N3-C2-O2 | 5.71 | 126.20 | 122.20 |
| 36 | A1 | 333 | G | C4-C5-N7 | -5.71 | 108.52 | 110.80 |
| 37 | A3 | 83 | U | C5-C6-N1 | -5.71 | 119.85 | 122.70 |
| 53 | BP | 131 | ARG | NE-CZ-NH2 | 5.71 | 123.15 | 120.30 |
| 36 | A5 | 2320 | A | N9-C4-C5 | 5.71 | 108.08 | 105.80 |
| 53 | DP | 24 | VAL | CB-CA-C | -5.71 | 100.56 | 111.40 |
| 36 | A1 | 2882 | U | C2-N3-C4 | -5.71 | 123.58 | 127.00 |
| 36 | A5 | 563 | U | N3-C2-O2 | -5.71 | 118.21 | 122.20 |
| 1 | A2 | 92 | A | C6-N1-C2 | -5.70 | 115.18 | 118.60 |
| 1 | A2 | 831 | U | C2-N1-C1' | 5.70 | 124.55 | 117.70 |
| 1 | A2 | 1075 | C | N3-C2-O2 | 5.70 | 125.89 | 121.90 |
| 36 | A1 | 517 | G | C5-N7-C8 | -5.70 | 101.45 | 104.30 |
| 36 | A1 | 1374 | G | C6-C5-N7 | -5.70 | 126.98 | 130.40 |
| 36 | A1 | 1392 | G | N9-C4-C5 | -5.70 | 103.12 | 105.40 |
| 36 | A1 | 1932 | A | C5-C6-N1 | 5.70 | 120.55 | 117.70 |
| 36 | A1 | 2571 | U | N3-C2-O2 | -5.70 | 118.21 | 122.20 |
| 36 | A1 | 2634 | U | C5-C6-N1 | -5.70 | 119.85 | 122.70 |
| 80 | A6 | 826 | U | C2-N1-C1' | 5.70 | 124.55 | 117.70 |
| 36 | A5 | 1163 | A | C5-C6-N1 | 5.70 | 120.55 | 117.70 |
| 36 | A5 | 2836 | C | C5-C4-N4 | 5.70 | 124.19 | 120.20 |
| 36 | A1 | 2329 | C | C6-N1-C1' | 5.70 | 127.64 | 120.80 |
| 36 | A1 | 3137 | C | C5-C6-N1 | 5.70 | 123.85 | 121.00 |
| 80 | A6 | 1025 | A | C5-C6-N1 | -5.70 | 114.85 | 117.70 |
| 36 | A5 | 2293 | C | N1-C2-O2 | 5.70 | 122.32 | 118.90 |
| 36 | A5 | 2866 | U | C2-N3-C4 | -5.70 | 123.58 | 127.00 |
| 1 | A2 | 612 | U | N3-C4-O4 | -5.70 | 115.41 | 119.40 |
| 1 | A2 | 1489 | U | N3-C2-O2 | -5.70 | 118.21 | 122.20 |
| 36 | A1 | 859 | G | N9-C4-C5 | -5.70 | 103.12 | 105.40 |
| 36 | A1 | 2310 | U | C6-N1-C2 | -5.70 | 117.58 | 121.00 |
| 36 | A1 | 2606 | G | N3-C2-N2 | 5.70 | 123.89 | 119.90 |
| 36 | A5 | 2552 | C | N3-C4-N4 | -5.70 | 114.01 | 118.00 |
| 36 | A1 | 967 | A | N1-C6-N6 | -5.70 | 115.18 | 118.60 |
| 36 | A1 | 1141 | C | N3-C4-C5 | -5.70 | 119.62 | 121.90 |
| 36 | A1 | 1787 | A | N7-C8-N9 | -5.70 | 110.95 | 113.80 |
| 73 | Bj | 72 | ARG | NE-CZ-NH1 | 5.70 | 123.15 | 120.30 |
| 80 | A6 | 1015 | U | C2-N3-C4 | 5.70 | 130.42 | 127.00 |
| 36 | A5 | 971 | G | N9-C4-C5 | 5.70 | 107.68 | 105.40 |
| 36 | A5 | 1840 | U | N1-C2-O2 | 5.70 | 126.79 | 122.80 |
| 36 | A1 | 2202 | C | C5-C6-N1 | -5.70 | 118.15 | 121.00 |
| 36 | A1 | 2735 | U | N3-C4-O4 | -5.70 | 115.41 | 119.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 38 | A8 | 20 | U | C5-C6-N1 | -5.70 | 119.85 | 122.70 |
| 1 | A2 | 539 | G | C5-N7-C8 | -5.70 | 101.45 | 104.30 |
| 36 | A1 | 3071 | U | N1-C2-O2 | -5.70 | 118.81 | 122.80 |
| 80 | A6 | 11 | A | C8-N9-C4 | 5.70 | 108.08 | 105.80 |
| 80 | A6 | 1127 | G | C6-N1-C2 | -5.70 | 121.68 | 125.10 |
| 36 | A5 | 665 | A | N9-C4-C5 | -5.70 | 103.52 | 105.80 |
| 36 | A5 | 3006 | A | N9-C4-C5 | 5.70 | 108.08 | 105.80 |
| 54 | DQ | 127 | LEU | CA-CB-CG | 5.70 | 128.40 | 115.30 |
| 1 | A2 | 741 | C | N1-C2-O2 | -5.69 | 115.48 | 118.90 |
| 80 | A6 | 1643 | U | N3-C4-O4 | -5.69 | 115.41 | 119.40 |
| 36 | A5 | 1639 | C | C6-N1-C2 | -5.69 | 118.02 | 120.30 |
| 1 | A2 | 1282 | U | N1-C2-N3 | 5.69 | 118.32 | 114.90 |
| 36 | A1 | 1514 | G | N3-C4-C5 | -5.69 | 125.75 | 128.60 |
| 36 | A1 | 2571 | U | C2-N1-C1' | 5.69 | 124.53 | 117.70 |
| 36 | A1 | 2760 | C | N3-C4-C5 | -5.69 | 119.62 | 121.90 |
| 80 | A6 | 411 | C | N3-C2-O2 | -5.69 | 117.92 | 121.90 |
| 36 | A5 | 276 | U | C4-C5-C6 | 5.69 | 123.11 | 119.70 |
| 36 | A5 | 1466 | G | N3-C4-N9 | -5.69 | 122.58 | 126.00 |
| 36 | A5 | 1589 | A | C5-C6-N1 | 5.69 | 120.55 | 117.70 |
| 36 | A5 | 1652 | G | C4-C5-N7 | -5.69 | 108.52 | 110.80 |
| 36 | A5 | 2330 | C | C4-C5-C6 | 5.69 | 120.25 | 117.40 |
| 36 | A1 | 87 | U | N3-C4-O4 | -5.69 | 115.42 | 119.40 |
| 36 | A1 | 233 | C | C6-N1-C2 | 5.69 | 122.58 | 120.30 |
| 36 | A1 | 655 | C | C2-N3-C4 | -5.69 | 117.06 | 119.90 |
| 36 | A1 | 678 | G | C5-C6-O6 | -5.69 | 125.19 | 128.60 |
| 36 | A1 | 1331 | U | C2-N3-C4 | -5.69 | 123.59 | 127.00 |
| 36 | A1 | 1507 | G | C4-C5-N7 | -5.69 | 108.52 | 110.80 |
| 36 | A1 | 2438 | A | C8-N9-C4 | 5.69 | 108.08 | 105.80 |
| 36 | A1 | 2865 | U | C2-N3-C4 | -5.69 | 123.59 | 127.00 |
| 62 | BY | 60 | ARG | NE-CZ-NH1 | -5.69 | 117.45 | 120.30 |
| 80 | A6 | 1421 | A | C8-N9-C4 | 5.69 | 108.08 | 105.80 |
| 36 | A5 | 2400 | G | C4-C5-N7 | 5.69 | 113.08 | 110.80 |
| 38 | A8 | 26 | U | C2-N1-C1' | 5.69 | 124.53 | 117.70 |
| 38 | A8 | 34 | U | C5-C6-N1 | -5.69 | 119.86 | 122.70 |
| 46 | DH | 151 | VAL | CB-CA-C | -5.69 | 100.59 | 111.40 |
| 52 | DO | 163[B] | ARG | NE-CZ-NH2 | -5.69 | 117.45 | 120.30 |
| 1 | A2 | 92 | A | N3-C4-C5 | -5.69 | 122.82 | 126.80 |
| 1 | A2 | 494 | U | N3-C2-O2 | -5.69 | 118.22 | 122.20 |
| 36 | A1 | 272 | G | C5-N7-C8 | 5.69 | 107.14 | 104.30 |
| 36 | A1 | 1502 | C | C4-C5-C6 | 5.69 | 120.25 | 117.40 |
| 36 | A5 | 582 | G | N1-C6-O6 | -5.69 | 116.49 | 119.90 |
| 36 | A1 | 3052 | G | N1-C6-O6 | -5.69 | 116.49 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 24 | G | C5-C6-O6 | -5.69 | 125.19 | 128.60 |
| 36 | A5 | 580 | C | N3-C4-C5 | -5.69 | 119.62 | 121.90 |
| 36 | A5 | 1726 | C | C5-C6-N1 | -5.69 | 118.16 | 121.00 |
| 36 | A5 | 1849 | C | N3-C2-O2 | -5.69 | 117.92 | 121.90 |
| 36 | A5 | 3200 | G | C5-C6-O6 | -5.69 | 125.19 | 128.60 |
| 36 | A1 | 2984 | C | C5-C4-N4 | 5.69 | 124.18 | 120.20 |
| 36 | A1 | 3010 | U | N3-C2-O2 | -5.69 | 118.22 | 122.20 |
| 80 | A6 | 864 | U | C2-N1-C1' | 5.69 | 124.52 | 117.70 |
| 36 | A5 | 2123 | G | C5-C6-N1 | 5.69 | 114.34 | 111.50 |
| 38 | A8 | 95 | G | C4-N9-C1' | -5.69 | 119.11 | 126.50 |
| 1 | A2 | 1781 | A | C5-C6-N1 | -5.68 | 114.86 | 117.70 |
| 36 | A1 | 2147 | A | C5-C6-N6 | -5.68 | 119.15 | 123.70 |
| 36 | A1 | 3110 | C | N1-C2-O2 | 5.68 | 122.31 | 118.90 |
| 36 | A1 | 3188 | G | N3-C4-N9 | 5.68 | 129.41 | 126.00 |
| 36 | A1 | 3235 | C | C6-N1-C2 | -5.68 | 118.03 | 120.30 |
| 36 | A1 | 3293 | U | C5-C4-O4 | -5.68 | 122.49 | 125.90 |
| 38 | A4 | 113 | U | C6-N1-C1' | 5.68 | 129.16 | 121.20 |
| 36 | A5 | 79 | U | C5-C4-O4 | -5.68 | 122.49 | 125.90 |
| 37 | A7 | 8 | G | C8-N9-C4 | -5.68 | 104.13 | 106.40 |
| 36 | A1 | 68 | C | N3-C2-O2 | -5.68 | 117.92 | 121.90 |
| 80 | A6 | 1143 | A | C2-N3-C4 | 5.68 | 113.44 | 110.60 |
| 80 | A6 | 1572 | G | C5-N7-C8 | -5.68 | 101.46 | 104.30 |
| 36 | A5 | 1429 | G | C6-C5-N7 | -5.68 | 126.99 | 130.40 |
| 36 | A5 | 1458 | U | N3-C4-C5 | 5.68 | 118.01 | 114.60 |
| 36 | A1 | 70 | A | C8-N9-C4 | 5.68 | 108.07 | 105.80 |
| 36 | A1 | 1191 | U | C2-N3-C4 | -5.68 | 123.59 | 127.00 |
| 36 | A1 | 1209 | G | N3-C4-C5 | -5.68 | 125.76 | 128.60 |
| 36 | A1 | 2749 | G | N1-C6-O6 | 5.68 | 123.31 | 119.90 |
| 80 | A6 | 66 | U | C4-C5-C6 | 5.68 | 123.11 | 119.70 |
| 80 | A6 | 385 | A | N7-C8-N9 | -5.68 | 110.96 | 113.80 |
| 36 | A5 | 1159 | A | N9-C4-C5 | -5.68 | 103.53 | 105.80 |
| 36 | A5 | 1371 | G | C5-N7-C8 | 5.68 | 107.14 | 104.30 |
| 36 | A5 | 1448 | U | C4-C5-C6 | 5.68 | 123.11 | 119.70 |
| 37 | A7 | 103 | A | C5-C6-N6 | -5.68 | 119.16 | 123.70 |
| 1 | A2 | 1361 | U | N3-C2-O2 | -5.68 | 118.22 | 122.20 |
| 1 | A2 | 1749 | A | C4-C5-N7 | 5.68 | 113.54 | 110.70 |
| 36 | A1 | 574 | U | N3-C4-C5 | 5.68 | 118.01 | 114.60 |
| 80 | A6 | 1118 | G | C6-N1-C2 | -5.68 | 121.69 | 125.10 |
| 36 | A5 | 39 | A | C2-N3-C4 | 5.68 | 113.44 | 110.60 |
| 36 | A5 | 3290 | G | N7-C8-N9 | 5.68 | 115.94 | 113.10 |
| 37 | A7 | 38 | U | C2-N1-C1' | 5.68 | 124.52 | 117.70 |
| 36 | A1 | 62 | A | C5-C6-N6 | -5.68 | 119.16 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-------|------|-----------|-------|-------------|----------|
| 36 | A1 | 2772 | C | C5-C6-N1 | 5.68 | 123.84 | 121.00 |
| 36 | A1 | 2944 | U | N3-C4-O4 | -5.68 | 115.42 | 119.40 |
| 36 | A1 | 885 | U | N3-C2-O2 | -5.68 | 118.23 | 122.20 |
| 36 | A1 | 1170 | A | C6-N1-C2 | 5.68 | 122.00 | 118.60 |
| 80 | A6 | 1600 | A | N3-C4-C5 | 5.68 | 130.77 | 126.80 |
| 36 | A5 | 413 | U | N1-C2-N3 | 5.68 | 118.31 | 114.90 |
| 36 | A5 | 1405 | U | C2-N3-C4 | -5.68 | 123.59 | 127.00 |
| 36 | A5 | 2197 | C | C2-N1-C1' | -5.68 | 112.56 | 118.80 |
| 36 | A5 | 2584 | G | C5-C6-O6 | -5.68 | 125.19 | 128.60 |
| 36 | A5 | 2892 | A | N1-C6-N6 | -5.68 | 115.19 | 118.60 |
| 36 | A5 | 2988 | C | N3-C4-C5 | -5.68 | 119.63 | 121.90 |
| 36 | A5 | 3020 | U | N3-C2-O2 | 5.68 | 126.17 | 122.20 |
| 1 | A2 | 1458 | G | C4-N9-C1' | 5.67 | 133.88 | 126.50 |
| 36 | A1 | 588 | G | N3-C4-N9 | 5.67 | 129.41 | 126.00 |
| 36 | A1 | 643 | U | C2-N1-C1' | -5.67 | 110.89 | 117.70 |
| 36 | A1 | 2403 | G | N3-C4-N9 | 5.67 | 129.40 | 126.00 |
| 38 | A8 | 95 | G | C8-N9-C1' | 5.67 | 134.38 | 127.00 |
| 52 | DO | 23[B] | ILE | C-N-CA | -5.67 | 107.51 | 121.70 |
| 36 | A1 | 417 | A | C2-N3-C4 | -5.67 | 107.76 | 110.60 |
| 36 | A1 | 1156 | C | C6-N1-C2 | 5.67 | 122.57 | 120.30 |
| 80 | A6 | 109 | G | N7-C8-N9 | -5.67 | 110.26 | 113.10 |
| 80 | A6 | 194 | U | N3-C2-O2 | -5.67 | 118.23 | 122.20 |
| 36 | A5 | 334 | A | C2-N3-C4 | 5.67 | 113.44 | 110.60 |
| 36 | A5 | 819 | U | N3-C4-O4 | 5.67 | 123.37 | 119.40 |
| 1 | A2 | 507 | U | C6-N1-C2 | -5.67 | 117.60 | 121.00 |
| 36 | A1 | 1417 | G | N7-C8-N9 | -5.67 | 110.27 | 113.10 |
| 36 | A1 | 1546 | A | C5-C6-N6 | 5.67 | 128.24 | 123.70 |
| 36 | A5 | 2326 | A | C2-N3-C4 | 5.67 | 113.44 | 110.60 |
| 38 | A8 | 113 | U | C6-N1-C1' | -5.67 | 113.26 | 121.20 |
| 80 | A6 | 389 | G | N3-C4-C5 | -5.67 | 125.77 | 128.60 |
| 80 | A6 | 987 | G | N1-C6-O6 | 5.67 | 123.30 | 119.90 |
| 80 | A6 | 1421 | A | N9-C4-C5 | -5.67 | 103.53 | 105.80 |
| 36 | A5 | 953 | G | N3-C4-N9 | -5.67 | 122.60 | 126.00 |
| 36 | A5 | 1314 | C | N3-C4-C5 | 5.67 | 124.17 | 121.90 |
| 36 | A5 | 2733 | A | C2-N3-C4 | -5.67 | 107.77 | 110.60 |
| 38 | A8 | 109 | A | C8-N9-C4 | -5.67 | 103.53 | 105.80 |
| 36 | A1 | 86 | G | C4-C5-N7 | -5.67 | 108.53 | 110.80 |
| 36 | A1 | 652 | G | N1-C6-O6 | -5.67 | 116.50 | 119.90 |
| 36 | A1 | 658 | G | N3-C4-C5 | -5.67 | 125.77 | 128.60 |
| 36 | A1 | 1919 | G | C8-N9-C4 | -5.67 | 104.13 | 106.40 |
| 80 | A6 | 328 | A | N9-C4-C5 | 5.67 | 108.07 | 105.80 |
| 36 | A5 | 248 | U | C2-N1-C1' | 5.67 | 124.50 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 998 | A | N1-C2-N3 | 5.67 | 132.13 | 129.30 |
| 36 | A5 | 1127 | G | N9-C4-C5 | -5.67 | 103.13 | 105.40 |
| 36 | A5 | 1940 | G | C8-N9-C4 | 5.67 | 108.67 | 106.40 |
| 36 | A5 | 2848 | G | C4-C5-C6 | 5.67 | 122.20 | 118.80 |
| 1 | A2 | 279 | G | N7-C8-N9 | 5.67 | 115.93 | 113.10 |
| 36 | A1 | 1434 | G | C4-C5-N7 | -5.67 | 108.53 | 110.80 |
| 36 | A1 | 3228 | C | N1-C2-O2 | 5.67 | 122.30 | 118.90 |
| 80 | A6 | 814 | A | N7-C8-N9 | 5.67 | 116.63 | 113.80 |
| 36 | A5 | 905 | U | N3-C4-O4 | 5.67 | 123.37 | 119.40 |
| 36 | A5 | 958 | C | N3-C4-C5 | 5.67 | 124.17 | 121.90 |
| 36 | A5 | 1321 | G | N1-C6-O6 | 5.67 | 123.30 | 119.90 |
| 36 | A5 | 2748 | A | C5-C6-N6 | -5.67 | 119.17 | 123.70 |
| 36 | A5 | 2832 | C | C6-N1-C2 | 5.67 | 122.57 | 120.30 |
| 36 | A5 | 2979 | U | C5-C6-N1 | -5.67 | 119.87 | 122.70 |
| 41 | DC | 136 | LEU | CA-CB-CG | 5.67 | 128.34 | 115.30 |
| 36 | A1 | 324 | A | N1-C2-N3 | 5.67 | 132.13 | 129.30 |
| 36 | A1 | 2967 | A | C5-N7-C8 | 5.67 | 106.73 | 103.90 |
| 36 | A1 | 3096 | C | C2-N3-C4 | -5.67 | 117.07 | 119.90 |
| 36 | A1 | 1156 | C | N1-C2-O2 | 5.66 | 122.30 | 118.90 |
| 36 | A1 | 1858 | A | C4-C5-C6 | 5.66 | 119.83 | 117.00 |
| 36 | A1 | 3060 | C | N3-C2-O2 | 5.66 | 125.86 | 121.90 |
| 36 | A5 | 65 | A | P-O3'-C3' | 5.66 | 126.50 | 119.70 |
| 36 | A5 | 824 | C | N3-C4-C5 | -5.66 | 119.64 | 121.90 |
| 36 | A5 | 948 | C | N3-C4-N4 | 5.66 | 121.97 | 118.00 |
| 36 | A5 | 1525 | G | C8-N9-C1' | -5.66 | 119.64 | 127.00 |
| 36 | A5 | 2191 | U | C5-C6-N1 | -5.66 | 119.87 | 122.70 |
| 36 | A5 | 2865 | U | N1-C2-O2 | 5.66 | 126.76 | 122.80 |
| 36 | A5 | 3285 | C | N1-C2-O2 | 5.66 | 122.30 | 118.90 |
| 36 | A1 | 1003 | A | C4-C5-C6 | 5.66 | 119.83 | 117.00 |
| 36 | A1 | 2197 | C | C4-C5-C6 | -5.66 | 114.57 | 117.40 |
| 73 | Bj | 73 | ARG | NE-CZ-NH1 | 5.66 | 123.13 | 120.30 |
| 80 | A6 | 1764 | C | N3-C4-N4 | -5.66 | 114.04 | 118.00 |
| 1 | A2 | 810 | G | C4-C5-N7 | 5.66 | 113.06 | 110.80 |
| 36 | A1 | 22 | G | N1-C6-O6 | -5.66 | 116.50 | 119.90 |
| 36 | A1 | 969 | C | N3-C4-C5 | 5.66 | 124.16 | 121.90 |
| 36 | A1 | 1349 | G | N3-C4-C5 | -5.66 | 125.77 | 128.60 |
| 36 | A1 | 1381 | A | N1-C6-N6 | 5.66 | 122.00 | 118.60 |
| 36 | A1 | 1518 | U | C4-C5-C6 | 5.66 | 123.10 | 119.70 |
| 36 | A1 | 2385 | G | C2-N3-C4 | -5.66 | 109.07 | 111.90 |
| 36 | A1 | 2888 | U | C5-C6-N1 | -5.66 | 119.87 | 122.70 |
| 36 | A5 | 39 | A | C5-N7-C8 | 5.66 | 106.73 | 103.90 |
| 36 | A5 | 114 | A | N1-C6-N6 | 5.66 | 122.00 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 326 | U | C4-C5-C6 | -5.66 | 116.30 | 119.70 |
| 36 | A5 | 1284 | C | C5-C6-N1 | 5.66 | 123.83 | 121.00 |
| 36 | A5 | 3010 | U | N3-C4-O4 | -5.66 | 115.44 | 119.40 |
| 36 | A1 | 192 | C | C2-N1-C1' | 5.66 | 125.02 | 118.80 |
| 36 | A1 | 435 | C | N3-C2-O2 | 5.66 | 125.86 | 121.90 |
| 36 | A1 | 2306 | C | C5-C6-N1 | 5.66 | 123.83 | 121.00 |
| 36 | A1 | 3204 | C | N3-C4-N4 | -5.66 | 114.04 | 118.00 |
| 38 | A4 | 145 | U | C2-N3-C4 | -5.66 | 123.61 | 127.00 |
| 36 | A5 | 769 | G | N7-C8-N9 | -5.66 | 110.27 | 113.10 |
| 36 | A5 | 2951 | G | C5-C6-N1 | 5.66 | 114.33 | 111.50 |
| 1 | A2 | 712 | G | C8-N9-C4 | -5.66 | 104.14 | 106.40 |
| 36 | A1 | 1309 | U | N3-C4-O4 | 5.66 | 123.36 | 119.40 |
| 36 | A5 | 2400 | G | N1-C6-O6 | 5.66 | 123.29 | 119.90 |
| 36 | A1 | 2121 | G | N1-C6-O6 | -5.66 | 116.51 | 119.90 |
| 36 | A5 | 1285 | G | N7-C8-N9 | -5.66 | 110.27 | 113.10 |
| 36 | A5 | 2293 | C | C2-N1-C1' | 5.66 | 125.02 | 118.80 |
| 36 | A5 | 3006 | A | C8-N9-C4 | -5.66 | 103.54 | 105.80 |
| 36 | A5 | 3054 | U | N3-C4-C5 | -5.66 | 111.21 | 114.60 |
| 38 | A4 | 9 | A | N1-C6-N6 | -5.65 | 115.21 | 118.60 |
| 36 | A5 | 625 | G | C8-N9-C4 | -5.65 | 104.14 | 106.40 |
| 1 | A2 | 1644 | C | N1-C2-O2 | -5.65 | 115.51 | 118.90 |
| 36 | A1 | 824 | C | N3-C4-N4 | -5.65 | 114.04 | 118.00 |
| 36 | A1 | 1428 | A | C8-N9-C4 | -5.65 | 103.54 | 105.80 |
| 38 | A4 | 88 | A | N1-C6-N6 | 5.65 | 121.99 | 118.60 |
| 38 | A4 | 103 | G | C8-N9-C4 | -5.65 | 104.14 | 106.40 |
| 52 | BO | 3[B] | SER | CA-C-N | -5.65 | 104.77 | 117.20 |
| 36 | A5 | 1300 | G | C6-C5-N7 | -5.65 | 127.01 | 130.40 |
| 36 | A1 | 197 | G | N1-C2-N2 | 5.65 | 121.29 | 116.20 |
| 36 | A1 | 1196 | C | C6-N1-C2 | 5.65 | 122.56 | 120.30 |
| 36 | A1 | 1349 | G | N3-C4-N9 | 5.65 | 129.39 | 126.00 |
| 36 | A5 | 1603 | A | N9-C4-C5 | 5.65 | 108.06 | 105.80 |
| 37 | A7 | 80 | G | N3-C4-N9 | 5.65 | 129.39 | 126.00 |
| 1 | A2 | 627 | C | N1-C2-O2 | -5.65 | 115.51 | 118.90 |
| 1 | A2 | 1600 | A | C4-C5-N7 | 5.65 | 113.53 | 110.70 |
| 36 | A5 | 925 | A | N1-C6-N6 | 5.65 | 121.99 | 118.60 |
| 36 | A5 | 2237 | C | N3-C2-O2 | -5.65 | 117.95 | 121.90 |
| 36 | A5 | 2341 | A | C5-N7-C8 | 5.65 | 106.72 | 103.90 |
| 36 | A5 | 2415 | C | C6-N1-C2 | 5.65 | 122.56 | 120.30 |
| 36 | A5 | 2904 | U | C2-N3-C4 | -5.65 | 123.61 | 127.00 |
| 36 | A1 | 2257 | C | C6-N1-C2 | -5.65 | 118.04 | 120.30 |
| 36 | A1 | 2368 | A | N1-C2-N3 | 5.65 | 132.12 | 129.30 |
| 41 | BC | 230 | VAL | CB-CA-C | -5.65 | 100.67 | 111.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 80 | A6 | 339 | C | C6-N1-C2 | -5.65 | 118.04 | 120.30 |
| 36 | A5 | 880 | G | C2-N3-C4 | 5.65 | 114.72 | 111.90 |
| 36 | A1 | 1002 | A | C4-C5-C6 | -5.65 | 114.18 | 117.00 |
| 36 | A1 | 1048 | A | C4-C5-C6 | -5.65 | 114.18 | 117.00 |
| 36 | A1 | 1168 | U | N3-C2-O2 | -5.65 | 118.25 | 122.20 |
| 36 | A1 | 1770 | G | N7-C8-N9 | 5.65 | 115.92 | 113.10 |
| 36 | A1 | 2142 | A | C4-C5-C6 | 5.65 | 119.82 | 117.00 |
| 36 | A1 | 3373 | U | C6-N1-C2 | 5.65 | 124.39 | 121.00 |
| 36 | A5 | 2955 | U | N1-C2-N3 | 5.65 | 118.29 | 114.90 |
| 36 | A1 | 304 | G | N1-C2-N3 | -5.64 | 120.51 | 123.90 |
| 36 | A1 | 2282 | U | N3-C4-C5 | 5.64 | 117.99 | 114.60 |
| 36 | A1 | 2885 | C | C5-C6-N1 | -5.64 | 118.18 | 121.00 |
| 38 | A4 | 113 | U | C2-N1-C1' | -5.64 | 110.93 | 117.70 |
| 80 | A6 | 587 | C | C2-N3-C4 | -5.64 | 117.08 | 119.90 |
| 36 | A5 | 1434 | G | C1'-O4'-C4' | -5.64 | 105.38 | 109.90 |
| 36 | A5 | 1883 | A | C8-N9-C4 | -5.64 | 103.54 | 105.80 |
| 1 | A2 | 355 | G | N3-C4-C5 | -5.64 | 125.78 | 128.60 |
| 1 | A2 | 402 | C | C2-N1-C1' | -5.64 | 112.59 | 118.80 |
| 36 | A1 | 1125 | U | C5-C6-N1 | -5.64 | 119.88 | 122.70 |
| 36 | A1 | 1483 | G | N3-C2-N2 | 5.64 | 123.85 | 119.90 |
| 36 | A1 | 2920 | U | C5-C6-N1 | -5.64 | 119.88 | 122.70 |
| 80 | A6 | 940 | A | C2-N3-C4 | -5.64 | 107.78 | 110.60 |
| 80 | A6 | 1620 | C | N3-C2-O2 | -5.64 | 117.95 | 121.90 |
| 36 | A5 | 53 | G | N3-C2-N2 | 5.64 | 123.85 | 119.90 |
| 36 | A5 | 1210 | U | N1-C2-O2 | 5.64 | 126.75 | 122.80 |
| 36 | A5 | 1832 | C | C6-N1-C2 | 5.64 | 122.56 | 120.30 |
| 80 | A6 | 194 | U | C5-C6-N1 | 5.64 | 125.52 | 122.70 |
| 36 | A5 | 1192 | C | C5-C6-N1 | -5.64 | 118.18 | 121.00 |
| 36 | A5 | 1331 | U | C5-C4-O4 | -5.64 | 122.52 | 125.90 |
| 1 | A2 | 382 | C | N3-C4-C5 | 5.64 | 124.16 | 121.90 |
| 36 | A1 | 686 | G | C5-C6-O6 | 5.64 | 131.98 | 128.60 |
| 36 | A1 | 1169 | A | N3-C4-N9 | 5.64 | 131.91 | 127.40 |
| 36 | A1 | 2679 | A | C4-C5-C6 | 5.64 | 119.82 | 117.00 |
| 38 | A4 | 53 | A | N3-C4-C5 | -5.64 | 122.85 | 126.80 |
| 36 | A5 | 1370 | G | N3-C4-N9 | 5.64 | 129.38 | 126.00 |
| 36 | A5 | 3007 | U | C5-C4-O4 | -5.64 | 122.52 | 125.90 |
| 1 | A2 | 1782 | A | C4-C5-N7 | -5.64 | 107.88 | 110.70 |
| 36 | A1 | 44 | U | C2-N3-C4 | -5.64 | 123.62 | 127.00 |
| 36 | A1 | 1514 | G | N1-C2-N2 | -5.64 | 111.13 | 116.20 |
| 80 | A6 | 310 | C | C2-N3-C4 | -5.64 | 117.08 | 119.90 |
| 80 | A6 | 612 | U | C5-C4-O4 | 5.64 | 129.28 | 125.90 |
| 36 | A5 | 574 | U | C5-C4-O4 | -5.64 | 122.52 | 125.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 2257 | C | N1-C2-O2 | 5.64 | 122.28 | 118.90 |
| 36 | A5 | 2816 | G | C4-N9-C1' | -5.64 | 119.17 | 126.50 |
| 64 | Da | 46 | ASP | N-CA-C | -5.64 | 95.78 | 111.00 |
| 36 | A1 | 34 | A | C5-C6-N6 | -5.63 | 119.19 | 123.70 |
| 36 | A1 | 109 | A | N1-C6-N6 | -5.63 | 115.22 | 118.60 |
| 36 | A1 | 157 | A | N1-C2-N3 | 5.63 | 132.12 | 129.30 |
| 36 | A1 | 880 | G | N1-C6-O6 | -5.63 | 116.52 | 119.90 |
| 36 | A1 | 970 | A | C2-N3-C4 | -5.63 | 107.78 | 110.60 |
| 36 | A1 | 3065 | G | N7-C8-N9 | -5.63 | 110.28 | 113.10 |
| 36 | A1 | 3105 | U | N3-C4-C5 | 5.63 | 117.98 | 114.60 |
| 36 | A1 | 3343 | G | N3-C2-N2 | 5.63 | 123.84 | 119.90 |
| 36 | A5 | 873 | C | C4-C5-C6 | 5.63 | 120.22 | 117.40 |
| 36 | A1 | 2787 | G | N3-C4-C5 | -5.63 | 125.78 | 128.60 |
| 24 | CW | 129 | VAL | CB-CA-C | -5.63 | 100.70 | 111.40 |
| 36 | A5 | 634 | C | C2-N3-C4 | -5.63 | 117.08 | 119.90 |
| 36 | A5 | 1909 | A | C4-C5-C6 | -5.63 | 114.18 | 117.00 |
| 36 | A1 | 1849 | C | N1-C2-O2 | -5.63 | 115.52 | 118.90 |
| 80 | A6 | 993 | A | C8-N9-C4 | -5.63 | 103.55 | 105.80 |
| 36 | A5 | 825 | U | N3-C4-O4 | -5.63 | 115.46 | 119.40 |
| 36 | A5 | 2277 | C | N1-C2-O2 | 5.63 | 122.28 | 118.90 |
| 36 | A5 | 2631 | U | N1-C2-O2 | -5.63 | 118.86 | 122.80 |
| 36 | A5 | 2717 | U | C2-N3-C4 | -5.63 | 123.62 | 127.00 |
| 36 | A5 | 3200 | G | N3-C2-N2 | -5.63 | 115.96 | 119.90 |
| 36 | A1 | 3142 | A | C2-N3-C4 | -5.63 | 107.78 | 110.60 |
| 36 | A5 | 359 | U | C5-C6-N1 | -5.63 | 119.89 | 122.70 |
| 36 | A5 | 2389 | C | C5-C4-N4 | -5.63 | 116.26 | 120.20 |
| 1 | A2 | 498 | G | N3-C4-C5 | -5.63 | 125.79 | 128.60 |
| 36 | A1 | 279 | U | N1-C2-N3 | 5.63 | 118.28 | 114.90 |
| 36 | A1 | 1444 | G | N9-C4-C5 | -5.63 | 103.15 | 105.40 |
| 36 | A1 | 2369 | G | C4-N9-C1' | 5.63 | 133.82 | 126.50 |
| 36 | A1 | 3269 | U | N3-C4-O4 | -5.63 | 115.46 | 119.40 |
| 80 | A6 | 158 | U | P-O3'-C3' | 5.63 | 126.45 | 119.70 |
| 36 | A5 | 842 | G | N1-C6-O6 | 5.63 | 123.28 | 119.90 |
| 36 | A5 | 916 | G | N9-C4-C5 | 5.63 | 107.65 | 105.40 |
| 36 | A5 | 3313 | U | N3-C4-O4 | -5.63 | 115.46 | 119.40 |
| 43 | DE | 31 | ARG | NE-CZ-NH2 | -5.63 | 117.49 | 120.30 |
| 36 | A1 | 933 | A | N7-C8-N9 | 5.63 | 116.61 | 113.80 |
| 36 | A1 | 1126 | G | C8-N9-C4 | 5.63 | 108.65 | 106.40 |
| 36 | A1 | 1439 | U | C2-N3-C4 | -5.63 | 123.62 | 127.00 |
| 36 | A1 | 1834 | U | C2-N1-C1' | -5.63 | 110.95 | 117.70 |
| 36 | A1 | 2145 | A | C5-C6-N1 | 5.63 | 120.51 | 117.70 |
| 38 | A4 | 85 | G | N3-C4-C5 | -5.63 | 125.79 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 80 | A6 | 1173 | C | C6-N1-C2 | -5.63 | 118.05 | 120.30 |
| 36 | A5 | 355 | A | N1-C6-N6 | 5.63 | 121.98 | 118.60 |
| 36 | A5 | 946 | U | N1-C2-O2 | 5.63 | 126.74 | 122.80 |
| 36 | A5 | 1146 | C | C2-N3-C4 | -5.63 | 117.09 | 119.90 |
| 36 | A5 | 1163 | A | C4-C5-N7 | -5.63 | 107.89 | 110.70 |
| 36 | A5 | 1381 | A | N9-C4-C5 | -5.63 | 103.55 | 105.80 |
| 1 | A2 | 397 | A | C5-C6-N6 | 5.62 | 128.20 | 123.70 |
| 1 | A2 | 1052 | U | N3-C2-O2 | -5.62 | 118.26 | 122.20 |
| 36 | A1 | 418 | A | C2-N3-C4 | -5.62 | 107.79 | 110.60 |
| 36 | A1 | 1849 | C | C5-C4-N4 | -5.62 | 116.26 | 120.20 |
| 38 | A4 | 31 | G | N3-C2-N2 | 5.62 | 123.84 | 119.90 |
| 80 | A6 | 84 | A | C5-N7-C8 | 5.62 | 106.71 | 103.90 |
| 36 | A5 | 636 | C | C2-N3-C4 | -5.62 | 117.09 | 119.90 |
| 36 | A5 | 1365 | G | N1-C2-N3 | 5.62 | 127.28 | 123.90 |
| 36 | A1 | 1156 | C | C5-C6-N1 | -5.62 | 118.19 | 121.00 |
| 36 | A1 | 1357 | G | C6-C5-N7 | -5.62 | 127.03 | 130.40 |
| 36 | A1 | 1451 | C | C5-C6-N1 | -5.62 | 118.19 | 121.00 |
| 36 | A5 | 2434 | U | C2-N3-C4 | -5.62 | 123.63 | 127.00 |
| 1 | A2 | 951 | A | C8-N9-C4 | 5.62 | 108.05 | 105.80 |
| 36 | A1 | 313 | A | N1-C2-N3 | 5.62 | 132.11 | 129.30 |
| 36 | A1 | 2882 | U | N3-C4-C5 | 5.62 | 117.97 | 114.60 |
| 80 | A6 | 153 | G | N3-C4-C5 | 5.62 | 131.41 | 128.60 |
| 80 | A6 | 968 | U | C4-C5-C6 | -5.62 | 116.33 | 119.70 |
| 36 | A5 | 966 | U | N3-C4-C5 | 5.62 | 117.97 | 114.60 |
| 36 | A5 | 2188 | A | N1-C2-N3 | 5.62 | 132.11 | 129.30 |
| 36 | A5 | 2606 | G | C4-C5-C6 | 5.62 | 122.17 | 118.80 |
| 38 | A8 | 15 | G | C5-C6-O6 | -5.62 | 125.23 | 128.60 |
| 1 | A2 | 74 | U | C3'-C2'-C1' | -5.62 | 97.00 | 101.50 |
| 1 | A2 | 1052 | U | N1-C2-O2 | 5.62 | 126.73 | 122.80 |
| 36 | A1 | 1065 | A | C5-N7-C8 | 5.62 | 106.71 | 103.90 |
| 36 | A1 | 1294 | A | C2-N3-C4 | 5.62 | 113.41 | 110.60 |
| 36 | A1 | 2528 | G | C8-N9-C4 | 5.62 | 108.65 | 106.40 |
| 80 | A6 | 129 | U | N1-C2-N3 | 5.62 | 118.27 | 114.90 |
| 80 | A6 | 472 | U | C2-N3-C4 | -5.62 | 123.63 | 127.00 |
| 36 | A5 | 1845 | G | N7-C8-N9 | -5.62 | 110.29 | 113.10 |
| 36 | A5 | 1914 | G | N1-C6-O6 | -5.62 | 116.53 | 119.90 |
| 36 | A5 | 2217 | U | N3-C2-O2 | -5.62 | 118.27 | 122.20 |
| 37 | A7 | 25 | G | N1-C2-N2 | 5.62 | 121.26 | 116.20 |
| 36 | A1 | 1329 | U | C6-N1-C2 | -5.62 | 117.63 | 121.00 |
| 36 | A5 | 2719 | U | N1-C2-O2 | -5.62 | 118.87 | 122.80 |
| 36 | A5 | 2744 | U | C5-C4-O4 | 5.62 | 129.27 | 125.90 |
| 1 | A2 | 1745 | G | N3-C4-C5 | -5.62 | 125.79 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 80 | A6 | 470 | A | C8-N9-C4 | -5.62 | 103.55 | 105.80 |
| 80 | A6 | 711 | U | C2-N1-C1' | 5.62 | 124.44 | 117.70 |
| 36 | A5 | 666 | A | N7-C8-N9 | -5.62 | 110.99 | 113.80 |
| 36 | A5 | 1206 | G | C5-C6-O6 | 5.62 | 131.97 | 128.60 |
| 36 | A5 | 2616 | C | N3-C4-C5 | 5.62 | 124.15 | 121.90 |
| 36 | A5 | 2742 | C | N3-C4-C5 | 5.62 | 124.15 | 121.90 |
| 1 | A2 | 444 | C | C2-N3-C4 | 5.61 | 122.71 | 119.90 |
| 1 | A2 | 1119 | G | N9-C4-C5 | 5.61 | 107.65 | 105.40 |
| 36 | A1 | 794 | U | N1-C2-N3 | 5.61 | 118.27 | 114.90 |
| 36 | A5 | 180 | C | C6-N1-C2 | -5.61 | 118.05 | 120.30 |
| 36 | A5 | 3197 | G | N3-C2-N2 | -5.61 | 115.97 | 119.90 |
| 68 | De | 105 | ARG | NE-CZ-NH2 | -5.61 | 117.49 | 120.30 |
| 1 | A2 | 109 | G | C5-C6-O6 | -5.61 | 125.23 | 128.60 |
| 36 | A1 | 23 | A | C2-N3-C4 | 5.61 | 113.41 | 110.60 |
| 36 | A1 | 1788 | C | C5-C4-N4 | -5.61 | 116.27 | 120.20 |
| 36 | A1 | 2819 | A | C5-N7-C8 | 5.61 | 106.71 | 103.90 |
| 36 | A1 | 3294 | A | N7-C8-N9 | 5.61 | 116.61 | 113.80 |
| 80 | A6 | 825 | U | N3-C2-O2 | 5.61 | 126.13 | 122.20 |
| 36 | A5 | 1485 | G | C4-C5-N7 | -5.61 | 108.56 | 110.80 |
| 36 | A5 | 2116 | G | C4-C5-C6 | 5.61 | 122.17 | 118.80 |
| 36 | A5 | 2180 | G | N3-C2-N2 | 5.61 | 123.83 | 119.90 |
| 36 | A5 | 2363 | A | N7-C8-N9 | 5.61 | 116.61 | 113.80 |
| 1 | A2 | 453 | U | C5-C4-O4 | 5.61 | 129.27 | 125.90 |
| 36 | A1 | 2639 | G | C5-C6-N1 | 5.61 | 114.31 | 111.50 |
| 36 | A1 | 3137 | C | C6-N1-C2 | -5.61 | 118.06 | 120.30 |
| 80 | A6 | 51 | A | N1-C2-N3 | 5.61 | 132.10 | 129.30 |
| 36 | A5 | 145 | G | N9-C4-C5 | 5.61 | 107.64 | 105.40 |
| 36 | A5 | 217 | U | C2-N3-C4 | -5.61 | 123.63 | 127.00 |
| 36 | A5 | 903 | U | N1-C2-O2 | 5.61 | 126.73 | 122.80 |
| 36 | A5 | 1744 | G | C5-C6-N1 | 5.61 | 114.31 | 111.50 |
| 36 | A5 | 2249 | G | C8-N9-C4 | -5.61 | 104.16 | 106.40 |
| 36 | A5 | 2870 | C | C5-C4-N4 | 5.61 | 124.13 | 120.20 |
| 50 | DM | 77 | ARG | NE-CZ-NH1 | -5.61 | 117.50 | 120.30 |
| 1 | A2 | 1646 | C | C6-N1-C2 | -5.61 | 118.06 | 120.30 |
| 36 | A1 | 3269 | U | C6-N1-C2 | -5.61 | 117.63 | 121.00 |
| 80 | A6 | 96 | G | N1-C2-N3 | 5.61 | 127.27 | 123.90 |
| 36 | A5 | 909 | G | N1-C6-O6 | -5.61 | 116.53 | 119.90 |
| 36 | A5 | 1510 | G | N1-C2-N3 | 5.61 | 127.27 | 123.90 |
| 36 | A5 | 3003 | G | C5-N7-C8 | -5.61 | 101.50 | 104.30 |
| 36 | A5 | 3219 | G | N3-C2-N2 | 5.61 | 123.83 | 119.90 |
| 37 | A7 | 38 | U | N3-C4-C5 | 5.61 | 117.97 | 114.60 |
| 38 | A8 | 100 | U | C2-N1-C1' | 5.61 | 124.43 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A2 | 1761 | U | N3-C4-C5 | -5.61 | 111.24 | 114.60 |
| 36 | A1 | 1360 | C | C5-C6-N1 | -5.61 | 118.20 | 121.00 |
| 36 | A1 | 2606 | G | N3-C4-N9 | 5.61 | 129.36 | 126.00 |
| 80 | A6 | 553 | G | C4-N9-C1' | 5.61 | 133.79 | 126.50 |
| 80 | A6 | 1423 | U | N1-C2-O2 | -5.61 | 118.88 | 122.80 |
| 36 | A5 | 280 | U | N3-C4-C5 | 5.61 | 117.96 | 114.60 |
| 36 | A5 | 282 | G | C2'-C3'-O3' | 5.61 | 122.67 | 113.70 |
| 36 | A5 | 1307 | G | N1-C6-O6 | -5.61 | 116.53 | 119.90 |
| 36 | A5 | 1451 | C | C2-N3-C4 | -5.61 | 117.10 | 119.90 |
| 36 | A5 | 1773 | C | C5-C6-N1 | -5.61 | 118.20 | 121.00 |
| 36 | A5 | 2630 | C | N1-C2-O2 | -5.61 | 115.54 | 118.90 |
| 37 | A7 | 5 | G | C5-C6-N1 | -5.61 | 108.70 | 111.50 |
| 44 | DF | 229 | PHE | CB-CG-CD1 | 5.61 | 124.73 | 120.80 |
| 1 | A2 | 401 | A | N1-C6-N6 | 5.61 | 121.96 | 118.60 |
| 1 | A2 | 1642 | G | N3-C4-C5 | -5.61 | 125.80 | 128.60 |
| 36 | A1 | 649 | A | C2-N3-C4 | -5.61 | 107.80 | 110.60 |
| 36 | A1 | 1391 | C | C4-C5-C6 | 5.61 | 120.20 | 117.40 |
| 36 | A1 | 1448 | U | C5-C4-O4 | -5.61 | 122.54 | 125.90 |
| 36 | A1 | 2227 | C | C3'-C2'-C1' | -5.61 | 97.02 | 101.50 |
| 36 | A1 | 2390 | A | C5-C6-N6 | -5.61 | 119.22 | 123.70 |
| 41 | BC | 327 | LEU | CA-CB-CG | 5.61 | 128.19 | 115.30 |
| 80 | A6 | 359 | A | C8-N9-C4 | 5.61 | 108.04 | 105.80 |
| 80 | A6 | 1773 | C | C2-N3-C4 | 5.61 | 122.70 | 119.90 |
| 36 | A5 | 2683 | U | C2-N1-C1' | 5.61 | 124.43 | 117.70 |
| 1 | A2 | 966 | A | N9-C4-C5 | -5.60 | 103.56 | 105.80 |
| 36 | A1 | 62 | A | N3-C4-N9 | 5.60 | 131.88 | 127.40 |
| 36 | A1 | 317 | A | C8-N9-C4 | -5.60 | 103.56 | 105.80 |
| 36 | A1 | 651 | G | C2-N3-C4 | 5.60 | 114.70 | 111.90 |
| 80 | A6 | 1534 | G | N3-C4-C5 | -5.60 | 125.80 | 128.60 |
| 36 | A5 | 106 | A | C8-N9-C4 | 5.60 | 108.04 | 105.80 |
| 1 | A2 | 131 | C | C5-C6-N1 | 5.60 | 123.80 | 121.00 |
| 1 | A2 | 380 | U | N1-C2-O2 | 5.60 | 126.72 | 122.80 |
| 36 | A1 | 412 | G | C8-N9-C4 | -5.60 | 104.16 | 106.40 |
| 36 | A1 | 634 | C | C2-N1-C1' | -5.60 | 112.64 | 118.80 |
| 36 | A5 | 934 | G | N1-C2-N2 | 5.60 | 121.24 | 116.20 |
| 36 | A5 | 1942 | U | N3-C4-O4 | 5.60 | 123.32 | 119.40 |
| 36 | A1 | 2430 | A | N1-C2-N3 | 5.60 | 132.10 | 129.30 |
| 80 | A6 | 1100 | G | N3-C4-C5 | -5.60 | 125.80 | 128.60 |
| 36 | A5 | 1601 | U | N1-C2-N3 | -5.60 | 111.54 | 114.90 |
| 36 | A5 | 1942 | U | N1-C2-N3 | 5.60 | 118.26 | 114.90 |
| 36 | A5 | 3173 | G | C5-C6-N1 | 5.60 | 114.30 | 111.50 |
| 1 | A2 | 1153 | G | N1-C6-O6 | -5.60 | 116.54 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 147 | U | N3-C2-O2 | -5.60 | 118.28 | 122.20 |
| 36 | A1 | 1548 | C | C6-N1-C2 | -5.60 | 118.06 | 120.30 |
| 36 | A1 | 2860 | U | C5-C6-N1 | 5.60 | 125.50 | 122.70 |
| 36 | A1 | 2933 | A | C5-N7-C8 | -5.60 | 101.10 | 103.90 |
| 36 | A1 | 3029 | A | C8-N9-C4 | -5.60 | 103.56 | 105.80 |
| 80 | A6 | 272 | U | P-O3'-C3' | 5.60 | 126.42 | 119.70 |
| 80 | A6 | 624 | G | N7-C8-N9 | -5.60 | 110.30 | 113.10 |
| 80 | A6 | 1343 | U | N3-C4-O4 | 5.60 | 123.32 | 119.40 |
| 36 | A5 | 347 | G | C8-N9-C4 | 5.60 | 108.64 | 106.40 |
| 36 | A5 | 635 | G | N1-C2-N2 | 5.60 | 121.24 | 116.20 |
| 36 | A5 | 658 | G | N1-C6-O6 | 5.60 | 123.26 | 119.90 |
| 38 | A8 | 37 | A | N1-C6-N6 | -5.60 | 115.24 | 118.60 |
| 1 | A2 | 1749 | A | N3-C4-C5 | 5.60 | 130.72 | 126.80 |
| 36 | A1 | 52 | A | C5-C6-N1 | -5.60 | 114.90 | 117.70 |
| 36 | A1 | 631 | U | C5-C6-N1 | -5.60 | 119.90 | 122.70 |
| 25 | CX | 132 | LEU | CB-CG-CD1 | -5.60 | 101.48 | 111.00 |
| 36 | A5 | 796 | U | N1-C2-O2 | 5.60 | 126.72 | 122.80 |
| 36 | A5 | 950 | G | N9-C4-C5 | -5.60 | 103.16 | 105.40 |
| 36 | A5 | 1343 | A | C8-N9-C4 | -5.60 | 103.56 | 105.80 |
| 36 | A5 | 2828 | G | N1-C6-O6 | -5.60 | 116.54 | 119.90 |
| 36 | A5 | 2889 | C | N3-C4-N4 | -5.60 | 114.08 | 118.00 |
| 36 | A1 | 1796 | G | N1-C6-O6 | -5.60 | 116.54 | 119.90 |
| 80 | A6 | 390 | G | N3-C4-C5 | -5.60 | 125.80 | 128.60 |
| 11 | CJ | 99 | LEU | CA-CB-CG | 5.60 | 128.17 | 115.30 |
| 36 | A1 | 148 | G | C6-C5-N7 | -5.59 | 127.04 | 130.40 |
| 36 | A1 | 890 | C | N3-C4-N4 | -5.59 | 114.08 | 118.00 |
| 36 | A1 | 2646 | C | C2-N3-C4 | -5.59 | 117.10 | 119.90 |
| 80 | A6 | 512 | A | N9-C4-C5 | -5.59 | 103.56 | 105.80 |
| 36 | A5 | 369 | A | N1-C6-N6 | -5.59 | 115.24 | 118.60 |
| 36 | A5 | 911 | C | C4-C5-C6 | 5.59 | 120.20 | 117.40 |
| 36 | A5 | 1844 | C | N1-C2-N3 | 5.59 | 123.12 | 119.20 |
| 1 | A2 | 1445 | G | N1-C6-O6 | 5.59 | 123.26 | 119.90 |
| 1 | A2 | 1796 | C | C6-N1-C2 | -5.59 | 118.06 | 120.30 |
| 36 | A1 | 97 | U | C2-N1-C1' | -5.59 | 110.99 | 117.70 |
| 36 | A1 | 2623 | G | C8-N9-C4 | 5.59 | 108.64 | 106.40 |
| 1 | A2 | 453 | U | C6-N1-C1' | -5.59 | 113.37 | 121.20 |
| 1 | A2 | 852 | C | C4-C5-C6 | -5.59 | 114.60 | 117.40 |
| 1 | A2 | 1145 | U | N1-C2-O2 | -5.59 | 118.89 | 122.80 |
| 36 | A1 | 416 | A | C4-C5-N7 | -5.59 | 107.91 | 110.70 |
| 36 | A1 | 2633 | U | N3-C4-O4 | -5.59 | 115.49 | 119.40 |
| 36 | A1 | 3056 | U | N1-C2-N3 | 5.59 | 118.25 | 114.90 |
| 40 | BB | 305 | ILE | CB-CA-C | -5.59 | 100.42 | 111.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 80 | A6 | 432 | G | N9-C4-C5 | 5.59 | 107.64 | 105.40 |
| 36 | A5 | 1171 | G | C8-N9-C4 | -5.59 | 104.16 | 106.40 |
| 36 | A5 | 3140 | G | C6-C5-N7 | -5.59 | 127.05 | 130.40 |
| 68 | De | 4 | LEU | C-N-CA | -5.59 | 98.52 | 122.00 |
| 1 | A2 | 334 | G | N3-C4-C5 | 5.59 | 131.40 | 128.60 |
| 36 | A1 | 34 | A | N1-C6-N6 | 5.59 | 121.95 | 118.60 |
| 36 | A1 | 658 | G | C4-C5-C6 | 5.59 | 122.15 | 118.80 |
| 36 | A1 | 1224 | C | C6-N1-C2 | -5.59 | 118.06 | 120.30 |
| 36 | A1 | 2547 | A | C4-N9-C1' | 5.59 | 136.36 | 126.30 |
| 37 | A3 | 21 | G | C8-N9-C4 | 5.59 | 108.64 | 106.40 |
| 80 | A6 | 359 | A | C6-C5-N7 | 5.59 | 136.21 | 132.30 |
| 36 | A5 | 1315 | U | C6-N1-C1' | -5.59 | 113.38 | 121.20 |
| 36 | A5 | 3252 | G | C8-N9-C4 | 5.59 | 108.64 | 106.40 |
| 37 | A7 | 46 | A | N9-C4-C5 | 5.59 | 108.04 | 105.80 |
| 1 | A2 | 1633 | A | C4-C5-N7 | -5.59 | 107.91 | 110.70 |
| 36 | A1 | 903 | U | N1-C2-N3 | 5.59 | 118.25 | 114.90 |
| 36 | A5 | 637 | C | C5-C6-N1 | -5.59 | 118.21 | 121.00 |
| 36 | A5 | 743 | C | C6-N1-C2 | -5.59 | 118.06 | 120.30 |
| 36 | A5 | 1872 | C | N3-C2-O2 | -5.59 | 117.99 | 121.90 |
| 37 | A7 | 79 | A | N7-C8-N9 | 5.59 | 116.59 | 113.80 |
| 1 | A2 | 1279 | C | C6-N1-C2 | -5.59 | 118.06 | 120.30 |
| 36 | A1 | 126 | U | N1-C2-N3 | 5.59 | 118.25 | 114.90 |
| 36 | A1 | 726 | G | N7-C8-N9 | 5.59 | 115.89 | 113.10 |
| 36 | A1 | 974 | G | C4-N9-C1' | 5.59 | 133.76 | 126.50 |
| 36 | A1 | 3052 | G | N9-C4-C5 | 5.59 | 107.64 | 105.40 |
| 36 | A1 | 3188 | G | C8-N9-C1' | -5.59 | 119.74 | 127.00 |
| 80 | A6 | 102 | U | N3-C4-O4 | 5.59 | 123.31 | 119.40 |
| 80 | A6 | 1260 | U | N3-C2-O2 | -5.59 | 118.29 | 122.20 |
| 36 | A5 | 363 | G | C4-C5-N7 | -5.59 | 108.56 | 110.80 |
| 36 | A5 | 546 | C | C6-N1-C2 | -5.59 | 118.07 | 120.30 |
| 36 | A5 | 1207 | G | N1-C6-O6 | -5.59 | 116.55 | 119.90 |
| 36 | A5 | 1926 | C | N1-C2-O2 | -5.59 | 115.55 | 118.90 |
| 36 | A1 | 47 | C | N3-C4-C5 | -5.58 | 119.67 | 121.90 |
| 36 | A1 | 154 | U | N3-C4-O4 | -5.58 | 115.49 | 119.40 |
| 36 | A1 | 2305 | G | N3-C4-N9 | 5.58 | 129.35 | 126.00 |
| 36 | A5 | 1754 | G | N1-C2-N2 | -5.58 | 111.17 | 116.20 |
| 36 | A5 | 2999 | U | C5-C6-N1 | -5.58 | 119.91 | 122.70 |
| 63 | DZ | 135 | ARG | NE-CZ-NH2 | 5.58 | 123.09 | 120.30 |
| 1 | A2 | 1456 | C | N1-C2-N3 | 5.58 | 123.11 | 119.20 |
| 36 | A1 | 332 | C | C2-N3-C4 | -5.58 | 117.11 | 119.90 |
| 36 | A1 | 420 | G | N3-C2-N2 | 5.58 | 123.81 | 119.90 |
| 36 | A1 | 776 | U | N3-C4-C5 | -5.58 | 111.25 | 114.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 36 | A1 | 1409 | G | C4-C5-N7 | -5.58 | 108.57 | 110.80 |
| 36 | A1 | 2161 | G | N9-C4-C5 | 5.58 | 107.63 | 105.40 |
| 36 | A1 | 2950 | G | C5-C6-N1 | 5.58 | 114.29 | 111.50 |
| 62 | BY | 126 | LEU | CA-CB-CG | 5.58 | 128.14 | 115.30 |
| 80 | A6 | 254 | A | C8-N9-C4 | 5.58 | 108.03 | 105.80 |
| 36 | A5 | 340 | C | N1-C2-N3 | 5.58 | 123.11 | 119.20 |
| 36 | A5 | 960 | U | C4-C5-C6 | 5.58 | 123.05 | 119.70 |
| 45 | DG | 69 | LEU | CA-CB-CG | 5.58 | 128.14 | 115.30 |
| 1 | A2 | 74 | U | C1'-O4'-C4' | -5.58 | 105.44 | 109.90 |
| 36 | A1 | 592 | A | C8-N9-C4 | 5.58 | 108.03 | 105.80 |
| 36 | A1 | 960 | U | C5-C4-O4 | -5.58 | 122.55 | 125.90 |
| 36 | A1 | 2173 | U | N1-C2-O2 | -5.58 | 118.89 | 122.80 |
| 37 | A3 | 68 | C | C6-N1-C2 | 5.58 | 122.53 | 120.30 |
| 80 | A6 | 99 | C | C5-C4-N4 | -5.58 | 116.29 | 120.20 |
| 10 | CI | 58 | LEU | CB-CG-CD1 | -5.58 | 101.51 | 111.00 |
| 36 | A5 | 911 | C | C5-C6-N1 | -5.58 | 118.21 | 121.00 |
| 36 | A5 | 1144 | U | C2-N3-C4 | -5.58 | 123.65 | 127.00 |
| 36 | A5 | 2343 | C | C5-C4-N4 | -5.58 | 116.29 | 120.20 |
| 1 | A2 | 42 | G | C8-N9-C4 | 5.58 | 108.63 | 106.40 |
| 1 | A2 | 1536 | G | C8-N9-C1' | -5.58 | 119.75 | 127.00 |
| 36 | A1 | 345 | G | C6-N1-C2 | -5.58 | 121.75 | 125.10 |
| 36 | A1 | 2343 | C | C5-C6-N1 | -5.58 | 118.21 | 121.00 |
| 36 | A1 | 2552 | C | N1-C2-O2 | 5.58 | 122.25 | 118.90 |
| 40 | BB | 316 | GLU | N-CA-C | 5.58 | 126.07 | 111.00 |
| 80 | A6 | 687 | G | N3-C4-C5 | 5.58 | 131.39 | 128.60 |
| 36 | A5 | 234 | G | N1-C6-O6 | 5.58 | 123.25 | 119.90 |
| 36 | A5 | 405 | U | C5-C4-O4 | -5.58 | 122.55 | 125.90 |
| 36 | A5 | 1403 | C | C2-N3-C4 | -5.58 | 117.11 | 119.90 |
| 36 | A1 | 20 | A | N1-C6-N6 | -5.58 | 115.25 | 118.60 |
| 36 | A1 | 206 | G | C2-N3-C4 | 5.58 | 114.69 | 111.90 |
| 36 | A1 | 1548 | C | N3-C4-N4 | 5.58 | 121.91 | 118.00 |
| 36 | A1 | 2200 | U | C5-C6-N1 | 5.58 | 125.49 | 122.70 |
| 36 | A1 | 2740 | A | C8-N9-C4 | -5.58 | 103.57 | 105.80 |
| 36 | A1 | 3173 | G | N7-C8-N9 | 5.58 | 115.89 | 113.10 |
| 36 | A5 | 2239 | G | N3-C2-N2 | 5.58 | 123.80 | 119.90 |
| 36 | A5 | 3287 | U | N3-C2-O2 | -5.58 | 118.30 | 122.20 |
| 36 | A1 | 350 | C | N1-C2-N3 | 5.58 | 123.10 | 119.20 |
| 36 | A1 | 835 | G | N7-C8-N9 | -5.58 | 110.31 | 113.10 |
| 36 | A1 | 1110 | U | C4-C5-C6 | -5.58 | 116.35 | 119.70 |
| 36 | A1 | 2138 | A | N7-C8-N9 | 5.58 | 116.59 | 113.80 |
| 36 | A5 | 1797 | A | C4-C5-N7 | -5.58 | 107.91 | 110.70 |
| 36 | A5 | 2307 | G | N3-C2-N2 | 5.58 | 123.80 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 36 | A5 | 2729 | U | C4-C5-C6 | -5.58 | 116.35 | 119.70 |
| 37 | A7 | 1 | G | C6-C5-N7 | -5.58 | 127.05 | 130.40 |
| 38 | A8 | 147 | U | N3-C4-C5 | 5.58 | 117.95 | 114.60 |
| 78 | Do | 41 | ARG | NE-CZ-NH2 | -5.58 | 117.51 | 120.30 |
| 1 | A2 | 1650 | U | C5-C6-N1 | -5.58 | 119.91 | 122.70 |
| 36 | A1 | 1439 | U | N1-C2-N3 | 5.58 | 118.25 | 114.90 |
| 36 | A1 | 2642 | A | N3-C4-C5 | 5.58 | 130.70 | 126.80 |
| 36 | A1 | 3328 | G | N7-C8-N9 | 5.58 | 115.89 | 113.10 |
| 80 | A6 | 352 | A | N3-C4-C5 | 5.58 | 130.70 | 126.80 |
| 80 | A6 | 1665 | U | C4-C5-C6 | -5.58 | 116.36 | 119.70 |
| 36 | A5 | 21 | G | N3-C4-C5 | 5.58 | 131.39 | 128.60 |
| 36 | A5 | 1183 | C | N3-C4-C5 | 5.58 | 124.13 | 121.90 |
| 36 | A5 | 2974 | U | C5-C4-O4 | 5.58 | 129.25 | 125.90 |
| 1 | A2 | 1280 | C | C4-C5-C6 | 5.57 | 120.19 | 117.40 |
| 18 | AQ | 69 | VAL | CB-CA-C | -5.57 | 100.81 | 111.40 |
| 36 | A1 | 2435 | G | N3-C4-C5 | -5.57 | 125.81 | 128.60 |
| 80 | A6 | 13 | C | C4-C5-C6 | 5.57 | 120.19 | 117.40 |
| 80 | A6 | 1763 | A | C8-N9-C4 | 5.57 | 108.03 | 105.80 |
| 36 | A5 | 1586 | G | C6-N1-C2 | -5.57 | 121.76 | 125.10 |
| 36 | A5 | 2642 | A | C8-N9-C4 | 5.57 | 108.03 | 105.80 |
| 36 | A5 | 2830 | G | N1-C6-O6 | -5.57 | 116.56 | 119.90 |
| 38 | A8 | 13 | A | C5-N7-C8 | -5.57 | 101.11 | 103.90 |
| 36 | A1 | 425 | G | N1-C2-N3 | 5.57 | 127.24 | 123.90 |
| 36 | A5 | 2914 | G | N1-C6-O6 | -5.57 | 116.56 | 119.90 |
| 36 | A1 | 44 | U | C2-N1-C1' | -5.57 | 111.02 | 117.70 |
| 36 | A1 | 2678 | A | C5-C6-N6 | 5.57 | 128.16 | 123.70 |
| 70 | Bg | 71 | THR | CB-CA-C | -5.57 | 96.56 | 111.60 |
| 80 | A6 | 356 | G | N7-C8-N9 | -5.57 | 110.31 | 113.10 |
| 36 | A5 | 436 | A | C4-C5-N7 | 5.57 | 113.48 | 110.70 |
| 36 | A5 | 935 | U | C2-N3-C4 | -5.57 | 123.66 | 127.00 |
| 36 | A5 | 1365 | G | C4-N9-C1' | 5.57 | 133.74 | 126.50 |
| 36 | A5 | 3152 | U | C5-C6-N1 | -5.57 | 119.91 | 122.70 |
| 36 | A1 | 1480 | G | C6-C5-N7 | -5.57 | 127.06 | 130.40 |
| 36 | A1 | 2692 | A | C6-C5-N7 | -5.57 | 128.40 | 132.30 |
| 36 | A5 | 2139 | A | C5-C6-N6 | 5.57 | 128.16 | 123.70 |
| 1 | A2 | 542 | A | C8-N9-C4 | -5.57 | 103.57 | 105.80 |
| 36 | A1 | 142 | C | C5-C6-N1 | 5.57 | 123.78 | 121.00 |
| 36 | A1 | 226 | C | C2-N3-C4 | -5.57 | 117.12 | 119.90 |
| 36 | A1 | 2513 | U | C3'-C2'-C1' | 5.57 | 105.95 | 101.50 |
| 38 | A4 | 85 | G | C5-C6-O6 | -5.57 | 125.26 | 128.60 |
| 80 | A6 | 1153 | G | N3-C4-C5 | 5.57 | 131.38 | 128.60 |
| 80 | A6 | 1745 | G | C8-N9-C4 | 5.57 | 108.63 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 2287 | C | C6-N1-C2 | -5.57 | 118.07 | 120.30 |
| 36 | A5 | 2605 | G | C2-N3-C4 | 5.57 | 114.68 | 111.90 |
| 36 | A5 | 367 | A | N3-C4-C5 | 5.57 | 130.69 | 126.80 |
| 36 | A5 | 2975 | U | N3-C4-O4 | -5.57 | 115.50 | 119.40 |
| 38 | A8 | 12 | A | C4-C5-C6 | -5.57 | 114.22 | 117.00 |
| 36 | A1 | 1899 | G | C8-N9-C4 | -5.56 | 104.17 | 106.40 |
| 36 | A1 | 2134 | G | C5-C6-N1 | 5.56 | 114.28 | 111.50 |
| 36 | A1 | 2137 | U | N3-C4-O4 | 5.56 | 123.30 | 119.40 |
| 36 | A5 | 1670 | C | C6-N1-C2 | 5.56 | 122.53 | 120.30 |
| 36 | A5 | 1909 | A | N1-C6-N6 | -5.56 | 115.26 | 118.60 |
| 1 | A2 | 1277 | G | N3-C4-N9 | -5.56 | 122.66 | 126.00 |
| 36 | A1 | 431 | U | N3-C2-O2 | -5.56 | 118.31 | 122.20 |
| 36 | A1 | 1930 | A | C2-N3-C4 | -5.56 | 107.82 | 110.60 |
| 36 | A1 | 3013 | U | C5-C6-N1 | 5.56 | 125.48 | 122.70 |
| 80 | A6 | 580 | A | N9-C4-C5 | 5.56 | 108.03 | 105.80 |
| 36 | A5 | 957 | C | C5-C6-N1 | -5.56 | 118.22 | 121.00 |
| 36 | A5 | 1170 | A | C8-N9-C4 | 5.56 | 108.03 | 105.80 |
| 36 | A5 | 2975 | U | C4-C5-C6 | -5.56 | 116.36 | 119.70 |
| 36 | A5 | 3010 | U | C5-C4-O4 | 5.56 | 129.24 | 125.90 |
| 80 | A6 | 1361 | U | C2-N1-C1' | 5.56 | 124.37 | 117.70 |
| 36 | A5 | 33 | G | C5-C6-N1 | 5.56 | 114.28 | 111.50 |
| 36 | A5 | 728 | G | N7-C8-N9 | -5.56 | 110.32 | 113.10 |
| 38 | A8 | 112 | U | C6-N1-C1' | 5.56 | 128.99 | 121.20 |
| 1 | A2 | 1486 | G | C6-C5-N7 | -5.56 | 127.06 | 130.40 |
| 36 | A1 | 212 | G | C8-N9-C4 | 5.56 | 108.62 | 106.40 |
| 36 | A1 | 290 | G | N1-C2-N3 | -5.56 | 120.56 | 123.90 |
| 36 | A1 | 1802 | C | N3-C2-O2 | 5.56 | 125.79 | 121.90 |
| 36 | A1 | 2130 | G | N3-C2-N2 | 5.56 | 123.79 | 119.90 |
| 36 | A1 | 2821 | C | N3-C4-C5 | -5.56 | 119.68 | 121.90 |
| 36 | A5 | 648 | C | C2-N1-C1' | 5.56 | 124.92 | 118.80 |
| 36 | A5 | 2327 | U | C2-N1-C1' | -5.56 | 111.03 | 117.70 |
| 36 | A5 | 3059 | G | C8-N9-C4 | 5.56 | 108.62 | 106.40 |
| 37 | A7 | 69 | C | N3-C4-C5 | 5.56 | 124.12 | 121.90 |
| 36 | A1 | 105 | C | C5-C6-N1 | -5.56 | 118.22 | 121.00 |
| 36 | A1 | 787 | G | C4-C5-N7 | -5.56 | 108.58 | 110.80 |
| 36 | A1 | 2131 | A | C2-N3-C4 | -5.56 | 107.82 | 110.60 |
| 36 | A1 | 3171 | U | C6-N1-C2 | 5.56 | 124.33 | 121.00 |
| 36 | A1 | 3362 | A | C8-N9-C1' | -5.56 | 117.70 | 127.70 |
| 36 | A5 | 42 | C | N1-C2-O2 | 5.56 | 122.23 | 118.90 |
| 36 | A5 | 335 | G | N1-C6-O6 | -5.56 | 116.57 | 119.90 |
| 36 | A5 | 1658 | G | N1-C6-O6 | -5.56 | 116.56 | 119.90 |
| 36 | A5 | 1670 | C | C5-C4-N4 | -5.56 | 116.31 | 120.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 1773 | C | C4-C5-C6 | 5.56 | 120.18 | 117.40 |
| 36 | A5 | 1901 | A | C6-C5-N7 | -5.56 | 128.41 | 132.30 |
| 36 | A1 | 1841 | A | C8-N9-C4 | -5.56 | 103.58 | 105.80 |
| 36 | A5 | 1444 | G | C8-N9-C4 | 5.56 | 108.62 | 106.40 |
| 36 | A5 | 1905 | G | N1-C6-O6 | -5.56 | 116.57 | 119.90 |
| 1 | A2 | 435 | C | C2-N3-C4 | 5.55 | 122.68 | 119.90 |
| 80 | A6 | 110 | U | N1-C2-O2 | 5.55 | 126.69 | 122.80 |
| 80 | A6 | 1235 | C | C6-N1-C2 | -5.55 | 118.08 | 120.30 |
| 36 | A5 | 715 | A | C5-C6-N1 | 5.55 | 120.48 | 117.70 |
| 36 | A1 | 2371 | G | N1-C6-O6 | 5.55 | 123.23 | 119.90 |
| 36 | A5 | 1360 | C | C2-N3-C4 | -5.55 | 117.12 | 119.90 |
| 36 | A5 | 2158 | A | C6-N1-C2 | -5.55 | 115.27 | 118.60 |
| 36 | A5 | 2293 | C | C5-C4-N4 | -5.55 | 116.31 | 120.20 |
| 1 | A2 | 696 | C | C6-N1-C2 | -5.55 | 118.08 | 120.30 |
| 1 | A2 | 1127 | G | N9-C4-C5 | 5.55 | 107.62 | 105.40 |
| 1 | A2 | 1636 | C | N3-C4-N4 | 5.55 | 121.89 | 118.00 |
| 36 | A1 | 65 | A | P-O3'-C3' | 5.55 | 126.36 | 119.70 |
| 36 | A1 | 695 | C | C5-C4-N4 | 5.55 | 124.09 | 120.20 |
| 36 | A1 | 1131 | G | N1-C2-N2 | -5.55 | 111.20 | 116.20 |
| 36 | A1 | 1158 | A | C5-C6-N6 | -5.55 | 119.26 | 123.70 |
| 80 | A6 | 54 | C | N3-C4-C5 | 5.55 | 124.12 | 121.90 |
| 80 | A6 | 987 | G | N1-C2-N2 | 5.55 | 121.20 | 116.20 |
| 36 | A5 | 367 | A | C5-C6-N6 | 5.55 | 128.14 | 123.70 |
| 36 | A5 | 3055 | U | C2-N1-C1' | 5.55 | 124.36 | 117.70 |
| 36 | A1 | 880 | G | C4-N9-C1' | -5.55 | 119.29 | 126.50 |
| 36 | A1 | 1365 | G | N3-C4-C5 | -5.55 | 125.83 | 128.60 |
| 36 | A1 | 1480 | G | C8-N9-C1' | -5.55 | 119.78 | 127.00 |
| 36 | A1 | 2645 | G | C6-N1-C2 | -5.55 | 121.77 | 125.10 |
| 36 | A1 | 2806 | U | N1-C2-N3 | 5.55 | 118.23 | 114.90 |
| 36 | A1 | 2814 | G | N9-C4-C5 | -5.55 | 103.18 | 105.40 |
| 36 | A1 | 3362 | A | N9-C4-C5 | -5.55 | 103.58 | 105.80 |
| 80 | A6 | 750 | U | C6-N1-C2 | 5.55 | 124.33 | 121.00 |
| 36 | A5 | 431 | U | C2-N3-C4 | -5.55 | 123.67 | 127.00 |
| 36 | A5 | 914 | A | N1-C2-N3 | 5.55 | 132.07 | 129.30 |
| 36 | A5 | 2658 | G | N3-C2-N2 | -5.55 | 116.02 | 119.90 |
| 36 | A5 | 2717 | U | N3-C2-O2 | -5.55 | 118.31 | 122.20 |
| 36 | A5 | 3179 | U | N3-C4-C5 | 5.55 | 117.93 | 114.60 |
| 36 | A1 | 2940 | A | C5-N7-C8 | 5.55 | 106.67 | 103.90 |
| 80 | A6 | 2 | A | C8-N9-C4 | 5.55 | 108.02 | 105.80 |
| 36 | A5 | 3336 | A | C4-C5-C6 | 5.55 | 119.77 | 117.00 |
| 1 | A2 | 1560 | U | N1-C2-O2 | 5.55 | 126.68 | 122.80 |
| 36 | A1 | 579 | G | N1-C6-O6 | -5.55 | 116.57 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-------|------|-----------|-------|-------------|----------|
| 36 | A5 | 98 | G | C8-N9-C4 | 5.55 | 108.62 | 106.40 |
| 36 | A5 | 1086 | C | C5-C6-N1 | 5.55 | 123.77 | 121.00 |
| 36 | A5 | 1847 | A | C2-N3-C4 | -5.55 | 107.83 | 110.60 |
| 36 | A5 | 3395 | G | N1-C6-O6 | 5.55 | 123.23 | 119.90 |
| 36 | A1 | 2273 | G | C4-N9-C1' | -5.54 | 119.29 | 126.50 |
| 36 | A5 | 1305 | U | C6-N1-C2 | 5.54 | 124.33 | 121.00 |
| 36 | A5 | 3103 | A | C5-C6-N1 | 5.54 | 120.47 | 117.70 |
| 1 | A2 | 258 | C | N3-C4-C5 | 5.54 | 124.12 | 121.90 |
| 1 | A2 | 342 | C | C6-N1-C2 | 5.54 | 122.52 | 120.30 |
| 36 | A1 | 51 | A | N1-C6-N6 | 5.54 | 121.93 | 118.60 |
| 36 | A1 | 1869 | C | N1-C2-O2 | 5.54 | 122.23 | 118.90 |
| 80 | A6 | 385 | A | C5-C6-N6 | 5.54 | 128.13 | 123.70 |
| 37 | A7 | 1 | G | N3-C4-N9 | 5.54 | 129.33 | 126.00 |
| 64 | Da | 17 | ALA | C-N-CA | -5.54 | 110.66 | 122.30 |
| 1 | A2 | 115 | G | N1-C6-O6 | 5.54 | 123.22 | 119.90 |
| 1 | A2 | 144 | U | C5-C4-O4 | 5.54 | 129.22 | 125.90 |
| 1 | A2 | 613 | G | N1-C6-O6 | -5.54 | 116.58 | 119.90 |
| 36 | A1 | 639 | G | C2-N3-C4 | -5.54 | 109.13 | 111.90 |
| 36 | A1 | 949 | C | C2-N3-C4 | -5.54 | 117.13 | 119.90 |
| 36 | A1 | 2773 | C | C5-C4-N4 | -5.54 | 116.32 | 120.20 |
| 80 | A6 | 647 | G | C8-N9-C4 | -5.54 | 104.18 | 106.40 |
| 36 | A5 | 347 | G | N7-C8-N9 | -5.54 | 110.33 | 113.10 |
| 36 | A5 | 395 | A | N7-C8-N9 | 5.54 | 116.57 | 113.80 |
| 36 | A5 | 1125 | U | N3-C4-O4 | -5.54 | 115.52 | 119.40 |
| 36 | A5 | 1189 | C | N3-C2-O2 | 5.54 | 125.78 | 121.90 |
| 36 | A5 | 1215 | U | N3-C2-O2 | 5.54 | 126.08 | 122.20 |
| 36 | A5 | 1441 | G | C5-C6-N1 | 5.54 | 114.27 | 111.50 |
| 36 | A5 | 2706 | G | N3-C4-C5 | -5.54 | 125.83 | 128.60 |
| 36 | A5 | 3326 | G | C5-C6-O6 | 5.54 | 131.93 | 128.60 |
| 36 | A1 | 2340 | U | C4-C5-C6 | -5.54 | 116.38 | 119.70 |
| 36 | A1 | 3375 | A | C4-C5-C6 | 5.54 | 119.77 | 117.00 |
| 36 | A5 | 1843 | C | C5-C6-N1 | 5.54 | 123.77 | 121.00 |
| 36 | A5 | 3052 | G | C4-N9-C1' | -5.54 | 119.30 | 126.50 |
| 52 | DO | 23[B] | ILE | CA-C-N | -5.54 | 105.01 | 117.20 |
| 1 | A2 | 323 | A | N9-C4-C5 | 5.54 | 108.02 | 105.80 |
| 36 | A1 | 970 | A | N9-C4-C5 | 5.54 | 108.02 | 105.80 |
| 36 | A5 | 390 | G | N9-C4-C5 | -5.54 | 103.19 | 105.40 |
| 36 | A5 | 1797 | A | C8-N9-C4 | 5.54 | 108.02 | 105.80 |
| 36 | A5 | 1906 | G | C2-N3-C4 | -5.54 | 109.13 | 111.90 |
| 36 | A1 | 362 | U | N3-C4-O4 | -5.54 | 115.52 | 119.40 |
| 36 | A5 | 1380 | G | C8-N9-C4 | 5.54 | 108.61 | 106.40 |
| 36 | A5 | 1724 | U | N3-C2-O2 | -5.54 | 118.32 | 122.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 1741 | A | N7-C8-N9 | 5.54 | 116.57 | 113.80 |
| 36 | A1 | 1910 | A | N9-C4-C5 | -5.54 | 103.58 | 105.80 |
| 36 | A1 | 3193 | C | N1-C2-O2 | -5.54 | 115.58 | 118.90 |
| 43 | BE | 64 | LEU | CA-CB-CG | 5.54 | 128.03 | 115.30 |
| 80 | A6 | 306 | U | C5-C4-O4 | -5.54 | 122.58 | 125.90 |
| 36 | A5 | 46 | U | C2-N3-C4 | 5.54 | 130.32 | 127.00 |
| 36 | A5 | 1165 | A | N7-C8-N9 | -5.54 | 111.03 | 113.80 |
| 36 | A5 | 1305 | U | C6-N1-C1' | -5.54 | 113.45 | 121.20 |
| 36 | A5 | 2289 | U | C5-C4-O4 | 5.54 | 129.22 | 125.90 |
| 36 | A5 | 2309 | A | C8-N9-C4 | 5.54 | 108.01 | 105.80 |
| 36 | A5 | 2335 | G | C6-N1-C2 | -5.54 | 121.78 | 125.10 |
| 36 | A1 | 847 | A | C4-C5-N7 | 5.53 | 113.47 | 110.70 |
| 36 | A1 | 1048 | A | C2-N3-C4 | 5.53 | 113.37 | 110.60 |
| 36 | A5 | 1887 | A | N9-C4-C5 | -5.53 | 103.59 | 105.80 |
| 36 | A5 | 2870 | C | C2-N1-C1' | -5.53 | 112.71 | 118.80 |
| 36 | A1 | 2350 | C | C5-C6-N1 | -5.53 | 118.23 | 121.00 |
| 1 | A2 | 36 | C | C5-C4-N4 | -5.53 | 116.33 | 120.20 |
| 1 | A2 | 1129 | U | C2-N3-C4 | -5.53 | 123.68 | 127.00 |
| 1 | A2 | 1503 | A | N7-C8-N9 | 5.53 | 116.56 | 113.80 |
| 36 | A1 | 45 | A | N7-C8-N9 | -5.53 | 111.03 | 113.80 |
| 36 | A1 | 56 | G | C4-C5-N7 | 5.53 | 113.01 | 110.80 |
| 36 | A1 | 810 | A | N9-C4-C5 | 5.53 | 108.01 | 105.80 |
| 36 | A1 | 926 | A | C4-C5-C6 | -5.53 | 114.23 | 117.00 |
| 36 | A1 | 3203 | U | N3-C2-O2 | -5.53 | 118.33 | 122.20 |
| 36 | A5 | 266 | A | N1-C2-N3 | 5.53 | 132.06 | 129.30 |
| 36 | A5 | 285 | A | C8-N9-C4 | -5.53 | 103.59 | 105.80 |
| 36 | A5 | 517 | G | C4-C5-C6 | 5.53 | 122.12 | 118.80 |
| 36 | A5 | 953 | G | N3-C4-C5 | 5.53 | 131.37 | 128.60 |
| 36 | A5 | 954 | U | C6-N1-C2 | -5.53 | 117.68 | 121.00 |
| 36 | A5 | 2966 | G | C5-C6-N1 | 5.53 | 114.27 | 111.50 |
| 36 | A5 | 2996 | U | C6-N1-C1' | -5.53 | 113.46 | 121.20 |
| 80 | A6 | 1400 | A | C2-N3-C4 | 5.53 | 113.36 | 110.60 |
| 36 | A5 | 969 | C | C5-C6-N1 | -5.53 | 118.24 | 121.00 |
| 36 | A1 | 190 | U | N3-C4-O4 | -5.53 | 115.53 | 119.40 |
| 36 | A1 | 642 | U | N3-C4-C5 | -5.53 | 111.28 | 114.60 |
| 36 | A1 | 1415 | U | N3-C4-O4 | -5.53 | 115.53 | 119.40 |
| 80 | A6 | 1678 | A | C8-N9-C4 | -5.53 | 103.59 | 105.80 |
| 36 | A5 | 39 | A | N7-C8-N9 | -5.53 | 111.04 | 113.80 |
| 36 | A5 | 814 | U | N1-C2-N3 | -5.53 | 111.58 | 114.90 |
| 36 | A5 | 3394 | U | N3-C4-O4 | -5.53 | 115.53 | 119.40 |
| 38 | A8 | 87 | G | C5-C6-O6 | -5.53 | 125.28 | 128.60 |
| 36 | A1 | 1421 | G | C8-N9-C4 | 5.53 | 108.61 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 359 | U | N3-C4-C5 | 5.53 | 117.92 | 114.60 |
| 36 | A5 | 844 | G | N7-C8-N9 | -5.53 | 110.34 | 113.10 |
| 36 | A5 | 1178 | G | N7-C8-N9 | 5.53 | 115.86 | 113.10 |
| 36 | A5 | 1295 | G | C5-C6-O6 | 5.53 | 131.92 | 128.60 |
| 36 | A5 | 2182 | A | C4-C5-C6 | -5.53 | 114.24 | 117.00 |
| 36 | A5 | 3064 | U | N1-C2-N3 | 5.53 | 118.22 | 114.90 |
| 1 | A2 | 1614 | A | C6-C5-N7 | -5.52 | 128.43 | 132.30 |
| 36 | A1 | 795 | G | N7-C8-N9 | -5.52 | 110.34 | 113.10 |
| 36 | A1 | 1211 | U | N3-C4-C5 | 5.52 | 117.91 | 114.60 |
| 80 | A6 | 1170 | G | C8-N9-C1' | -5.52 | 119.82 | 127.00 |
| 1 | A2 | 145 | A | N9-C4-C5 | 5.52 | 108.01 | 105.80 |
| 1 | A2 | 386 | G | C4-C5-N7 | -5.52 | 108.59 | 110.80 |
| 36 | A1 | 620 | U | N1-C2-N3 | 5.52 | 118.21 | 114.90 |
| 36 | A1 | 1335 | C | C5-C6-N1 | -5.52 | 118.24 | 121.00 |
| 72 | Bi | 27 | SER | N-CA-C | -5.52 | 96.09 | 111.00 |
| 80 | A6 | 96 | G | C5-C6-O6 | 5.52 | 131.91 | 128.60 |
| 80 | A6 | 418 | G | C4-C5-C6 | 5.52 | 122.11 | 118.80 |
| 80 | A6 | 1292 | G | N1-C6-O6 | 5.52 | 123.21 | 119.90 |
| 80 | A6 | 1340 | U | C5-C4-O4 | 5.52 | 129.21 | 125.90 |
| 36 | A5 | 1938 | U | C5-C6-N1 | -5.52 | 119.94 | 122.70 |
| 36 | A5 | 2172 | A | N1-C6-N6 | 5.52 | 121.91 | 118.60 |
| 36 | A5 | 2346 | C | N3-C4-C5 | 5.52 | 124.11 | 121.90 |
| 36 | A5 | 2549 | G | N7-C8-N9 | 5.52 | 115.86 | 113.10 |
| 36 | A5 | 2699 | G | N3-C4-N9 | 5.52 | 129.31 | 126.00 |
| 38 | A8 | 104 | A | N1-C2-N3 | -5.52 | 126.54 | 129.30 |
| 36 | A1 | 34 | A | C5-N7-C8 | -5.52 | 101.14 | 103.90 |
| 36 | A1 | 1543 | G | C5-C6-O6 | -5.52 | 125.29 | 128.60 |
| 36 | A1 | 2376 | G | C4-N9-C1' | 5.52 | 133.68 | 126.50 |
| 1 | A2 | 639 | U | N3-C4-C5 | 5.52 | 117.91 | 114.60 |
| 36 | A1 | 346 | C | C5-C6-N1 | -5.52 | 118.24 | 121.00 |
| 36 | A1 | 386 | A | C8-N9-C1' | -5.52 | 117.77 | 127.70 |
| 36 | A1 | 658 | G | N1-C6-O6 | 5.52 | 123.21 | 119.90 |
| 36 | A1 | 1917 | C | C6-N1-C2 | 5.52 | 122.51 | 120.30 |
| 80 | A6 | 767 | U | N3-C2-O2 | -5.52 | 118.34 | 122.20 |
| 36 | A5 | 419 | G | C4-C5-N7 | 5.52 | 113.01 | 110.80 |
| 36 | A5 | 1441 | G | C5-N7-C8 | 5.52 | 107.06 | 104.30 |
| 36 | A5 | 1869 | C | C6-N1-C2 | 5.52 | 122.51 | 120.30 |
| 36 | A5 | 2607 | G | C8-N9-C4 | -5.52 | 104.19 | 106.40 |
| 64 | Da | 4 | ARG | NE-CZ-NH1 | -5.52 | 117.54 | 120.30 |
| 36 | A1 | 408 | A | C5-C6-N6 | 5.52 | 128.11 | 123.70 |
| 36 | A1 | 1507 | G | N3-C4-C5 | -5.52 | 125.84 | 128.60 |
| 36 | A1 | 3138 | U | C5-C6-N1 | -5.52 | 119.94 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 80 | A6 | 633 | U | N1-C2-N3 | -5.52 | 111.59 | 114.90 |
| 80 | A6 | 1401 | A | N1-C6-N6 | -5.52 | 115.29 | 118.60 |
| 80 | A6 | 1773 | C | N3-C2-O2 | 5.52 | 125.76 | 121.90 |
| 36 | A5 | 590 | G | C8-N9-C4 | -5.52 | 104.19 | 106.40 |
| 36 | A5 | 2843 | U | N3-C2-O2 | -5.52 | 118.34 | 122.20 |
| 36 | A5 | 3042 | U | N1-C2-N3 | 5.52 | 118.21 | 114.90 |
| 80 | A6 | 756 | A | C5-N7-C8 | -5.52 | 101.14 | 103.90 |
| 36 | A5 | 1007 | U | C6-N1-C2 | 5.52 | 124.31 | 121.00 |
| 36 | A5 | 1869 | C | N3-C4-C5 | 5.52 | 124.11 | 121.90 |
| 1 | A2 | 599 | A | C5-N7-C8 | 5.51 | 106.66 | 103.90 |
| 59 | BV | 80 | ARG | NE-CZ-NH1 | 5.51 | 123.06 | 120.30 |
| 80 | A6 | 409 | C | C5-C4-N4 | -5.51 | 116.34 | 120.20 |
| 36 | A5 | 1183 | C | C5-C6-N1 | -5.51 | 118.24 | 121.00 |
| 80 | A6 | 387 | A | C4-C5-N7 | -5.51 | 107.94 | 110.70 |
| 36 | A5 | 1176 | C | C4-C5-C6 | 5.51 | 120.16 | 117.40 |
| 36 | A5 | 2654 | C | C2-N3-C4 | -5.51 | 117.14 | 119.90 |
| 36 | A1 | 220 | G | N3-C4-N9 | 5.51 | 129.31 | 126.00 |
| 36 | A1 | 1537 | A | C2-N3-C4 | -5.51 | 107.84 | 110.60 |
| 36 | A1 | 2184 | U | C5-C4-O4 | -5.51 | 122.59 | 125.90 |
| 36 | A1 | 3114 | A | C8-N9-C4 | 5.51 | 108.00 | 105.80 |
| 36 | A1 | 3355 | U | C2-N1-C1' | 5.51 | 124.31 | 117.70 |
| 80 | A6 | 146 | U | N3-C2-O2 | -5.51 | 118.34 | 122.20 |
| 80 | A6 | 1269 | U | C5-C4-O4 | 5.51 | 129.21 | 125.90 |
| 36 | A5 | 631 | U | N1-C2-O2 | 5.51 | 126.66 | 122.80 |
| 36 | A5 | 1878 | G | C4-N9-C1' | 5.51 | 133.66 | 126.50 |
| 36 | A5 | 2396 | G | N1-C6-O6 | -5.51 | 116.59 | 119.90 |
| 36 | A1 | 437 | G | C4-N9-C1' | -5.51 | 119.34 | 126.50 |
| 36 | A1 | 910 | G | C8-N9-C4 | -5.51 | 104.20 | 106.40 |
| 36 | A1 | 2618 | G | C2-N3-C4 | 5.51 | 114.66 | 111.90 |
| 36 | A1 | 2794 | G | N9-C4-C5 | 5.51 | 107.60 | 105.40 |
| 38 | A4 | 14 | C | N3-C4-C5 | 5.51 | 124.10 | 121.90 |
| 36 | A5 | 745 | C | N1-C2-O2 | -5.51 | 115.59 | 118.90 |
| 36 | A5 | 1178 | G | C6-N1-C2 | -5.51 | 121.79 | 125.10 |
| 36 | A5 | 1338 | C | C4-C5-C6 | 5.51 | 120.16 | 117.40 |
| 48 | BJ | 112 | LEU | CA-CB-CG | 5.51 | 127.97 | 115.30 |
| 36 | A5 | 1841 | A | C8-N9-C4 | -5.51 | 103.60 | 105.80 |
| 36 | A5 | 2177 | G | C8-N9-C4 | -5.51 | 104.20 | 106.40 |
| 36 | A5 | 2777 | G | C8-N9-C4 | -5.51 | 104.20 | 106.40 |
| 36 | A5 | 3318 | G | C4-C5-N7 | -5.51 | 108.60 | 110.80 |
| 37 | A7 | 8 | G | N3-C2-N2 | 5.51 | 123.76 | 119.90 |
| 36 | A1 | 347 | G | N1-C6-O6 | 5.51 | 123.20 | 119.90 |
| 36 | A1 | 1497 | C | C6-N1-C2 | -5.51 | 118.10 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 2891 | U | N3-C4-C5 | 5.51 | 117.90 | 114.60 |
| 36 | A1 | 3201 | C | N3-C2-O2 | -5.51 | 118.05 | 121.90 |
| 80 | A6 | 418 | G | N1-C6-O6 | 5.51 | 123.20 | 119.90 |
| 80 | A6 | 1177 | C | C2-N1-C1' | -5.51 | 112.74 | 118.80 |
| 36 | A5 | 666 | A | N1-C2-N3 | 5.51 | 132.05 | 129.30 |
| 36 | A5 | 1140 | G | C5-C6-N1 | 5.51 | 114.25 | 111.50 |
| 36 | A5 | 2134 | G | N3-C4-N9 | 5.51 | 129.30 | 126.00 |
| 36 | A5 | 2665 | U | C4-C5-C6 | -5.51 | 116.40 | 119.70 |
| 36 | A5 | 3043 | C | N3-C4-N4 | -5.51 | 114.15 | 118.00 |
| 1 | A2 | 838 | G | N7-C8-N9 | -5.50 | 110.35 | 113.10 |
| 36 | A1 | 2819 | A | N3-C4-C5 | -5.50 | 122.95 | 126.80 |
| 54 | BQ | 66 | ARG | NE-CZ-NH1 | -5.50 | 117.55 | 120.30 |
| 80 | A6 | 681 | U | N3-C2-O2 | -5.50 | 118.35 | 122.20 |
| 36 | A5 | 96 | G | C4-C5-N7 | -5.50 | 108.60 | 110.80 |
| 36 | A5 | 1115 | G | C6-N1-C2 | -5.50 | 121.80 | 125.10 |
| 36 | A5 | 2181 | C | C6-N1-C2 | -5.50 | 118.10 | 120.30 |
| 1 | A2 | 1024 | U | N1-C2-O2 | 5.50 | 126.65 | 122.80 |
| 1 | A2 | 1207 | C | C6-N1-C2 | 5.50 | 122.50 | 120.30 |
| 36 | A1 | 1144 | U | N3-C2-O2 | -5.50 | 118.35 | 122.20 |
| 36 | A1 | 1475 | A | C5-C6-N1 | 5.50 | 120.45 | 117.70 |
| 36 | A1 | 2252 | A | N7-C8-N9 | 5.50 | 116.55 | 113.80 |
| 36 | A1 | 2257 | C | C5-C4-N4 | 5.50 | 124.05 | 120.20 |
| 36 | A1 | 2358 | A | N7-C8-N9 | -5.50 | 111.05 | 113.80 |
| 36 | A1 | 2795 | U | C5-C6-N1 | -5.50 | 119.95 | 122.70 |
| 80 | A6 | 1650 | U | C5-C6-N1 | -5.50 | 119.95 | 122.70 |
| 36 | A5 | 3350 | C | C6-N1-C2 | -5.50 | 118.10 | 120.30 |
| 36 | A1 | 437 | G | N3-C4-C5 | 5.50 | 131.35 | 128.60 |
| 36 | A1 | 1411 | C | N3-C4-C5 | 5.50 | 124.10 | 121.90 |
| 36 | A1 | 2286 | U | C5-C6-N1 | -5.50 | 119.95 | 122.70 |
| 39 | BA | 247 | ARG | NE-CZ-NH1 | 5.50 | 123.05 | 120.30 |
| 80 | A6 | 425 | A | N1-C6-N6 | -5.50 | 115.30 | 118.60 |
| 80 | A6 | 1078 | C | N3-C4-N4 | -5.50 | 114.15 | 118.00 |
| 36 | A5 | 1792 | C | C4-C5-C6 | 5.50 | 120.15 | 117.40 |
| 36 | A5 | 2344 | U | C2-N3-C4 | -5.50 | 123.70 | 127.00 |
| 36 | A5 | 2369 | G | C8-N9-C4 | 5.50 | 108.60 | 106.40 |
| 37 | A7 | 101 | G | N9-C4-C5 | -5.50 | 103.20 | 105.40 |
| 36 | A1 | 49 | A | C6-N1-C2 | 5.50 | 121.90 | 118.60 |
| 36 | A1 | 637 | C | N3-C4-N4 | -5.50 | 114.15 | 118.00 |
| 36 | A1 | 2323 | G | N3-C2-N2 | 5.50 | 123.75 | 119.90 |
| 36 | A5 | 54 | C | N3-C4-N4 | -5.50 | 114.15 | 118.00 |
| 1 | A2 | 393 | C | C2-N3-C4 | -5.50 | 117.15 | 119.90 |
| 36 | A1 | 898 | U | C5-C6-N1 | -5.50 | 119.95 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 1049 | C | C5-C6-N1 | 5.50 | 123.75 | 121.00 |
| 36 | A5 | 1931 | U | C5-C4-O4 | 5.50 | 129.20 | 125.90 |
| 1 | A2 | 995 | A | C8-N9-C4 | 5.50 | 108.00 | 105.80 |
| 36 | A1 | 224 | C | C6-N1-C2 | -5.50 | 118.10 | 120.30 |
| 36 | A1 | 672 | A | C6-C5-N7 | -5.50 | 128.45 | 132.30 |
| 36 | A1 | 1824 | U | N3-C2-O2 | -5.50 | 118.35 | 122.20 |
| 36 | A1 | 1923 | C | C5-C6-N1 | -5.50 | 118.25 | 121.00 |
| 80 | A6 | 622 | A | N3-C4-C5 | -5.50 | 122.95 | 126.80 |
| 80 | A6 | 1573 | A | C2-N3-C4 | 5.50 | 113.35 | 110.60 |
| 36 | A5 | 1508 | C | N1-C2-O2 | 5.50 | 122.20 | 118.90 |
| 36 | A1 | 1041 | U | C6-N1-C2 | 5.50 | 124.30 | 121.00 |
| 36 | A1 | 1578 | C | C5-C6-N1 | 5.50 | 123.75 | 121.00 |
| 36 | A1 | 1646 | G | N1-C6-O6 | 5.50 | 123.20 | 119.90 |
| 36 | A1 | 2290 | C | N3-C2-O2 | -5.50 | 118.05 | 121.90 |
| 36 | A1 | 2819 | A | C4-C5-C6 | 5.50 | 119.75 | 117.00 |
| 36 | A1 | 3101 | G | C6-C5-N7 | 5.50 | 133.70 | 130.40 |
| 36 | A5 | 1495 | U | C6-N1-C2 | -5.50 | 117.70 | 121.00 |
| 36 | A5 | 1937 | U | C5-C6-N1 | -5.50 | 119.95 | 122.70 |
| 1 | A2 | 938 | G | N1-C2-N2 | -5.49 | 111.26 | 116.20 |
| 1 | A2 | 1270 | G | C2-N3-C4 | 5.49 | 114.65 | 111.90 |
| 36 | A1 | 965 | A | N9-C4-C5 | 5.49 | 108.00 | 105.80 |
| 36 | A1 | 2422 | C | N3-C2-O2 | -5.49 | 118.06 | 121.90 |
| 41 | BC | 76 | ARG | CG-CD-NE | -5.49 | 100.26 | 111.80 |
| 80 | A6 | 1455 | G | C4-C5-N7 | -5.49 | 108.60 | 110.80 |
| 36 | A5 | 1365 | G | N1-C2-N2 | -5.49 | 111.26 | 116.20 |
| 36 | A5 | 2112 | U | C6-N1-C2 | -5.49 | 117.70 | 121.00 |
| 36 | A5 | 3028 | G | N3-C2-N2 | 5.49 | 123.75 | 119.90 |
| 1 | A2 | 829 | A | C2-N3-C4 | 5.49 | 113.35 | 110.60 |
| 1 | A2 | 1462 | G | C5-C6-O6 | -5.49 | 125.31 | 128.60 |
| 36 | A1 | 106 | A | N1-C2-N3 | 5.49 | 132.05 | 129.30 |
| 36 | A1 | 929 | A | C4-C5-C6 | 5.49 | 119.75 | 117.00 |
| 38 | A8 | 19 | C | N3-C4-C5 | -5.49 | 119.70 | 121.90 |
| 38 | A8 | 156 | U | C5-C6-N1 | 5.49 | 125.45 | 122.70 |
| 1 | A2 | 42 | G | N7-C8-N9 | -5.49 | 110.36 | 113.10 |
| 1 | A2 | 566 | C | N3-C2-O2 | -5.49 | 118.06 | 121.90 |
| 36 | A1 | 606 | C | N3-C4-C5 | -5.49 | 119.70 | 121.90 |
| 36 | A1 | 694 | C | C2-N3-C4 | -5.49 | 117.15 | 119.90 |
| 47 | BI | 24 | ARG | NE-CZ-NH2 | -5.49 | 117.56 | 120.30 |
| 54 | BQ | 38 | ARG | NE-CZ-NH2 | -5.49 | 117.56 | 120.30 |
| 80 | A6 | 448 | C | N1-C2-N3 | 5.49 | 123.04 | 119.20 |
| 36 | A5 | 620 | U | C2-N1-C1' | 5.49 | 124.29 | 117.70 |
| 37 | A7 | 8 | G | N1-C2-N2 | -5.49 | 111.26 | 116.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 64 | Da | 9 | ARG | NE-CZ-NH1 | -5.49 | 117.56 | 120.30 |
| 36 | A1 | 1345 | G | C4-N9-C1' | 5.49 | 133.63 | 126.50 |
| 80 | A6 | 351 | C | C6-N1-C1' | -5.49 | 114.22 | 120.80 |
| 36 | A5 | 3387 | U | N1-C2-O2 | 5.49 | 126.64 | 122.80 |
| 1 | A2 | 380 | U | N3-C2-O2 | -5.49 | 118.36 | 122.20 |
| 36 | A1 | 740 | G | N1-C6-O6 | -5.49 | 116.61 | 119.90 |
| 36 | A1 | 1326 | A | N7-C8-N9 | -5.49 | 111.06 | 113.80 |
| 36 | A1 | 2126 | A | C2-N3-C4 | 5.49 | 113.34 | 110.60 |
| 80 | A6 | 557 | G | N3-C4-C5 | -5.49 | 125.86 | 128.60 |
| 36 | A5 | 828 | A | N1-C6-N6 | -5.49 | 115.31 | 118.60 |
| 36 | A5 | 2109 | U | N3-C4-O4 | -5.49 | 115.56 | 119.40 |
| 1 | A2 | 972 | G | C4-C5-N7 | -5.49 | 108.61 | 110.80 |
| 36 | A1 | 332 | C | C5-C6-N1 | -5.49 | 118.26 | 121.00 |
| 36 | A1 | 514 | G | N1-C2-N3 | 5.49 | 127.19 | 123.90 |
| 36 | A1 | 947 | G | N1-C6-O6 | -5.49 | 116.61 | 119.90 |
| 36 | A1 | 1681 | U | N1-C2-O2 | 5.49 | 126.64 | 122.80 |
| 36 | A1 | 2957 | G | C8-N9-C4 | 5.49 | 108.59 | 106.40 |
| 80 | A6 | 72 | A | N1-C6-N6 | -5.49 | 115.31 | 118.60 |
| 80 | A6 | 542 | A | C5-N7-C8 | -5.49 | 101.16 | 103.90 |
| 36 | A5 | 3341 | U | N3-C2-O2 | -5.49 | 118.36 | 122.20 |
| 36 | A5 | 3350 | C | C5-C6-N1 | 5.49 | 123.74 | 121.00 |
| 1 | A2 | 992 | A | C4-C5-N7 | 5.48 | 113.44 | 110.70 |
| 36 | A1 | 1802 | C | N3-C4-N4 | 5.48 | 121.84 | 118.00 |
| 68 | Be | 105 | ARG | NE-CZ-NH1 | 5.48 | 123.04 | 120.30 |
| 80 | A6 | 1354 | G | N7-C8-N9 | 5.48 | 115.84 | 113.10 |
| 1 | A2 | 1455 | G | C4-C5-C6 | 5.48 | 122.09 | 118.80 |
| 36 | A1 | 1133 | A | C5-C6-N1 | 5.48 | 120.44 | 117.70 |
| 36 | A1 | 3149 | G | N3-C4-N9 | -5.48 | 122.71 | 126.00 |
| 80 | A6 | 782 | U | N3-C2-O2 | -5.48 | 118.36 | 122.20 |
| 36 | A5 | 411 | U | C2-N3-C4 | -5.48 | 123.71 | 127.00 |
| 36 | A5 | 997 | A | N7-C8-N9 | 5.48 | 116.54 | 113.80 |
| 36 | A5 | 2321 | A | C5-C6-N1 | 5.48 | 120.44 | 117.70 |
| 36 | A5 | 2728 | G | N1-C2-N2 | 5.48 | 121.13 | 116.20 |
| 1 | A2 | 377 | G | C4-N9-C1' | -5.48 | 119.38 | 126.50 |
| 36 | A1 | 45 | A | C5-N7-C8 | 5.48 | 106.64 | 103.90 |
| 36 | A1 | 2730 | G | C5-C6-N1 | -5.48 | 108.76 | 111.50 |
| 36 | A1 | 3244 | A | C8-N9-C4 | 5.48 | 107.99 | 105.80 |
| 80 | A6 | 751 | G | N3-C4-C5 | -5.48 | 125.86 | 128.60 |
| 36 | A5 | 25 | U | N1-C2-N3 | 5.48 | 118.19 | 114.90 |
| 36 | A5 | 229 | G | N1-C6-O6 | 5.48 | 123.19 | 119.90 |
| 37 | A7 | 90 | U | C6-N1-C2 | 5.48 | 124.29 | 121.00 |
| 36 | A1 | 334 | A | N1-C6-N6 | 5.48 | 121.89 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 2756 | C | C6-N1-C2 | -5.48 | 118.11 | 120.30 |
| 36 | A5 | 3336 | A | C5-C6-N1 | -5.48 | 114.96 | 117.70 |
| 37 | A7 | 37 | G | N9-C4-C5 | -5.48 | 103.21 | 105.40 |
| 36 | A1 | 2135 | U | N1-C2-O2 | 5.48 | 126.64 | 122.80 |
| 36 | A1 | 2272 | G | N1-C6-O6 | 5.48 | 123.19 | 119.90 |
| 80 | A6 | 1308 | G | N1-C6-O6 | 5.48 | 123.19 | 119.90 |
| 37 | A7 | 105 | C | N3-C4-C5 | -5.48 | 119.71 | 121.90 |
| 1 | A2 | 42 | G | N1-C6-O6 | -5.48 | 116.61 | 119.90 |
| 36 | A1 | 1330 | A | C4-C5-N7 | 5.47 | 113.44 | 110.70 |
| 36 | A1 | 1877 | U | C5-C6-N1 | -5.47 | 119.96 | 122.70 |
| 36 | A1 | 2361 | A | N3-C4-C5 | -5.47 | 122.97 | 126.80 |
| 36 | A1 | 2770 | G | C8-N9-C4 | -5.47 | 104.21 | 106.40 |
| 36 | A1 | 3109 | G | C5-C6-O6 | -5.47 | 125.32 | 128.60 |
| 36 | A5 | 961 | C | C4-C5-C6 | 5.47 | 120.14 | 117.40 |
| 38 | A8 | 43 | A | C8-N9-C4 | -5.47 | 103.61 | 105.80 |
| 36 | A1 | 1331 | U | C6-N1-C1' | -5.47 | 113.54 | 121.20 |
| 36 | A1 | 2329 | C | C2-N1-C1' | -5.47 | 112.78 | 118.80 |
| 38 | A4 | 60 | U | C2-N3-C4 | -5.47 | 123.72 | 127.00 |
| 36 | A5 | 282 | G | N7-C8-N9 | 5.47 | 115.84 | 113.10 |
| 36 | A5 | 1187 | C | N3-C4-N4 | -5.47 | 114.17 | 118.00 |
| 36 | A5 | 2430 | A | N1-C2-N3 | 5.47 | 132.04 | 129.30 |
| 36 | A5 | 3015 | G | N1-C6-O6 | -5.47 | 116.62 | 119.90 |
| 36 | A1 | 634 | C | N1-C2-O2 | 5.47 | 122.18 | 118.90 |
| 36 | A1 | 3192 | U | N3-C4-C5 | 5.47 | 117.88 | 114.60 |
| 36 | A5 | 810 | A | C5-C6-N6 | 5.47 | 128.08 | 123.70 |
| 1 | A2 | 703 | G | N7-C8-N9 | 5.47 | 115.83 | 113.10 |
| 36 | A1 | 2309 | A | C8-N9-C4 | 5.47 | 107.99 | 105.80 |
| 36 | A1 | 2550 | U | C4-C5-C6 | 5.47 | 122.98 | 119.70 |
| 36 | A1 | 2990 | G | C5-N7-C8 | 5.47 | 107.03 | 104.30 |
| 36 | A1 | 3000 | A | C2-N3-C4 | -5.47 | 107.86 | 110.60 |
| 6 | CE | 77 | ARG | NE-CZ-NH1 | 5.47 | 123.03 | 120.30 |
| 36 | A5 | 996 | A | C5-C6-N1 | 5.47 | 120.43 | 117.70 |
| 36 | A5 | 1191 | U | C5-C6-N1 | -5.47 | 119.97 | 122.70 |
| 69 | Df | 91 | ALA | N-CA-CB | 5.47 | 117.76 | 110.10 |
| 36 | A5 | 2119 | A | C6-N1-C2 | -5.47 | 115.32 | 118.60 |
| 36 | A5 | 2800 | G | C4-C5-N7 | -5.47 | 108.61 | 110.80 |
| 1 | A2 | 1386 | G | C4-C5-N7 | -5.47 | 108.61 | 110.80 |
| 1 | A2 | 1491 | U | N3-C2-O2 | -5.47 | 118.37 | 122.20 |
| 36 | A1 | 1459 | C | C5-C6-N1 | -5.47 | 118.27 | 121.00 |
| 80 | A6 | 639 | U | N3-C4-O4 | -5.47 | 115.57 | 119.40 |
| 80 | A6 | 790 | U | N3-C2-O2 | -5.47 | 118.37 | 122.20 |
| 36 | A5 | 422 | A | C8-N9-C4 | 5.47 | 107.99 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 37 | A7 | 82 | G | N9-C4-C5 | 5.47 | 107.59 | 105.40 |
| 1 | A2 | 1097 | U | C6-N1-C1' | -5.46 | 113.55 | 121.20 |
| 1 | A2 | 1754 | A | N3-C4-C5 | 5.46 | 130.63 | 126.80 |
| 36 | A1 | 200 | C | C2-N1-C1' | 5.46 | 124.81 | 118.80 |
| 36 | A1 | 1307 | G | C8-N9-C4 | -5.46 | 104.21 | 106.40 |
| 36 | A1 | 1926 | C | C2-N3-C4 | -5.46 | 117.17 | 119.90 |
| 36 | A1 | 2384 | A | N9-C4-C5 | -5.46 | 103.61 | 105.80 |
| 36 | A1 | 3029 | A | C6-C5-N7 | -5.46 | 128.47 | 132.30 |
| 80 | A6 | 1078 | C | C5-C4-N4 | 5.46 | 124.03 | 120.20 |
| 36 | A5 | 809 | G | C5-N7-C8 | 5.46 | 107.03 | 104.30 |
| 36 | A5 | 811 | U | N1-C2-N3 | 5.46 | 118.18 | 114.90 |
| 36 | A1 | 2782 | U | C5-C4-O4 | 5.46 | 129.18 | 125.90 |
| 36 | A5 | 98 | G | N9-C4-C5 | -5.46 | 103.22 | 105.40 |
| 36 | A5 | 3215 | A | C5-C6-N1 | -5.46 | 114.97 | 117.70 |
| 36 | A1 | 1119 | C | N3-C2-O2 | -5.46 | 118.08 | 121.90 |
| 36 | A1 | 2786 | G | N9-C4-C5 | 5.46 | 107.58 | 105.40 |
| 36 | A5 | 1190 | A | C5-N7-C8 | 5.46 | 106.63 | 103.90 |
| 36 | A5 | 1380 | G | C2-N3-C4 | -5.46 | 109.17 | 111.90 |
| 36 | A5 | 2608 | G | N1-C6-O6 | -5.46 | 116.62 | 119.90 |
| 36 | A5 | 2808 | A | C6-C5-N7 | -5.46 | 128.48 | 132.30 |
| 36 | A5 | 2948 | C | N3-C4-C5 | 5.46 | 124.08 | 121.90 |
| 36 | A1 | 1868 | G | C6-C5-N7 | -5.46 | 127.12 | 130.40 |
| 36 | A1 | 2408 | U | C2-N1-C1' | 5.46 | 124.25 | 117.70 |
| 36 | A1 | 2662 | G | C2-N3-C4 | -5.46 | 109.17 | 111.90 |
| 36 | A1 | 2902 | A | N1-C6-N6 | 5.46 | 121.88 | 118.60 |
| 80 | A6 | 991 | G | C5-C6-N1 | 5.46 | 114.23 | 111.50 |
| 80 | A6 | 1097 | U | P-O3'-C3' | 5.46 | 126.25 | 119.70 |
| 49 | DL | 47 | ALA | C-N-CD | 5.46 | 139.87 | 128.40 |
| 1 | A2 | 1185 | U | C6-N1-C1' | -5.46 | 113.56 | 121.20 |
| 36 | A1 | 1081 | U | C2-N1-C1' | 5.46 | 124.25 | 117.70 |
| 80 | A6 | 1019 | A | C8-N9-C4 | 5.46 | 107.98 | 105.80 |
| 80 | A6 | 1111 | G | C6-C5-N7 | -5.46 | 127.12 | 130.40 |
| 36 | A5 | 1239 | C | C6-N1-C2 | -5.46 | 118.12 | 120.30 |
| 1 | A2 | 1027 | A | C5-N7-C8 | -5.46 | 101.17 | 103.90 |
| 36 | A1 | 280 | U | C5-C6-N1 | 5.46 | 125.43 | 122.70 |
| 36 | A1 | 1528 | G | N9-C4-C5 | 5.46 | 107.58 | 105.40 |
| 36 | A1 | 1949 | G | N1-C6-O6 | 5.46 | 123.17 | 119.90 |
| 36 | A1 | 2368 | A | C8-N9-C4 | -5.46 | 103.62 | 105.80 |
| 36 | A1 | 2855 | U | C5-C6-N1 | -5.46 | 119.97 | 122.70 |
| 80 | A6 | 1284 | C | N3-C2-O2 | -5.46 | 118.08 | 121.90 |
| 80 | A6 | 1654 | G | C6-N1-C2 | -5.46 | 121.83 | 125.10 |
| 80 | A6 | 1678 | A | N7-C8-N9 | 5.46 | 116.53 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 36 | A5 | 414 | U | N3-C4-O4 | 5.46 | 123.22 | 119.40 |
| 36 | A5 | 2904 | U | N1-C2-N3 | 5.46 | 118.17 | 114.90 |
| 37 | A7 | 105 | C | C2-N3-C4 | 5.46 | 122.63 | 119.90 |
| 52 | DO | 197[B] | PHE | CA-C-N | -5.46 | 105.29 | 116.20 |
| 36 | A5 | 41 | G | C6-C5-N7 | -5.46 | 127.13 | 130.40 |
| 36 | A5 | 2379 | U | N1-C2-N3 | 5.46 | 118.17 | 114.90 |
| 36 | A1 | 1906 | G | N1-C6-O6 | 5.45 | 123.17 | 119.90 |
| 36 | A1 | 3110 | C | N3-C2-O2 | -5.45 | 118.08 | 121.90 |
| 80 | A6 | 300 | A | C8-N9-C4 | 5.45 | 107.98 | 105.80 |
| 80 | A6 | 426 | G | N3-C4-N9 | 5.45 | 129.27 | 126.00 |
| 80 | A6 | 1642 | G | C5-C6-N1 | 5.45 | 114.23 | 111.50 |
| 36 | A5 | 879 | U | C6-N1-C1' | -5.45 | 113.57 | 121.20 |
| 36 | A5 | 1045 | C | C2-N3-C4 | -5.45 | 117.17 | 119.90 |
| 36 | A5 | 1242 | G | N3-C4-C5 | -5.45 | 125.87 | 128.60 |
| 36 | A5 | 2632 | G | N1-C2-N3 | -5.45 | 120.63 | 123.90 |
| 38 | A8 | 17 | A | C5-N7-C8 | -5.45 | 101.17 | 103.90 |
| 38 | A8 | 103 | G | C5-C6-N1 | 5.45 | 114.23 | 111.50 |
| 36 | A1 | 708 | G | C4-C5-N7 | 5.45 | 112.98 | 110.80 |
| 36 | A1 | 1591 | G | C5-C6-O6 | 5.45 | 131.87 | 128.60 |
| 36 | A1 | 3007 | U | C4-C5-C6 | 5.45 | 122.97 | 119.70 |
| 36 | A5 | 266 | A | C4-C5-C6 | 5.45 | 119.73 | 117.00 |
| 36 | A5 | 2524 | A | N3-C4-C5 | 5.45 | 130.62 | 126.80 |
| 36 | A5 | 3035 | A | C8-N9-C4 | 5.45 | 107.98 | 105.80 |
| 36 | A5 | 3302 | U | N3-C4-C5 | 5.45 | 117.87 | 114.60 |
| 36 | A1 | 797 | U | C5-C6-N1 | -5.45 | 119.97 | 122.70 |
| 36 | A1 | 1100 | U | N1-C2-O2 | -5.45 | 118.98 | 122.80 |
| 36 | A1 | 3172 | A | N1-C6-N6 | 5.45 | 121.87 | 118.60 |
| 38 | A4 | 125 | U | N3-C2-O2 | -5.45 | 118.38 | 122.20 |
| 80 | A6 | 1332 | C | N1-C2-O2 | 5.45 | 122.17 | 118.90 |
| 37 | A7 | 61 | G | C8-N9-C4 | 5.45 | 108.58 | 106.40 |
| 37 | A7 | 100 | C | N3-C4-C5 | 5.45 | 124.08 | 121.90 |
| 36 | A1 | 748 | U | N3-C4-C5 | 5.45 | 117.87 | 114.60 |
| 36 | A1 | 785 | G | N3-C4-N9 | 5.45 | 129.27 | 126.00 |
| 36 | A1 | 1791 | C | N3-C4-C5 | 5.45 | 124.08 | 121.90 |
| 36 | A1 | 3127 | A | C8-N9-C4 | -5.45 | 103.62 | 105.80 |
| 38 | A4 | 23 | U | N1-C2-O2 | -5.45 | 118.99 | 122.80 |
| 80 | A6 | 30 | G | N9-C4-C5 | 5.45 | 107.58 | 105.40 |
| 36 | A5 | 341 | G | C5-N7-C8 | -5.45 | 101.58 | 104.30 |
| 36 | A5 | 1176 | C | C6-N1-C2 | 5.45 | 122.48 | 120.30 |
| 36 | A1 | 2850 | G | C8-N9-C1' | -5.45 | 119.92 | 127.00 |
| 36 | A5 | 844 | G | C8-N9-C4 | 5.45 | 108.58 | 106.40 |
| 36 | A5 | 1127 | G | N3-C4-N9 | 5.45 | 129.27 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 2958 | A | N1-C6-N6 | -5.45 | 115.33 | 118.60 |
| 36 | A5 | 3263 | G | N1-C6-O6 | -5.45 | 116.63 | 119.90 |
| 37 | A7 | 19 | C | N3-C4-C5 | 5.45 | 124.08 | 121.90 |
| 1 | A2 | 1662 | G | C8-N9-C4 | -5.45 | 104.22 | 106.40 |
| 36 | A1 | 283 | G | C8-N9-C1' | -5.45 | 119.92 | 127.00 |
| 36 | A1 | 2400 | G | N3-C2-N2 | -5.45 | 116.09 | 119.90 |
| 36 | A5 | 1306 | G | C5-C6-N1 | 5.45 | 114.22 | 111.50 |
| 36 | A5 | 2754 | G | N3-C4-N9 | 5.45 | 129.27 | 126.00 |
| 36 | A1 | 416 | A | N9-C4-C5 | 5.44 | 107.98 | 105.80 |
| 36 | A1 | 2805 | G | N3-C4-C5 | -5.44 | 125.88 | 128.60 |
| 80 | A6 | 403 | G | N9-C4-C5 | -5.44 | 103.22 | 105.40 |
| 36 | A5 | 63 | A | N9-C4-C5 | -5.44 | 103.62 | 105.80 |
| 36 | A5 | 648 | C | C4-C5-C6 | 5.44 | 120.12 | 117.40 |
| 36 | A5 | 2522 | G | N9-C4-C5 | -5.44 | 103.22 | 105.40 |
| 41 | DC | 73 | ARG | CB-CG-CD | -5.44 | 97.44 | 111.60 |
| 1 | A2 | 264 | G | N3-C4-N9 | -5.44 | 122.73 | 126.00 |
| 36 | A1 | 821 | U | N1-C2-O2 | 5.44 | 126.61 | 122.80 |
| 36 | A1 | 859 | G | C5-C6-N1 | -5.44 | 108.78 | 111.50 |
| 36 | A1 | 2414 | G | N3-C2-N2 | -5.44 | 116.09 | 119.90 |
| 36 | A1 | 2727 | A | N3-C4-C5 | -5.44 | 122.99 | 126.80 |
| 36 | A1 | 3192 | U | C2-N3-C4 | -5.44 | 123.73 | 127.00 |
| 80 | A6 | 1306 | C | C6-N1-C2 | -5.44 | 118.12 | 120.30 |
| 36 | A5 | 277 | G | C5-C6-O6 | 5.44 | 131.87 | 128.60 |
| 36 | A5 | 498 | A | N1-C6-N6 | -5.44 | 115.33 | 118.60 |
| 36 | A5 | 516 | A | C5-C6-N6 | -5.44 | 119.35 | 123.70 |
| 36 | A5 | 1335 | C | C6-N1-C2 | -5.44 | 118.12 | 120.30 |
| 36 | A5 | 2123 | G | N3-C4-C5 | -5.44 | 125.88 | 128.60 |
| 1 | A2 | 1330 | G | C4-N9-C1' | -5.44 | 119.43 | 126.50 |
| 36 | A1 | 104 | G | N9-C4-C5 | -5.44 | 103.22 | 105.40 |
| 36 | A1 | 649 | A | N7-C8-N9 | -5.44 | 111.08 | 113.80 |
| 36 | A1 | 2178 | A | C5-C6-N1 | -5.44 | 114.98 | 117.70 |
| 36 | A5 | 339 | C | C6-N1-C2 | -5.44 | 118.12 | 120.30 |
| 36 | A5 | 2433 | U | C5-C6-N1 | -5.44 | 119.98 | 122.70 |
| 36 | A5 | 3052 | G | C6-C5-N7 | 5.44 | 133.66 | 130.40 |
| 36 | A5 | 3083 | G | N1-C2-N3 | 5.44 | 127.16 | 123.90 |
| 1 | A2 | 529 | A | C8-N9-C4 | 5.44 | 107.98 | 105.80 |
| 36 | A1 | 121 | A | N7-C8-N9 | -5.44 | 111.08 | 113.80 |
| 36 | A1 | 1514 | G | C5-C6-N1 | 5.44 | 114.22 | 111.50 |
| 1 | A2 | 42 | G | C5-C6-N1 | 5.44 | 114.22 | 111.50 |
| 1 | A2 | 1458 | G | C8-N9-C1' | -5.44 | 119.93 | 127.00 |
| 36 | A1 | 794 | U | C6-N1-C2 | -5.44 | 117.74 | 121.00 |
| 36 | A1 | 2996 | U | C2-N1-C1' | 5.44 | 124.22 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 80 | A6 | 647 | G | C5-N7-C8 | -5.44 | 101.58 | 104.30 |
| 80 | A6 | 1537 | C | N3-C2-O2 | 5.44 | 125.71 | 121.90 |
| 36 | A5 | 519 | A | C6-C5-N7 | -5.44 | 128.49 | 132.30 |
| 36 | A5 | 3112 | G | C8-N9-C4 | 5.44 | 108.58 | 106.40 |
| 36 | A5 | 3143 | C | N3-C2-O2 | 5.44 | 125.71 | 121.90 |
| 36 | A1 | 1269 | U | N3-C2-O2 | -5.44 | 118.39 | 122.20 |
| 36 | A1 | 1503 | A | N3-C4-N9 | -5.44 | 123.05 | 127.40 |
| 36 | A1 | 1858 | A | C8-N9-C1' | -5.44 | 117.92 | 127.70 |
| 36 | A1 | 3326 | G | C8-N9-C4 | 5.44 | 108.58 | 106.40 |
| 36 | A5 | 2197 | C | C6-N1-C1' | 5.44 | 127.32 | 120.80 |
| 36 | A5 | 2757 | U | C5-C4-O4 | -5.44 | 122.64 | 125.90 |
| 36 | A1 | 25 | U | N3-C4-O4 | 5.43 | 123.20 | 119.40 |
| 36 | A1 | 504 | A | C2-N3-C4 | -5.43 | 107.88 | 110.60 |
| 36 | A1 | 864 | G | N3-C2-N2 | 5.43 | 123.70 | 119.90 |
| 36 | A1 | 1313 | G | C4-C5-N7 | 5.43 | 112.97 | 110.80 |
| 36 | A1 | 1882 | G | N3-C4-N9 | -5.43 | 122.74 | 126.00 |
| 36 | A1 | 2553 | U | C5-C6-N1 | -5.43 | 119.98 | 122.70 |
| 36 | A1 | 3055 | U | C5-C4-O4 | -5.43 | 122.64 | 125.90 |
| 36 | A1 | 3245 | A | C5-N7-C8 | -5.43 | 101.18 | 103.90 |
| 70 | Bg | 8 | ARG | NE-CZ-NH2 | -5.43 | 117.58 | 120.30 |
| 80 | A6 | 720 | G | C2-N3-C4 | 5.43 | 114.62 | 111.90 |
| 36 | A5 | 1041 | U | C5-C6-N1 | -5.43 | 119.98 | 122.70 |
| 36 | A5 | 2323 | G | C8-N9-C4 | -5.43 | 104.23 | 106.40 |
| 36 | A5 | 2386 | A | C5-N7-C8 | -5.43 | 101.18 | 103.90 |
| 36 | A5 | 3049 | A | C8-N9-C4 | 5.43 | 107.97 | 105.80 |
| 36 | A1 | 76 | G | N3-C4-C5 | -5.43 | 125.88 | 128.60 |
| 36 | A1 | 1658 | G | N1-C6-O6 | -5.43 | 116.64 | 119.90 |
| 36 | A1 | 2129 | U | N3-C2-O2 | -5.43 | 118.40 | 122.20 |
| 36 | A1 | 2621 | G | C8-N9-C4 | -5.43 | 104.23 | 106.40 |
| 37 | A3 | 96 | U | C2-N3-C4 | -5.43 | 123.74 | 127.00 |
| 38 | A4 | 23 | U | C2-N3-C4 | -5.43 | 123.74 | 127.00 |
| 80 | A6 | 381 | C | C2-N3-C4 | -5.43 | 117.18 | 119.90 |
| 80 | A6 | 1028 | C | C2-N3-C4 | -5.43 | 117.18 | 119.90 |
| 4 | CC | 229 | LEU | CA-CB-CG | 5.43 | 127.80 | 115.30 |
| 36 | A5 | 2634 | U | N3-C2-O2 | 5.43 | 126.00 | 122.20 |
| 36 | A5 | 3064 | U | C2-N3-C4 | -5.43 | 123.74 | 127.00 |
| 36 | A5 | 3366 | G | N1-C6-O6 | -5.43 | 116.64 | 119.90 |
| 64 | Da | 28 | HIS | CB-CA-C | -5.43 | 99.54 | 110.40 |
| 36 | A1 | 628 | A | N1-C6-N6 | 5.43 | 121.86 | 118.60 |
| 36 | A1 | 3142 | A | C5-N7-C8 | -5.43 | 101.18 | 103.90 |
| 36 | A5 | 923 | C | C5-C6-N1 | -5.43 | 118.28 | 121.00 |
| 38 | A8 | 11 | C | N1-C2-O2 | 5.43 | 122.16 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A2 | 1560 | U | C6-N1-C2 | -5.43 | 117.74 | 121.00 |
| 36 | A1 | 347 | G | C8-N9-C1' | -5.43 | 119.94 | 127.00 |
| 37 | A3 | 53 | U | N1-C2-N3 | 5.43 | 118.16 | 114.90 |
| 52 | BO | 3[B] | SER | C-N-CA | -5.43 | 108.13 | 121.70 |
| 80 | A6 | 153 | G | C2-N3-C4 | -5.43 | 109.19 | 111.90 |
| 36 | A5 | 591 | G | C6-C5-N7 | -5.43 | 127.14 | 130.40 |
| 36 | A5 | 706 | A | N9-C4-C5 | -5.43 | 103.63 | 105.80 |
| 36 | A5 | 1359 | C | N3-C4-N4 | 5.43 | 121.80 | 118.00 |
| 36 | A5 | 2355 | G | C5-C6-O6 | -5.43 | 125.34 | 128.60 |
| 36 | A5 | 2635 | A | N1-C6-N6 | -5.43 | 115.34 | 118.60 |
| 37 | A7 | 1 | G | C8-N9-C1' | -5.43 | 119.94 | 127.00 |
| 37 | A7 | 93 | C | N3-C4-C5 | 5.43 | 124.07 | 121.90 |
| 1 | A2 | 396 | G | C5-C6-O6 | -5.43 | 125.34 | 128.60 |
| 1 | A2 | 767 | U | N3-C2-O2 | -5.43 | 118.40 | 122.20 |
| 36 | A1 | 105 | C | N1-C2-N3 | 5.43 | 123.00 | 119.20 |
| 36 | A1 | 967 | A | C8-N9-C4 | 5.43 | 107.97 | 105.80 |
| 36 | A1 | 2366 | C | C5-C6-N1 | 5.43 | 123.71 | 121.00 |
| 80 | A6 | 1724 | U | N3-C4-C5 | 5.43 | 117.86 | 114.60 |
| 36 | A5 | 2375 | G | C4-C5-N7 | 5.43 | 112.97 | 110.80 |
| 36 | A5 | 3031 | G | C5-C6-O6 | -5.43 | 125.34 | 128.60 |
| 1 | A2 | 268 | C | C6-N1-C2 | -5.43 | 118.13 | 120.30 |
| 36 | A1 | 892 | U | N3-C4-O4 | -5.43 | 115.60 | 119.40 |
| 36 | A1 | 3048 | A | C5-N7-C8 | -5.43 | 101.19 | 103.90 |
| 80 | A6 | 647 | G | C2-N3-C4 | -5.43 | 109.19 | 111.90 |
| 36 | A5 | 1491 | A | C4-C5-C6 | 5.43 | 119.71 | 117.00 |
| 36 | A5 | 2149 | A | N9-C4-C5 | 5.43 | 107.97 | 105.80 |
| 36 | A5 | 2174 | G | N1-C2-N3 | 5.43 | 127.16 | 123.90 |
| 36 | A5 | 2549 | G | C5-C6-N1 | -5.43 | 108.79 | 111.50 |
| 1 | A2 | 396 | G | N1-C6-O6 | 5.42 | 123.16 | 119.90 |
| 1 | A2 | 407 | A | C5-N7-C8 | 5.42 | 106.61 | 103.90 |
| 36 | A1 | 328 | U | N1-C2-O2 | 5.42 | 126.60 | 122.80 |
| 36 | A1 | 342 | A | C8-N9-C4 | 5.42 | 107.97 | 105.80 |
| 36 | A1 | 944 | C | C5-C6-N1 | 5.42 | 123.71 | 121.00 |
| 36 | A1 | 1385 | C | C6-N1-C2 | -5.42 | 118.13 | 120.30 |
| 36 | A1 | 1658 | G | N9-C4-C5 | 5.42 | 107.57 | 105.40 |
| 36 | A1 | 1836 | C | N3-C4-C5 | 5.42 | 124.07 | 121.90 |
| 36 | A1 | 2359 | C | N3-C4-C5 | 5.42 | 124.07 | 121.90 |
| 36 | A5 | 930 | U | N1-C2-O2 | 5.42 | 126.60 | 122.80 |
| 36 | A5 | 1007 | U | C5-C4-O4 | -5.42 | 122.64 | 125.90 |
| 36 | A5 | 1724 | U | N1-C2-N3 | 5.42 | 118.16 | 114.90 |
| 36 | A5 | 2385 | G | C8-N9-C1' | 5.42 | 134.05 | 127.00 |
| 36 | A5 | 3115 | C | N1-C2-N3 | 5.42 | 123.00 | 119.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 36 | A1 | 731 | U | C5-C6-N1 | -5.42 | 119.99 | 122.70 |
| 36 | A1 | 1173 | U | C6-N1-C2 | 5.42 | 124.25 | 121.00 |
| 36 | A1 | 2647 | A | C5-C6-N1 | 5.42 | 120.41 | 117.70 |
| 38 | A4 | 78 | G | N3-C2-N2 | 5.42 | 123.70 | 119.90 |
| 36 | A5 | 2744 | U | N3-C4-O4 | -5.42 | 115.60 | 119.40 |
| 36 | A5 | 3008 | A | C8-N9-C4 | 5.42 | 107.97 | 105.80 |
| 36 | A5 | 3377 | G | C6-N1-C2 | -5.42 | 121.85 | 125.10 |
| 37 | A7 | 33 | U | N1-C2-O2 | 5.42 | 126.60 | 122.80 |
| 36 | A1 | 24 | G | N7-C8-N9 | -5.42 | 110.39 | 113.10 |
| 36 | A1 | 370 | U | C6-N1-C2 | -5.42 | 117.75 | 121.00 |
| 36 | A1 | 934 | G | C2-N3-C4 | 5.42 | 114.61 | 111.90 |
| 36 | A1 | 1496 | C | C4-C5-C6 | -5.42 | 114.69 | 117.40 |
| 56 | DS | 167 | ARG | NE-CZ-NH2 | -5.42 | 117.59 | 120.30 |
| 1 | A2 | 1679 | G | C2-N3-C4 | 5.42 | 114.61 | 111.90 |
| 36 | A1 | 582 | G | C8-N9-C1' | 5.42 | 134.05 | 127.00 |
| 80 | A6 | 1124 | A | C4-C5-C6 | -5.42 | 114.29 | 117.00 |
| 36 | A5 | 616 | G | C2-N3-C4 | 5.42 | 114.61 | 111.90 |
| 36 | A5 | 2257 | C | C5-C6-N1 | 5.42 | 123.71 | 121.00 |
| 36 | A1 | 376 | G | N3-C4-C5 | -5.42 | 125.89 | 128.60 |
| 36 | A1 | 506 | U | C2-N1-C1' | -5.42 | 111.20 | 117.70 |
| 36 | A1 | 1518 | U | N1-C2-O2 | -5.42 | 119.01 | 122.80 |
| 36 | A1 | 3112 | G | N9-C4-C5 | -5.42 | 103.23 | 105.40 |
| 80 | A6 | 1649 | G | N1-C6-O6 | -5.42 | 116.65 | 119.90 |
| 36 | A5 | 675 | C | N1-C2-O2 | -5.42 | 115.65 | 118.90 |
| 36 | A5 | 1510 | G | C2-N3-C4 | -5.42 | 109.19 | 111.90 |
| 36 | A5 | 1858 | A | C4-N9-C1' | 5.42 | 136.05 | 126.30 |
| 36 | A5 | 2145 | A | C6-N1-C2 | -5.42 | 115.35 | 118.60 |
| 36 | A5 | 2320 | A | N7-C8-N9 | -5.42 | 111.09 | 113.80 |
| 36 | A5 | 2434 | U | N3-C2-O2 | -5.42 | 118.41 | 122.20 |
| 36 | A5 | 2810 | C | C6-N1-C2 | -5.42 | 118.13 | 120.30 |
| 36 | A5 | 2837 | A | C8-N9-C4 | 5.42 | 107.97 | 105.80 |
| 36 | A1 | 547 | G | C3'-C2'-C1' | 5.42 | 105.83 | 101.50 |
| 36 | A1 | 1902 | G | C4-N9-C1' | 5.42 | 133.54 | 126.50 |
| 80 | A6 | 336 | G | C5-N7-C8 | 5.42 | 107.01 | 104.30 |
| 80 | A6 | 491 | C | C2-N1-C1' | 5.42 | 124.76 | 118.80 |
| 36 | A5 | 1081 | U | C5-C6-N1 | 5.42 | 125.41 | 122.70 |
| 36 | A5 | 3021 | A | N1-C6-N6 | -5.42 | 115.35 | 118.60 |
| 36 | A5 | 1399 | A | N9-C4-C5 | -5.42 | 103.63 | 105.80 |
| 36 | A5 | 3362 | A | C4-C5-N7 | 5.42 | 113.41 | 110.70 |
| 1 | A2 | 426 | G | C4-N9-C1' | 5.41 | 133.54 | 126.50 |
| 36 | A1 | 3140 | G | N3-C4-N9 | 5.41 | 129.25 | 126.00 |
| 36 | A5 | 1427 | U | N3-C4-O4 | -5.41 | 115.61 | 119.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 1538 | G | N9-C4-C5 | -5.41 | 103.23 | 105.40 |
| 36 | A5 | 2377 | G | N3-C4-C5 | -5.41 | 125.89 | 128.60 |
| 1 | A2 | 1146 | G | C4-N9-C1' | 5.41 | 133.53 | 126.50 |
| 36 | A1 | 386 | A | C4-C5-C6 | 5.41 | 119.71 | 117.00 |
| 36 | A1 | 1447 | G | C4-C5-N7 | -5.41 | 108.64 | 110.80 |
| 40 | BB | 4 | ARG | NE-CZ-NH2 | -5.41 | 117.59 | 120.30 |
| 36 | A5 | 1905 | G | N9-C4-C5 | 5.41 | 107.56 | 105.40 |
| 36 | A5 | 2980 | U | N3-C2-O2 | -5.41 | 118.41 | 122.20 |
| 36 | A1 | 406 | G | C4-N9-C1' | -5.41 | 119.47 | 126.50 |
| 36 | A1 | 529 | A | C8-N9-C4 | -5.41 | 103.64 | 105.80 |
| 36 | A1 | 2830 | G | N9-C4-C5 | 5.41 | 107.56 | 105.40 |
| 36 | A1 | 2975 | U | N1-C2-O2 | 5.41 | 126.59 | 122.80 |
| 36 | A5 | 632 | G | C5-C6-N1 | 5.41 | 114.20 | 111.50 |
| 36 | A5 | 1159 | A | C4-C5-C6 | -5.41 | 114.30 | 117.00 |
| 36 | A5 | 2374 | C | N3-C4-N4 | -5.41 | 114.21 | 118.00 |
| 36 | A5 | 2767 | U | N3-C4-O4 | -5.41 | 115.61 | 119.40 |
| 36 | A1 | 1363 | A | N1-C6-N6 | -5.41 | 115.36 | 118.60 |
| 36 | A1 | 1507 | G | N1-C2-N3 | 5.41 | 127.14 | 123.90 |
| 36 | A5 | 288 | C | C6-N1-C2 | 5.41 | 122.46 | 120.30 |
| 36 | A5 | 987 | U | C5-C4-O4 | 5.41 | 129.15 | 125.90 |
| 36 | A5 | 1144 | U | C4-C5-C6 | 5.41 | 122.94 | 119.70 |
| 36 | A5 | 1660 | C | N1-C2-O2 | -5.41 | 115.66 | 118.90 |
| 36 | A1 | 1450 | G | C5-C6-O6 | -5.41 | 125.36 | 128.60 |
| 36 | A1 | 2227 | C | C2-N3-C4 | -5.41 | 117.20 | 119.90 |
| 36 | A1 | 2915 | U | N3-C4-C5 | 5.41 | 117.84 | 114.60 |
| 80 | A6 | 1241 | G | C4-C5-N7 | 5.41 | 112.96 | 110.80 |
| 36 | A5 | 1191 | U | C4-C5-C6 | 5.41 | 122.94 | 119.70 |
| 1 | A2 | 557 | G | N1-C2-N2 | -5.41 | 111.33 | 116.20 |
| 36 | A1 | 22 | G | C5-C6-N1 | 5.41 | 114.20 | 111.50 |
| 36 | A1 | 1337 | A | N1-C6-N6 | -5.41 | 115.36 | 118.60 |
| 80 | A6 | 372 | G | N7-C8-N9 | -5.41 | 110.40 | 113.10 |
| 80 | A6 | 988 | A | N9-C4-C5 | 5.41 | 107.96 | 105.80 |
| 80 | A6 | 1541 | G | C2-N3-C4 | 5.41 | 114.60 | 111.90 |
| 18 | CQ | 69 | VAL | CB-CA-C | -5.41 | 101.13 | 111.40 |
| 36 | A5 | 600 | G | C4-N9-C1' | 5.41 | 133.53 | 126.50 |
| 36 | A5 | 646 | A | N1-C2-N3 | 5.41 | 132.00 | 129.30 |
| 36 | A5 | 1209 | G | N1-C2-N2 | 5.41 | 121.06 | 116.20 |
| 36 | A5 | 2242 | A | N9-C4-C5 | 5.41 | 107.96 | 105.80 |
| 36 | A5 | 2524 | A | C5-C6-N1 | -5.41 | 115.00 | 117.70 |
| 36 | A5 | 848 | A | N1-C2-N3 | 5.40 | 132.00 | 129.30 |
| 36 | A5 | 1447 | G | N7-C8-N9 | 5.40 | 115.80 | 113.10 |
| 36 | A5 | 2665 | U | N1-C2-O2 | 5.40 | 126.58 | 122.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | A2 | 393 | C | C5-C6-N1 | -5.40 | 118.30 | 121.00 |
| 1 | A2 | 469 | C | N3-C2-O2 | 5.40 | 125.68 | 121.90 |
| 1 | A2 | 1170 | G | C6-C5-N7 | -5.40 | 127.16 | 130.40 |
| 1 | A2 | 1666 | U | C5-C6-N1 | 5.40 | 125.40 | 122.70 |
| 36 | A1 | 364 | G | C5-N7-C8 | -5.40 | 101.60 | 104.30 |
| 36 | A1 | 931 | C | N3-C2-O2 | -5.40 | 118.12 | 121.90 |
| 36 | A1 | 1377 | G | N1-C6-O6 | -5.40 | 116.66 | 119.90 |
| 36 | A1 | 3230 | G | C5-C6-N1 | 5.40 | 114.20 | 111.50 |
| 37 | A3 | 97 | A | N9-C4-C5 | 5.40 | 107.96 | 105.80 |
| 80 | A6 | 232 | U | N1-C2-O2 | 5.40 | 126.58 | 122.80 |
| 80 | A6 | 1035 | G | N7-C8-N9 | -5.40 | 110.40 | 113.10 |
| 80 | A6 | 1549 | C | C4-C5-C6 | 5.40 | 120.10 | 117.40 |
| 36 | A5 | 1925 | U | N1-C2-N3 | 5.40 | 118.14 | 114.90 |
| 36 | A5 | 2184 | U | N3-C4-C5 | 5.40 | 117.84 | 114.60 |
| 36 | A5 | 3350 | C | N1-C2-O2 | 5.40 | 122.14 | 118.90 |
| 62 | DY | 14 | LYS | CD-CE-NZ | 5.40 | 124.13 | 111.70 |
| 1 | A2 | 1768 | G | C8-N9-C1' | 5.40 | 134.02 | 127.00 |
| 36 | A1 | 80 | G | N1-C2-N2 | -5.40 | 111.34 | 116.20 |
| 36 | A1 | 89 | A | C8-N9-C4 | -5.40 | 103.64 | 105.80 |
| 36 | A1 | 503 | C | N3-C4-C5 | 5.40 | 124.06 | 121.90 |
| 36 | A1 | 1382 | G | N7-C8-N9 | -5.40 | 110.40 | 113.10 |
| 36 | A1 | 2835 | U | C5-C6-N1 | -5.40 | 120.00 | 122.70 |
| 36 | A1 | 3345 | G | C8-N9-C4 | 5.40 | 108.56 | 106.40 |
| 52 | BO | 104[B] | ILE | CA-C-N | -5.40 | 105.32 | 117.20 |
| 36 | A5 | 852 | U | N1-C2-N3 | 5.40 | 118.14 | 114.90 |
| 36 | A5 | 1447 | G | N9-C4-C5 | 5.40 | 107.56 | 105.40 |
| 36 | A5 | 2794 | G | C5-C6-O6 | -5.40 | 125.36 | 128.60 |
| 36 | A5 | 2894 | C | C2-N3-C4 | -5.40 | 117.20 | 119.90 |
| 39 | DA | 207 | VAL | CB-CA-C | -5.40 | 101.14 | 111.40 |
| 18 | AQ | 40 | GLU | C-N-CA | 5.40 | 144.68 | 122.00 |
| 36 | A5 | 1164 | G | C2-N3-C4 | -5.40 | 109.20 | 111.90 |
| 36 | A5 | 3113 | A | C6-N1-C2 | -5.40 | 115.36 | 118.60 |
| 1 | A2 | 523 | G | N1-C6-O6 | -5.40 | 116.66 | 119.90 |
| 1 | A2 | 790 | U | N1-C2-N3 | 5.40 | 118.14 | 114.90 |
| 1 | A2 | 966 | A | N7-C8-N9 | -5.40 | 111.10 | 113.80 |
| 36 | A1 | 637 | C | C2-N3-C4 | -5.40 | 117.20 | 119.90 |
| 36 | A1 | 950 | G | N9-C4-C5 | -5.40 | 103.24 | 105.40 |
| 36 | A1 | 2958 | A | C6-C5-N7 | 5.40 | 136.08 | 132.30 |
| 36 | A1 | 3256 | G | N1-C2-N3 | -5.40 | 120.66 | 123.90 |
| 38 | A4 | 109 | A | C5-C6-N6 | -5.40 | 119.38 | 123.70 |
| 36 | A5 | 1505 | C | C4-C5-C6 | 5.40 | 120.10 | 117.40 |
| 36 | A5 | 2148 | U | N3-C4-C5 | 5.40 | 117.84 | 114.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 2904 | U | N3-C2-O2 | -5.40 | 118.42 | 122.20 |
| 36 | A1 | 158 | G | N3-C4-N9 | -5.40 | 122.76 | 126.00 |
| 36 | A1 | 1482 | A | C4-C5-N7 | -5.40 | 108.00 | 110.70 |
| 36 | A1 | 2197 | C | C5-C6-N1 | 5.40 | 123.70 | 121.00 |
| 70 | Bg | 8 | ARG | NE-CZ-NH1 | 5.40 | 123.00 | 120.30 |
| 36 | A5 | 2655 | U | N3-C4-C5 | 5.40 | 117.84 | 114.60 |
| 36 | A1 | 1499 | C | C6-N1-C2 | -5.39 | 118.14 | 120.30 |
| 36 | A1 | 1834 | U | C5-C4-O4 | 5.39 | 129.14 | 125.90 |
| 38 | A4 | 23 | U | C5-C4-O4 | -5.39 | 122.66 | 125.90 |
| 80 | A6 | 1043 | A | N1-C6-N6 | 5.39 | 121.84 | 118.60 |
| 80 | A6 | 1198 | G | C6-C5-N7 | 5.39 | 133.64 | 130.40 |
| 36 | A5 | 339 | C | C6-N1-C1' | 5.39 | 127.27 | 120.80 |
| 36 | A5 | 1808 | G | C5-C6-O6 | -5.39 | 125.36 | 128.60 |
| 1 | A2 | 307 | G | C8-N9-C4 | 5.39 | 108.56 | 106.40 |
| 36 | A1 | 506 | U | C2-N3-C4 | -5.39 | 123.77 | 127.00 |
| 36 | A1 | 653 | A | C5-C6-N6 | -5.39 | 119.39 | 123.70 |
| 36 | A1 | 743 | C | C5-C6-N1 | -5.39 | 118.30 | 121.00 |
| 36 | A1 | 1948 | G | C8-N9-C1' | -5.39 | 119.99 | 127.00 |
| 36 | A1 | 2787 | G | C5-C6-N1 | 5.39 | 114.20 | 111.50 |
| 80 | A6 | 366 | A | C2-N3-C4 | -5.39 | 107.90 | 110.60 |
| 80 | A6 | 1484 | G | N3-C4-C5 | -5.39 | 125.90 | 128.60 |
| 36 | A5 | 91 | G | N9-C4-C5 | 5.39 | 107.56 | 105.40 |
| 1 | A2 | 1361 | U | C2-N1-C1' | 5.39 | 124.17 | 117.70 |
| 36 | A1 | 1053 | A | C8-N9-C4 | 5.39 | 107.96 | 105.80 |
| 36 | A1 | 2692 | A | C4-C5-C6 | 5.39 | 119.69 | 117.00 |
| 38 | A4 | 103 | G | C5-C6-O6 | 5.39 | 131.84 | 128.60 |
| 36 | A5 | 1396 | C | C6-N1-C2 | 5.39 | 122.46 | 120.30 |
| 36 | A5 | 3245 | A | C4-C5-C6 | 5.39 | 119.69 | 117.00 |
| 1 | A2 | 1192 | C | N1-C2-O2 | -5.39 | 115.67 | 118.90 |
| 36 | A1 | 593 | C | N1-C2-N3 | 5.39 | 122.97 | 119.20 |
| 36 | A1 | 1654 | A | N1-C2-N3 | -5.39 | 126.61 | 129.30 |
| 36 | A5 | 998 | A | C5-N7-C8 | 5.39 | 106.59 | 103.90 |
| 36 | A5 | 1389 | G | C8-N9-C4 | 5.39 | 108.56 | 106.40 |
| 36 | A5 | 2658 | G | C8-N9-C4 | 5.39 | 108.56 | 106.40 |
| 36 | A1 | 327 | A | N1-C6-N6 | 5.39 | 121.83 | 118.60 |
| 36 | A5 | 1170 | A | N9-C4-C5 | -5.39 | 103.64 | 105.80 |
| 1 | A2 | 336 | G | C6-C5-N7 | -5.39 | 127.17 | 130.40 |
| 1 | A2 | 1389 | C | N3-C2-O2 | -5.39 | 118.13 | 121.90 |
| 12 | AK | 63 | TYR | N-CA-C | 5.39 | 125.55 | 111.00 |
| 36 | A1 | 412 | G | N1-C2-N3 | 5.39 | 127.13 | 123.90 |
| 36 | A1 | 1379 | G | N1-C2-N3 | 5.39 | 127.13 | 123.90 |
| 36 | A1 | 1610 | G | C5-C6-N1 | -5.39 | 108.81 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 36 | A1 | 2685 | C | N1-C2-O2 | -5.39 | 115.67 | 118.90 |
| 36 | A1 | 2963 | C | N3-C4-C5 | -5.39 | 119.75 | 121.90 |
| 36 | A1 | 3107 | U | N3-C2-O2 | -5.39 | 118.43 | 122.20 |
| 80 | A6 | 69 | G | C8-N9-C4 | 5.39 | 108.56 | 106.40 |
| 21 | CT | 57 | ARG | NE-CZ-NH1 | 5.39 | 122.99 | 120.30 |
| 36 | A5 | 363 | G | C5-N7-C8 | 5.39 | 106.99 | 104.30 |
| 36 | A5 | 1534 | A | C6-N1-C2 | -5.39 | 115.37 | 118.60 |
| 36 | A5 | 2399 | A | C5-C6-N6 | -5.39 | 119.39 | 123.70 |
| 36 | A5 | 2820 | A | N9-C4-C5 | 5.39 | 107.95 | 105.80 |
| 36 | A5 | 2955 | U | C6-N1-C2 | -5.39 | 117.77 | 121.00 |
| 36 | A5 | 3374 | U | C6-N1-C2 | 5.39 | 124.23 | 121.00 |
| 36 | A1 | 857 | G | N9-C4-C5 | -5.38 | 103.25 | 105.40 |
| 36 | A1 | 1178 | G | C5-C6-O6 | 5.38 | 131.83 | 128.60 |
| 36 | A5 | 3193 | C | C4-C5-C6 | 5.38 | 120.09 | 117.40 |
| 1 | A2 | 719 | U | C6-N1-C1' | -5.38 | 113.66 | 121.20 |
| 36 | A1 | 3147 | G | N1-C2-N2 | -5.38 | 111.36 | 116.20 |
| 36 | A1 | 3209 | A | C4-C5-N7 | 5.38 | 113.39 | 110.70 |
| 36 | A5 | 696 | C | C2-N1-C1' | 5.38 | 124.72 | 118.80 |
| 36 | A5 | 2429 | G | N9-C4-C5 | 5.38 | 107.55 | 105.40 |
| 36 | A1 | 200 | C | N3-C2-O2 | -5.38 | 118.13 | 121.90 |
| 36 | A1 | 339 | C | C6-N1-C2 | -5.38 | 118.15 | 120.30 |
| 36 | A1 | 3362 | A | O4'-C1'-N9 | 5.38 | 112.51 | 108.20 |
| 80 | A6 | 1320 | U | C5-C6-N1 | 5.38 | 125.39 | 122.70 |
| 80 | A6 | 1615 | C | N1-C2-O2 | -5.38 | 115.67 | 118.90 |
| 36 | A5 | 1192 | C | N1-C2-N3 | 5.38 | 122.97 | 119.20 |
| 80 | A6 | 418 | G | C5-N7-C8 | -5.38 | 101.61 | 104.30 |
| 1 | A2 | 392 | G | C5-C6-O6 | -5.38 | 125.37 | 128.60 |
| 36 | A1 | 1369 | A | C6-N1-C2 | 5.38 | 121.83 | 118.60 |
| 36 | A1 | 2426 | U | C5-C4-O4 | 5.38 | 129.13 | 125.90 |
| 36 | A5 | 388 | G | N3-C2-N2 | -5.38 | 116.14 | 119.90 |
| 36 | A5 | 806 | A | C8-N9-C4 | 5.38 | 107.95 | 105.80 |
| 36 | A5 | 2621 | G | N1-C2-N2 | 5.38 | 121.04 | 116.20 |
| 36 | A1 | 66 | A | N3-C4-C5 | 5.38 | 130.56 | 126.80 |
| 36 | A1 | 324 | A | C6-N1-C2 | -5.38 | 115.37 | 118.60 |
| 36 | A1 | 1819 | U | C5-C6-N1 | 5.38 | 125.39 | 122.70 |
| 36 | A1 | 1832 | C | C2-N3-C4 | -5.38 | 117.21 | 119.90 |
| 36 | A1 | 2621 | G | N1-C2-N2 | 5.38 | 121.04 | 116.20 |
| 36 | A1 | 2981 | U | C2-N3-C4 | -5.38 | 123.77 | 127.00 |
| 38 | A4 | 31 | G | N3-C4-C5 | 5.38 | 131.29 | 128.60 |
| 80 | A6 | 524 | U | N3-C4-O4 | -5.38 | 115.64 | 119.40 |
| 80 | A6 | 814 | A | C5-N7-C8 | -5.38 | 101.21 | 103.90 |
| 36 | A5 | 2393 | G | C8-N9-C1' | -5.38 | 120.01 | 127.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 3243 | A | C4-C5-C6 | 5.38 | 119.69 | 117.00 |
| 37 | A7 | 48 | U | C5-C6-N1 | -5.38 | 120.01 | 122.70 |
| 43 | DE | 173 | MET | CB-CG-SD | -5.38 | 96.27 | 112.40 |
| 80 | A6 | 879 | G | N9-C4-C5 | 5.38 | 107.55 | 105.40 |
| 36 | A5 | 706 | A | N1-C6-N6 | 5.38 | 121.83 | 118.60 |
| 1 | A2 | 1324 | G | N1-C2-N2 | 5.37 | 121.04 | 116.20 |
| 36 | A1 | 1000 | C | C5-C6-N1 | 5.37 | 123.69 | 121.00 |
| 36 | A1 | 1308 | A | N1-C2-N3 | 5.37 | 131.99 | 129.30 |
| 36 | A1 | 1929 | G | C4-C5-N7 | 5.37 | 112.95 | 110.80 |
| 36 | A1 | 2148 | U | C5-C6-N1 | -5.37 | 120.01 | 122.70 |
| 36 | A1 | 2156 | C | C2-N3-C4 | -5.37 | 117.21 | 119.90 |
| 36 | A1 | 2400 | G | C4-N9-C1' | -5.37 | 119.52 | 126.50 |
| 36 | A1 | 2639 | G | C6-N1-C2 | -5.37 | 121.88 | 125.10 |
| 36 | A1 | 3055 | U | C6-N1-C1' | -5.37 | 113.68 | 121.20 |
| 80 | A6 | 558 | U | C6-N1-C1' | -5.37 | 113.68 | 121.20 |
| 36 | A5 | 1804 | A | C8-N9-C4 | 5.37 | 107.95 | 105.80 |
| 36 | A5 | 1828 | A | C8-N9-C4 | -5.37 | 103.65 | 105.80 |
| 36 | A5 | 1870 | C | N1-C2-O2 | -5.37 | 115.68 | 118.90 |
| 36 | A5 | 1885 | U | N1-C2-O2 | -5.37 | 119.04 | 122.80 |
| 36 | A5 | 1907 | C | C6-N1-C1' | 5.37 | 127.25 | 120.80 |
| 36 | A5 | 2639 | G | C6-N1-C2 | -5.37 | 121.88 | 125.10 |
| 36 | A5 | 3047 | U | N3-C2-O2 | -5.37 | 118.44 | 122.20 |
| 36 | A5 | 3189 | G | C6-N1-C2 | -5.37 | 121.88 | 125.10 |
| 36 | A5 | 3336 | A | C2-N3-C4 | -5.37 | 107.91 | 110.60 |
| 36 | A5 | 3346 | U | C5-C6-N1 | -5.37 | 120.01 | 122.70 |
| 36 | A1 | 386 | A | C4-N9-C1' | 5.37 | 135.97 | 126.30 |
| 36 | A1 | 1773 | C | C6-N1-C2 | 5.37 | 122.45 | 120.30 |
| 36 | A1 | 2157 | G | C2-N3-C4 | 5.37 | 114.59 | 111.90 |
| 36 | A1 | 2275 | A | C5-C6-N1 | -5.37 | 115.01 | 117.70 |
| 36 | A1 | 2722 | U | C4-C5-C6 | 5.37 | 122.92 | 119.70 |
| 36 | A1 | 2787 | G | C6-N1-C2 | -5.37 | 121.88 | 125.10 |
| 38 | A4 | 1 | A | N1-C6-N6 | 5.37 | 121.82 | 118.60 |
| 38 | A4 | 41 | A | N1-C2-N3 | 5.37 | 131.99 | 129.30 |
| 44 | BF | 100 | ARG | NE-CZ-NH1 | -5.37 | 117.61 | 120.30 |
| 36 | A5 | 51 | A | N1-C6-N6 | 5.37 | 121.82 | 118.60 |
| 36 | A5 | 965 | A | N1-C2-N3 | -5.37 | 126.61 | 129.30 |
| 36 | A5 | 2134 | G | N3-C2-N2 | 5.37 | 123.66 | 119.90 |
| 36 | A5 | 2376 | G | C8-N9-C1' | -5.37 | 120.02 | 127.00 |
| 36 | A5 | 3003 | G | N3-C4-N9 | -5.37 | 122.78 | 126.00 |
| 1 | A2 | 1422 | A | N7-C8-N9 | -5.37 | 111.11 | 113.80 |
| 1 | A2 | 1481 | C | C5-C6-N1 | 5.37 | 123.69 | 121.00 |
| 36 | A1 | 1556 | C | N1-C2-O2 | 5.37 | 122.12 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 3083 | G | C5-N7-C8 | 5.37 | 106.98 | 104.30 |
| 36 | A1 | 3319 | U | N1-C2-O2 | 5.37 | 126.56 | 122.80 |
| 21 | CT | 57 | ARG | NE-CZ-NH2 | -5.37 | 117.61 | 120.30 |
| 36 | A5 | 799 | G | C6-N1-C2 | -5.37 | 121.88 | 125.10 |
| 36 | A5 | 1409 | G | N9-C4-C5 | 5.37 | 107.55 | 105.40 |
| 36 | A5 | 1844 | C | C6-N1-C2 | -5.37 | 118.15 | 120.30 |
| 1 | A2 | 864 | U | C2-N1-C1' | 5.37 | 124.14 | 117.70 |
| 36 | A1 | 2288 | G | C2-N3-C4 | 5.37 | 114.58 | 111.90 |
| 49 | BL | 57 | VAL | N-CA-C | -5.37 | 96.51 | 111.00 |
| 80 | A6 | 328 | A | N1-C6-N6 | -5.37 | 115.38 | 118.60 |
| 80 | A6 | 385 | A | C5-C6-N1 | -5.37 | 115.02 | 117.70 |
| 80 | A6 | 491 | C | N1-C2-O2 | 5.37 | 122.12 | 118.90 |
| 80 | A6 | 538 | A | C8-N9-C4 | -5.37 | 103.65 | 105.80 |
| 80 | A6 | 1144 | U | N3-C2-O2 | -5.37 | 118.44 | 122.20 |
| 8 | CG | 108 | VAL | CB-CA-C | -5.37 | 101.20 | 111.40 |
| 36 | A5 | 1300 | G | N1-C6-O6 | 5.37 | 123.12 | 119.90 |
| 36 | A5 | 2915 | U | N3-C4-O4 | -5.37 | 115.64 | 119.40 |
| 36 | A5 | 3043 | C | N1-C2-O2 | 5.37 | 122.12 | 118.90 |
| 38 | A8 | 6 | U | C5-C4-O4 | -5.37 | 122.68 | 125.90 |
| 38 | A8 | 29 | U | C5-C6-N1 | -5.37 | 120.02 | 122.70 |
| 36 | A5 | 76 | G | N1-C6-O6 | 5.37 | 123.12 | 119.90 |
| 1 | A2 | 1504 | G | C5-C6-O6 | 5.37 | 131.82 | 128.60 |
| 1 | A2 | 1762 | A | N9-C4-C5 | -5.37 | 103.65 | 105.80 |
| 10 | AI | 29 | LEU | CA-CB-CG | 5.37 | 127.64 | 115.30 |
| 29 | Ab | 29 | ARG | NE-CZ-NH1 | 5.37 | 122.98 | 120.30 |
| 36 | A1 | 126 | U | C4-C5-C6 | 5.37 | 122.92 | 119.70 |
| 36 | A1 | 972 | A | C5-C6-N1 | -5.37 | 115.02 | 117.70 |
| 36 | A1 | 1372 | C | N3-C4-C5 | 5.37 | 124.05 | 121.90 |
| 36 | A1 | 2305 | G | C4-N9-C1' | 5.37 | 133.48 | 126.50 |
| 36 | A1 | 3014 | U | C5-C6-N1 | -5.37 | 120.02 | 122.70 |
| 38 | A4 | 151 | C | N3-C4-C5 | -5.37 | 119.75 | 121.90 |
| 36 | A5 | 419 | G | C5-C6-N1 | 5.37 | 114.18 | 111.50 |
| 36 | A5 | 555 | U | N1-C2-O2 | -5.37 | 119.04 | 122.80 |
| 36 | A5 | 1374 | G | N1-C2-N2 | -5.37 | 111.37 | 116.20 |
| 36 | A5 | 2614 | G | C4-N9-C1' | 5.37 | 133.47 | 126.50 |
| 36 | A5 | 3101 | G | N1-C2-N2 | -5.37 | 111.37 | 116.20 |
| 1 | A2 | 628 | G | N3-C4-C5 | 5.36 | 131.28 | 128.60 |
| 1 | A2 | 1148 | C | C6-N1-C2 | 5.36 | 122.45 | 120.30 |
| 36 | A1 | 362 | U | N3-C4-C5 | 5.36 | 117.82 | 114.60 |
| 36 | A1 | 714 | G | C8-N9-C4 | 5.36 | 108.55 | 106.40 |
| 36 | A1 | 2273 | G | C2-N3-C4 | 5.36 | 114.58 | 111.90 |
| 36 | A1 | 2777 | G | N7-C8-N9 | 5.36 | 115.78 | 113.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 80 | A6 | 1297 | G | N7-C8-N9 | -5.36 | 110.42 | 113.10 |
| 36 | A5 | 227 | G | C5-C6-O6 | -5.36 | 125.38 | 128.60 |
| 36 | A5 | 356 | C | C5-C6-N1 | -5.36 | 118.32 | 121.00 |
| 36 | A5 | 536 | U | N3-C4-O4 | -5.36 | 115.65 | 119.40 |
| 36 | A5 | 1128 | U | C2-N3-C4 | -5.36 | 123.78 | 127.00 |
| 36 | A5 | 2231 | C | C2-N1-C1' | 5.36 | 124.70 | 118.80 |
| 36 | A5 | 3028 | G | C8-N9-C1' | -5.36 | 120.03 | 127.00 |
| 36 | A1 | 2809 | C | N3-C4-C5 | 5.36 | 124.05 | 121.90 |
| 80 | A6 | 477 | A | N9-C4-C5 | -5.36 | 103.66 | 105.80 |
| 37 | A7 | 83 | U | N3-C4-O4 | -5.36 | 115.65 | 119.40 |
| 53 | DP | 127 | ARG | NE-CZ-NH2 | -5.36 | 117.62 | 120.30 |
| 1 | A2 | 554 | C | C6-N1-C1' | -5.36 | 114.37 | 120.80 |
| 1 | A2 | 1642 | G | N3-C4-N9 | 5.36 | 129.22 | 126.00 |
| 36 | A1 | 1445 | U | C6-N1-C2 | 5.36 | 124.22 | 121.00 |
| 56 | BS | 115 | ARG | NE-CZ-NH2 | -5.36 | 117.62 | 120.30 |
| 80 | A6 | 434 | G | N1-C6-O6 | -5.36 | 116.68 | 119.90 |
| 80 | A6 | 991 | G | C6-N1-C2 | -5.36 | 121.88 | 125.10 |
| 80 | A6 | 1085 | G | N1-C2-N2 | -5.36 | 111.38 | 116.20 |
| 36 | A5 | 1838 | G | C6-N1-C2 | -5.36 | 121.88 | 125.10 |
| 36 | A5 | 1889 | G | C4-C5-N7 | -5.36 | 108.66 | 110.80 |
| 36 | A5 | 2609 | A | N7-C8-N9 | -5.36 | 111.12 | 113.80 |
| 36 | A5 | 3179 | U | N1-C2-O2 | 5.36 | 126.55 | 122.80 |
| 36 | A5 | 322 | U | C2-N3-C4 | -5.36 | 123.78 | 127.00 |
| 36 | A5 | 948 | C | C4-C5-C6 | 5.36 | 120.08 | 117.40 |
| 36 | A5 | 1312 | C | C5-C4-N4 | 5.36 | 123.95 | 120.20 |
| 36 | A5 | 1319 | G | N1-C2-N2 | -5.36 | 111.38 | 116.20 |
| 36 | A5 | 2836 | C | N1-C2-O2 | -5.36 | 115.68 | 118.90 |
| 1 | A2 | 350 | U | C5-C6-N1 | -5.36 | 120.02 | 122.70 |
| 1 | A2 | 720 | G | P-O3'-C3' | 5.36 | 126.13 | 119.70 |
| 36 | A1 | 367 | A | C5-C6-N1 | -5.36 | 115.02 | 117.70 |
| 36 | A1 | 640 | U | N1-C2-O2 | 5.36 | 126.55 | 122.80 |
| 36 | A1 | 805 | G | C5-C6-N1 | 5.36 | 114.18 | 111.50 |
| 36 | A1 | 2674 | A | N1-C6-N6 | -5.36 | 115.39 | 118.60 |
| 36 | A1 | 2871 | G | N3-C4-C5 | 5.36 | 131.28 | 128.60 |
| 80 | A6 | 3 | U | N3-C4-O4 | -5.36 | 115.65 | 119.40 |
| 80 | A6 | 93 | A | N9-C4-C5 | -5.36 | 103.66 | 105.80 |
| 80 | A6 | 146 | U | N1-C2-O2 | 5.36 | 126.55 | 122.80 |
| 80 | A6 | 1724 | U | C5-C4-O4 | -5.36 | 122.69 | 125.90 |
| 80 | A6 | 1783 | C | N3-C4-C5 | -5.36 | 119.76 | 121.90 |
| 36 | A5 | 408 | A | C2-N3-C4 | -5.36 | 107.92 | 110.60 |
| 36 | A5 | 1143 | A | C2-N3-C4 | -5.36 | 107.92 | 110.60 |
| 36 | A5 | 2369 | G | N3-C2-N2 | 5.36 | 123.65 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 2755 | C | N1-C2-O2 | -5.36 | 115.69 | 118.90 |
| 36 | A5 | 3112 | G | N7-C8-N9 | -5.36 | 110.42 | 113.10 |
| 1 | A2 | 932 | U | C6-N1-C1' | 5.36 | 128.70 | 121.20 |
| 1 | A2 | 1524 | A | N1-C6-N6 | -5.36 | 115.39 | 118.60 |
| 36 | A1 | 2345 | A | C2-N3-C4 | -5.36 | 107.92 | 110.60 |
| 80 | A6 | 1458 | G | C8-N9-C1' | -5.36 | 120.04 | 127.00 |
| 36 | A5 | 3138 | U | N3-C2-O2 | 5.36 | 125.95 | 122.20 |
| 36 | A5 | 3246 | G | N1-C6-O6 | 5.36 | 123.11 | 119.90 |
| 37 | A7 | 115 | G | C8-N9-C4 | -5.36 | 104.26 | 106.40 |
| 1 | A2 | 1769 | U | C5-C4-O4 | 5.35 | 129.11 | 125.90 |
| 36 | A1 | 701 | G | C5-N7-C8 | -5.35 | 101.62 | 104.30 |
| 36 | A1 | 843 | A | C8-N9-C4 | 5.35 | 107.94 | 105.80 |
| 36 | A1 | 1362 | G | N7-C8-N9 | -5.35 | 110.42 | 113.10 |
| 80 | A6 | 1100 | G | N1-C2-N3 | 5.35 | 127.11 | 123.90 |
| 36 | A1 | 73 | C | C4-C5-C6 | 5.35 | 120.08 | 117.40 |
| 36 | A1 | 1164 | G | C2-N3-C4 | -5.35 | 109.22 | 111.90 |
| 36 | A1 | 1506 | A | N1-C2-N3 | 5.35 | 131.98 | 129.30 |
| 36 | A1 | 1512 | U | N1-C2-N3 | 5.35 | 118.11 | 114.90 |
| 36 | A1 | 2315 | G | C5-C6-O6 | 5.35 | 131.81 | 128.60 |
| 36 | A1 | 2884 | C | C5-C4-N4 | -5.35 | 116.45 | 120.20 |
| 80 | A6 | 148 | A | C8-N9-C4 | -5.35 | 103.66 | 105.80 |
| 36 | A5 | 14 | U | N3-C4-C5 | 5.35 | 117.81 | 114.60 |
| 36 | A5 | 590 | G | C2-N3-C4 | 5.35 | 114.58 | 111.90 |
| 36 | A5 | 702 | C | N3-C4-C5 | 5.35 | 124.04 | 121.90 |
| 36 | A5 | 1152 | G | N9-C4-C5 | 5.35 | 107.54 | 105.40 |
| 36 | A1 | 276 | U | C2-N3-C4 | -5.35 | 123.79 | 127.00 |
| 36 | A1 | 1180 | A | C4-C5-C6 | 5.35 | 119.68 | 117.00 |
| 36 | A1 | 1472 | U | C5-C4-O4 | -5.35 | 122.69 | 125.90 |
| 36 | A1 | 2244 | A | N1-C6-N6 | -5.35 | 115.39 | 118.60 |
| 36 | A5 | 3227 | A | C2-N3-C4 | -5.35 | 107.92 | 110.60 |
| 38 | A8 | 135 | G | C4-C5-N7 | -5.35 | 108.66 | 110.80 |
| 40 | DB | 4 | ARG | NE-CZ-NH2 | -5.35 | 117.62 | 120.30 |
| 36 | A1 | 1183 | C | C6-N1-C2 | 5.35 | 122.44 | 120.30 |
| 36 | A1 | 2233 | A | N1-C6-N6 | -5.35 | 115.39 | 118.60 |
| 36 | A1 | 3111 | U | C6-N1-C2 | 5.35 | 124.21 | 121.00 |
| 38 | A4 | 88 | A | C4-C5-N7 | 5.35 | 113.38 | 110.70 |
| 80 | A6 | 866 | G | N1-C6-O6 | -5.35 | 116.69 | 119.90 |
| 36 | A5 | 283 | G | C5-C6-O6 | -5.35 | 125.39 | 128.60 |
| 36 | A5 | 354 | U | C5-C6-N1 | -5.35 | 120.03 | 122.70 |
| 36 | A5 | 372 | A | N1-C6-N6 | 5.35 | 121.81 | 118.60 |
| 36 | A5 | 564 | G | C5-N7-C8 | 5.35 | 106.97 | 104.30 |
| 36 | A5 | 688 | G | N3-C4-N9 | -5.35 | 122.79 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 810 | A | C4-C5-N7 | -5.35 | 108.03 | 110.70 |
| 36 | A5 | 1838 | G | C4-C5-N7 | -5.35 | 108.66 | 110.80 |
| 36 | A5 | 2342 | U | N3-C4-C5 | 5.35 | 117.81 | 114.60 |
| 36 | A5 | 2891 | U | N1-C2-N3 | 5.35 | 118.11 | 114.90 |
| 36 | A5 | 3368 | U | C2-N1-C1' | -5.35 | 111.28 | 117.70 |
| 1 | A2 | 313 | U | C5-C4-O4 | 5.35 | 129.11 | 125.90 |
| 1 | A2 | 343 | C | C6-N1-C2 | -5.35 | 118.16 | 120.30 |
| 17 | AP | 60 | LEU | CA-CB-CG | 5.35 | 127.60 | 115.30 |
| 36 | A1 | 1388 | U | N1-C2-O2 | -5.35 | 119.06 | 122.80 |
| 80 | A6 | 336 | G | N7-C8-N9 | -5.35 | 110.43 | 113.10 |
| 36 | A5 | 909 | G | N7-C8-N9 | -5.35 | 110.43 | 113.10 |
| 36 | A5 | 1321 | G | C8-N9-C4 | 5.35 | 108.54 | 106.40 |
| 36 | A5 | 1506 | A | N9-C4-C5 | 5.35 | 107.94 | 105.80 |
| 36 | A5 | 3055 | U | C6-N1-C1' | -5.35 | 113.71 | 121.20 |
| 36 | A5 | 3347 | A | C8-N9-C4 | 5.35 | 107.94 | 105.80 |
| 36 | A5 | 3078 | U | C2-N1-C1' | 5.35 | 124.11 | 117.70 |
| 1 | A2 | 1461 | C | C6-N1-C2 | 5.34 | 122.44 | 120.30 |
| 36 | A1 | 715 | A | C8-N9-C4 | -5.34 | 103.66 | 105.80 |
| 36 | A1 | 806 | A | C8-N9-C4 | 5.34 | 107.94 | 105.80 |
| 36 | A1 | 857 | G | N1-C2-N2 | -5.34 | 111.39 | 116.20 |
| 36 | A1 | 2644 | C | N1-C2-N3 | 5.34 | 122.94 | 119.20 |
| 80 | A6 | 1227 | A | P-O3'-C3' | 5.34 | 126.11 | 119.70 |
| 80 | A6 | 1400 | A | C5-C6-N1 | 5.34 | 120.37 | 117.70 |
| 80 | A6 | 1764 | C | N3-C4-C5 | 5.34 | 124.04 | 121.90 |
| 36 | A5 | 859 | G | N3-C4-C5 | -5.34 | 125.93 | 128.60 |
| 36 | A5 | 1017 | C | C2-N1-C1' | 5.34 | 124.68 | 118.80 |
| 56 | BS | 117 | ARG | NE-CZ-NH2 | 5.34 | 122.97 | 120.30 |
| 36 | A5 | 1239 | C | C2-N1-C1' | 5.34 | 124.68 | 118.80 |
| 36 | A5 | 1375 | G | C8-N9-C4 | -5.34 | 104.26 | 106.40 |
| 36 | A5 | 1628 | C | C6-N1-C2 | -5.34 | 118.16 | 120.30 |
| 36 | A1 | 582 | G | N1-C6-O6 | -5.34 | 116.69 | 119.90 |
| 36 | A1 | 960 | U | N3-C2-O2 | 5.34 | 125.94 | 122.20 |
| 36 | A1 | 1113 | G | N3-C2-N2 | -5.34 | 116.16 | 119.90 |
| 36 | A1 | 2278 | C | C5-C4-N4 | 5.34 | 123.94 | 120.20 |
| 36 | A1 | 2412 | G | C8-N9-C4 | -5.34 | 104.26 | 106.40 |
| 77 | Bn | 6 | ARG | NE-CZ-NH2 | -5.34 | 117.63 | 120.30 |
| 80 | A6 | 124 | A | C6-N1-C2 | 5.34 | 121.81 | 118.60 |
| 11 | CJ | 149 | ARG | NE-CZ-NH1 | 5.34 | 122.97 | 120.30 |
| 36 | A5 | 496 | C | N3-C2-O2 | -5.34 | 118.16 | 121.90 |
| 36 | A5 | 1433 | A | C6-N1-C2 | 5.34 | 121.81 | 118.60 |
| 36 | A5 | 2261 | G | N7-C8-N9 | -5.34 | 110.43 | 113.10 |
| 36 | A5 | 2319 | U | C5-C6-N1 | -5.34 | 120.03 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 3048 | A | C6-N1-C2 | -5.34 | 115.40 | 118.60 |
| 1 | A2 | 1679 | G | N1-C6-O6 | -5.34 | 116.70 | 119.90 |
| 36 | A1 | 115 | A | C5-C6-N6 | 5.34 | 127.97 | 123.70 |
| 36 | A1 | 867 | G | C6-N1-C2 | -5.34 | 121.90 | 125.10 |
| 36 | A1 | 2377 | G | C2-N3-C4 | -5.34 | 109.23 | 111.90 |
| 36 | A1 | 2719 | U | C6-N1-C1' | 5.34 | 128.67 | 121.20 |
| 80 | A6 | 1329 | A | C6-C5-N7 | -5.34 | 128.56 | 132.30 |
| 80 | A6 | 1419 | G | C5-C6-N1 | -5.34 | 108.83 | 111.50 |
| 36 | A5 | 1129 | A | C5-C6-N1 | 5.34 | 120.37 | 117.70 |
| 36 | A5 | 2930 | A | C5-C6-N1 | 5.34 | 120.37 | 117.70 |
| 36 | A1 | 1187 | C | C6-N1-C2 | -5.34 | 118.17 | 120.30 |
| 36 | A1 | 2710 | C | C2-N3-C4 | -5.34 | 117.23 | 119.90 |
| 36 | A1 | 2965 | U | C6-N1-C2 | 5.34 | 124.20 | 121.00 |
| 38 | A8 | 3 | A | C5-C6-N1 | 5.34 | 120.37 | 117.70 |
| 38 | A8 | 87 | G | C4-C5-N7 | 5.34 | 112.94 | 110.80 |
| 1 | A2 | 527 | A | N7-C8-N9 | 5.34 | 116.47 | 113.80 |
| 36 | A1 | 318 | A | N1-C6-N6 | 5.34 | 121.80 | 118.60 |
| 36 | A1 | 857 | G | C8-N9-C4 | 5.34 | 108.53 | 106.40 |
| 36 | A1 | 2607 | G | N3-C2-N2 | 5.34 | 123.64 | 119.90 |
| 36 | A1 | 2786 | G | C2-N3-C4 | 5.34 | 114.57 | 111.90 |
| 38 | A4 | 121 | U | C5-C4-O4 | 5.34 | 129.10 | 125.90 |
| 80 | A6 | 542 | A | C8-N9-C1' | -5.34 | 118.10 | 127.70 |
| 80 | A6 | 1185 | U | C2-N1-C1' | 5.34 | 124.10 | 117.70 |
| 80 | A6 | 1458 | G | C4-C5-N7 | 5.34 | 112.94 | 110.80 |
| 36 | A5 | 524 | U | C2-N1-C1' | -5.34 | 111.30 | 117.70 |
| 36 | A5 | 1376 | C | C6-N1-C2 | 5.34 | 122.43 | 120.30 |
| 36 | A5 | 2300 | G | C5-C6-N1 | 5.34 | 114.17 | 111.50 |
| 36 | A5 | 2361 | A | N9-C4-C5 | 5.34 | 107.93 | 105.80 |
| 36 | A1 | 109 | A | C5-C6-N6 | 5.33 | 127.97 | 123.70 |
| 80 | A6 | 1060 | U | N3-C2-O2 | -5.33 | 118.47 | 122.20 |
| 36 | A5 | 509 | U | N3-C4-C5 | 5.33 | 117.80 | 114.60 |
| 36 | A5 | 514 | G | N9-C4-C5 | -5.33 | 103.27 | 105.40 |
| 36 | A5 | 972 | A | C4-C5-C6 | 5.33 | 119.67 | 117.00 |
| 36 | A5 | 2636 | A | N1-C6-N6 | -5.33 | 115.40 | 118.60 |
| 36 | A5 | 3247 | G | C5-C6-O6 | 5.33 | 131.80 | 128.60 |
| 1 | A2 | 274 | G | C8-N9-C4 | -5.33 | 104.27 | 106.40 |
| 1 | A2 | 1145 | U | N3-C2-O2 | 5.33 | 125.93 | 122.20 |
| 36 | A1 | 1037 | C | C6-N1-C2 | -5.33 | 118.17 | 120.30 |
| 36 | A1 | 1882 | G | N9-C4-C5 | 5.33 | 107.53 | 105.40 |
| 36 | A1 | 2932 | U | N3-C4-O4 | -5.33 | 115.67 | 119.40 |
| 41 | BC | 60 | THR | CB-CA-C | -5.33 | 97.20 | 111.60 |
| 80 | A6 | 411 | C | C5-C6-N1 | -5.33 | 118.33 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 80 | A6 | 1230 | A | N7-C8-N9 | 5.33 | 116.47 | 113.80 |
| 20 | CS | 15 | LEU | CA-CB-CG | 5.33 | 127.57 | 115.30 |
| 36 | A5 | 90 | C | C6-N1-C2 | -5.33 | 118.17 | 120.30 |
| 36 | A5 | 1906 | G | C6-N1-C2 | -5.33 | 121.90 | 125.10 |
| 36 | A5 | 1927 | G | C8-N9-C4 | -5.33 | 104.27 | 106.40 |
| 36 | A5 | 2167 | A | C5-C6-N1 | 5.33 | 120.37 | 117.70 |
| 36 | A1 | 18 | G | C8-N9-C4 | -5.33 | 104.27 | 106.40 |
| 36 | A1 | 1142 | G | C4-N9-C1' | 5.33 | 133.43 | 126.50 |
| 36 | A1 | 2362 | C | N3-C4-N4 | 5.33 | 121.73 | 118.00 |
| 36 | A1 | 2549 | G | N3-C4-C5 | -5.33 | 125.94 | 128.60 |
| 36 | A1 | 3140 | G | N3-C4-C5 | -5.33 | 125.93 | 128.60 |
| 36 | A1 | 3214 | U | C4-C5-C6 | 5.33 | 122.90 | 119.70 |
| 80 | A6 | 547 | U | N3-C4-C5 | 5.33 | 117.80 | 114.60 |
| 80 | A6 | 1110 | G | C5-N7-C8 | 5.33 | 106.97 | 104.30 |
| 80 | A6 | 1522 | U | N1-C2-N3 | 5.33 | 118.10 | 114.90 |
| 36 | A5 | 98 | G | C4-C5-N7 | 5.33 | 112.93 | 110.80 |
| 36 | A5 | 1150 | A | C5-N7-C8 | -5.33 | 101.23 | 103.90 |
| 1 | A2 | 1052 | U | C2-N1-C1' | 5.33 | 124.10 | 117.70 |
| 36 | A1 | 1124 | U | C5-C4-O4 | -5.33 | 122.70 | 125.90 |
| 36 | A1 | 1607 | U | P-O3'-C3' | 5.33 | 126.10 | 119.70 |
| 36 | A1 | 2411 | U | N3-C4-O4 | -5.33 | 115.67 | 119.40 |
| 80 | A6 | 484 | C | C2-N1-C1' | 5.33 | 124.66 | 118.80 |
| 36 | A5 | 2664 | C | C4-C5-C6 | -5.33 | 114.73 | 117.40 |
| 36 | A1 | 1690 | C | C4-C5-C6 | 5.33 | 120.06 | 117.40 |
| 36 | A1 | 2244 | A | N7-C8-N9 | -5.33 | 111.14 | 113.80 |
| 36 | A1 | 2912 | G | C5-C6-N1 | 5.33 | 114.16 | 111.50 |
| 36 | A1 | 3293 | U | N3-C2-O2 | 5.33 | 125.93 | 122.20 |
| 37 | A3 | 52 | G | C3'-C2'-C1' | -5.33 | 97.24 | 101.50 |
| 80 | A6 | 1130 | G | N1-C2-N3 | 5.33 | 127.10 | 123.90 |
| 36 | A5 | 1788 | C | C4-C5-C6 | 5.33 | 120.06 | 117.40 |
| 36 | A5 | 1869 | C | C5-C6-N1 | -5.33 | 118.33 | 121.00 |
| 36 | A5 | 2639 | G | N1-C6-O6 | 5.33 | 123.10 | 119.90 |
| 36 | A5 | 3174 | A | N1-C6-N6 | 5.33 | 121.80 | 118.60 |
| 36 | A1 | 429 | U | C5-C6-N1 | -5.33 | 120.04 | 122.70 |
| 80 | A6 | 1749 | A | C6-C5-N7 | -5.33 | 128.57 | 132.30 |
| 36 | A5 | 800 | G | N9-C4-C5 | -5.33 | 103.27 | 105.40 |
| 36 | A5 | 1307 | G | N3-C2-N2 | 5.33 | 123.63 | 119.90 |
| 36 | A5 | 1722 | U | N1-C2-O2 | -5.33 | 119.07 | 122.80 |
| 36 | A5 | 1939 | G | C8-N9-C1' | -5.33 | 120.08 | 127.00 |
| 36 | A5 | 2897 | A | C5-N7-C8 | 5.33 | 106.56 | 103.90 |
| 36 | A5 | 2928 | C | N3-C4-C5 | -5.33 | 119.77 | 121.90 |
| 36 | A5 | 3045 | G | N3-C4-C5 | -5.33 | 125.94 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A2 | 190 | C | C6-N1-C2 | 5.33 | 122.43 | 120.30 |
| 1 | A2 | 393 | C | C2-N1-C1' | -5.33 | 112.94 | 118.80 |
| 1 | A2 | 1315 | U | C5-C4-O4 | -5.33 | 122.70 | 125.90 |
| 1 | A2 | 1778 | G | N1-C6-O6 | -5.33 | 116.70 | 119.90 |
| 36 | A1 | 72 | C | N1-C2-O2 | -5.33 | 115.70 | 118.90 |
| 36 | A1 | 280 | U | C4-C5-C6 | -5.33 | 116.50 | 119.70 |
| 36 | A1 | 2730 | G | C2-N3-C4 | -5.33 | 109.24 | 111.90 |
| 36 | A1 | 2786 | G | C4-C5-N7 | -5.33 | 108.67 | 110.80 |
| 36 | A1 | 2814 | G | C5-N7-C8 | 5.33 | 106.96 | 104.30 |
| 36 | A5 | 1054 | A | N9-C4-C5 | -5.33 | 103.67 | 105.80 |
| 36 | A5 | 2625 | C | N3-C4-C5 | 5.33 | 124.03 | 121.90 |
| 36 | A5 | 3045 | G | C4-C5-N7 | -5.33 | 108.67 | 110.80 |
| 36 | A1 | 381 | U | C5-C6-N1 | -5.32 | 120.04 | 122.70 |
| 36 | A1 | 994 | G | C6-N1-C2 | -5.32 | 121.91 | 125.10 |
| 36 | A1 | 1743 | G | N7-C8-N9 | -5.32 | 110.44 | 113.10 |
| 36 | A1 | 3181 | C | C2-N3-C4 | -5.32 | 117.24 | 119.90 |
| 40 | BB | 7 | GLU | CB-CA-C | 5.32 | 121.05 | 110.40 |
| 80 | A6 | 232 | U | C5-C6-N1 | 5.32 | 125.36 | 122.70 |
| 1 | A2 | 323 | A | N7-C8-N9 | 5.32 | 116.46 | 113.80 |
| 36 | A1 | 1399 | A | C5-C6-N1 | -5.32 | 115.04 | 117.70 |
| 36 | A1 | 1609 | C | N3-C4-N4 | 5.32 | 121.73 | 118.00 |
| 36 | A1 | 2165 | G | C6-C5-N7 | -5.32 | 127.21 | 130.40 |
| 80 | A6 | 85 | A | C8-N9-C4 | -5.32 | 103.67 | 105.80 |
| 80 | A6 | 1099 | U | N3-C4-O4 | -5.32 | 115.67 | 119.40 |
| 36 | A5 | 3141 | A | N1-C2-N3 | 5.32 | 131.96 | 129.30 |
| 1 | A2 | 969 | C | N3-C4-C5 | 5.32 | 124.03 | 121.90 |
| 36 | A1 | 83 | U | C6-N1-C2 | 5.32 | 124.19 | 121.00 |
| 36 | A1 | 428 | A | C6-N1-C2 | -5.32 | 115.41 | 118.60 |
| 36 | A1 | 963 | G | N3-C4-N9 | 5.32 | 129.19 | 126.00 |
| 36 | A1 | 1154 | A | C5-C6-N1 | -5.32 | 115.04 | 117.70 |
| 41 | BC | 235 | LEU | CB-CG-CD2 | -5.32 | 101.95 | 111.00 |
| 80 | A6 | 958 | U | N3-C2-O2 | 5.32 | 125.92 | 122.20 |
| 36 | A5 | 1107 | C | N3-C4-C5 | 5.32 | 124.03 | 121.90 |
| 36 | A5 | 1131 | G | N1-C2-N3 | 5.32 | 127.09 | 123.90 |
| 36 | A5 | 1490 | A | C6-C5-N7 | -5.32 | 128.58 | 132.30 |
| 36 | A5 | 2998 | U | C2-N3-C4 | -5.32 | 123.81 | 127.00 |
| 36 | A1 | 1899 | G | C4-C5-N7 | 5.32 | 112.93 | 110.80 |
| 36 | A5 | 2976 | A | C5-C6-N1 | 5.32 | 120.36 | 117.70 |
| 36 | A5 | 3025 | C | N3-C2-O2 | -5.32 | 118.18 | 121.90 |
| 36 | A5 | 3323 | A | N1-C2-N3 | 5.32 | 131.96 | 129.30 |
| 1 | A2 | 811 | A | C4-N9-C1' | 5.32 | 135.87 | 126.30 |
| 1 | A2 | 1541 | G | N3-C4-C5 | -5.32 | 125.94 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A2 | 1754 | A | C4-C5-C6 | -5.32 | 114.34 | 117.00 |
| 36 | A1 | 635 | G | N9-C4-C5 | -5.32 | 103.27 | 105.40 |
| 36 | A1 | 638 | C | C2-N3-C4 | -5.32 | 117.24 | 119.90 |
| 36 | A1 | 682 | U | N1-C2-N3 | 5.32 | 118.09 | 114.90 |
| 36 | A1 | 1546 | A | C5-C6-N1 | -5.32 | 115.04 | 117.70 |
| 36 | A1 | 2970 | C | N1-C2-O2 | -5.32 | 115.71 | 118.90 |
| 36 | A1 | 2993 | G | C6-C5-N7 | 5.32 | 133.59 | 130.40 |
| 36 | A1 | 3375 | A | N9-C4-C5 | 5.32 | 107.93 | 105.80 |
| 38 | A4 | 107 | G | C8-N9-C4 | 5.32 | 108.53 | 106.40 |
| 80 | A6 | 163 | G | C6-C5-N7 | -5.32 | 127.21 | 130.40 |
| 36 | A5 | 806 | A | C6-N1-C2 | 5.32 | 121.79 | 118.60 |
| 36 | A5 | 887 | G | C4-C5-C6 | 5.32 | 121.99 | 118.80 |
| 36 | A5 | 1161 | G | C6-C5-N7 | 5.32 | 133.59 | 130.40 |
| 36 | A5 | 1317 | A | N9-C4-C5 | -5.32 | 103.67 | 105.80 |
| 36 | A5 | 1483 | G | N1-C6-O6 | -5.32 | 116.71 | 119.90 |
| 1 | A2 | 214 | G | C8-N9-C1' | 5.32 | 133.91 | 127.00 |
| 1 | A2 | 1537 | C | C5-C4-N4 | -5.32 | 116.48 | 120.20 |
| 36 | A1 | 425 | G | N7-C8-N9 | 5.32 | 115.76 | 113.10 |
| 36 | A1 | 2134 | G | N3-C4-N9 | 5.32 | 129.19 | 126.00 |
| 36 | A1 | 2853 | A | C6-C5-N7 | -5.32 | 128.58 | 132.30 |
| 38 | A4 | 77 | A | C2-N3-C4 | -5.32 | 107.94 | 110.60 |
| 54 | BQ | 179 | ARG | NE-CZ-NH2 | -5.32 | 117.64 | 120.30 |
| 80 | A6 | 396 | G | N3-C4-N9 | 5.32 | 129.19 | 126.00 |
| 36 | A5 | 588 | G | C5-C6-N1 | 5.32 | 114.16 | 111.50 |
| 36 | A5 | 1346 | G | C8-N9-C4 | 5.32 | 108.53 | 106.40 |
| 36 | A5 | 1833 | G | N1-C2-N2 | -5.32 | 111.42 | 116.20 |
| 36 | A5 | 2942 | C | N1-C2-O2 | -5.32 | 115.71 | 118.90 |
| 36 | A5 | 3019 | U | C6-N1-C2 | 5.32 | 124.19 | 121.00 |
| 36 | A1 | 78 | U | C4-C5-C6 | 5.31 | 122.89 | 119.70 |
| 36 | A1 | 89 | A | C4-C5-C6 | 5.31 | 119.66 | 117.00 |
| 1 | A2 | 557 | G | N3-C4-C5 | -5.31 | 125.94 | 128.60 |
| 36 | A1 | 276 | U | N3-C2-O2 | -5.31 | 118.48 | 122.20 |
| 36 | A1 | 2634 | U | N1-C2-O2 | -5.31 | 119.08 | 122.80 |
| 36 | A1 | 2977 | G | C5-N7-C8 | 5.31 | 106.96 | 104.30 |
| 80 | A6 | 65 | A | C6-C5-N7 | -5.31 | 128.58 | 132.30 |
| 80 | A6 | 571 | G | C8-N9-C4 | -5.31 | 104.28 | 106.40 |
| 80 | A6 | 1087 | A | N1-C2-N3 | 5.31 | 131.96 | 129.30 |
| 36 | A5 | 1011 | A | C2-N3-C4 | -5.31 | 107.94 | 110.60 |
| 36 | A5 | 1786 | G | N3-C4-C5 | -5.31 | 125.94 | 128.60 |
| 36 | A5 | 2987 | A | N7-C8-N9 | -5.31 | 111.14 | 113.80 |
| 36 | A5 | 3307 | A | C6-N1-C2 | 5.31 | 121.79 | 118.60 |
| 36 | A5 | 3369 | G | C5-C6-N1 | 5.31 | 114.16 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 38 | A8 | 126 | A | N7-C8-N9 | 5.31 | 116.46 | 113.80 |
| 43 | DE | 26 | ARG | NE-CZ-NH2 | -5.31 | 117.64 | 120.30 |
| 36 | A1 | 1331 | U | C5-C4-O4 | -5.31 | 122.71 | 125.90 |
| 36 | A1 | 1524 | A | N1-C2-N3 | 5.31 | 131.96 | 129.30 |
| 80 | A6 | 1649 | G | N1-C2-N2 | -5.31 | 111.42 | 116.20 |
| 36 | A5 | 1442 | U | C2-N3-C4 | -5.31 | 123.81 | 127.00 |
| 36 | A5 | 1586 | G | C6-C5-N7 | -5.31 | 127.21 | 130.40 |
| 36 | A1 | 31 | C | C2-N3-C4 | -5.31 | 117.25 | 119.90 |
| 36 | A1 | 635 | G | C6-N1-C2 | -5.31 | 121.91 | 125.10 |
| 36 | A1 | 1851 | G | C4-C5-C6 | 5.31 | 121.99 | 118.80 |
| 36 | A1 | 1851 | G | N1-C2-N3 | 5.31 | 127.08 | 123.90 |
| 36 | A1 | 2306 | C | C2-N3-C4 | 5.31 | 122.55 | 119.90 |
| 36 | A1 | 2862 | U | C5-C6-N1 | -5.31 | 120.05 | 122.70 |
| 36 | A1 | 3041 | U | C2-N3-C4 | -5.31 | 123.81 | 127.00 |
| 36 | A5 | 641 | C | C6-N1-C2 | -5.31 | 118.18 | 120.30 |
| 36 | A5 | 969 | C | C6-N1-C2 | 5.31 | 122.42 | 120.30 |
| 36 | A5 | 1085 | A | C4-C5-N7 | 5.31 | 113.36 | 110.70 |
| 36 | A5 | 3110 | C | C5-C6-N1 | -5.31 | 118.34 | 121.00 |
| 1 | A2 | 1524 | A | N1-C2-N3 | 5.31 | 131.95 | 129.30 |
| 36 | A1 | 785 | G | C5-N7-C8 | 5.31 | 106.95 | 104.30 |
| 36 | A1 | 2328 | U | N1-C2-O2 | 5.31 | 126.52 | 122.80 |
| 36 | A1 | 2644 | C | C2-N3-C4 | -5.31 | 117.25 | 119.90 |
| 80 | A6 | 447 | U | N3-C2-O2 | -5.31 | 118.48 | 122.20 |
| 80 | A6 | 794 | U | N1-C2-O2 | 5.31 | 126.52 | 122.80 |
| 36 | A5 | 147 | U | C5-C4-O4 | 5.31 | 129.09 | 125.90 |
| 36 | A5 | 3046 | A | N1-C6-N6 | -5.31 | 115.42 | 118.60 |
| 36 | A5 | 3259 | U | C6-N1-C2 | -5.31 | 117.81 | 121.00 |
| 38 | A4 | 140 | G | N3-C4-C5 | -5.31 | 125.95 | 128.60 |
| 80 | A6 | 1241 | G | C5-N7-C8 | -5.31 | 101.65 | 104.30 |
| 80 | A6 | 1457 | C | C4-C5-C6 | 5.31 | 120.05 | 117.40 |
| 36 | A5 | 799 | G | C5-C6-N1 | 5.31 | 114.15 | 111.50 |
| 36 | A5 | 1110 | U | N1-C2-N3 | -5.31 | 111.72 | 114.90 |
| 36 | A5 | 2175 | U | C2-N1-C1' | -5.31 | 111.33 | 117.70 |
| 36 | A1 | 249 | U | N3-C2-O2 | -5.30 | 118.49 | 122.20 |
| 36 | A1 | 626 | U | N3-C4-C5 | 5.30 | 117.78 | 114.60 |
| 36 | A1 | 1877 | U | N3-C4-C5 | 5.30 | 117.78 | 114.60 |
| 37 | A3 | 29 | C | C6-N1-C2 | -5.30 | 118.18 | 120.30 |
| 80 | A6 | 944 | A | C2-N3-C4 | -5.30 | 107.95 | 110.60 |
| 20 | CS | 116 | LEU | CA-CB-CG | 5.30 | 127.50 | 115.30 |
| 36 | A5 | 587 | U | N3-C4-O4 | -5.30 | 115.69 | 119.40 |
| 36 | A5 | 637 | C | C2-N3-C4 | -5.30 | 117.25 | 119.90 |
| 36 | A5 | 924 | G | C5-C6-O6 | -5.30 | 125.42 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 36 | A5 | 2572 | C | C6-N1-C1' | -5.30 | 114.44 | 120.80 |
| 36 | A5 | 3173 | G | C4-C5-N7 | 5.30 | 112.92 | 110.80 |
| 38 | A8 | 95 | G | N3-C4-N9 | -5.30 | 122.82 | 126.00 |
| 80 | A6 | 1244 | A | C2-N3-C4 | 5.30 | 113.25 | 110.60 |
| 7 | CF | 70 | VAL | CB-CA-C | -5.30 | 101.32 | 111.40 |
| 36 | A5 | 1846 | C | C6-N1-C2 | 5.30 | 122.42 | 120.30 |
| 24 | AW | 93 | LEU | CA-CB-CG | 5.30 | 127.49 | 115.30 |
| 36 | A1 | 16 | A | C2-N3-C4 | -5.30 | 107.95 | 110.60 |
| 36 | A1 | 428 | A | N1-C2-N3 | 5.30 | 131.95 | 129.30 |
| 36 | A1 | 1201 | C | N3-C4-C5 | -5.30 | 119.78 | 121.90 |
| 36 | A1 | 1387 | G | C5-C6-N1 | -5.30 | 108.85 | 111.50 |
| 36 | A1 | 1513 | G | C5-C6-N1 | 5.30 | 114.15 | 111.50 |
| 36 | A1 | 2147 | A | C6-N1-C2 | -5.30 | 115.42 | 118.60 |
| 36 | A1 | 2311 | G | C5-N7-C8 | -5.30 | 101.65 | 104.30 |
| 80 | A6 | 1035 | G | C6-C5-N7 | 5.30 | 133.58 | 130.40 |
| 36 | A5 | 1315 | U | C6-N1-C2 | 5.30 | 124.18 | 121.00 |
| 36 | A5 | 1378 | U | N3-C4-C5 | 5.30 | 117.78 | 114.60 |
| 36 | A5 | 2279 | A | C2-N3-C4 | -5.30 | 107.95 | 110.60 |
| 36 | A5 | 3385 | U | C5-C6-N1 | -5.30 | 120.05 | 122.70 |
| 1 | A2 | 583 | C | C2-N1-C1' | 5.30 | 124.63 | 118.80 |
| 36 | A1 | 921 | A | C5-C6-N6 | -5.30 | 119.46 | 123.70 |
| 36 | A1 | 1209 | G | C4-C5-N7 | -5.30 | 108.68 | 110.80 |
| 36 | A1 | 1887 | A | C2-N3-C4 | -5.30 | 107.95 | 110.60 |
| 36 | A1 | 2615 | G | N3-C2-N2 | -5.30 | 116.19 | 119.90 |
| 37 | A3 | 96 | U | N3-C4-C5 | 5.30 | 117.78 | 114.60 |
| 80 | A6 | 1754 | A | N9-C4-C5 | 5.30 | 107.92 | 105.80 |
| 36 | A5 | 2632 | G | N3-C2-N2 | 5.30 | 123.61 | 119.90 |
| 36 | A5 | 2884 | C | C5-C4-N4 | -5.30 | 116.49 | 120.20 |
| 51 | DN | 174 | ILE | CG1-CB-CG2 | -5.30 | 99.74 | 111.40 |
| 1 | A2 | 1119 | G | N3-C4-C5 | -5.30 | 125.95 | 128.60 |
| 36 | A1 | 726 | G | C8-N9-C4 | -5.30 | 104.28 | 106.40 |
| 36 | A1 | 2361 | A | N7-C8-N9 | 5.30 | 116.45 | 113.80 |
| 36 | A1 | 2940 | A | C4-C5-N7 | -5.30 | 108.05 | 110.70 |
| 36 | A5 | 637 | C | C6-N1-C1' | 5.30 | 127.16 | 120.80 |
| 36 | A5 | 961 | C | C5-C6-N1 | -5.30 | 118.35 | 121.00 |
| 36 | A1 | 221 | A | N1-C2-N3 | 5.30 | 131.95 | 129.30 |
| 36 | A1 | 1929 | G | N7-C8-N9 | -5.30 | 110.45 | 113.10 |
| 80 | A6 | 1272 | U | N3-C4-C5 | -5.30 | 111.42 | 114.60 |
| 36 | A5 | 661 | G | C5-C6-O6 | 5.30 | 131.78 | 128.60 |
| 36 | A5 | 1741 | A | N1-C2-N3 | 5.30 | 131.95 | 129.30 |
| 36 | A5 | 2893 | C | N3-C2-O2 | 5.30 | 125.61 | 121.90 |
| 37 | A7 | 35 | C | N1-C2-O2 | -5.30 | 115.72 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 62 | DY | 103 | LYS | CD-CE-NZ | -5.30 | 99.52 | 111.70 |
| 80 | A6 | 1072 | C | N3-C4-C5 | 5.29 | 124.02 | 121.90 |
| 36 | A5 | 979 | U | C2-N1-C1' | 5.29 | 124.05 | 117.70 |
| 36 | A5 | 2213 | A | N7-C8-N9 | -5.29 | 111.15 | 113.80 |
| 1 | A2 | 1763 | A | C5-N7-C8 | -5.29 | 101.25 | 103.90 |
| 36 | A1 | 895 | A | C6-N1-C2 | 5.29 | 121.78 | 118.60 |
| 36 | A1 | 2177 | G | C6-N1-C2 | -5.29 | 121.92 | 125.10 |
| 36 | A1 | 2435 | G | C2-N3-C4 | 5.29 | 114.55 | 111.90 |
| 36 | A1 | 2678 | A | C8-N9-C4 | -5.29 | 103.68 | 105.80 |
| 36 | A5 | 656 | A | C5-N7-C8 | 5.29 | 106.55 | 103.90 |
| 36 | A5 | 960 | U | C6-N1-C1' | -5.29 | 113.79 | 121.20 |
| 36 | A5 | 1050 | U | C5-C4-O4 | 5.29 | 129.08 | 125.90 |
| 36 | A5 | 1126 | G | C5-C6-N1 | -5.29 | 108.85 | 111.50 |
| 36 | A5 | 1140 | G | N3-C4-N9 | 5.29 | 129.18 | 126.00 |
| 36 | A5 | 1846 | C | N1-C2-N3 | 5.29 | 122.91 | 119.20 |
| 36 | A5 | 1917 | C | C4-C5-C6 | 5.29 | 120.05 | 117.40 |
| 36 | A5 | 2359 | C | N3-C4-N4 | -5.29 | 114.30 | 118.00 |
| 37 | A7 | 14 | U | N1-C2-N3 | 5.29 | 118.08 | 114.90 |
| 1 | A2 | 319 | U | N1-C2-N3 | -5.29 | 111.73 | 114.90 |
| 36 | A1 | 817 | A | N3-C4-C5 | -5.29 | 123.10 | 126.80 |
| 54 | BQ | 138 | LEU | CA-CB-CG | 5.29 | 127.47 | 115.30 |
| 6 | CE | 38 | LEU | CA-CB-CG | 5.29 | 127.47 | 115.30 |
| 36 | A5 | 381 | U | C5-C6-N1 | -5.29 | 120.05 | 122.70 |
| 36 | A5 | 2279 | A | C5-N7-C8 | -5.29 | 101.25 | 103.90 |
| 36 | A5 | 2525 | G | C8-N9-C4 | 5.29 | 108.52 | 106.40 |
| 36 | A5 | 2665 | U | C5-C6-N1 | 5.29 | 125.35 | 122.70 |
| 36 | A5 | 2721 | A | N3-C4-C5 | -5.29 | 123.10 | 126.80 |
| 36 | A5 | 2882 | U | N3-C4-O4 | -5.29 | 115.69 | 119.40 |
| 1 | A2 | 1086 | A | C5-C6-N1 | 5.29 | 120.34 | 117.70 |
| 36 | A1 | 517 | G | C2-N3-C4 | 5.29 | 114.55 | 111.90 |
| 36 | A1 | 2364 | G | N1-C6-O6 | 5.29 | 123.07 | 119.90 |
| 36 | A1 | 2400 | G | N1-C6-O6 | 5.29 | 123.07 | 119.90 |
| 36 | A5 | 1369 | A | N1-C2-N3 | -5.29 | 126.66 | 129.30 |
| 36 | A5 | 2370 | G | N3-C4-N9 | 5.29 | 129.17 | 126.00 |
| 1 | A2 | 12 | U | N3-C2-O2 | -5.29 | 118.50 | 122.20 |
| 1 | A2 | 1200 | G | C8-N9-C4 | -5.29 | 104.28 | 106.40 |
| 1 | A2 | 1370 | U | C2-N1-C1' | 5.29 | 124.05 | 117.70 |
| 36 | A1 | 794 | U | C5-C4-O4 | 5.29 | 129.07 | 125.90 |
| 36 | A1 | 931 | C | N1-C2-N3 | 5.29 | 122.90 | 119.20 |
| 36 | A1 | 1904 | C | C5-C6-N1 | 5.29 | 123.64 | 121.00 |
| 36 | A1 | 2651 | G | N7-C8-N9 | -5.29 | 110.46 | 113.10 |
| 46 | BH | 166 | ARG | CG-CD-NE | 5.29 | 122.91 | 111.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 80 | A6 | 296 | U | N3-C4-C5 | 5.29 | 117.77 | 114.60 |
| 80 | A6 | 420 | A | C5-N7-C8 | -5.29 | 101.26 | 103.90 |
| 80 | A6 | 1000 | C | N1-C2-N3 | 5.29 | 122.90 | 119.20 |
| 36 | A5 | 905 | U | C2-N3-C4 | -5.29 | 123.83 | 127.00 |
| 36 | A5 | 1220 | U | C5-C6-N1 | -5.29 | 120.06 | 122.70 |
| 1 | A2 | 387 | A | N1-C6-N6 | -5.29 | 115.43 | 118.60 |
| 36 | A1 | 639 | G | C4-C5-C6 | 5.29 | 121.97 | 118.80 |
| 36 | A1 | 1565 | G | N7-C8-N9 | 5.29 | 115.74 | 113.10 |
| 36 | A1 | 2395 | G | C5-N7-C8 | 5.29 | 106.94 | 104.30 |
| 36 | A1 | 2989 | U | N1-C2-N3 | 5.29 | 118.07 | 114.90 |
| 36 | A5 | 929 | A | C5-N7-C8 | 5.29 | 106.54 | 103.90 |
| 36 | A5 | 992 | A | C8-N9-C4 | 5.29 | 107.92 | 105.80 |
| 36 | A5 | 1929 | G | C2-N3-C4 | -5.29 | 109.26 | 111.90 |
| 36 | A5 | 3171 | U | C6-N1-C2 | 5.29 | 124.17 | 121.00 |
| 1 | A2 | 151 | G | C5-C6-N1 | 5.29 | 114.14 | 111.50 |
| 36 | A1 | 811 | U | C2-N3-C4 | -5.29 | 123.83 | 127.00 |
| 36 | A1 | 835 | G | C5-C6-O6 | -5.29 | 125.43 | 128.60 |
| 36 | A1 | 3207 | U | C6-N1-C1' | 5.29 | 128.60 | 121.20 |
| 36 | A5 | 406 | G | O4'-C1'-N9 | 5.29 | 112.43 | 108.20 |
| 36 | A5 | 975 | C | N1-C2-N3 | 5.29 | 122.90 | 119.20 |
| 36 | A5 | 1828 | A | C2-N3-C4 | -5.29 | 107.96 | 110.60 |
| 36 | A5 | 2506 | U | C5-C6-N1 | 5.29 | 125.34 | 122.70 |
| 36 | A5 | 2648 | G | N9-C4-C5 | -5.29 | 103.29 | 105.40 |
| 1 | A2 | 1520 | U | C5-C6-N1 | -5.28 | 120.06 | 122.70 |
| 36 | A1 | 1587 | A | C5-C6-N1 | 5.28 | 120.34 | 117.70 |
| 80 | A6 | 251 | A | C2-N3-C4 | -5.28 | 107.96 | 110.60 |
| 80 | A6 | 1466 | G | C5-C6-N1 | -5.28 | 108.86 | 111.50 |
| 12 | CK | 88 | PRO | N-CA-CB | 5.28 | 109.64 | 103.30 |
| 36 | A5 | 1190 | A | C4-N9-C1' | 5.28 | 135.81 | 126.30 |
| 36 | A5 | 1421 | G | N3-C4-C5 | 5.28 | 131.24 | 128.60 |
| 36 | A5 | 2374 | C | C5-C4-N4 | 5.28 | 123.90 | 120.20 |
| 36 | A5 | 1007 | U | N3-C4-C5 | 5.28 | 117.77 | 114.60 |
| 36 | A5 | 1445 | U | N1-C2-O2 | -5.28 | 119.10 | 122.80 |
| 36 | A5 | 2549 | G | C5-N7-C8 | -5.28 | 101.66 | 104.30 |
| 1 | A2 | 1200 | G | N7-C8-N9 | 5.28 | 115.74 | 113.10 |
| 36 | A1 | 355 | A | C8-N9-C4 | 5.28 | 107.91 | 105.80 |
| 36 | A1 | 796 | U | N3-C2-O2 | 5.28 | 125.90 | 122.20 |
| 36 | A1 | 1916 | U | N3-C4-C5 | 5.28 | 117.77 | 114.60 |
| 36 | A1 | 3208 | G | N3-C2-N2 | -5.28 | 116.20 | 119.90 |
| 36 | A1 | 3334 | U | N1-C2-N3 | 5.28 | 118.07 | 114.90 |
| 37 | A3 | 120 | C | C6-N1-C2 | 5.28 | 122.41 | 120.30 |
| 80 | A6 | 1455 | G | N3-C2-N2 | -5.28 | 116.20 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 2422 | C | N3-C4-C5 | 5.28 | 124.01 | 121.90 |
| 36 | A5 | 2763 | U | C5-C4-O4 | -5.28 | 122.73 | 125.90 |
| 36 | A5 | 2956 | A | C5-C6-N1 | -5.28 | 115.06 | 117.70 |
| 36 | A1 | 3101 | G | N1-C6-O6 | -5.28 | 116.73 | 119.90 |
| 36 | A1 | 3103 | A | C2-N3-C4 | -5.28 | 107.96 | 110.60 |
| 36 | A1 | 3127 | A | N9-C4-C5 | 5.28 | 107.91 | 105.80 |
| 36 | A5 | 1180 | A | C2-N3-C4 | -5.28 | 107.96 | 110.60 |
| 36 | A5 | 2279 | A | N1-C6-N6 | 5.28 | 121.77 | 118.60 |
| 1 | A2 | 1334 | U | N1-C2-N3 | 5.28 | 118.07 | 114.90 |
| 36 | A1 | 702 | C | N3-C4-N4 | 5.28 | 121.69 | 118.00 |
| 36 | A1 | 811 | U | C5-C6-N1 | -5.28 | 120.06 | 122.70 |
| 36 | A1 | 1005 | G | C8-N9-C4 | -5.28 | 104.29 | 106.40 |
| 36 | A1 | 1369 | A | C2-N3-C4 | -5.28 | 107.96 | 110.60 |
| 36 | A1 | 2124 | G | C5-C6-O6 | -5.28 | 125.43 | 128.60 |
| 36 | A1 | 2192 | C | C4-C5-C6 | 5.28 | 120.04 | 117.40 |
| 36 | A1 | 3256 | G | C2-N3-C4 | 5.28 | 114.54 | 111.90 |
| 38 | A4 | 1 | A | C5-N7-C8 | -5.28 | 101.26 | 103.90 |
| 80 | A6 | 800 | U | C5-C4-O4 | 5.28 | 129.07 | 125.90 |
| 80 | A6 | 1389 | C | N1-C2-O2 | 5.28 | 122.07 | 118.90 |
| 80 | A6 | 1780 | G | C4-C5-N7 | 5.28 | 112.91 | 110.80 |
| 36 | A5 | 35 | A | N1-C2-N3 | 5.28 | 131.94 | 129.30 |
| 36 | A5 | 1080 | A | N1-C2-N3 | 5.28 | 131.94 | 129.30 |
| 36 | A5 | 1500 | G | N7-C8-N9 | -5.28 | 110.46 | 113.10 |
| 36 | A5 | 2144 | A | N1-C6-N6 | 5.28 | 121.77 | 118.60 |
| 36 | A5 | 2364 | G | C4-C5-N7 | -5.28 | 108.69 | 110.80 |
| 1 | A2 | 1086 | A | N1-C6-N6 | -5.28 | 115.44 | 118.60 |
| 1 | A2 | 1195 | C | P-O3'-C3' | 5.28 | 126.03 | 119.70 |
| 36 | A1 | 600 | G | C6-C5-N7 | -5.28 | 127.23 | 130.40 |
| 36 | A1 | 1132 | C | N3-C2-O2 | -5.28 | 118.21 | 121.90 |
| 36 | A1 | 1517 | G | C4-C5-N7 | -5.28 | 108.69 | 110.80 |
| 36 | A1 | 1660 | C | N1-C2-O2 | -5.28 | 115.73 | 118.90 |
| 36 | A1 | 1899 | G | C5-N7-C8 | -5.28 | 101.66 | 104.30 |
| 36 | A1 | 2209 | U | C5-C6-N1 | 5.28 | 125.34 | 122.70 |
| 38 | A4 | 60 | U | N1-C2-N3 | 5.28 | 118.06 | 114.90 |
| 54 | BQ | 24 | VAL | CB-CA-C | -5.28 | 101.38 | 111.40 |
| 80 | A6 | 1456 | C | C5-C6-N1 | -5.28 | 118.36 | 121.00 |
| 80 | A6 | 1547 | A | N1-C6-N6 | -5.28 | 115.44 | 118.60 |
| 51 | DN | 201 | ARG | NE-CZ-NH1 | 5.28 | 122.94 | 120.30 |
| 36 | A1 | 3147 | G | N1-C6-O6 | -5.27 | 116.74 | 119.90 |
| 80 | A6 | 946 | U | N3-C4-C5 | -5.27 | 111.44 | 114.60 |
| 36 | A5 | 1203 | A | N1-C6-N6 | 5.27 | 121.77 | 118.60 |
| 36 | A5 | 2755 | C | C4-C5-C6 | 5.27 | 120.04 | 117.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 37 | A7 | 48 | U | N3-C2-O2 | 5.27 | 125.89 | 122.20 |
| 1 | A2 | 1170 | G | C5-C6-O6 | -5.27 | 125.44 | 128.60 |
| 36 | A1 | 313 | A | C6-N1-C2 | -5.27 | 115.44 | 118.60 |
| 36 | A1 | 344 | A | C2-N3-C4 | 5.27 | 113.24 | 110.60 |
| 36 | A1 | 1131 | G | N9-C4-C5 | -5.27 | 103.29 | 105.40 |
| 36 | A1 | 1550 | C | N1-C2-O2 | -5.27 | 115.74 | 118.90 |
| 36 | A1 | 1897 | G | C4-C5-C6 | 5.27 | 121.96 | 118.80 |
| 36 | A1 | 2413 | A | C6-N1-C2 | 5.27 | 121.76 | 118.60 |
| 36 | A1 | 3325 | G | C4-C5-N7 | -5.27 | 108.69 | 110.80 |
| 80 | A6 | 1295 | G | N3-C2-N2 | -5.27 | 116.21 | 119.90 |
| 1 | A2 | 1761 | U | N1-C2-N3 | 5.27 | 118.06 | 114.90 |
| 36 | A1 | 1182 | A | N1-C6-N6 | 5.27 | 121.76 | 118.60 |
| 51 | BN | 85 | THR | CB-CA-C | -5.27 | 97.37 | 111.60 |
| 1 | A2 | 1614 | A | N1-C6-N6 | 5.27 | 121.76 | 118.60 |
| 36 | A1 | 1691 | U | C5-C6-N1 | -5.27 | 120.06 | 122.70 |
| 36 | A1 | 1751 | G | N1-C6-O6 | -5.27 | 116.74 | 119.90 |
| 36 | A1 | 1893 | A | N9-C4-C5 | 5.27 | 107.91 | 105.80 |
| 36 | A1 | 2413 | A | C2-N3-C4 | 5.27 | 113.23 | 110.60 |
| 36 | A1 | 2909 | U | C4-C5-C6 | 5.27 | 122.86 | 119.70 |
| 42 | BD | 41 | LYS | CD-CE-NZ | 5.27 | 123.82 | 111.70 |
| 80 | A6 | 1031 | U | N3-C2-O2 | 5.27 | 125.89 | 122.20 |
| 80 | A6 | 1094 | G | N3-C4-C5 | -5.27 | 125.97 | 128.60 |
| 80 | A6 | 1423 | U | C2-N3-C4 | -5.27 | 123.84 | 127.00 |
| 36 | A5 | 1714 | A | C2-N3-C4 | -5.27 | 107.97 | 110.60 |
| 36 | A5 | 2158 | A | C5-C6-N1 | 5.27 | 120.33 | 117.70 |
| 36 | A5 | 2191 | U | C4-C5-C6 | 5.27 | 122.86 | 119.70 |
| 36 | A5 | 2321 | A | C8-N9-C4 | 5.27 | 107.91 | 105.80 |
| 36 | A5 | 2524 | A | C2-N3-C4 | -5.27 | 107.97 | 110.60 |
| 36 | A5 | 2921 | U | N1-C2-N3 | 5.27 | 118.06 | 114.90 |
| 36 | A5 | 2928 | C | C2-N1-C1' | 5.27 | 124.60 | 118.80 |
| 36 | A5 | 3052 | G | C5-N7-C8 | 5.27 | 106.94 | 104.30 |
| 1 | A2 | 1297 | G | C4-N9-C1' | -5.27 | 119.65 | 126.50 |
| 36 | A1 | 375 | A | C5-N7-C8 | -5.27 | 101.27 | 103.90 |
| 36 | A1 | 761 | A | N1-C2-N3 | 5.27 | 131.93 | 129.30 |
| 36 | A1 | 1506 | A | C8-N9-C4 | -5.27 | 103.69 | 105.80 |
| 80 | A6 | 1114 | G | N3-C4-N9 | 5.27 | 129.16 | 126.00 |
| 36 | A5 | 813 | G | N3-C4-C5 | -5.27 | 125.97 | 128.60 |
| 36 | A5 | 1724 | U | P-O3'-C3' | 5.27 | 126.02 | 119.70 |
| 36 | A5 | 2211 | U | C6-N1-C2 | -5.27 | 117.84 | 121.00 |
| 36 | A5 | 2606 | G | C6-C5-N7 | -5.27 | 127.24 | 130.40 |
| 36 | A5 | 2692 | A | C4-C5-N7 | -5.27 | 108.07 | 110.70 |
| 36 | A5 | 3309 | G | C2-N3-C4 | 5.27 | 114.53 | 111.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 1227 | C | C6-N1-C2 | -5.27 | 118.19 | 120.30 |
| 36 | A5 | 997 | A | C8-N9-C4 | -5.27 | 103.69 | 105.80 |
| 36 | A5 | 2163 | C | N3-C4-C5 | 5.27 | 124.01 | 121.90 |
| 1 | A2 | 1245 | G | N3-C4-N9 | -5.26 | 122.84 | 126.00 |
| 36 | A1 | 658 | G | N3-C2-N2 | -5.26 | 116.22 | 119.90 |
| 36 | A1 | 1358 | C | C6-N1-C2 | 5.26 | 122.41 | 120.30 |
| 80 | A6 | 449 | C | C5-C6-N1 | -5.26 | 118.37 | 121.00 |
| 80 | A6 | 1675 | C | C4-C5-C6 | 5.26 | 120.03 | 117.40 |
| 36 | A5 | 141 | C | C6-N1-C2 | -5.26 | 118.19 | 120.30 |
| 36 | A5 | 186 | U | N1-C2-O2 | 5.26 | 126.49 | 122.80 |
| 36 | A5 | 1305 | U | C5-C6-N1 | -5.26 | 120.07 | 122.70 |
| 36 | A5 | 1310 | G | C5-C6-N1 | 5.26 | 114.13 | 111.50 |
| 36 | A5 | 2798 | C | N3-C4-C5 | -5.26 | 119.79 | 121.90 |
| 36 | A1 | 21 | G | N3-C4-C5 | -5.26 | 125.97 | 128.60 |
| 36 | A1 | 1343 | A | N1-C2-N3 | 5.26 | 131.93 | 129.30 |
| 36 | A5 | 1939 | G | C4-N9-C1' | 5.26 | 133.34 | 126.50 |
| 37 | A7 | 37 | G | C8-N9-C4 | 5.26 | 108.50 | 106.40 |
| 1 | A2 | 542 | A | C5-C6-N1 | -5.26 | 115.07 | 117.70 |
| 36 | A1 | 1332 | A | C6-N1-C2 | 5.26 | 121.76 | 118.60 |
| 36 | A1 | 2214 | A | C5-C6-N1 | -5.26 | 115.07 | 117.70 |
| 36 | A1 | 2286 | U | C2-N3-C4 | -5.26 | 123.84 | 127.00 |
| 36 | A1 | 2415 | C | N3-C4-C5 | 5.26 | 124.00 | 121.90 |
| 80 | A6 | 358 | U | N1-C2-N3 | 5.26 | 118.06 | 114.90 |
| 80 | A6 | 769 | A | N1-C6-N6 | -5.26 | 115.44 | 118.60 |
| 80 | A6 | 1455 | G | C8-N9-C4 | -5.26 | 104.30 | 106.40 |
| 25 | CX | 23 | ARG | CG-CD-NE | 5.26 | 122.85 | 111.80 |
| 36 | A5 | 1137 | C | N3-C4-C5 | -5.26 | 119.80 | 121.90 |
| 15 | AN | 22 | ALA | C-N-CA | 5.26 | 144.09 | 122.00 |
| 36 | A1 | 373 | A | N1-C6-N6 | -5.26 | 115.44 | 118.60 |
| 36 | A1 | 2608 | G | C8-N9-C4 | 5.26 | 108.50 | 106.40 |
| 40 | BB | 25 | ILE | CB-CA-C | -5.26 | 101.08 | 111.60 |
| 80 | A6 | 1634 | C | N3-C2-O2 | -5.26 | 118.22 | 121.90 |
| 36 | A5 | 282 | G | C5-C6-N1 | -5.26 | 108.87 | 111.50 |
| 36 | A5 | 2164 | A | C4-C5-C6 | 5.26 | 119.63 | 117.00 |
| 36 | A5 | 2790 | A | C5-C6-N1 | 5.26 | 120.33 | 117.70 |
| 38 | A8 | 147 | U | C2-N3-C4 | -5.26 | 123.84 | 127.00 |
| 1 | A2 | 1542 | G | N1-C6-O6 | -5.26 | 116.75 | 119.90 |
| 36 | A1 | 426 | G | C8-N9-C1' | -5.26 | 120.17 | 127.00 |
| 36 | A1 | 636 | C | C4-C5-C6 | 5.26 | 120.03 | 117.40 |
| 36 | A1 | 931 | C | N3-C4-C5 | 5.26 | 124.00 | 121.90 |
| 36 | A1 | 2940 | A | N1-C2-N3 | 5.26 | 131.93 | 129.30 |
| 36 | A1 | 3242 | G | C4-C5-N7 | -5.26 | 108.70 | 110.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 38 | A4 | 102 | U | N1-C2-N3 | 5.26 | 118.06 | 114.90 |
| 36 | A5 | 693 | A | C5-C6-N6 | 5.26 | 127.91 | 123.70 |
| 1 | A2 | 971 | A | N1-C2-N3 | 5.26 | 131.93 | 129.30 |
| 1 | A2 | 1600 | A | N3-C4-C5 | 5.26 | 130.48 | 126.80 |
| 36 | A1 | 1049 | C | C2-N3-C4 | -5.26 | 117.27 | 119.90 |
| 36 | A1 | 1409 | G | C5-C6-N1 | 5.26 | 114.13 | 111.50 |
| 37 | A3 | 93 | C | C2-N3-C4 | -5.26 | 117.27 | 119.90 |
| 38 | A4 | 151 | C | C6-N1-C2 | -5.26 | 118.20 | 120.30 |
| 80 | A6 | 1317 | C | C6-N1-C2 | -5.26 | 118.20 | 120.30 |
| 36 | A5 | 327 | A | N1-C2-N3 | -5.26 | 126.67 | 129.30 |
| 36 | A5 | 1178 | G | C5-C6-O6 | -5.26 | 125.45 | 128.60 |
| 36 | A5 | 1327 | C | C5-C4-N4 | 5.26 | 123.88 | 120.20 |
| 36 | A5 | 3294 | A | N1-C2-N3 | 5.26 | 131.93 | 129.30 |
| 36 | A1 | 301 | G | C5-C6-O6 | 5.25 | 131.75 | 128.60 |
| 36 | A1 | 984 | G | C6-C5-N7 | -5.25 | 127.25 | 130.40 |
| 36 | A1 | 1171 | G | C5-C6-N1 | 5.25 | 114.13 | 111.50 |
| 36 | A5 | 1516 | C | C4-C5-C6 | 5.25 | 120.03 | 117.40 |
| 41 | DC | 190 | GLY | N-CA-C | 5.25 | 126.24 | 113.10 |
| 36 | A1 | 1389 | G | N9-C4-C5 | -5.25 | 103.30 | 105.40 |
| 36 | A1 | 1431 | G | N1-C6-O6 | -5.25 | 116.75 | 119.90 |
| 36 | A1 | 2606 | G | C6-C5-N7 | -5.25 | 127.25 | 130.40 |
| 36 | A1 | 2619 | G | C5-C6-N1 | 5.25 | 114.13 | 111.50 |
| 36 | A5 | 413 | U | C5-C4-O4 | -5.25 | 122.75 | 125.90 |
| 36 | A5 | 494 | G | N1-C6-O6 | -5.25 | 116.75 | 119.90 |
| 36 | A5 | 515 | C | C5-C4-N4 | -5.25 | 116.52 | 120.20 |
| 36 | A5 | 802 | C | N3-C2-O2 | -5.25 | 118.22 | 121.90 |
| 36 | A5 | 1856 | C | N3-C2-O2 | -5.25 | 118.22 | 121.90 |
| 36 | A5 | 2271 | A | C6-C5-N7 | 5.25 | 135.98 | 132.30 |
| 36 | A5 | 2724 | U | N3-C4-O4 | -5.25 | 115.72 | 119.40 |
| 36 | A5 | 2965 | U | N3-C4-O4 | 5.25 | 123.08 | 119.40 |
| 36 | A5 | 3005 | A | C8-N9-C4 | -5.25 | 103.70 | 105.80 |
| 1 | A2 | 972 | G | N1-C6-O6 | -5.25 | 116.75 | 119.90 |
| 1 | A2 | 1648 | A | N1-C6-N6 | -5.25 | 115.45 | 118.60 |
| 36 | A1 | 54 | C | C4-C5-C6 | -5.25 | 114.77 | 117.40 |
| 36 | A1 | 1421 | G | N7-C8-N9 | -5.25 | 110.47 | 113.10 |
| 36 | A1 | 1515 | A | N1-C2-N3 | 5.25 | 131.93 | 129.30 |
| 36 | A1 | 2805 | G | C2-N3-C4 | 5.25 | 114.53 | 111.90 |
| 36 | A1 | 3100 | U | N3-C4-C5 | -5.25 | 111.45 | 114.60 |
| 80 | A6 | 1129 | U | C6-N1-C2 | 5.25 | 124.15 | 121.00 |
| 8 | CG | 193 | LEU | CA-CB-CG | 5.25 | 127.38 | 115.30 |
| 36 | A5 | 831 | G | C5-C6-O6 | -5.25 | 125.45 | 128.60 |
| 36 | A5 | 1158 | A | N9-C4-C5 | -5.25 | 103.70 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 36 | A5 | 1925 | U | N3-C4-C5 | 5.25 | 117.75 | 114.60 |
| 36 | A5 | 2979 | U | N1-C2-N3 | -5.25 | 111.75 | 114.90 |
| 36 | A1 | 2381 | G | C5-N7-C8 | 5.25 | 106.92 | 104.30 |
| 36 | A1 | 2645 | G | N3-C2-N2 | -5.25 | 116.22 | 119.90 |
| 80 | A6 | 864 | U | N1-C2-N3 | 5.25 | 118.05 | 114.90 |
| 36 | A5 | 365 | A | C4-C5-N7 | 5.25 | 113.33 | 110.70 |
| 36 | A5 | 1792 | C | C5-C6-N1 | -5.25 | 118.38 | 121.00 |
| 36 | A1 | 655 | C | N1-C2-N3 | 5.25 | 122.87 | 119.20 |
| 36 | A1 | 804 | C | C6-N1-C1' | 5.25 | 127.10 | 120.80 |
| 36 | A1 | 1807 | G | N7-C8-N9 | 5.25 | 115.72 | 113.10 |
| 36 | A1 | 2912 | G | C5-C6-O6 | -5.25 | 125.45 | 128.60 |
| 36 | A1 | 2996 | U | N3-C2-O2 | -5.25 | 118.53 | 122.20 |
| 80 | A6 | 576 | G | N3-C4-C5 | -5.25 | 125.97 | 128.60 |
| 5 | CD | 202 | LEU | CA-CB-CG | 5.25 | 127.37 | 115.30 |
| 36 | A5 | 318 | A | N1-C2-N3 | -5.25 | 126.67 | 129.30 |
| 36 | A5 | 2851 | A | C2-N3-C4 | -5.25 | 107.98 | 110.60 |
| 36 | A5 | 3339 | A | N1-C6-N6 | 5.25 | 121.75 | 118.60 |
| 52 | DO | 182[B] | SER | CA-C-N | 5.25 | 128.75 | 117.20 |
| 36 | A1 | 1156 | C | N3-C2-O2 | -5.25 | 118.23 | 121.90 |
| 41 | BC | 198 | ARG | NE-CZ-NH2 | -5.25 | 117.68 | 120.30 |
| 36 | A5 | 1100 | U | N3-C4-C5 | 5.25 | 117.75 | 114.60 |
| 36 | A5 | 1208 | U | N1-C2-O2 | 5.25 | 126.47 | 122.80 |
| 36 | A5 | 1432 | C | C2-N1-C1' | 5.25 | 124.57 | 118.80 |
| 1 | A2 | 582 | U | C5-C6-N1 | 5.25 | 125.32 | 122.70 |
| 36 | A1 | 1131 | G | N3-C2-N2 | 5.25 | 123.57 | 119.90 |
| 36 | A1 | 2644 | C | N3-C2-O2 | -5.25 | 118.23 | 121.90 |
| 68 | Be | 16 | LYS | CD-CE-NZ | 5.25 | 123.76 | 111.70 |
| 80 | A6 | 106 | U | N3-C4-C5 | 5.25 | 117.75 | 114.60 |
| 36 | A5 | 496 | C | N1-C2-O2 | 5.25 | 122.05 | 118.90 |
| 36 | A5 | 928 | C | C6-N1-C2 | -5.25 | 118.20 | 120.30 |
| 36 | A5 | 2207 | A | C4-C5-N7 | 5.25 | 113.32 | 110.70 |
| 47 | DI | 99 | ILE | CB-CA-C | -5.25 | 101.11 | 111.60 |
| 1 | A2 | 1454 | G | C4-C5-N7 | -5.24 | 108.70 | 110.80 |
| 36 | A1 | 801 | A | C6-N1-C2 | 5.24 | 121.75 | 118.60 |
| 36 | A1 | 1337 | A | N1-C2-N3 | -5.24 | 126.68 | 129.30 |
| 80 | A6 | 876 | G | C4-C5-C6 | 5.24 | 121.95 | 118.80 |
| 80 | A6 | 1282 | U | N3-C2-O2 | 5.24 | 125.87 | 122.20 |
| 36 | A5 | 404 | G | C4-C5-N7 | -5.24 | 108.70 | 110.80 |
| 36 | A5 | 1603 | A | C5-C6-N1 | -5.24 | 115.08 | 117.70 |
| 36 | A5 | 1901 | A | C8-N9-C1' | -5.24 | 118.26 | 127.70 |
| 38 | A8 | 77 | A | C2-N3-C4 | -5.24 | 107.98 | 110.60 |
| 38 | A8 | 79 | A | C4-C5-N7 | 5.24 | 113.32 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A2 | 608 | U | C5-C6-N1 | -5.24 | 120.08 | 122.70 |
| 36 | A1 | 1160 | C | C2-N3-C4 | 5.24 | 122.52 | 119.90 |
| 36 | A1 | 1549 | U | C6-N1-C1' | -5.24 | 113.86 | 121.20 |
| 80 | A6 | 1328 | G | N9-C4-C5 | -5.24 | 103.30 | 105.40 |
| 36 | A5 | 3335 | A | C5-N7-C8 | -5.24 | 101.28 | 103.90 |
| 16 | AO | 107 | ARG | NE-CZ-NH2 | 5.24 | 122.92 | 120.30 |
| 36 | A1 | 111 | C | C6-N1-C2 | 5.24 | 122.40 | 120.30 |
| 36 | A1 | 158 | G | C2-N3-C4 | -5.24 | 109.28 | 111.90 |
| 36 | A1 | 696 | C | C4-C5-C6 | -5.24 | 114.78 | 117.40 |
| 80 | A6 | 232 | U | N3-C2-O2 | -5.24 | 118.53 | 122.20 |
| 80 | A6 | 870 | C | C5-C6-N1 | -5.24 | 118.38 | 121.00 |
| 36 | A5 | 218 | G | N1-C6-O6 | -5.24 | 116.75 | 119.90 |
| 36 | A5 | 719 | U | N3-C2-O2 | -5.24 | 118.53 | 122.20 |
| 36 | A5 | 1834 | U | C5-C6-N1 | -5.24 | 120.08 | 122.70 |
| 36 | A5 | 2403 | G | N3-C4-N9 | 5.24 | 129.14 | 126.00 |
| 36 | A5 | 2604 | U | N3-C4-C5 | -5.24 | 111.45 | 114.60 |
| 1 | A2 | 1148 | C | N3-C4-C5 | 5.24 | 124.00 | 121.90 |
| 36 | A1 | 1303 | A | N1-C2-N3 | -5.24 | 126.68 | 129.30 |
| 36 | A1 | 2888 | U | C6-N1-C2 | 5.24 | 124.14 | 121.00 |
| 36 | A1 | 3072 | C | N3-C2-O2 | -5.24 | 118.23 | 121.90 |
| 36 | A5 | 576 | C | C2-N3-C4 | -5.24 | 117.28 | 119.90 |
| 36 | A5 | 1116 | G | C5-C6-N1 | -5.24 | 108.88 | 111.50 |
| 36 | A5 | 1545 | A | C8-N9-C4 | 5.24 | 107.90 | 105.80 |
| 36 | A5 | 2852 | C | N1-C2-O2 | -5.24 | 115.76 | 118.90 |
| 37 | A7 | 100 | C | C2-N3-C4 | -5.24 | 117.28 | 119.90 |
| 36 | A1 | 53 | G | C2-N3-C4 | -5.24 | 109.28 | 111.90 |
| 36 | A1 | 1848 | G | N1-C2-N3 | 5.24 | 127.04 | 123.90 |
| 36 | A1 | 2602 | G | N7-C8-N9 | -5.24 | 110.48 | 113.10 |
| 1 | A2 | 1015 | U | N1-C2-O2 | 5.24 | 126.47 | 122.80 |
| 80 | A6 | 379 | U | N1-C2-O2 | -5.24 | 119.14 | 122.80 |
| 80 | A6 | 561 | G | C8-N9-C4 | -5.24 | 104.31 | 106.40 |
| 36 | A5 | 784 | A | C4-C5-N7 | 5.24 | 113.32 | 110.70 |
| 36 | A5 | 808 | A | C6-N1-C2 | 5.24 | 121.74 | 118.60 |
| 36 | A5 | 1325 | U | N1-C2-N3 | 5.24 | 118.04 | 114.90 |
| 36 | A5 | 2213 | A | C5-N7-C8 | 5.24 | 106.52 | 103.90 |
| 38 | A8 | 113 | U | C5-C4-O4 | -5.24 | 122.76 | 125.90 |
| 36 | A5 | 568 | G | N1-C6-O6 | -5.23 | 116.76 | 119.90 |
| 36 | A5 | 2344 | U | N1-C2-N3 | 5.23 | 118.04 | 114.90 |
| 36 | A5 | 3094 | A | C5-N7-C8 | 5.23 | 106.52 | 103.90 |
| 37 | A7 | 1 | G | C4-C5-N7 | 5.23 | 112.89 | 110.80 |
| 1 | A2 | 938 | G | N3-C2-N2 | 5.23 | 123.56 | 119.90 |
| 1 | A2 | 1258 | U | N1-C2-N3 | 5.23 | 118.04 | 114.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 1391 | C | C2-N3-C4 | -5.23 | 117.28 | 119.90 |
| 36 | A1 | 2184 | U | C6-N1-C1' | -5.23 | 113.87 | 121.20 |
| 36 | A1 | 2533 | G | N3-C4-C5 | -5.23 | 125.98 | 128.60 |
| 36 | A1 | 2606 | G | C8-N9-C1' | -5.23 | 120.20 | 127.00 |
| 80 | A6 | 794 | U | N3-C2-O2 | -5.23 | 118.54 | 122.20 |
| 36 | A5 | 1693 | C | N1-C2-O2 | -5.23 | 115.76 | 118.90 |
| 36 | A5 | 2118 | C | C5-C4-N4 | 5.23 | 123.86 | 120.20 |
| 36 | A5 | 2930 | A | N1-C2-N3 | -5.23 | 126.68 | 129.30 |
| 55 | DR | 42 | ARG | NE-CZ-NH2 | -5.23 | 117.68 | 120.30 |
| 36 | A1 | 643 | U | C5-C6-N1 | 5.23 | 125.32 | 122.70 |
| 36 | A1 | 2169 | G | N9-C4-C5 | 5.23 | 107.49 | 105.40 |
| 36 | A1 | 2776 | C | C5-C4-N4 | -5.23 | 116.54 | 120.20 |
| 80 | A6 | 484 | C | C5-C4-N4 | -5.23 | 116.54 | 120.20 |
| 80 | A6 | 1274 | C | C5-C4-N4 | 5.23 | 123.86 | 120.20 |
| 80 | A6 | 1638 | G | C4-C5-N7 | -5.23 | 108.71 | 110.80 |
| 36 | A5 | 432 | G | N3-C2-N2 | 5.23 | 123.56 | 119.90 |
| 36 | A5 | 804 | C | C2-N1-C1' | -5.23 | 113.05 | 118.80 |
| 36 | A5 | 1404 | G | N1-C2-N2 | -5.23 | 111.49 | 116.20 |
| 36 | A5 | 1603 | A | C4-C5-C6 | 5.23 | 119.61 | 117.00 |
| 36 | A5 | 1655 | G | C5-N7-C8 | -5.23 | 101.69 | 104.30 |
| 36 | A5 | 2897 | A | N7-C8-N9 | -5.23 | 111.19 | 113.80 |
| 48 | DJ | 10 | ARG | NE-CZ-NH2 | -5.23 | 117.69 | 120.30 |
| 54 | DQ | 178 | ARG | NE-CZ-NH2 | -5.23 | 117.69 | 120.30 |
| 1 | A2 | 440 | U | N1-C2-O2 | 5.23 | 126.46 | 122.80 |
| 1 | A2 | 1188 | G | C8-N9-C4 | 5.23 | 108.49 | 106.40 |
| 36 | A1 | 22 | G | C6-N1-C2 | -5.23 | 121.96 | 125.10 |
| 36 | A1 | 806 | A | N9-C4-C5 | -5.23 | 103.71 | 105.80 |
| 38 | A4 | 74 | U | N1-C2-N3 | 5.23 | 118.04 | 114.90 |
| 80 | A6 | 1605 | G | N1-C6-O6 | -5.23 | 116.76 | 119.90 |
| 36 | A5 | 227 | G | N1-C6-O6 | 5.23 | 123.04 | 119.90 |
| 1 | A2 | 647 | G | C8-N9-C4 | -5.23 | 104.31 | 106.40 |
| 1 | A2 | 971 | A | C2-N3-C4 | -5.23 | 107.99 | 110.60 |
| 1 | A2 | 1116 | A | N1-C6-N6 | 5.23 | 121.74 | 118.60 |
| 36 | A1 | 72 | C | C5-C6-N1 | -5.23 | 118.39 | 121.00 |
| 36 | A1 | 652 | G | N3-C4-C5 | -5.23 | 125.99 | 128.60 |
| 36 | A1 | 1578 | C | C6-N1-C2 | -5.23 | 118.21 | 120.30 |
| 36 | A1 | 2350 | C | N1-C2-N3 | 5.23 | 122.86 | 119.20 |
| 36 | A1 | 2887 | A | C4-C5-N7 | 5.23 | 113.31 | 110.70 |
| 80 | A6 | 1300 | A | N1-C6-N6 | -5.23 | 115.46 | 118.60 |
| 36 | A5 | 299 | G | C5-C6-N1 | 5.23 | 114.11 | 111.50 |
| 36 | A5 | 333 | G | C2-N3-C4 | -5.23 | 109.29 | 111.90 |
| 36 | A5 | 894 | G | C4-C5-N7 | 5.23 | 112.89 | 110.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 2772 | C | P-O3'-C3' | 5.23 | 125.97 | 119.70 |
| 1 | A2 | 139 | C | C4-C5-C6 | 5.23 | 120.01 | 117.40 |
| 36 | A1 | 363 | G | N1-C6-O6 | 5.23 | 123.04 | 119.90 |
| 36 | A1 | 1878 | G | N1-C6-O6 | 5.23 | 123.04 | 119.90 |
| 36 | A1 | 2725 | U | N3-C4-O4 | -5.23 | 115.74 | 119.40 |
| 80 | A6 | 1260 | U | N1-C2-O2 | 5.23 | 126.46 | 122.80 |
| 36 | A5 | 46 | U | N1-C2-N3 | -5.23 | 111.76 | 114.90 |
| 36 | A5 | 75 | G | C5-C6-N1 | 5.23 | 114.11 | 111.50 |
| 36 | A5 | 903 | U | N3-C4-C5 | 5.23 | 117.73 | 114.60 |
| 36 | A5 | 2245 | C | N1-C2-N3 | 5.23 | 122.86 | 119.20 |
| 64 | Da | 15 | VAL | N-CA-C | -5.23 | 96.89 | 111.00 |
| 36 | A1 | 378 | A | C4-C5-C6 | 5.22 | 119.61 | 117.00 |
| 36 | A1 | 1044 | U | N3-C4-C5 | 5.22 | 117.73 | 114.60 |
| 37 | A3 | 71 | G | N3-C2-N2 | 5.22 | 123.56 | 119.90 |
| 80 | A6 | 1681 | A | C5-N7-C8 | -5.22 | 101.29 | 103.90 |
| 80 | A6 | 1730 | A | C5-C6-N6 | -5.22 | 119.52 | 123.70 |
| 36 | A5 | 857 | G | N1-C2-N2 | -5.22 | 111.50 | 116.20 |
| 36 | A5 | 1828 | A | N7-C8-N9 | 5.22 | 116.41 | 113.80 |
| 36 | A5 | 2391 | G | C5-C6-O6 | 5.22 | 131.73 | 128.60 |
| 36 | A5 | 3247 | G | C4-C5-N7 | -5.22 | 108.71 | 110.80 |
| 38 | A8 | 121 | U | N3-C2-O2 | -5.22 | 118.54 | 122.20 |
| 1 | A2 | 308 | C | C6-N1-C2 | 5.22 | 122.39 | 120.30 |
| 1 | A2 | 1363 | U | N3-C2-O2 | -5.22 | 118.54 | 122.20 |
| 1 | A2 | 1462 | G | N3-C4-N9 | 5.22 | 129.13 | 126.00 |
| 1 | A2 | 1600 | A | C6-C5-N7 | -5.22 | 128.64 | 132.30 |
| 1 | A2 | 1600 | A | N1-C2-N3 | 5.22 | 131.91 | 129.30 |
| 36 | A1 | 28 | C | C5-C6-N1 | -5.22 | 118.39 | 121.00 |
| 64 | Ba | 55 | LYS | CD-CE-NZ | -5.22 | 99.69 | 111.70 |
| 36 | A5 | 1114 | U | C2-N3-C4 | -5.22 | 123.87 | 127.00 |
| 36 | A5 | 1733 | G | C6-C5-N7 | -5.22 | 127.27 | 130.40 |
| 36 | A5 | 2148 | U | N1-C2-N3 | 5.22 | 118.03 | 114.90 |
| 36 | A1 | 335 | G | N7-C8-N9 | 5.22 | 115.71 | 113.10 |
| 36 | A1 | 346 | C | N3-C2-O2 | -5.22 | 118.25 | 121.90 |
| 36 | A1 | 1313 | G | C6-N1-C2 | -5.22 | 121.97 | 125.10 |
| 80 | A6 | 539 | G | C2-N3-C4 | -5.22 | 109.29 | 111.90 |
| 14 | CM | 58 | LEU | CA-CB-CG | 5.22 | 127.31 | 115.30 |
| 1 | A2 | 137 | U | N3-C2-O2 | -5.22 | 118.55 | 122.20 |
| 1 | A2 | 987 | G | C8-N9-C4 | 5.22 | 108.49 | 106.40 |
| 1 | A2 | 1293 | U | N3-C2-O2 | -5.22 | 118.55 | 122.20 |
| 36 | A1 | 1337 | A | C8-N9-C4 | -5.22 | 103.71 | 105.80 |
| 36 | A1 | 2190 | U | N3-C4-C5 | 5.22 | 117.73 | 114.60 |
| 36 | A1 | 2238 | G | C5-C6-O6 | -5.22 | 125.47 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 2984 | C | N3-C2-O2 | -5.22 | 118.25 | 121.90 |
| 71 | Bh | 69 | LEU | CA-CB-CG | 5.22 | 127.30 | 115.30 |
| 80 | A6 | 791 | A | N7-C8-N9 | 5.22 | 116.41 | 113.80 |
| 80 | A6 | 1310 | U | N3-C4-O4 | -5.22 | 115.75 | 119.40 |
| 36 | A5 | 2139 | A | N1-C6-N6 | -5.22 | 115.47 | 118.60 |
| 36 | A5 | 2228 | A | N7-C8-N9 | 5.22 | 116.41 | 113.80 |
| 36 | A5 | 2379 | U | C5-C6-N1 | -5.22 | 120.09 | 122.70 |
| 36 | A5 | 3028 | G | N1-C2-N2 | -5.22 | 111.50 | 116.20 |
| 38 | A8 | 109 | A | C5-C6-N1 | 5.22 | 120.31 | 117.70 |
| 36 | A5 | 197 | G | C4-N9-C1' | 5.22 | 133.28 | 126.50 |
| 36 | A5 | 341 | G | C4-C5-N7 | 5.22 | 112.89 | 110.80 |
| 36 | A5 | 682 | U | C2-N3-C4 | -5.22 | 123.87 | 127.00 |
| 36 | A5 | 972 | A | C5-N7-C8 | 5.22 | 106.51 | 103.90 |
| 36 | A5 | 1167 | U | N3-C2-O2 | 5.22 | 125.85 | 122.20 |
| 1 | A2 | 1611 | A | C6-C5-N7 | -5.22 | 128.65 | 132.30 |
| 36 | A1 | 2953 | U | C5-C6-N1 | -5.22 | 120.09 | 122.70 |
| 36 | A1 | 3298 | C | N3-C2-O2 | 5.22 | 125.55 | 121.90 |
| 36 | A5 | 815 | G | N3-C4-C5 | -5.22 | 125.99 | 128.60 |
| 36 | A5 | 868 | C | C6-N1-C2 | 5.22 | 122.39 | 120.30 |
| 36 | A5 | 1149 | G | C4-C5-N7 | -5.22 | 108.71 | 110.80 |
| 36 | A5 | 1324 | U | N3-C2-O2 | -5.22 | 118.55 | 122.20 |
| 36 | A5 | 1604 | G | N3-C4-C5 | -5.22 | 125.99 | 128.60 |
| 36 | A5 | 2716 | U | C5-C4-O4 | 5.22 | 129.03 | 125.90 |
| 36 | A5 | 2841 | G | N3-C2-N2 | 5.22 | 123.55 | 119.90 |
| 37 | A7 | 41 | G | C4-C5-N7 | 5.22 | 112.89 | 110.80 |
| 36 | A1 | 1010 | G | C2-N3-C4 | 5.21 | 114.51 | 111.90 |
| 36 | A1 | 1310 | G | C4-C5-N7 | 5.21 | 112.89 | 110.80 |
| 36 | A1 | 2279 | A | N3-C4-N9 | 5.21 | 131.57 | 127.40 |
| 36 | A1 | 2965 | U | C5-C6-N1 | -5.21 | 120.09 | 122.70 |
| 80 | A6 | 300 | A | N7-C8-N9 | -5.21 | 111.19 | 113.80 |
| 36 | A5 | 1527 | C | N1-C2-O2 | 5.21 | 122.03 | 118.90 |
| 36 | A5 | 2375 | G | C5-N7-C8 | -5.21 | 101.69 | 104.30 |
| 36 | A5 | 2721 | A | C5-C6-N1 | 5.21 | 120.31 | 117.70 |
| 1 | A2 | 63 | G | C5-C6-O6 | 5.21 | 131.73 | 128.60 |
| 80 | A6 | 1108 | G | N1-C6-O6 | -5.21 | 116.77 | 119.90 |
| 80 | A6 | 1522 | U | C2-N1-C1' | -5.21 | 111.44 | 117.70 |
| 36 | A5 | 84 | U | N3-C4-O4 | 5.21 | 123.05 | 119.40 |
| 36 | A5 | 307 | A | N9-C4-C5 | 5.21 | 107.89 | 105.80 |
| 36 | A5 | 625 | G | N3-C4-N9 | -5.21 | 122.87 | 126.00 |
| 36 | A5 | 1153 | A | C5-C6-N6 | -5.21 | 119.53 | 123.70 |
| 36 | A5 | 3106 | A | C8-N9-C4 | -5.21 | 103.72 | 105.80 |
| 1 | A2 | 687 | G | N3-C4-N9 | -5.21 | 122.87 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 634 | C | C5-C6-N1 | -5.21 | 118.39 | 121.00 |
| 36 | A1 | 880 | G | C8-N9-C1' | 5.21 | 133.77 | 127.00 |
| 36 | A1 | 912 | G | C5-C6-O6 | -5.21 | 125.47 | 128.60 |
| 36 | A1 | 1075 | A | C8-N9-C4 | 5.21 | 107.89 | 105.80 |
| 36 | A1 | 1173 | U | N3-C4-O4 | -5.21 | 115.75 | 119.40 |
| 36 | A1 | 1640 | G | C4-C5-N7 | 5.21 | 112.88 | 110.80 |
| 36 | A1 | 2596 | U | C5-C4-O4 | -5.21 | 122.77 | 125.90 |
| 36 | A1 | 2794 | G | C8-N9-C1' | 5.21 | 133.78 | 127.00 |
| 36 | A1 | 3110 | C | C2-N1-C1' | 5.21 | 124.53 | 118.80 |
| 36 | A1 | 3318 | G | C4-C5-C6 | 5.21 | 121.93 | 118.80 |
| 80 | A6 | 611 | U | N1-C2-O2 | -5.21 | 119.15 | 122.80 |
| 36 | A5 | 410 | U | C5-C6-N1 | -5.21 | 120.09 | 122.70 |
| 36 | A5 | 817 | A | N9-C4-C5 | 5.21 | 107.89 | 105.80 |
| 36 | A5 | 2629 | U | C2-N3-C4 | -5.21 | 123.87 | 127.00 |
| 38 | A8 | 45 | C | C4-C5-C6 | 5.21 | 120.01 | 117.40 |
| 1 | A2 | 811 | A | N3-C4-C5 | -5.21 | 123.15 | 126.80 |
| 49 | BL | 36 | ARG | NE-CZ-NH1 | -5.21 | 117.69 | 120.30 |
| 36 | A5 | 329 | U | C6-N1-C2 | 5.21 | 124.13 | 121.00 |
| 37 | A7 | 88 | G | N1-C6-O6 | -5.21 | 116.77 | 119.90 |
| 1 | A2 | 7 | G | N9-C4-C5 | 5.21 | 107.48 | 105.40 |
| 36 | A1 | 1345 | G | N7-C8-N9 | 5.21 | 115.70 | 113.10 |
| 36 | A1 | 1780 | G | C8-N9-C1' | -5.21 | 120.23 | 127.00 |
| 80 | A6 | 628 | G | N1-C6-O6 | -5.21 | 116.78 | 119.90 |
| 80 | A6 | 1000 | C | C2-N3-C4 | -5.21 | 117.30 | 119.90 |
| 80 | A6 | 1123 | C | N3-C4-C5 | 5.21 | 123.98 | 121.90 |
| 80 | A6 | 1483 | A | N1-C6-N6 | 5.21 | 121.72 | 118.60 |
| 80 | A6 | 1665 | U | C5-C6-N1 | 5.21 | 125.31 | 122.70 |
| 36 | A5 | 1518 | U | C4-C5-C6 | -5.21 | 116.57 | 119.70 |
| 36 | A5 | 2934 | A | N1-C6-N6 | -5.21 | 115.47 | 118.60 |
| 36 | A5 | 3103 | A | C6-N1-C2 | -5.21 | 115.47 | 118.60 |
| 36 | A5 | 3381 | U | C5-C6-N1 | -5.21 | 120.09 | 122.70 |
| 1 | A2 | 1648 | A | C5-C6-N1 | 5.21 | 120.30 | 117.70 |
| 36 | A1 | 500 | C | N1-C2-N3 | 5.21 | 122.84 | 119.20 |
| 36 | A1 | 3042 | U | C5-C6-N1 | -5.21 | 120.10 | 122.70 |
| 36 | A5 | 689 | U | N3-C4-C5 | 5.21 | 117.72 | 114.60 |
| 36 | A5 | 1013 | G | C4-N9-C1' | 5.21 | 133.27 | 126.50 |
| 36 | A5 | 3098 | G | N3-C2-N2 | 5.21 | 123.55 | 119.90 |
| 36 | A5 | 3124 | G | C4-C5-N7 | -5.21 | 108.72 | 110.80 |
| 36 | A5 | 3315 | G | C4-C5-N7 | -5.21 | 108.72 | 110.80 |
| 38 | A8 | 99 | C | C5-C6-N1 | -5.21 | 118.40 | 121.00 |
| 1 | A2 | 1784 | C | N3-C4-C5 | 5.21 | 123.98 | 121.90 |
| 36 | A5 | 1704 | A | C8-N9-C4 | 5.21 | 107.88 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 2732 | G | C5-N7-C8 | 5.21 | 106.90 | 104.30 |
| 37 | A7 | 40 | C | C2-N3-C4 | -5.21 | 117.30 | 119.90 |
| 1 | A2 | 391 | A | C4-C5-C6 | -5.20 | 114.40 | 117.00 |
| 36 | A1 | 1817 | G | C4-N9-C1' | -5.20 | 119.74 | 126.50 |
| 36 | A1 | 3203 | U | N1-C2-O2 | 5.20 | 126.44 | 122.80 |
| 38 | A4 | 137 | C | C6-N1-C2 | 5.20 | 122.38 | 120.30 |
| 49 | BL | 27 | ASP | CB-CG-OD2 | 5.20 | 122.98 | 118.30 |
| 80 | A6 | 941 | A | C5-C6-N6 | 5.20 | 127.86 | 123.70 |
| 36 | A5 | 2386 | A | C4-C5-N7 | 5.20 | 113.30 | 110.70 |
| 36 | A1 | 1316 | C | N1-C2-N3 | 5.20 | 122.84 | 119.20 |
| 36 | A1 | 1419 | A | C5-N7-C8 | 5.20 | 106.50 | 103.90 |
| 36 | A5 | 1833 | G | C5-C6-O6 | 5.20 | 131.72 | 128.60 |
| 37 | A7 | 11 | A | C5-C6-N1 | -5.20 | 115.10 | 117.70 |
| 36 | A1 | 338 | A | N1-C6-N6 | 5.20 | 121.72 | 118.60 |
| 36 | A1 | 641 | C | C5-C6-N1 | -5.20 | 118.40 | 121.00 |
| 36 | A1 | 644 | G | N3-C4-N9 | -5.20 | 122.88 | 126.00 |
| 36 | A1 | 1549 | U | N3-C2-O2 | -5.20 | 118.56 | 122.20 |
| 80 | A6 | 1414 | U | C2-N3-C4 | -5.20 | 123.88 | 127.00 |
| 80 | A6 | 1609 | U | N1-C2-O2 | -5.20 | 119.16 | 122.80 |
| 36 | A5 | 735 | A | N7-C8-N9 | 5.20 | 116.40 | 113.80 |
| 36 | A5 | 861 | C | N3-C4-N4 | 5.20 | 121.64 | 118.00 |
| 36 | A5 | 1458 | U | C5-C4-O4 | -5.20 | 122.78 | 125.90 |
| 36 | A5 | 1876 | U | C6-N1-C2 | -5.20 | 117.88 | 121.00 |
| 36 | A5 | 3302 | U | C5-C6-N1 | -5.20 | 120.10 | 122.70 |
| 41 | DC | 98 | ARG | NE-CZ-NH2 | -5.20 | 117.70 | 120.30 |
| 1 | A2 | 149 | C | C6-N1-C2 | 5.20 | 122.38 | 120.30 |
| 1 | A2 | 1330 | G | C8-N9-C1' | 5.20 | 133.76 | 127.00 |
| 36 | A1 | 39 | A | N1-C6-N6 | 5.20 | 121.72 | 118.60 |
| 36 | A1 | 343 | U | C2-N3-C4 | -5.20 | 123.88 | 127.00 |
| 36 | A1 | 1082 | U | N3-C2-O2 | -5.20 | 118.56 | 122.20 |
| 36 | A1 | 1481 | A | C4-C5-C6 | 5.20 | 119.60 | 117.00 |
| 80 | A6 | 452 | A | C8-N9-C4 | 5.20 | 107.88 | 105.80 |
| 36 | A5 | 881 | C | C5-C6-N1 | 5.20 | 123.60 | 121.00 |
| 36 | A5 | 999 | G | C5-C6-N1 | 5.20 | 114.10 | 111.50 |
| 36 | A5 | 1183 | C | N3-C4-N4 | -5.20 | 114.36 | 118.00 |
| 36 | A5 | 2364 | G | C8-N9-C4 | -5.20 | 104.32 | 106.40 |
| 36 | A5 | 2416 | U | N1-C2-N3 | 5.20 | 118.02 | 114.90 |
| 36 | A5 | 3075 | G | C5-N7-C8 | 5.20 | 106.90 | 104.30 |
| 36 | A5 | 3101 | G | N3-C2-N2 | 5.20 | 123.54 | 119.90 |
| 36 | A5 | 3177 | G | C2-N3-C4 | -5.20 | 109.30 | 111.90 |
| 37 | A7 | 50 | U | C6-N1-C2 | -5.20 | 117.88 | 121.00 |
| 1 | A2 | 192 | U | C5-C6-N1 | 5.20 | 125.30 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A2 | 1000 | C | C6-N1-C2 | 5.20 | 122.38 | 120.30 |
| 36 | A1 | 28 | C | N1-C2-O2 | 5.20 | 122.02 | 118.90 |
| 36 | A1 | 809 | G | C5-C6-O6 | -5.20 | 125.48 | 128.60 |
| 36 | A1 | 864 | G | N3-C4-N9 | 5.20 | 129.12 | 126.00 |
| 80 | A6 | 108 | A | C6-N1-C2 | -5.20 | 115.48 | 118.60 |
| 36 | A5 | 376 | G | N3-C4-C5 | -5.20 | 126.00 | 128.60 |
| 36 | A5 | 559 | A | C8-N9-C4 | -5.20 | 103.72 | 105.80 |
| 36 | A5 | 595 | G | C5-C6-O6 | 5.20 | 131.72 | 128.60 |
| 36 | A5 | 2632 | G | C6-N1-C2 | 5.20 | 128.22 | 125.10 |
| 1 | A2 | 577 | G | C2-N3-C4 | -5.20 | 109.30 | 111.90 |
| 36 | A1 | 981 | U | C5-C6-N1 | 5.20 | 125.30 | 122.70 |
| 36 | A1 | 1362 | G | N9-C4-C5 | -5.20 | 103.32 | 105.40 |
| 36 | A1 | 1857 | C | N1-C2-N3 | 5.20 | 122.84 | 119.20 |
| 38 | A4 | 48 | A | C4-C5-C6 | 5.20 | 119.60 | 117.00 |
| 80 | A6 | 1190 | C | N3-C2-O2 | 5.20 | 125.54 | 121.90 |
| 36 | A5 | 421 | G | C5-C6-N1 | 5.20 | 114.10 | 111.50 |
| 36 | A5 | 424 | G | C5-C6-N1 | 5.20 | 114.10 | 111.50 |
| 36 | A5 | 635 | G | N3-C4-C5 | 5.20 | 131.20 | 128.60 |
| 36 | A5 | 2349 | U | N1-C2-O2 | 5.20 | 126.44 | 122.80 |
| 36 | A5 | 2406 | C | C4-C5-C6 | 5.20 | 120.00 | 117.40 |
| 36 | A5 | 2737 | C | N1-C2-O2 | -5.20 | 115.78 | 118.90 |
| 38 | A8 | 12 | A | C8-N9-C4 | -5.20 | 103.72 | 105.80 |
| 1 | A2 | 871 | G | N3-C4-N9 | 5.19 | 129.12 | 126.00 |
| 36 | A1 | 2197 | C | N1-C2-N3 | -5.19 | 115.56 | 119.20 |
| 80 | A6 | 628 | G | C5-C6-O6 | 5.19 | 131.72 | 128.60 |
| 80 | A6 | 1170 | G | C4-N9-C1' | 5.19 | 133.25 | 126.50 |
| 36 | A5 | 1402 | C | N1-C2-O2 | 5.19 | 122.02 | 118.90 |
| 36 | A5 | 2960 | C | C2-N3-C4 | -5.19 | 117.30 | 119.90 |
| 36 | A5 | 3373 | U | C2-N3-C4 | -5.19 | 123.88 | 127.00 |
| 1 | A2 | 361 | C | C5-C6-N1 | 5.19 | 123.60 | 121.00 |
| 1 | A2 | 460 | A | C4-C5-C6 | -5.19 | 114.40 | 117.00 |
| 1 | A2 | 555 | A | N9-C4-C5 | 5.19 | 107.88 | 105.80 |
| 1 | A2 | 605 | A | C8-N9-C4 | 5.19 | 107.88 | 105.80 |
| 36 | A1 | 3028 | G | N3-C4-N9 | 5.19 | 129.12 | 126.00 |
| 36 | A1 | 3180 | A | N7-C8-N9 | 5.19 | 116.40 | 113.80 |
| 80 | A6 | 1787 | C | N3-C4-C5 | -5.19 | 119.82 | 121.90 |
| 36 | A5 | 267 | G | N7-C8-N9 | -5.19 | 110.50 | 113.10 |
| 36 | A5 | 1597 | C | N3-C4-C5 | -5.19 | 119.82 | 121.90 |
| 36 | A5 | 2112 | U | N1-C2-N3 | 5.19 | 118.02 | 114.90 |
| 1 | A2 | 380 | U | C6-N1-C2 | -5.19 | 117.89 | 121.00 |
| 36 | A1 | 59 | G | N9-C4-C5 | -5.19 | 103.32 | 105.40 |
| 36 | A1 | 271 | C | N3-C2-O2 | -5.19 | 118.27 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 36 | A1 | 614 | C | C5-C6-N1 | -5.19 | 118.41 | 121.00 |
| 36 | A1 | 652 | G | C5-C6-N1 | 5.19 | 114.10 | 111.50 |
| 36 | A1 | 2937 | G | C4-C5-N7 | -5.19 | 108.72 | 110.80 |
| 36 | A1 | 3355 | U | C5-C6-N1 | 5.19 | 125.30 | 122.70 |
| 80 | A6 | 691 | C | C2-N1-C1' | 5.19 | 124.51 | 118.80 |
| 80 | A6 | 1185 | U | N3-C2-O2 | -5.19 | 118.57 | 122.20 |
| 36 | A5 | 367 | A | C2-N3-C4 | -5.19 | 108.00 | 110.60 |
| 36 | A5 | 418 | A | C4-C5-C6 | 5.19 | 119.59 | 117.00 |
| 36 | A5 | 943 | U | C5-C4-O4 | -5.19 | 122.79 | 125.90 |
| 36 | A5 | 2193 | U | N1-C2-N3 | 5.19 | 118.02 | 114.90 |
| 36 | A5 | 2804 | A | C2-N3-C4 | -5.19 | 108.00 | 110.60 |
| 36 | A5 | 3387 | U | N3-C2-O2 | -5.19 | 118.57 | 122.20 |
| 44 | DF | 232 | ARG | NE-CZ-NH1 | -5.19 | 117.70 | 120.30 |
| 36 | A1 | 616 | G | C6-N1-C2 | -5.19 | 121.99 | 125.10 |
| 36 | A1 | 1081 | U | C5-C4-O4 | -5.19 | 122.79 | 125.90 |
| 36 | A1 | 1482 | A | N3-C4-C5 | -5.19 | 123.17 | 126.80 |
| 36 | A5 | 1513 | G | N1-C6-O6 | -5.19 | 116.79 | 119.90 |
| 36 | A5 | 3333 | G | C4-C5-N7 | 5.19 | 112.88 | 110.80 |
| 1 | A2 | 1245 | G | N3-C4-C5 | 5.19 | 131.19 | 128.60 |
| 36 | A1 | 586 | C | N1-C2-O2 | -5.19 | 115.79 | 118.90 |
| 36 | A1 | 958 | C | C2-N3-C4 | -5.19 | 117.31 | 119.90 |
| 36 | A1 | 1000 | C | C4-C5-C6 | -5.19 | 114.81 | 117.40 |
| 36 | A1 | 1580 | A | C3'-C2'-C1' | 5.19 | 105.65 | 101.50 |
| 36 | A1 | 2377 | G | C5-C6-N1 | -5.19 | 108.91 | 111.50 |
| 36 | A1 | 2757 | U | N1-C2-O2 | -5.19 | 119.17 | 122.80 |
| 36 | A1 | 2868 | U | N3-C4-O4 | -5.19 | 115.77 | 119.40 |
| 37 | A3 | 96 | U | C6-N1-C2 | 5.19 | 124.11 | 121.00 |
| 38 | A4 | 36 | G | N9-C4-C5 | 5.19 | 107.47 | 105.40 |
| 80 | A6 | 95 | G | N7-C8-N9 | 5.19 | 115.69 | 113.10 |
| 80 | A6 | 113 | U | N3-C2-O2 | 5.19 | 125.83 | 122.20 |
| 80 | A6 | 610 | G | N3-C4-N9 | 5.19 | 129.11 | 126.00 |
| 80 | A6 | 613 | G | N9-C4-C5 | -5.19 | 103.33 | 105.40 |
| 36 | A5 | 83 | U | C6-N1-C1' | -5.19 | 113.94 | 121.20 |
| 36 | A5 | 582 | G | C4-C5-N7 | -5.19 | 108.72 | 110.80 |
| 36 | A5 | 872 | U | N3-C4-O4 | -5.19 | 115.77 | 119.40 |
| 36 | A5 | 1485 | G | N9-C4-C5 | 5.19 | 107.47 | 105.40 |
| 36 | A5 | 2899 | C | C2-N3-C4 | -5.19 | 117.31 | 119.90 |
| 37 | A7 | 51 | A | C2-N3-C4 | 5.19 | 113.19 | 110.60 |
| 36 | A1 | 187 | A | C8-N9-C4 | -5.19 | 103.73 | 105.80 |
| 80 | A6 | 317 | C | C5-C6-N1 | -5.19 | 118.41 | 121.00 |
| 36 | A5 | 340 | C | N3-C2-O2 | -5.19 | 118.27 | 121.90 |
| 36 | A5 | 2695 | A | C5-N7-C8 | -5.19 | 101.31 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-------|------|-----------|-------|-------------|----------|
| 1 | A2 | 445 | A | N1-C2-N3 | -5.18 | 126.71 | 129.30 |
| 36 | A1 | 1420 | C | C4-C5-C6 | 5.18 | 119.99 | 117.40 |
| 36 | A1 | 2307 | G | C5-N7-C8 | 5.18 | 106.89 | 104.30 |
| 36 | A1 | 2831 | G | N1-C6-O6 | 5.18 | 123.01 | 119.90 |
| 36 | A5 | 2303 | A | C5-C6-N1 | 5.18 | 120.29 | 117.70 |
| 36 | A5 | 2724 | U | N3-C2-O2 | -5.18 | 118.57 | 122.20 |
| 36 | A5 | 3107 | U | N1-C2-O2 | 5.18 | 126.43 | 122.80 |
| 52 | DO | 27[B] | VAL | CA-C-N | 5.18 | 128.61 | 117.20 |
| 63 | DZ | 121 | ARG | NE-CZ-NH1 | 5.18 | 122.89 | 120.30 |
| 1 | A2 | 139 | C | P-O3'-C3' | 5.18 | 125.92 | 119.70 |
| 1 | A2 | 337 | G | N3-C4-C5 | -5.18 | 126.01 | 128.60 |
| 1 | A2 | 704 | C | C5-C6-N1 | 5.18 | 123.59 | 121.00 |
| 36 | A1 | 90 | C | C5-C6-N1 | -5.18 | 118.41 | 121.00 |
| 37 | A3 | 3 | U | C2-N3-C4 | -5.18 | 123.89 | 127.00 |
| 80 | A6 | 997 | G | C5-C6-O6 | 5.18 | 131.71 | 128.60 |
| 80 | A6 | 1272 | U | C5-C4-O4 | 5.18 | 129.01 | 125.90 |
| 80 | A6 | 1396 | U | C5-C6-N1 | 5.18 | 125.29 | 122.70 |
| 80 | A6 | 1661 | U | C2-N3-C4 | -5.18 | 123.89 | 127.00 |
| 36 | A5 | 28 | C | C6-N1-C2 | 5.18 | 122.37 | 120.30 |
| 36 | A5 | 926 | A | C4-C5-C6 | -5.18 | 114.41 | 117.00 |
| 36 | A5 | 1120 | A | N1-C6-N6 | -5.18 | 115.49 | 118.60 |
| 36 | A5 | 1205 | A | C5-N7-C8 | -5.18 | 101.31 | 103.90 |
| 36 | A5 | 1242 | G | C8-N9-C1' | -5.18 | 120.26 | 127.00 |
| 36 | A5 | 1312 | C | C6-N1-C1' | 5.18 | 127.02 | 120.80 |
| 36 | A5 | 1805 | C | C6-N1-C2 | 5.18 | 122.37 | 120.30 |
| 36 | A5 | 2942 | C | C5-C4-N4 | -5.18 | 116.57 | 120.20 |
| 36 | A5 | 3048 | A | C5-C6-N1 | 5.18 | 120.29 | 117.70 |
| 38 | A8 | 32 | C | N3-C2-O2 | 5.18 | 125.53 | 121.90 |
| 52 | DO | 16[B] | LEU | O-C-N | -5.18 | 114.39 | 123.20 |
| 1 | A2 | 6 | G | N3-C4-N9 | 5.18 | 129.11 | 126.00 |
| 36 | A1 | 274 | G | C5-C6-O6 | 5.18 | 131.71 | 128.60 |
| 36 | A1 | 2727 | A | N1-C6-N6 | -5.18 | 115.49 | 118.60 |
| 80 | A6 | 777 | C | C6-N1-C2 | -5.18 | 118.23 | 120.30 |
| 36 | A1 | 500 | C | N3-C2-O2 | -5.18 | 118.27 | 121.90 |
| 36 | A1 | 929 | A | N9-C4-C5 | 5.18 | 107.87 | 105.80 |
| 36 | A1 | 999 | G | N3-C4-C5 | -5.18 | 126.01 | 128.60 |
| 36 | A1 | 1183 | C | C5-C6-N1 | -5.18 | 118.41 | 121.00 |
| 36 | A5 | 39 | A | N3-C4-C5 | -5.18 | 123.17 | 126.80 |
| 36 | A5 | 610 | G | C5-C6-N1 | 5.18 | 114.09 | 111.50 |
| 36 | A5 | 809 | G | C8-N9-C4 | 5.18 | 108.47 | 106.40 |
| 36 | A5 | 902 | G | N7-C8-N9 | -5.18 | 110.51 | 113.10 |
| 36 | A5 | 2833 | A | C6-C5-N7 | 5.18 | 135.93 | 132.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 37 | A7 | 90 | U | C2-N3-C4 | -5.18 | 123.89 | 127.00 |
| 38 | A8 | 34 | U | C2-N3-C4 | -5.18 | 123.89 | 127.00 |
| 38 | A8 | 109 | A | C5-N7-C8 | -5.18 | 101.31 | 103.90 |
| 68 | De | 33 | ARG | NE-CZ-NH2 | -5.18 | 117.71 | 120.30 |
| 36 | A1 | 874 | U | C6-N1-C2 | 5.18 | 124.11 | 121.00 |
| 36 | A1 | 2363 | A | C6-C5-N7 | 5.18 | 135.93 | 132.30 |
| 80 | A6 | 1305 | U | N1-C2-N3 | 5.18 | 118.01 | 114.90 |
| 41 | DC | 230 | VAL | CB-CA-C | -5.18 | 101.56 | 111.40 |
| 1 | A2 | 1171 | A | N1-C6-N6 | -5.18 | 115.49 | 118.60 |
| 1 | A2 | 1245 | G | C4-N9-C1' | -5.18 | 119.77 | 126.50 |
| 36 | A1 | 726 | G | C4-C5-N7 | 5.18 | 112.87 | 110.80 |
| 36 | A1 | 2222 | A | N1-C2-N3 | 5.18 | 131.89 | 129.30 |
| 36 | A1 | 2341 | A | C6-N1-C2 | -5.18 | 115.49 | 118.60 |
| 36 | A1 | 2733 | A | N7-C8-N9 | -5.18 | 111.21 | 113.80 |
| 36 | A1 | 2953 | U | N1-C2-O2 | -5.18 | 119.18 | 122.80 |
| 36 | A1 | 3176 | G | N3-C2-N2 | -5.18 | 116.28 | 119.90 |
| 80 | A6 | 90 | C | N3-C2-O2 | -5.18 | 118.28 | 121.90 |
| 80 | A6 | 109 | G | C5-N7-C8 | 5.18 | 106.89 | 104.30 |
| 80 | A6 | 110 | U | N3-C2-O2 | -5.18 | 118.58 | 122.20 |
| 80 | A6 | 209 | U | N1-C2-O2 | -5.18 | 119.18 | 122.80 |
| 80 | A6 | 1733 | C | C6-N1-C2 | -5.18 | 118.23 | 120.30 |
| 36 | A5 | 80 | G | C5-C6-O6 | 5.18 | 131.71 | 128.60 |
| 36 | A5 | 1377 | G | C8-N9-C4 | -5.18 | 104.33 | 106.40 |
| 36 | A5 | 2526 | C | C6-N1-C1' | -5.18 | 114.59 | 120.80 |
| 36 | A5 | 2884 | C | N3-C4-N4 | 5.18 | 121.62 | 118.00 |
| 1 | A2 | 1051 | G | C8-N9-C1' | -5.17 | 120.27 | 127.00 |
| 36 | A1 | 336 | A | C2-N3-C4 | 5.17 | 113.19 | 110.60 |
| 36 | A1 | 2686 | A | N1-C6-N6 | 5.17 | 121.70 | 118.60 |
| 36 | A1 | 2749 | G | C4-C5-N7 | 5.17 | 112.87 | 110.80 |
| 43 | BE | 26 | ARG | NE-CZ-NH2 | -5.17 | 117.71 | 120.30 |
| 80 | A6 | 583 | C | C6-N1-C2 | -5.17 | 118.23 | 120.30 |
| 80 | A6 | 1020 | A | C4-C5-C6 | 5.17 | 119.59 | 117.00 |
| 80 | A6 | 1654 | G | N3-C2-N2 | -5.17 | 116.28 | 119.90 |
| 36 | A5 | 114 | A | C5-C6-N1 | -5.17 | 115.11 | 117.70 |
| 36 | A5 | 928 | C | C2-N3-C4 | -5.17 | 117.31 | 119.90 |
| 36 | A5 | 2639 | G | C4-C5-C6 | 5.17 | 121.90 | 118.80 |
| 36 | A5 | 2693 | C | N3-C4-N4 | -5.17 | 114.38 | 118.00 |
| 36 | A5 | 2858 | U | C2-N1-C1' | 5.17 | 123.91 | 117.70 |
| 36 | A5 | 3173 | G | N3-C4-N9 | 5.17 | 129.10 | 126.00 |
| 36 | A1 | 1107 | C | C5-C4-N4 | -5.17 | 116.58 | 120.20 |
| 36 | A1 | 2573 | G | C8-N9-C4 | -5.17 | 104.33 | 106.40 |
| 36 | A1 | 3140 | G | C4-N9-C1' | 5.17 | 133.22 | 126.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 36 | A1 | 3306 | U | C4-C5-C6 | 5.17 | 122.80 | 119.70 |
| 36 | A5 | 2135 | U | N3-C4-C5 | 5.17 | 117.70 | 114.60 |
| 36 | A5 | 2584 | G | N7-C8-N9 | 5.17 | 115.69 | 113.10 |
| 36 | A1 | 282 | G | P-O3'-C3' | 5.17 | 125.91 | 119.70 |
| 36 | A1 | 1335 | C | C6-N1-C2 | 5.17 | 122.37 | 120.30 |
| 80 | A6 | 464 | A | C2-N3-C4 | -5.17 | 108.02 | 110.60 |
| 80 | A6 | 1428 | G | N7-C8-N9 | 5.17 | 115.69 | 113.10 |
| 36 | A5 | 102 | C | C4-C5-C6 | 5.17 | 119.99 | 117.40 |
| 36 | A5 | 434 | U | N1-C2-O2 | 5.17 | 126.42 | 122.80 |
| 36 | A5 | 852 | U | N3-C2-O2 | -5.17 | 118.58 | 122.20 |
| 36 | A5 | 968 | G | C6-N1-C2 | 5.17 | 128.20 | 125.10 |
| 36 | A5 | 1004 | U | N1-C2-N3 | -5.17 | 111.80 | 114.90 |
| 36 | A5 | 1633 | C | N3-C4-C5 | -5.17 | 119.83 | 121.90 |
| 36 | A5 | 3107 | U | N3-C4-O4 | -5.17 | 115.78 | 119.40 |
| 1 | A2 | 240 | U | N1-C2-O2 | 5.17 | 126.42 | 122.80 |
| 36 | A1 | 1940 | G | N1-C6-O6 | -5.17 | 116.80 | 119.90 |
| 36 | A1 | 2740 | A | N1-C6-N6 | -5.17 | 115.50 | 118.60 |
| 36 | A5 | 2169 | G | N9-C4-C5 | 5.17 | 107.47 | 105.40 |
| 36 | A5 | 2550 | U | N3-C2-O2 | -5.17 | 118.58 | 122.20 |
| 36 | A5 | 2686 | A | N1-C6-N6 | 5.17 | 121.70 | 118.60 |
| 36 | A5 | 2716 | U | N1-C2-N3 | 5.17 | 118.00 | 114.90 |
| 83 | Dq | 70 | LEU | CA-CB-CG | 5.17 | 127.19 | 115.30 |
| 1 | A2 | 49 | C | C6-N1-C2 | -5.17 | 118.23 | 120.30 |
| 1 | A2 | 783 | G | C8-N9-C1' | -5.17 | 120.28 | 127.00 |
| 1 | A2 | 1258 | U | C5-C6-N1 | -5.17 | 120.12 | 122.70 |
| 1 | A2 | 1448 | G | N1-C6-O6 | -5.17 | 116.80 | 119.90 |
| 1 | A2 | 1796 | C | C5-C4-N4 | 5.17 | 123.82 | 120.20 |
| 36 | A1 | 1507 | G | N3-C4-N9 | 5.17 | 129.10 | 126.00 |
| 36 | A1 | 2377 | G | C6-N1-C2 | 5.17 | 128.20 | 125.10 |
| 80 | A6 | 489 | C | C2-N1-C1' | 5.17 | 124.48 | 118.80 |
| 3 | CB | 106 | THR | N-CA-CB | 5.17 | 120.12 | 110.30 |
| 36 | A5 | 149 | U | N3-C2-O2 | -5.17 | 118.58 | 122.20 |
| 36 | A5 | 580 | C | N1-C2-N3 | 5.17 | 122.82 | 119.20 |
| 36 | A5 | 1466 | G | N1-C6-O6 | -5.17 | 116.80 | 119.90 |
| 36 | A5 | 1845 | G | C8-N9-C4 | 5.17 | 108.47 | 106.40 |
| 36 | A5 | 2366 | C | C2-N3-C4 | 5.17 | 122.48 | 119.90 |
| 36 | A5 | 3309 | G | C8-N9-C4 | -5.17 | 104.33 | 106.40 |
| 37 | A7 | 41 | G | C5-C6-N1 | 5.17 | 114.08 | 111.50 |
| 52 | DO | 104[B] | ILE | CA-C-N | -5.17 | 105.83 | 117.20 |
| 64 | Da | 14 | HIS | N-CA-C | -5.17 | 97.05 | 111.00 |
| 1 | A2 | 815 | G | C8-N9-C1' | 5.17 | 133.72 | 127.00 |
| 1 | A2 | 1503 | A | C5-C6-N1 | -5.17 | 115.12 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 654 | C | C5-C6-N1 | -5.17 | 118.42 | 121.00 |
| 36 | A1 | 949 | C | C4-C5-C6 | 5.17 | 119.98 | 117.40 |
| 36 | A1 | 1154 | A | C4-C5-C6 | 5.17 | 119.58 | 117.00 |
| 36 | A1 | 1903 | U | N3-C4-O4 | -5.17 | 115.78 | 119.40 |
| 37 | A3 | 22 | A | C5-C6-N6 | -5.17 | 119.57 | 123.70 |
| 80 | A6 | 934 | C | C2-N1-C1' | 5.17 | 124.48 | 118.80 |
| 80 | A6 | 1560 | U | N1-C2-O2 | 5.17 | 126.42 | 122.80 |
| 36 | A5 | 1695 | U | N3-C2-O2 | -5.17 | 118.58 | 122.20 |
| 36 | A5 | 1872 | C | N1-C2-N3 | 5.17 | 122.82 | 119.20 |
| 36 | A5 | 2340 | U | N3-C2-O2 | -5.17 | 118.58 | 122.20 |
| 38 | A8 | 14 | C | N1-C2-O2 | -5.17 | 115.80 | 118.90 |
| 1 | A2 | 1093 | A | C8-N9-C4 | 5.17 | 107.87 | 105.80 |
| 1 | A2 | 1454 | G | C5-N7-C8 | 5.17 | 106.88 | 104.30 |
| 36 | A1 | 187 | A | C4-C5-C6 | 5.17 | 119.58 | 117.00 |
| 36 | A1 | 679 | U | C5-C4-O4 | 5.17 | 129.00 | 125.90 |
| 80 | A6 | 984 | G | C8-N9-C4 | 5.17 | 108.47 | 106.40 |
| 36 | A5 | 340 | C | C4-C5-C6 | 5.17 | 119.98 | 117.40 |
| 36 | A5 | 3018 | C | C6-N1-C2 | -5.17 | 118.23 | 120.30 |
| 36 | A1 | 829 | U | N1-C2-N3 | 5.16 | 118.00 | 114.90 |
| 36 | A1 | 1006 | A | C8-N9-C4 | -5.16 | 103.73 | 105.80 |
| 36 | A1 | 1051 | U | N3-C4-O4 | -5.16 | 115.78 | 119.40 |
| 36 | A1 | 1131 | G | C6-C5-N7 | -5.16 | 127.30 | 130.40 |
| 36 | A1 | 1857 | C | C4-C5-C6 | 5.16 | 119.98 | 117.40 |
| 36 | A1 | 2551 | U | N1-C2-N3 | 5.16 | 118.00 | 114.90 |
| 80 | A6 | 1258 | U | N1-C2-O2 | 5.16 | 126.41 | 122.80 |
| 80 | A6 | 1457 | C | C5-C6-N1 | -5.16 | 118.42 | 121.00 |
| 36 | A5 | 110 | G | C5-C6-N1 | 5.16 | 114.08 | 111.50 |
| 36 | A5 | 234 | G | C5-C6-O6 | -5.16 | 125.50 | 128.60 |
| 36 | A5 | 1205 | A | C2-N3-C4 | 5.16 | 113.18 | 110.60 |
| 36 | A5 | 1658 | G | C5-C6-O6 | 5.16 | 131.70 | 128.60 |
| 36 | A5 | 2560 | C | N1-C2-O2 | 5.16 | 122.00 | 118.90 |
| 36 | A5 | 2635 | A | C8-N9-C4 | -5.16 | 103.73 | 105.80 |
| 36 | A5 | 3100 | U | N3-C2-O2 | -5.16 | 118.58 | 122.20 |
| 36 | A5 | 3215 | A | N9-C4-C5 | -5.16 | 103.73 | 105.80 |
| 1 | A2 | 1781 | A | C4-C5-N7 | -5.16 | 108.12 | 110.70 |
| 36 | A1 | 1408 | G | N1-C6-O6 | -5.16 | 116.80 | 119.90 |
| 36 | A1 | 2828 | G | N1-C2-N3 | -5.16 | 120.80 | 123.90 |
| 80 | A6 | 1543 | A | N1-C6-N6 | 5.16 | 121.70 | 118.60 |
| 36 | A5 | 2565 | U | C6-N1-C2 | -5.16 | 117.90 | 121.00 |
| 36 | A5 | 2731 | U | N1-C2-N3 | 5.16 | 118.00 | 114.90 |
| 36 | A5 | 2881 | C | N1-C2-N3 | 5.16 | 122.81 | 119.20 |
| 1 | A2 | 68 | A | N7-C8-N9 | 5.16 | 116.38 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 36 | A1 | 342 | A | C2-N3-C4 | -5.16 | 108.02 | 110.60 |
| 36 | A1 | 673 | U | N3-C4-C5 | 5.16 | 117.70 | 114.60 |
| 36 | A1 | 1143 | A | N7-C8-N9 | 5.16 | 116.38 | 113.80 |
| 36 | A1 | 1803 | C | N3-C4-N4 | 5.16 | 121.61 | 118.00 |
| 36 | A1 | 3042 | U | N3-C4-O4 | -5.16 | 115.79 | 119.40 |
| 36 | A1 | 3378 | C | C6-N1-C2 | 5.16 | 122.36 | 120.30 |
| 80 | A6 | 54 | C | C2-N3-C4 | -5.16 | 117.32 | 119.90 |
| 80 | A6 | 139 | C | C5-C4-N4 | 5.16 | 123.81 | 120.20 |
| 80 | A6 | 419 | G | C5-C6-O6 | 5.16 | 131.70 | 128.60 |
| 36 | A5 | 3202 | G | C5-C6-O6 | 5.16 | 131.70 | 128.60 |
| 51 | DN | 172 | ARG | NE-CZ-NH1 | -5.16 | 117.72 | 120.30 |
| 1 | A2 | 139 | C | N1-C2-N3 | 5.16 | 122.81 | 119.20 |
| 1 | A2 | 749 | U | C5-C6-N1 | 5.16 | 125.28 | 122.70 |
| 1 | A2 | 782 | U | P-O3'-C3' | 5.16 | 125.89 | 119.70 |
| 1 | A2 | 1189 | A | N7-C8-N9 | -5.16 | 111.22 | 113.80 |
| 1 | A2 | 1672 | G | N3-C4-C5 | -5.16 | 126.02 | 128.60 |
| 36 | A1 | 2522 | G | C8-N9-C1' | -5.16 | 120.29 | 127.00 |
| 36 | A1 | 3302 | U | N1-C2-N3 | -5.16 | 111.81 | 114.90 |
| 36 | A5 | 323 | A | N1-C2-N3 | 5.16 | 131.88 | 129.30 |
| 36 | A5 | 911 | C | C5-C4-N4 | -5.16 | 116.59 | 120.20 |
| 36 | A5 | 2142 | A | C5-C6-N6 | -5.16 | 119.57 | 123.70 |
| 36 | A5 | 2848 | G | C4-N9-C1' | 5.16 | 133.21 | 126.50 |
| 36 | A5 | 3386 | G | N1-C2-N3 | 5.16 | 127.00 | 123.90 |
| 37 | A7 | 77 | G | C6-C5-N7 | -5.16 | 127.31 | 130.40 |
| 38 | A8 | 8 | C | N1-C2-N3 | 5.16 | 122.81 | 119.20 |
| 38 | A8 | 24 | G | C5-C6-O6 | 5.16 | 131.69 | 128.60 |
| 1 | A2 | 140 | A | C4-N9-C1' | 5.16 | 135.58 | 126.30 |
| 36 | A1 | 1848 | G | C4-C5-N7 | 5.16 | 112.86 | 110.80 |
| 80 | A6 | 308 | C | C6-N1-C2 | 5.16 | 122.36 | 120.30 |
| 80 | A6 | 406 | U | C6-N1-C2 | 5.16 | 124.09 | 121.00 |
| 80 | A6 | 416 | A | N7-C8-N9 | 5.16 | 116.38 | 113.80 |
| 80 | A6 | 677 | G | C8-N9-C4 | 5.16 | 108.46 | 106.40 |
| 80 | A6 | 1186 | U | C2-N3-C4 | -5.16 | 123.91 | 127.00 |
| 80 | A6 | 1796 | C | C4-C5-C6 | 5.16 | 119.98 | 117.40 |
| 37 | A7 | 1 | G | N7-C8-N9 | 5.16 | 115.68 | 113.10 |
| 37 | A7 | 79 | A | C8-N9-C4 | -5.16 | 103.74 | 105.80 |
| 36 | A1 | 596 | C | C4-C5-C6 | 5.16 | 119.98 | 117.40 |
| 36 | A1 | 659 | G | N1-C6-O6 | -5.16 | 116.81 | 119.90 |
| 76 | Bm | 106 | ARG | NE-CZ-NH2 | -5.16 | 117.72 | 120.30 |
| 36 | A5 | 1476 | G | N7-C8-N9 | -5.16 | 110.52 | 113.10 |
| 36 | A5 | 1607 | U | N3-C4-O4 | -5.16 | 115.79 | 119.40 |
| 36 | A5 | 2272 | G | O4'-C1'-N9 | 5.16 | 112.32 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 2855 | U | N3-C4-C5 | 5.16 | 117.69 | 114.60 |
| 36 | A5 | 3321 | C | C6-N1-C2 | 5.16 | 122.36 | 120.30 |
| 37 | A7 | 120 | C | C5-C6-N1 | -5.16 | 118.42 | 121.00 |
| 36 | A1 | 359 | U | N3-C2-O2 | -5.15 | 118.59 | 122.20 |
| 36 | A5 | 985 | U | C6-N1-C2 | 5.15 | 124.09 | 121.00 |
| 36 | A5 | 996 | A | N7-C8-N9 | -5.15 | 111.22 | 113.80 |
| 36 | A5 | 1087 | G | N1-C6-O6 | 5.15 | 122.99 | 119.90 |
| 36 | A5 | 1543 | G | N1-C6-O6 | -5.15 | 116.81 | 119.90 |
| 1 | A2 | 1033 | C | N3-C2-O2 | -5.15 | 118.29 | 121.90 |
| 1 | A2 | 1542 | G | N9-C4-C5 | 5.15 | 107.46 | 105.40 |
| 1 | A2 | 1736 | G | C8-N9-C4 | 5.15 | 108.46 | 106.40 |
| 36 | A1 | 398 | A | N1-C2-N3 | -5.15 | 126.72 | 129.30 |
| 36 | A1 | 821 | U | N3-C4-C5 | 5.15 | 117.69 | 114.60 |
| 36 | A1 | 1416 | C | N3-C4-C5 | 5.15 | 123.96 | 121.90 |
| 36 | A1 | 1845 | G | C5-C6-N1 | 5.15 | 114.08 | 111.50 |
| 36 | A1 | 2240 | G | C5-C6-O6 | -5.15 | 125.51 | 128.60 |
| 80 | A6 | 800 | U | N3-C2-O2 | -5.15 | 118.59 | 122.20 |
| 80 | A6 | 1415 | U | N3-C2-O2 | -5.15 | 118.59 | 122.20 |
| 36 | A5 | 1445 | U | C6-N1-C2 | 5.15 | 124.09 | 121.00 |
| 36 | A5 | 1832 | C | C5-C6-N1 | -5.15 | 118.42 | 121.00 |
| 36 | A5 | 2396 | G | C4-C5-N7 | -5.15 | 108.74 | 110.80 |
| 1 | A2 | 494 | U | C2-N1-C1' | 5.15 | 123.88 | 117.70 |
| 36 | A1 | 112 | U | C6-N1-C2 | -5.15 | 117.91 | 121.00 |
| 36 | A1 | 196 | G | C5-C6-O6 | -5.15 | 125.51 | 128.60 |
| 36 | A1 | 2892 | A | C5-C6-N6 | 5.15 | 127.82 | 123.70 |
| 38 | A4 | 6 | U | C5-C6-N1 | -5.15 | 120.12 | 122.70 |
| 36 | A5 | 2706 | G | N1-C6-O6 | -5.15 | 116.81 | 119.90 |
| 38 | A8 | 23 | U | N3-C2-O2 | -5.15 | 118.59 | 122.20 |
| 1 | A2 | 853 | G | C4-C5-N7 | 5.15 | 112.86 | 110.80 |
| 80 | A6 | 49 | C | C2-N3-C4 | -5.15 | 117.33 | 119.90 |
| 80 | A6 | 637 | C | C5-C4-N4 | -5.15 | 116.60 | 120.20 |
| 36 | A5 | 934 | G | C8-N9-C1' | -5.15 | 120.31 | 127.00 |
| 36 | A5 | 2351 | U | N1-C2-O2 | 5.15 | 126.40 | 122.80 |
| 36 | A5 | 2549 | G | C8-N9-C1' | -5.15 | 120.31 | 127.00 |
| 1 | A2 | 1270 | G | N1-C6-O6 | -5.15 | 116.81 | 119.90 |
| 36 | A1 | 249 | U | C6-N1-C2 | -5.15 | 117.91 | 121.00 |
| 36 | A1 | 592 | A | N1-C6-N6 | 5.15 | 121.69 | 118.60 |
| 36 | A1 | 774 | G | N1-C6-O6 | -5.15 | 116.81 | 119.90 |
| 36 | A1 | 2647 | A | N1-C6-N6 | -5.15 | 115.51 | 118.60 |
| 36 | A1 | 2754 | G | N1-C2-N3 | 5.15 | 126.99 | 123.90 |
| 36 | A1 | 2838 | A | C2-N3-C4 | -5.15 | 108.03 | 110.60 |
| 36 | A5 | 216 | G | N9-C4-C5 | -5.15 | 103.34 | 105.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 2634 | U | N3-C4-O4 | 5.15 | 123.00 | 119.40 |
| 38 | A8 | 95 | G | N3-C4-C5 | 5.15 | 131.17 | 128.60 |
| 1 | A2 | 766 | U | N1-C2-O2 | 5.15 | 126.40 | 122.80 |
| 36 | A1 | 223 | U | C2-N3-C4 | -5.15 | 123.91 | 127.00 |
| 80 | A6 | 45 | U | N3-C4-C5 | 5.15 | 117.69 | 114.60 |
| 80 | A6 | 1020 | A | N1-C2-N3 | 5.15 | 131.87 | 129.30 |
| 36 | A5 | 420 | G | C6-C5-N7 | -5.15 | 127.31 | 130.40 |
| 36 | A5 | 523 | A | N1-C6-N6 | -5.15 | 115.51 | 118.60 |
| 36 | A5 | 1851 | G | C4-N9-C1' | 5.15 | 133.19 | 126.50 |
| 1 | A2 | 944 | A | C2-N3-C4 | -5.14 | 108.03 | 110.60 |
| 1 | A2 | 992 | A | N7-C8-N9 | 5.14 | 116.37 | 113.80 |
| 36 | A1 | 23 | A | N3-C4-N9 | 5.14 | 131.51 | 127.40 |
| 36 | A1 | 74 | G | N3-C2-N2 | -5.14 | 116.30 | 119.90 |
| 36 | A1 | 557 | A | C8-N9-C4 | 5.14 | 107.86 | 105.80 |
| 36 | A1 | 793 | C | N3-C4-N4 | 5.14 | 121.60 | 118.00 |
| 36 | A1 | 2407 | C | C4-C5-C6 | 5.14 | 119.97 | 117.40 |
| 80 | A6 | 1428 | G | N1-C6-O6 | -5.14 | 116.81 | 119.90 |
| 80 | A6 | 1722 | A | N1-C6-N6 | -5.14 | 115.51 | 118.60 |
| 36 | A5 | 66 | A | N7-C8-N9 | -5.14 | 111.23 | 113.80 |
| 36 | A5 | 1942 | U | C4-C5-C6 | 5.14 | 122.79 | 119.70 |
| 36 | A5 | 2280 | A | C5-N7-C8 | -5.14 | 101.33 | 103.90 |
| 37 | A7 | 13 | A | C8-N9-C4 | -5.14 | 103.74 | 105.80 |
| 1 | A2 | 432 | G | C5-C6-N1 | 5.14 | 114.07 | 111.50 |
| 36 | A1 | 126 | U | C5-C6-N1 | -5.14 | 120.13 | 122.70 |
| 36 | A1 | 508 | U | C2-N3-C4 | -5.14 | 123.92 | 127.00 |
| 36 | A1 | 1305 | U | N3-C4-C5 | 5.14 | 117.69 | 114.60 |
| 36 | A1 | 2326 | A | C5-N7-C8 | -5.14 | 101.33 | 103.90 |
| 36 | A1 | 2638 | C | N3-C4-C5 | 5.14 | 123.96 | 121.90 |
| 36 | A1 | 3188 | G | C2-N3-C4 | 5.14 | 114.47 | 111.90 |
| 80 | A6 | 431 | C | N3-C2-O2 | -5.14 | 118.30 | 121.90 |
| 80 | A6 | 691 | C | N3-C2-O2 | -5.14 | 118.30 | 121.90 |
| 36 | A5 | 112 | U | N3-C4-O4 | 5.14 | 123.00 | 119.40 |
| 36 | A5 | 863 | C | C5-C4-N4 | 5.14 | 123.80 | 120.20 |
| 38 | A8 | 51 | G | N3-C2-N2 | -5.14 | 116.30 | 119.90 |
| 1 | A2 | 712 | G | N7-C8-N9 | 5.14 | 115.67 | 113.10 |
| 36 | A1 | 1548 | C | N3-C4-C5 | -5.14 | 119.84 | 121.90 |
| 37 | A3 | 4 | U | C5-C4-O4 | -5.14 | 122.81 | 125.90 |
| 80 | A6 | 1033 | C | N1-C2-O2 | -5.14 | 115.82 | 118.90 |
| 36 | A5 | 1013 | G | N3-C4-C5 | -5.14 | 126.03 | 128.60 |
| 1 | A2 | 7 | G | C5-C6-O6 | 5.14 | 131.68 | 128.60 |
| 36 | A1 | 917 | A | N9-C4-C5 | 5.14 | 107.86 | 105.80 |
| 36 | A1 | 1770 | G | C8-N9-C4 | -5.14 | 104.34 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 2176 | U | N3-C4-O4 | -5.14 | 115.80 | 119.40 |
| 73 | Bj | 21 | ARG | NE-CZ-NH1 | 5.14 | 122.87 | 120.30 |
| 80 | A6 | 138 | A | N1-C6-N6 | -5.14 | 115.52 | 118.60 |
| 80 | A6 | 308 | C | N3-C4-C5 | 5.14 | 123.96 | 121.90 |
| 80 | A6 | 871 | G | N3-C4-C5 | -5.14 | 126.03 | 128.60 |
| 80 | A6 | 1127 | G | N1-C2-N3 | 5.14 | 126.98 | 123.90 |
| 80 | A6 | 1735 | U | N3-C4-O4 | -5.14 | 115.80 | 119.40 |
| 36 | A5 | 341 | G | N3-C2-N2 | -5.14 | 116.30 | 119.90 |
| 36 | A5 | 1482 | A | C8-N9-C4 | -5.14 | 103.74 | 105.80 |
| 36 | A5 | 2831 | G | C2-N3-C4 | 5.14 | 114.47 | 111.90 |
| 36 | A5 | 2877 | G | C5-C6-O6 | 5.14 | 131.68 | 128.60 |
| 36 | A5 | 3318 | G | C5-C6-O6 | 5.14 | 131.68 | 128.60 |
| 36 | A1 | 365 | A | C6-C5-N7 | -5.14 | 128.70 | 132.30 |
| 36 | A1 | 580 | C | N3-C2-O2 | -5.14 | 118.30 | 121.90 |
| 36 | A1 | 974 | G | N3-C4-N9 | 5.14 | 129.08 | 126.00 |
| 36 | A1 | 2152 | A | C4-C5-N7 | -5.14 | 108.13 | 110.70 |
| 80 | A6 | 16 | G | C8-N9-C4 | 5.14 | 108.45 | 106.40 |
| 36 | A5 | 2122 | G | N7-C8-N9 | -5.14 | 110.53 | 113.10 |
| 1 | A2 | 266 | A | C2-N3-C4 | -5.14 | 108.03 | 110.60 |
| 1 | A2 | 1751 | C | C2-N3-C4 | -5.14 | 117.33 | 119.90 |
| 36 | A1 | 1400 | G | C8-N9-C1' | -5.14 | 120.32 | 127.00 |
| 36 | A1 | 2634 | U | C4-C5-C6 | 5.14 | 122.78 | 119.70 |
| 36 | A1 | 3318 | G | N7-C8-N9 | 5.14 | 115.67 | 113.10 |
| 37 | A3 | 7 | G | N3-C4-C5 | -5.14 | 126.03 | 128.60 |
| 47 | BI | 7 | ARG | NE-CZ-NH1 | -5.14 | 117.73 | 120.30 |
| 36 | A5 | 2145 | A | N3-C4-C5 | -5.14 | 123.20 | 126.80 |
| 36 | A5 | 2246 | G | C6-C5-N7 | 5.14 | 133.48 | 130.40 |
| 37 | A7 | 75 | G | N3-C2-N2 | -5.14 | 116.31 | 119.90 |
| 1 | A2 | 557 | G | C5-C6-N1 | -5.13 | 108.93 | 111.50 |
| 36 | A1 | 625 | G | N1-C6-O6 | -5.13 | 116.82 | 119.90 |
| 36 | A1 | 778 | U | N3-C2-O2 | -5.13 | 118.61 | 122.20 |
| 36 | A1 | 1891 | A | C4-N9-C1' | -5.13 | 117.06 | 126.30 |
| 36 | A1 | 2371 | G | C6-C5-N7 | -5.13 | 127.32 | 130.40 |
| 36 | A1 | 2776 | C | C5-C6-N1 | -5.13 | 118.43 | 121.00 |
| 36 | A1 | 2866 | U | C6-N1-C2 | -5.13 | 117.92 | 121.00 |
| 36 | A1 | 2905 | U | N3-C2-O2 | 5.13 | 125.80 | 122.20 |
| 41 | BC | 82 | THR | C-N-CA | -5.13 | 111.52 | 122.30 |
| 80 | A6 | 1111 | G | N9-C4-C5 | -5.13 | 103.35 | 105.40 |
| 80 | A6 | 1503 | A | C8-N9-C4 | -5.13 | 103.75 | 105.80 |
| 80 | A6 | 1652 | C | N3-C2-O2 | -5.13 | 118.31 | 121.90 |
| 36 | A5 | 1138 | U | N3-C4-O4 | -5.13 | 115.81 | 119.40 |
| 36 | A5 | 1813 | A | C8-N9-C4 | -5.13 | 103.75 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 3173 | G | C6-N1-C2 | -5.13 | 122.02 | 125.10 |
| 36 | A1 | 588 | G | C6-N1-C2 | -5.13 | 122.02 | 125.10 |
| 36 | A1 | 994 | G | C5-N7-C8 | 5.13 | 106.87 | 104.30 |
| 36 | A1 | 2279 | A | C6-C5-N7 | -5.13 | 128.71 | 132.30 |
| 36 | A1 | 2959 | C | C6-N1-C2 | -5.13 | 118.25 | 120.30 |
| 36 | A1 | 3256 | G | C4-C5-C6 | -5.13 | 115.72 | 118.80 |
| 80 | A6 | 1682 | U | C5-C6-N1 | 5.13 | 125.27 | 122.70 |
| 36 | A5 | 943 | U | C6-N1-C2 | 5.13 | 124.08 | 121.00 |
| 36 | A5 | 1938 | U | N3-C4-C5 | 5.13 | 117.68 | 114.60 |
| 1 | A2 | 142 | G | C5-C6-N1 | -5.13 | 108.93 | 111.50 |
| 1 | A2 | 572 | C | N3-C2-O2 | -5.13 | 118.31 | 121.90 |
| 36 | A1 | 819 | U | N1-C2-N3 | 5.13 | 117.98 | 114.90 |
| 36 | A1 | 2384 | A | C8-N9-C4 | 5.13 | 107.85 | 105.80 |
| 80 | A6 | 718 | U | C2-N1-C1' | 5.13 | 123.86 | 117.70 |
| 36 | A5 | 146 | U | C5-C6-N1 | -5.13 | 120.14 | 122.70 |
| 36 | A5 | 672 | A | C5-C6-N6 | -5.13 | 119.59 | 123.70 |
| 36 | A5 | 1938 | U | C2-N3-C4 | -5.13 | 123.92 | 127.00 |
| 36 | A5 | 2371 | G | N7-C8-N9 | -5.13 | 110.53 | 113.10 |
| 36 | A5 | 2988 | C | C5-C4-N4 | 5.13 | 123.79 | 120.20 |
| 36 | A5 | 3186 | A | N7-C8-N9 | 5.13 | 116.37 | 113.80 |
| 37 | A7 | 116 | C | C6-N1-C2 | 5.13 | 122.35 | 120.30 |
| 36 | A1 | 1367 | G | C4-C5-N7 | 5.13 | 112.85 | 110.80 |
| 75 | B1 | 45 | ARG | NE-CZ-NH2 | -5.13 | 117.73 | 120.30 |
| 36 | A5 | 2378 | C | C2-N3-C4 | 5.13 | 122.47 | 119.90 |
| 1 | A2 | 719 | U | N3-C2-O2 | -5.13 | 118.61 | 122.20 |
| 1 | A2 | 1441 | C | C6-N1-C2 | 5.13 | 122.35 | 120.30 |
| 36 | A1 | 1496 | C | C6-N1-C1' | -5.13 | 114.65 | 120.80 |
| 36 | A1 | 1640 | G | N1-C6-O6 | 5.13 | 122.98 | 119.90 |
| 36 | A1 | 3036 | G | N3-C4-C5 | -5.13 | 126.04 | 128.60 |
| 38 | A4 | 90 | U | C6-N1-C2 | 5.13 | 124.08 | 121.00 |
| 38 | A4 | 147 | U | N3-C4-O4 | 5.13 | 122.99 | 119.40 |
| 80 | A6 | 295 | A | C8-N9-C4 | 5.13 | 107.85 | 105.80 |
| 80 | A6 | 591 | A | C8-N9-C4 | 5.13 | 107.85 | 105.80 |
| 80 | A6 | 1031 | U | C5-C6-N1 | -5.13 | 120.14 | 122.70 |
| 80 | A6 | 1661 | U | C5-C6-N1 | -5.13 | 120.14 | 122.70 |
| 36 | A5 | 893 | C | N3-C2-O2 | 5.13 | 125.49 | 121.90 |
| 36 | A5 | 1938 | U | C6-N1-C2 | 5.13 | 124.08 | 121.00 |
| 1 | A2 | 866 | G | C8-N9-C4 | 5.13 | 108.45 | 106.40 |
| 1 | A2 | 1187 | U | N3-C2-O2 | -5.13 | 118.61 | 122.20 |
| 36 | A1 | 899 | U | C5-C4-O4 | 5.13 | 128.98 | 125.90 |
| 36 | A1 | 1057 | A | C8-N9-C4 | 5.13 | 107.85 | 105.80 |
| 36 | A1 | 1404 | G | N9-C4-C5 | -5.13 | 103.35 | 105.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 1588 | A | C8-N9-C4 | 5.13 | 107.85 | 105.80 |
| 60 | BW | 97 | LYS | C-N-CD | 5.13 | 139.17 | 128.40 |
| 80 | A6 | 32 | U | N3-C2-O2 | -5.13 | 118.61 | 122.20 |
| 36 | A5 | 919 | U | C5-C4-O4 | -5.13 | 122.82 | 125.90 |
| 36 | A5 | 1114 | U | C5-C4-O4 | -5.13 | 122.82 | 125.90 |
| 36 | A5 | 1137 | C | N3-C4-N4 | 5.13 | 121.59 | 118.00 |
| 36 | A5 | 3074 | G | N1-C2-N2 | -5.13 | 111.58 | 116.20 |
| 53 | DP | 23 | ARG | NE-CZ-NH1 | 5.13 | 122.86 | 120.30 |
| 1 | A2 | 294 | C | N1-C2-N3 | -5.12 | 115.61 | 119.20 |
| 1 | A2 | 994 | G | C4-C5-N7 | -5.12 | 108.75 | 110.80 |
| 36 | A1 | 1565 | G | C8-N9-C4 | -5.12 | 104.35 | 106.40 |
| 36 | A1 | 2960 | C | C5-C6-N1 | -5.12 | 118.44 | 121.00 |
| 36 | A1 | 3242 | G | C5-C6-O6 | 5.12 | 131.68 | 128.60 |
| 27 | CZ | 86 | GLU | N-CA-C | -5.12 | 97.16 | 111.00 |
| 36 | A5 | 973 | A | C6-N1-C2 | -5.12 | 115.53 | 118.60 |
| 36 | A5 | 2305 | G | N3-C4-N9 | 5.12 | 129.07 | 126.00 |
| 36 | A1 | 32 | U | C4-C5-C6 | 5.12 | 122.77 | 119.70 |
| 36 | A1 | 267 | G | C5-N7-C8 | 5.12 | 106.86 | 104.30 |
| 36 | A1 | 419 | G | N3-C2-N2 | 5.12 | 123.49 | 119.90 |
| 36 | A1 | 829 | U | C5-C6-N1 | -5.12 | 120.14 | 122.70 |
| 36 | A1 | 1923 | C | C6-N1-C2 | 5.12 | 122.35 | 120.30 |
| 80 | A6 | 1515 | A | N9-C4-C5 | 5.12 | 107.85 | 105.80 |
| 36 | A5 | 726 | G | N7-C8-N9 | 5.12 | 115.66 | 113.10 |
| 36 | A5 | 884 | A | C8-N9-C1' | 5.12 | 136.92 | 127.70 |
| 36 | A5 | 2600 | C | C2-N1-C1' | 5.12 | 124.44 | 118.80 |
| 37 | A7 | 89 | G | C5-C6-N1 | 5.12 | 114.06 | 111.50 |
| 1 | A2 | 885 | G | N1-C6-O6 | 5.12 | 122.97 | 119.90 |
| 36 | A1 | 101 | G | C8-N9-C1' | -5.12 | 120.34 | 127.00 |
| 36 | A1 | 437 | G | C4-C5-C6 | -5.12 | 115.73 | 118.80 |
| 36 | A1 | 588 | G | C2-N3-C4 | 5.12 | 114.46 | 111.90 |
| 36 | A1 | 1851 | G | C6-C5-N7 | -5.12 | 127.33 | 130.40 |
| 36 | A1 | 2650 | U | N3-C4-O4 | -5.12 | 115.81 | 119.40 |
| 36 | A1 | 2868 | U | N3-C4-C5 | 5.12 | 117.67 | 114.60 |
| 80 | A6 | 879 | G | N1-C6-O6 | -5.12 | 116.83 | 119.90 |
| 36 | A5 | 1822 | C | C6-N1-C2 | 5.12 | 122.35 | 120.30 |
| 36 | A5 | 2810 | C | C2-N3-C4 | -5.12 | 117.34 | 119.90 |
| 36 | A5 | 2820 | A | N3-C4-C5 | -5.12 | 123.22 | 126.80 |
| 1 | A2 | 502 | U | C5-C6-N1 | 5.12 | 125.26 | 122.70 |
| 36 | A1 | 374 | A | N1-C2-N3 | -5.12 | 126.74 | 129.30 |
| 36 | A1 | 1118 | C | N1-C2-N3 | 5.12 | 122.78 | 119.20 |
| 36 | A1 | 2184 | U | N1-C2-O2 | 5.12 | 126.38 | 122.80 |
| 36 | A1 | 2364 | G | C8-N9-C4 | 5.12 | 108.45 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 2399 | A | C2-N3-C4 | 5.12 | 113.16 | 110.60 |
| 36 | A1 | 2977 | G | C6-C5-N7 | 5.12 | 133.47 | 130.40 |
| 80 | A6 | 1066 | C | N3-C4-C5 | -5.12 | 119.85 | 121.90 |
| 36 | A5 | 1403 | C | N3-C4-C5 | 5.12 | 123.95 | 121.90 |
| 36 | A5 | 2344 | U | N1-C2-O2 | -5.12 | 119.22 | 122.80 |
| 1 | A2 | 378 | A | C4-C5-N7 | 5.12 | 113.26 | 110.70 |
| 10 | AI | 172 | ARG | NE-CZ-NH2 | -5.12 | 117.74 | 120.30 |
| 36 | A1 | 1308 | A | C4-C5-C6 | 5.12 | 119.56 | 117.00 |
| 36 | A1 | 1363 | A | C5-C6-N1 | 5.12 | 120.26 | 117.70 |
| 36 | A1 | 2931 | C | N3-C4-N4 | 5.12 | 121.58 | 118.00 |
| 36 | A1 | 3078 | U | N3-C2-O2 | -5.12 | 118.62 | 122.20 |
| 36 | A1 | 3119 | U | C5-C4-O4 | 5.12 | 128.97 | 125.90 |
| 36 | A5 | 887 | G | N1-C2-N2 | -5.12 | 111.59 | 116.20 |
| 36 | A5 | 943 | U | C2-N3-C4 | -5.12 | 123.93 | 127.00 |
| 36 | A5 | 1144 | U | N3-C2-O2 | -5.12 | 118.62 | 122.20 |
| 36 | A5 | 1316 | C | C5-C6-N1 | 5.12 | 123.56 | 121.00 |
| 36 | A5 | 2278 | C | P-O3'-C3' | 5.12 | 125.84 | 119.70 |
| 1 | A2 | 1321 | A | N1-C6-N6 | -5.12 | 115.53 | 118.60 |
| 36 | A1 | 225 | C | C5-C4-N4 | -5.12 | 116.62 | 120.20 |
| 36 | A5 | 1303 | A | C8-N9-C4 | 5.12 | 107.85 | 105.80 |
| 36 | A5 | 1901 | A | N1-C6-N6 | 5.12 | 121.67 | 118.60 |
| 36 | A5 | 2352 | A | C5-N7-C8 | 5.12 | 106.46 | 103.90 |
| 1 | A2 | 570 | A | C2-N3-C4 | 5.12 | 113.16 | 110.60 |
| 1 | A2 | 886 | U | N3-C2-O2 | -5.12 | 118.62 | 122.20 |
| 36 | A1 | 267 | G | N3-C4-C5 | -5.12 | 126.04 | 128.60 |
| 36 | A1 | 688 | G | C5-C6-O6 | 5.12 | 131.67 | 128.60 |
| 36 | A1 | 903 | U | C4-C5-C6 | 5.12 | 122.77 | 119.70 |
| 36 | A1 | 1116 | G | N9-C4-C5 | 5.12 | 107.45 | 105.40 |
| 36 | A1 | 1790 | G | C8-N9-C4 | -5.12 | 104.35 | 106.40 |
| 36 | A1 | 2222 | A | C4-C5-C6 | 5.12 | 119.56 | 117.00 |
| 36 | A1 | 2616 | C | N3-C4-C5 | 5.12 | 123.95 | 121.90 |
| 36 | A1 | 2659 | G | C8-N9-C4 | 5.12 | 108.45 | 106.40 |
| 36 | A1 | 2679 | A | N3-C4-C5 | 5.12 | 130.38 | 126.80 |
| 36 | A1 | 2703 | A | C8-N9-C4 | -5.12 | 103.75 | 105.80 |
| 13 | CL | 122 | ILE | N-CA-C | -5.12 | 97.19 | 111.00 |
| 36 | A5 | 2745 | G | C5-C6-N1 | 5.12 | 114.06 | 111.50 |
| 36 | A5 | 2913 | C | N3-C2-O2 | -5.12 | 118.32 | 121.90 |
| 39 | DA | 242 | ARG | NE-CZ-NH2 | -5.12 | 117.74 | 120.30 |
| 1 | A2 | 1761 | U | N3-C2-O2 | -5.11 | 118.62 | 122.20 |
| 36 | A1 | 518 | G | C4-C5-N7 | 5.11 | 112.84 | 110.80 |
| 36 | A1 | 639 | G | C5-C6-N1 | -5.11 | 108.94 | 111.50 |
| 36 | A1 | 812 | G | C8-N9-C4 | -5.11 | 104.35 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 36 | A1 | 2661 | G | N1-C6-O6 | 5.11 | 122.97 | 119.90 |
| 36 | A1 | 2859 | U | N1-C2-O2 | -5.11 | 119.22 | 122.80 |
| 38 | A4 | 144 | G | C8-N9-C4 | 5.11 | 108.45 | 106.40 |
| 80 | A6 | 432 | G | C8-N9-C4 | -5.11 | 104.35 | 106.40 |
| 36 | A5 | 433 | A | C8-N9-C4 | 5.11 | 107.84 | 105.80 |
| 36 | A5 | 802 | C | N1-C2-N3 | 5.11 | 122.78 | 119.20 |
| 36 | A5 | 2124 | G | N7-C8-N9 | -5.11 | 110.54 | 113.10 |
| 36 | A5 | 3255 | U | N3-C4-C5 | 5.11 | 117.67 | 114.60 |
| 1 | A2 | 1782 | A | C5-C6-N1 | -5.11 | 115.14 | 117.70 |
| 80 | A6 | 695 | U | N3-C2-O2 | -5.11 | 118.62 | 122.20 |
| 36 | A5 | 2848 | G | C8-N9-C4 | -5.11 | 104.36 | 106.40 |
| 36 | A5 | 3218 | A | N3-C4-N9 | -5.11 | 123.31 | 127.40 |
| 36 | A1 | 672 | A | C5-N7-C8 | -5.11 | 101.34 | 103.90 |
| 36 | A1 | 1787 | A | C5-N7-C8 | 5.11 | 106.46 | 103.90 |
| 36 | A1 | 1948 | G | C6-C5-N7 | -5.11 | 127.33 | 130.40 |
| 36 | A1 | 2154 | U | C2-N3-C4 | -5.11 | 123.93 | 127.00 |
| 36 | A1 | 2618 | G | N1-C6-O6 | -5.11 | 116.83 | 119.90 |
| 36 | A1 | 3180 | A | N3-C4-N9 | -5.11 | 123.31 | 127.40 |
| 36 | A1 | 3328 | G | C5-N7-C8 | -5.11 | 101.75 | 104.30 |
| 36 | A1 | 3375 | A | N1-C2-N3 | 5.11 | 131.85 | 129.30 |
| 38 | A4 | 88 | A | N9-C4-C5 | -5.11 | 103.76 | 105.80 |
| 36 | A5 | 1445 | U | N3-C2-O2 | 5.11 | 125.78 | 122.20 |
| 38 | A8 | 47 | C | N3-C2-O2 | -5.11 | 118.32 | 121.90 |
| 41 | DC | 60 | THR | CB-CA-C | -5.11 | 97.80 | 111.60 |
| 36 | A1 | 950 | G | C8-N9-C4 | 5.11 | 108.44 | 106.40 |
| 36 | A1 | 2160 | G | N3-C4-N9 | 5.11 | 129.06 | 126.00 |
| 36 | A1 | 2916 | U | C5-C4-O4 | -5.11 | 122.83 | 125.90 |
| 36 | A5 | 3019 | U | C5-C6-N1 | -5.11 | 120.15 | 122.70 |
| 1 | A2 | 20 | G | N1-C2-N2 | -5.11 | 111.60 | 116.20 |
| 36 | A1 | 339 | C | N1-C2-N3 | 5.11 | 122.78 | 119.20 |
| 36 | A1 | 854 | G | N1-C2-N3 | 5.11 | 126.96 | 123.90 |
| 36 | A1 | 1942 | U | N1-C2-N3 | 5.11 | 117.96 | 114.90 |
| 36 | A1 | 2201 | G | C4-C5-N7 | 5.11 | 112.84 | 110.80 |
| 36 | A1 | 2382 | G | N3-C4-C5 | -5.11 | 126.05 | 128.60 |
| 36 | A1 | 2830 | G | N1-C2-N3 | 5.11 | 126.96 | 123.90 |
| 80 | A6 | 383 | G | C8-N9-C4 | -5.11 | 104.36 | 106.40 |
| 80 | A6 | 430 | G | C6-N1-C2 | -5.11 | 122.04 | 125.10 |
| 80 | A6 | 695 | U | C6-N1-C2 | -5.11 | 117.94 | 121.00 |
| 36 | A5 | 284 | A | C8-N9-C4 | -5.11 | 103.76 | 105.80 |
| 36 | A5 | 1412 | G | N9-C4-C5 | 5.11 | 107.44 | 105.40 |
| 36 | A5 | 2290 | C | N1-C2-O2 | -5.11 | 115.83 | 118.90 |
| 36 | A5 | 3259 | U | N1-C2-N3 | 5.11 | 117.97 | 114.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 36 | A5 | 3294 | A | C5-C6-N6 | 5.11 | 127.79 | 123.70 |
| 1 | A2 | 422 | G | C8-N9-C4 | -5.11 | 104.36 | 106.40 |
| 1 | A2 | 1096 | C | C6-N1-C2 | -5.11 | 118.26 | 120.30 |
| 1 | A2 | 1376 | C | C6-N1-C2 | 5.11 | 122.34 | 120.30 |
| 24 | AW | 104 | LEU | CA-CB-CG | 5.11 | 127.04 | 115.30 |
| 36 | A1 | 354 | U | C5-C6-N1 | -5.11 | 120.15 | 122.70 |
| 36 | A1 | 1461 | A | C5-C6-N1 | 5.11 | 120.25 | 117.70 |
| 36 | A1 | 1482 | A | C4-C5-C6 | 5.11 | 119.55 | 117.00 |
| 36 | A1 | 3144 | G | C5-C6-N1 | 5.11 | 114.05 | 111.50 |
| 80 | A6 | 403 | G | C8-N9-C1' | -5.11 | 120.36 | 127.00 |
| 80 | A6 | 624 | G | C5-C6-N1 | 5.11 | 114.05 | 111.50 |
| 36 | A5 | 2271 | A | C5-C6-N6 | 5.11 | 127.78 | 123.70 |
| 36 | A5 | 2364 | G | C6-N1-C2 | -5.11 | 122.04 | 125.10 |
| 36 | A1 | 614 | C | C6-N1-C2 | 5.10 | 122.34 | 120.30 |
| 36 | A1 | 929 | A | C4-C5-N7 | -5.10 | 108.15 | 110.70 |
| 36 | A1 | 1395 | G | N3-C4-N9 | 5.10 | 129.06 | 126.00 |
| 36 | A1 | 2275 | A | N1-C2-N3 | 5.10 | 131.85 | 129.30 |
| 36 | A5 | 3056 | U | N1-C2-O2 | -5.10 | 119.23 | 122.80 |
| 38 | A8 | 100 | U | C6-N1-C1' | -5.10 | 114.06 | 121.20 |
| 1 | A2 | 597 | G | C8-N9-C4 | -5.10 | 104.36 | 106.40 |
| 36 | A1 | 282 | G | C2'-C3'-O3' | 5.10 | 121.86 | 113.70 |
| 36 | A1 | 2160 | G | C4-C5-N7 | 5.10 | 112.84 | 110.80 |
| 36 | A1 | 2727 | A | N9-C4-C5 | 5.10 | 107.84 | 105.80 |
| 36 | A1 | 2787 | G | C8-N9-C4 | -5.10 | 104.36 | 106.40 |
| 80 | A6 | 543 | C | C4-C5-C6 | 5.10 | 119.95 | 117.40 |
| 36 | A5 | 437 | G | C5-C6-O6 | -5.10 | 125.54 | 128.60 |
| 36 | A5 | 1468 | A | N7-C8-N9 | 5.10 | 116.35 | 113.80 |
| 36 | A5 | 3180 | A | C6-N1-C2 | -5.10 | 115.54 | 118.60 |
| 36 | A5 | 3378 | C | N3-C4-N4 | -5.10 | 114.43 | 118.00 |
| 1 | A2 | 564 | G | C5-C6-O6 | 5.10 | 131.66 | 128.60 |
| 36 | A1 | 643 | U | N1-C2-O2 | -5.10 | 119.23 | 122.80 |
| 36 | A1 | 889 | U | N1-C2-O2 | 5.10 | 126.37 | 122.80 |
| 36 | A1 | 2200 | U | C2-N1-C1' | 5.10 | 123.82 | 117.70 |
| 80 | A6 | 568 | G | N1-C6-O6 | -5.10 | 116.84 | 119.90 |
| 80 | A6 | 820 | U | N1-C2-N3 | -5.10 | 111.84 | 114.90 |
| 36 | A5 | 2830 | G | C8-N9-C4 | -5.10 | 104.36 | 106.40 |
| 37 | A7 | 57 | G | C5-C6-O6 | 5.10 | 131.66 | 128.60 |
| 36 | A1 | 275 | U | C4-C5-C6 | -5.10 | 116.64 | 119.70 |
| 36 | A1 | 2277 | C | N3-C4-N4 | -5.10 | 114.43 | 118.00 |
| 36 | A1 | 3083 | G | C5-C6-N1 | 5.10 | 114.05 | 111.50 |
| 37 | A3 | 97 | A | C8-N9-C4 | -5.10 | 103.76 | 105.80 |
| 80 | A6 | 118 | U | C2-N3-C4 | -5.10 | 123.94 | 127.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 80 | A6 | 1120 | U | N3-C4-C5 | 5.10 | 117.66 | 114.60 |
| 36 | A5 | 2392 | C | C2-N1-C1' | -5.10 | 113.19 | 118.80 |
| 51 | BN | 172 | ARG | NE-CZ-NH1 | -5.10 | 117.75 | 120.30 |
| 36 | A5 | 2128 | C | C6-N1-C2 | -5.10 | 118.26 | 120.30 |
| 36 | A5 | 2978 | U | C5-C4-O4 | 5.10 | 128.96 | 125.90 |
| 36 | A5 | 3241 | G | N1-C6-O6 | 5.10 | 122.96 | 119.90 |
| 1 | A2 | 1734 | U | C5-C4-O4 | 5.10 | 128.96 | 125.90 |
| 36 | A1 | 1183 | C | N3-C2-O2 | 5.10 | 125.47 | 121.90 |
| 36 | A5 | 583 | G | C8-N9-C4 | 5.10 | 108.44 | 106.40 |
| 36 | A5 | 2691 | A | N1-C2-N3 | 5.10 | 131.85 | 129.30 |
| 60 | DW | 39 | LEU | CA-CB-CG | 5.10 | 127.02 | 115.30 |
| 1 | A2 | 1431 | C | C6-N1-C2 | 5.09 | 122.34 | 120.30 |
| 36 | A1 | 51 | A | N9-C4-C5 | -5.09 | 103.76 | 105.80 |
| 36 | A1 | 214 | G | N7-C8-N9 | -5.09 | 110.55 | 113.10 |
| 36 | A1 | 718 | G | N7-C8-N9 | 5.09 | 115.65 | 113.10 |
| 36 | A1 | 1838 | G | C4-C5-C6 | 5.09 | 121.86 | 118.80 |
| 36 | A1 | 2363 | A | C5-C6-N6 | 5.09 | 127.78 | 123.70 |
| 36 | A1 | 2850 | G | N3-C4-N9 | 5.09 | 129.06 | 126.00 |
| 36 | A1 | 2969 | A | N9-C4-C5 | 5.09 | 107.84 | 105.80 |
| 36 | A1 | 3369 | G | C5-C6-O6 | -5.09 | 125.54 | 128.60 |
| 80 | A6 | 543 | C | N3-C4-N4 | -5.09 | 114.43 | 118.00 |
| 80 | A6 | 1527 | C | C2-N1-C1' | -5.09 | 113.20 | 118.80 |
| 36 | A5 | 102 | C | N1-C2-O2 | -5.09 | 115.84 | 118.90 |
| 36 | A5 | 284 | A | N1-C6-N6 | -5.09 | 115.54 | 118.60 |
| 36 | A5 | 613 | G | C4-C5-N7 | -5.09 | 108.76 | 110.80 |
| 36 | A5 | 2518 | C | C4-C5-C6 | 5.09 | 119.95 | 117.40 |
| 1 | A2 | 810 | G | C4-N9-C1' | 5.09 | 133.12 | 126.50 |
| 37 | A3 | 29 | C | C5-C4-N4 | 5.09 | 123.77 | 120.20 |
| 36 | A5 | 1100 | U | C5-C4-O4 | -5.09 | 122.84 | 125.90 |
| 1 | A2 | 359 | A | C4-C5-C6 | -5.09 | 114.45 | 117.00 |
| 1 | A2 | 647 | G | C8-N9-C1' | 5.09 | 133.62 | 127.00 |
| 36 | A1 | 905 | U | N1-C2-O2 | -5.09 | 119.24 | 122.80 |
| 36 | A1 | 983 | A | C4-C5-C6 | 5.09 | 119.55 | 117.00 |
| 36 | A1 | 1543 | G | N1-C6-O6 | 5.09 | 122.95 | 119.90 |
| 36 | A1 | 1617 | G | N7-C8-N9 | -5.09 | 110.56 | 113.10 |
| 36 | A1 | 2163 | C | C5-C6-N1 | -5.09 | 118.45 | 121.00 |
| 36 | A1 | 2368 | A | C2-N3-C4 | -5.09 | 108.05 | 110.60 |
| 36 | A1 | 2979 | U | C5-C4-O4 | 5.09 | 128.96 | 125.90 |
| 38 | A4 | 39 | G | C5-C6-O6 | 5.09 | 131.65 | 128.60 |
| 80 | A6 | 1507 | G | N1-C2-N2 | -5.09 | 111.62 | 116.20 |
| 36 | A5 | 183 | G | C3'-C2'-C1' | -5.09 | 97.43 | 101.50 |
| 36 | A5 | 436 | A | N1-C2-N3 | 5.09 | 131.85 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 979 | U | N1-C2-N3 | -5.09 | 111.84 | 114.90 |
| 36 | A5 | 1147 | G | C5-C6-O6 | 5.09 | 131.66 | 128.60 |
| 36 | A5 | 2317 | A | C5-N7-C8 | -5.09 | 101.35 | 103.90 |
| 36 | A5 | 2866 | U | N1-C2-N3 | 5.09 | 117.95 | 114.90 |
| 36 | A5 | 3154 | C | C6-N1-C2 | -5.09 | 118.26 | 120.30 |
| 38 | A8 | 31 | G | C5-N7-C8 | 5.09 | 106.85 | 104.30 |
| 1 | A2 | 111 | U | C6-N1-C2 | -5.09 | 117.95 | 121.00 |
| 36 | A1 | 74 | G | C8-N9-C4 | -5.09 | 104.36 | 106.40 |
| 36 | A1 | 218 | G | N9-C4-C5 | 5.09 | 107.44 | 105.40 |
| 36 | A1 | 1051 | U | N1-C2-N3 | 5.09 | 117.95 | 114.90 |
| 36 | A1 | 1452 | A | N9-C4-C5 | -5.09 | 103.76 | 105.80 |
| 36 | A1 | 1919 | G | N9-C4-C5 | 5.09 | 107.44 | 105.40 |
| 36 | A1 | 3304 | U | N1-C2-O2 | -5.09 | 119.24 | 122.80 |
| 36 | A1 | 3317 | U | C5-C6-N1 | 5.09 | 125.25 | 122.70 |
| 80 | A6 | 1792 | G | C5-N7-C8 | -5.09 | 101.75 | 104.30 |
| 36 | A5 | 959 | C | N3-C4-C5 | 5.09 | 123.94 | 121.90 |
| 36 | A5 | 2136 | C | C2-N3-C4 | -5.09 | 117.36 | 119.90 |
| 36 | A5 | 2283 | G | C8-N9-C4 | 5.09 | 108.44 | 106.40 |
| 36 | A5 | 2857 | C | C5-C6-N1 | -5.09 | 118.45 | 121.00 |
| 36 | A5 | 3313 | U | N1-C2-N3 | 5.09 | 117.95 | 114.90 |
| 1 | A2 | 586 | G | N1-C6-O6 | -5.09 | 116.85 | 119.90 |
| 36 | A1 | 1552 | G | C5-C6-O6 | -5.09 | 125.55 | 128.60 |
| 36 | A1 | 2143 | A | N1-C2-N3 | 5.09 | 131.84 | 129.30 |
| 36 | A1 | 2206 | G | C2-N3-C4 | 5.09 | 114.44 | 111.90 |
| 56 | DS | 167 | ARG | NE-CZ-NH1 | 5.09 | 122.84 | 120.30 |
| 1 | A2 | 553 | G | C2-N3-C4 | -5.09 | 109.36 | 111.90 |
| 36 | A1 | 32 | U | N1-C2-N3 | 5.09 | 117.95 | 114.90 |
| 36 | A1 | 292 | U | N1-C2-N3 | 5.09 | 117.95 | 114.90 |
| 36 | A1 | 748 | U | C5-C6-N1 | -5.09 | 120.16 | 122.70 |
| 36 | A1 | 1483 | G | C5-C6-O6 | 5.09 | 131.65 | 128.60 |
| 36 | A1 | 2349 | U | N3-C2-O2 | -5.09 | 118.64 | 122.20 |
| 37 | A3 | 39 | C | N1-C2-O2 | 5.09 | 121.95 | 118.90 |
| 80 | A6 | 794 | U | C5-C6-N1 | 5.09 | 125.24 | 122.70 |
| 80 | A6 | 1641 | C | C4-C5-C6 | 5.09 | 119.94 | 117.40 |
| 36 | A5 | 95 | A | C5-C6-N1 | 5.09 | 120.24 | 117.70 |
| 36 | A5 | 2614 | G | C2-N3-C4 | -5.09 | 109.36 | 111.90 |
| 36 | A1 | 1130 | A | N3-C4-C5 | -5.08 | 123.24 | 126.80 |
| 36 | A1 | 1916 | U | C2-N3-C4 | -5.08 | 123.95 | 127.00 |
| 36 | A5 | 2633 | U | C2-N3-C4 | -5.08 | 123.95 | 127.00 |
| 1 | A2 | 132 | U | C6-N1-C1' | 5.08 | 128.32 | 121.20 |
| 1 | A2 | 760 | A | N1-C6-N6 | 5.08 | 121.65 | 118.60 |
| 36 | A1 | 780 | A | N1-C6-N6 | -5.08 | 115.55 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 790 | U | N1-C2-N3 | 5.08 | 117.95 | 114.90 |
| 36 | A1 | 1049 | C | C6-N1-C2 | 5.08 | 122.33 | 120.30 |
| 36 | A1 | 1907 | C | C5-C4-N4 | 5.08 | 123.76 | 120.20 |
| 36 | A1 | 1947 | G | C4-N9-C1' | -5.08 | 119.89 | 126.50 |
| 36 | A1 | 2148 | U | C6-N1-C2 | 5.08 | 124.05 | 121.00 |
| 36 | A1 | 2549 | G | C2-N3-C4 | 5.08 | 114.44 | 111.90 |
| 36 | A1 | 2914 | G | C4-N9-C1' | 5.08 | 133.11 | 126.50 |
| 36 | A1 | 3126 | C | C5-C4-N4 | 5.08 | 123.76 | 120.20 |
| 37 | A3 | 102 | A | N9-C4-C5 | -5.08 | 103.77 | 105.80 |
| 73 | Bj | 79 | GLN | CB-CA-C | -5.08 | 100.23 | 110.40 |
| 80 | A6 | 358 | U | C2-N3-C4 | -5.08 | 123.95 | 127.00 |
| 80 | A6 | 381 | C | N1-C2-N3 | 5.08 | 122.76 | 119.20 |
| 36 | A5 | 1637 | A | N1-C6-N6 | -5.08 | 115.55 | 118.60 |
| 36 | A5 | 1788 | C | C6-N1-C2 | -5.08 | 118.27 | 120.30 |
| 36 | A5 | 2974 | U | C5-C6-N1 | -5.08 | 120.16 | 122.70 |
| 1 | A2 | 1311 | U | C6-N1-C2 | 5.08 | 124.05 | 121.00 |
| 36 | A1 | 1890 | U | C4-C5-C6 | 5.08 | 122.75 | 119.70 |
| 36 | A1 | 2310 | U | C5-C4-O4 | 5.08 | 128.95 | 125.90 |
| 36 | A1 | 2329 | C | N3-C2-O2 | 5.08 | 125.46 | 121.90 |
| 41 | BC | 328 | ASN | N-CA-C | 5.08 | 124.72 | 111.00 |
| 43 | BE | 77 | ARG | NE-CZ-NH2 | -5.08 | 117.76 | 120.30 |
| 69 | Bf | 49 | ILE | CB-CA-C | -5.08 | 101.44 | 111.60 |
| 80 | A6 | 87 | C | N1-C2-N3 | 5.08 | 122.76 | 119.20 |
| 36 | A5 | 1439 | U | C5-C4-O4 | -5.08 | 122.85 | 125.90 |
| 36 | A5 | 1473 | G | C8-N9-C4 | 5.08 | 108.43 | 106.40 |
| 36 | A5 | 2857 | C | C2-N3-C4 | -5.08 | 117.36 | 119.90 |
| 36 | A5 | 2883 | U | N1-C2-N3 | 5.08 | 117.95 | 114.90 |
| 36 | A5 | 2941 | A | C8-N9-C4 | 5.08 | 107.83 | 105.80 |
| 36 | A5 | 3010 | U | N1-C2-O2 | 5.08 | 126.36 | 122.80 |
| 36 | A5 | 3066 | U | N1-C2-O2 | 5.08 | 126.36 | 122.80 |
| 36 | A1 | 1307 | G | C5-C6-N1 | 5.08 | 114.04 | 111.50 |
| 36 | A5 | 1412 | G | N3-C2-N2 | -5.08 | 116.34 | 119.90 |
| 36 | A1 | 1482 | A | C5-N7-C8 | 5.08 | 106.44 | 103.90 |
| 36 | A1 | 2395 | G | C2-N3-C4 | 5.08 | 114.44 | 111.90 |
| 36 | A1 | 2945 | G | N9-C4-C5 | -5.08 | 103.37 | 105.40 |
| 36 | A1 | 3102 | G | N1-C6-O6 | -5.08 | 116.85 | 119.90 |
| 38 | A4 | 4 | C | C2-N3-C4 | -5.08 | 117.36 | 119.90 |
| 38 | A4 | 46 | G | C4-N9-C1' | 5.08 | 133.10 | 126.50 |
| 36 | A5 | 622 | A | C4-C5-N7 | 5.08 | 113.24 | 110.70 |
| 36 | A5 | 860 | G | N3-C4-C5 | -5.08 | 126.06 | 128.60 |
| 36 | A5 | 958 | C | C6-N1-C2 | 5.08 | 122.33 | 120.30 |
| 36 | A5 | 2190 | U | N3-C2-O2 | -5.08 | 118.65 | 122.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 2293 | C | N3-C2-O2 | -5.08 | 118.34 | 121.90 |
| 36 | A5 | 3132 | C | C6-N1-C2 | 5.08 | 122.33 | 120.30 |
| 36 | A1 | 699 | A | C2-N3-C4 | -5.08 | 108.06 | 110.60 |
| 36 | A1 | 2327 | U | N1-C2-N3 | 5.08 | 117.95 | 114.90 |
| 80 | A6 | 1156 | C | C6-N1-C2 | 5.08 | 122.33 | 120.30 |
| 80 | A6 | 1743 | U | C2-N3-C4 | -5.08 | 123.95 | 127.00 |
| 36 | A5 | 2198 | A | C8-N9-C4 | 5.08 | 107.83 | 105.80 |
| 36 | A5 | 3310 | A | C5-N7-C8 | 5.08 | 106.44 | 103.90 |
| 37 | A3 | 89 | G | C5-C6-O6 | -5.08 | 125.55 | 128.60 |
| 38 | A4 | 12 | A | N1-C6-N6 | -5.08 | 115.56 | 118.60 |
| 80 | A6 | 1027 | A | N9-C4-C5 | 5.08 | 107.83 | 105.80 |
| 36 | A5 | 1077 | U | N1-C2-O2 | -5.08 | 119.25 | 122.80 |
| 36 | A5 | 1100 | U | C6-N1-C2 | 5.08 | 124.05 | 121.00 |
| 36 | A5 | 1851 | G | C8-N9-C1' | -5.08 | 120.40 | 127.00 |
| 36 | A5 | 2748 | A | C5-C6-N1 | 5.08 | 120.24 | 117.70 |
| 36 | A5 | 3127 | A | C5-C6-N6 | 5.08 | 127.76 | 123.70 |
| 1 | A2 | 638 | U | C2-N3-C4 | -5.07 | 123.96 | 127.00 |
| 36 | A1 | 117 | U | N1-C2-O2 | -5.07 | 119.25 | 122.80 |
| 36 | A1 | 2551 | U | N3-C4-O4 | -5.07 | 115.85 | 119.40 |
| 38 | A4 | 41 | A | C6-N1-C2 | -5.07 | 115.56 | 118.60 |
| 80 | A6 | 569 | C | C6-N1-C2 | -5.07 | 118.27 | 120.30 |
| 80 | A6 | 1489 | U | C2-N3-C4 | -5.07 | 123.96 | 127.00 |
| 36 | A5 | 1301 | A | C6-C5-N7 | -5.07 | 128.75 | 132.30 |
| 36 | A5 | 1432 | C | N3-C2-O2 | -5.07 | 118.35 | 121.90 |
| 36 | A5 | 2138 | A | C5-C6-N1 | -5.07 | 115.16 | 117.70 |
| 36 | A5 | 3130 | A | C4-C5-C6 | 5.07 | 119.54 | 117.00 |
| 36 | A5 | 3273 | A | C5-N7-C8 | -5.07 | 101.36 | 103.90 |
| 1 | A2 | 1596 | C | N1-C2-O2 | 5.07 | 121.94 | 118.90 |
| 80 | A6 | 909 | U | N1-C2-O2 | -5.07 | 119.25 | 122.80 |
| 36 | A5 | 2162 | U | C5-C6-N1 | -5.07 | 120.16 | 122.70 |
| 1 | A2 | 63 | G | N1-C6-O6 | -5.07 | 116.86 | 119.90 |
| 1 | A2 | 158 | U | N1-C2-O2 | 5.07 | 126.35 | 122.80 |
| 1 | A2 | 26 | A | C8-N9-C4 | -5.07 | 103.77 | 105.80 |
| 36 | A1 | 395 | A | C8-N9-C4 | -5.07 | 103.77 | 105.80 |
| 36 | A1 | 574 | U | C5-C6-N1 | -5.07 | 120.17 | 122.70 |
| 36 | A1 | 3135 | U | C6-N1-C2 | 5.07 | 124.04 | 121.00 |
| 56 | BS | 12 | ARG | N-CA-C | 5.07 | 124.69 | 111.00 |
| 1 | A2 | 335 | U | N3-C2-O2 | 5.07 | 125.75 | 122.20 |
| 36 | A1 | 651 | G | C4-N9-C1' | 5.07 | 133.09 | 126.50 |
| 36 | A1 | 2917 | G | C5-N7-C8 | 5.07 | 106.83 | 104.30 |
| 80 | A6 | 22 | A | N7-C8-N9 | -5.07 | 111.27 | 113.80 |
| 80 | A6 | 1299 | G | C4-N9-C1' | 5.07 | 133.09 | 126.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 36 | A5 | 874 | U | C2-N1-C1' | -5.07 | 111.62 | 117.70 |
| 36 | A5 | 1142 | G | N3-C2-N2 | 5.07 | 123.45 | 119.90 |
| 36 | A5 | 1804 | A | N1-C6-N6 | 5.07 | 121.64 | 118.60 |
| 36 | A5 | 2407 | C | N3-C2-O2 | 5.07 | 125.45 | 121.90 |
| 37 | A7 | 83 | U | C6-N1-C1' | 5.07 | 128.29 | 121.20 |
| 1 | A2 | 1643 | U | C2-N3-C4 | -5.07 | 123.96 | 127.00 |
| 15 | AN | 114 | ARG | NE-CZ-NH1 | 5.07 | 122.83 | 120.30 |
| 36 | A1 | 340 | C | N1-C2-O2 | 5.07 | 121.94 | 118.90 |
| 36 | A1 | 808 | A | C5-N7-C8 | 5.07 | 106.43 | 103.90 |
| 36 | A1 | 1770 | G | C4-N9-C1' | 5.07 | 133.09 | 126.50 |
| 36 | A1 | 2280 | A | C4-C5-N7 | 5.07 | 113.23 | 110.70 |
| 36 | A1 | 2866 | U | N1-C2-N3 | 5.07 | 117.94 | 114.90 |
| 80 | A6 | 802 | G | C5-C6-O6 | -5.07 | 125.56 | 128.60 |
| 80 | A6 | 922 | G | N1-C6-O6 | -5.07 | 116.86 | 119.90 |
| 80 | A6 | 1772 | C | C2-N3-C4 | -5.07 | 117.37 | 119.90 |
| 36 | A5 | 1241 | U | C5-C6-N1 | 5.07 | 125.23 | 122.70 |
| 36 | A5 | 2386 | A | N1-C6-N6 | 5.07 | 121.64 | 118.60 |
| 36 | A5 | 2805 | G | C5-C6-N1 | 5.07 | 114.03 | 111.50 |
| 36 | A5 | 3377 | G | C6-C5-N7 | -5.07 | 127.36 | 130.40 |
| 1 | A2 | 1536 | G | N3-C4-C5 | -5.06 | 126.07 | 128.60 |
| 36 | A1 | 1215 | U | N1-C2-O2 | -5.06 | 119.25 | 122.80 |
| 36 | A1 | 2644 | C | C6-N1-C2 | -5.06 | 118.28 | 120.30 |
| 44 | BF | 177 | GLY | N-CA-C | -5.06 | 100.44 | 113.10 |
| 80 | A6 | 1031 | U | C2-N1-C1' | -5.06 | 111.62 | 117.70 |
| 36 | A5 | 1451 | C | C6-N1-C2 | 5.06 | 122.33 | 120.30 |
| 36 | A5 | 3030 | G | C5-C6-N1 | -5.06 | 108.97 | 111.50 |
| 1 | A2 | 704 | C | N3-C2-O2 | -5.06 | 118.36 | 121.90 |
| 1 | A2 | 1354 | G | C8-N9-C4 | -5.06 | 104.38 | 106.40 |
| 36 | A1 | 1791 | C | C5-C6-N1 | -5.06 | 118.47 | 121.00 |
| 71 | Bh | 31 | LEU | CA-CB-CG | 5.06 | 126.94 | 115.30 |
| 80 | A6 | 37 | U | N3-C2-O2 | 5.06 | 125.74 | 122.20 |
| 80 | A6 | 99 | C | C6-N1-C1' | -5.06 | 114.72 | 120.80 |
| 80 | A6 | 575 | C | N3-C4-C5 | -5.06 | 119.88 | 121.90 |
| 80 | A6 | 691 | C | N1-C2-O2 | 5.06 | 121.94 | 118.90 |
| 4 | CC | 107 | SER | N-CA-C | -5.06 | 97.33 | 111.00 |
| 36 | A5 | 346 | C | N3-C4-C5 | 5.06 | 123.92 | 121.90 |
| 36 | A5 | 1414 | G | C2-N3-C4 | -5.06 | 109.37 | 111.90 |
| 36 | A5 | 3137 | C | N3-C4-N4 | -5.06 | 114.46 | 118.00 |
| 36 | A5 | 3191 | G | N7-C8-N9 | -5.06 | 110.57 | 113.10 |
| 37 | A7 | 35 | C | C6-N1-C2 | 5.06 | 122.33 | 120.30 |
| 37 | A7 | 35 | C | N3-C4-C5 | 5.06 | 123.92 | 121.90 |
| 1 | A2 | 73 | U | C1'-O4'-C4' | -5.06 | 105.85 | 109.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A2 | 1541 | G | C2-N3-C4 | 5.06 | 114.43 | 111.90 |
| 36 | A5 | 2662 | G | N3-C4-C5 | -5.06 | 126.07 | 128.60 |
| 1 | A2 | 927 | C | C6-N1-C2 | -5.06 | 118.28 | 120.30 |
| 36 | A1 | 223 | U | C5-C6-N1 | -5.06 | 120.17 | 122.70 |
| 36 | A1 | 431 | U | N1-C2-N3 | 5.06 | 117.94 | 114.90 |
| 36 | A1 | 620 | U | C3'-C2'-C1' | 5.06 | 105.55 | 101.50 |
| 36 | A1 | 959 | C | C5-C4-N4 | -5.06 | 116.66 | 120.20 |
| 36 | A1 | 1640 | G | C5-C6-O6 | -5.06 | 125.56 | 128.60 |
| 37 | A3 | 94 | C | C5-C4-N4 | -5.06 | 116.66 | 120.20 |
| 38 | A4 | 30 | C | C6-N1-C2 | -5.06 | 118.28 | 120.30 |
| 38 | A4 | 31 | G | C2-N3-C4 | -5.06 | 109.37 | 111.90 |
| 80 | A6 | 1005 | A | C2-N3-C4 | -5.06 | 108.07 | 110.60 |
| 80 | A6 | 1246 | C | N1-C2-O2 | 5.06 | 121.94 | 118.90 |
| 36 | A5 | 627 | U | N3-C2-O2 | -5.06 | 118.66 | 122.20 |
| 36 | A5 | 880 | G | C6-N1-C2 | -5.06 | 122.06 | 125.10 |
| 36 | A5 | 2593 | A | P-O3'-C3' | 5.06 | 125.77 | 119.70 |
| 36 | A5 | 2754 | G | N3-C4-C5 | -5.06 | 126.07 | 128.60 |
| 44 | DF | 177 | GLY | N-CA-C | -5.06 | 100.45 | 113.10 |
| 1 | A2 | 1649 | G | N1-C2-N3 | 5.06 | 126.94 | 123.90 |
| 36 | A1 | 37 | U | N3-C2-O2 | 5.06 | 125.74 | 122.20 |
| 36 | A1 | 695 | C | C6-N1-C2 | 5.06 | 122.32 | 120.30 |
| 36 | A1 | 2142 | A | N9-C4-C5 | 5.06 | 107.82 | 105.80 |
| 37 | A3 | 109 | G | N9-C4-C5 | 5.06 | 107.42 | 105.40 |
| 36 | A5 | 2371 | G | N1-C2-N2 | -5.06 | 111.65 | 116.20 |
| 80 | A6 | 1119 | G | N1-C6-O6 | -5.06 | 116.87 | 119.90 |
| 36 | A5 | 813 | G | C4-N9-C1' | 5.06 | 133.07 | 126.50 |
| 1 | A2 | 1605 | G | N1-C2-N2 | -5.05 | 111.65 | 116.20 |
| 36 | A1 | 351 | A | C2-N3-C4 | -5.05 | 108.07 | 110.60 |
| 36 | A1 | 1150 | A | N3-C4-N9 | -5.05 | 123.36 | 127.40 |
| 36 | A1 | 1187 | C | C2-N3-C4 | -5.05 | 117.37 | 119.90 |
| 36 | A1 | 1313 | G | C5-C6-N1 | 5.05 | 114.03 | 111.50 |
| 36 | A1 | 1838 | G | C5-C6-N1 | -5.05 | 108.97 | 111.50 |
| 36 | A1 | 2751 | G | N1-C6-O6 | 5.05 | 122.93 | 119.90 |
| 36 | A5 | 578 | A | C2-N3-C4 | 5.05 | 113.13 | 110.60 |
| 36 | A5 | 1461 | A | C8-N9-C4 | 5.05 | 107.82 | 105.80 |
| 36 | A5 | 1660 | C | C2-N3-C4 | -5.05 | 117.37 | 119.90 |
| 36 | A5 | 2207 | A | C5-C6-N1 | -5.05 | 115.17 | 117.70 |
| 36 | A5 | 2309 | A | N1-C6-N6 | 5.05 | 121.63 | 118.60 |
| 36 | A5 | 2919 | A | C5-C6-N6 | 5.05 | 127.74 | 123.70 |
| 36 | A5 | 3217 | C | C2-N1-C1' | -5.05 | 113.24 | 118.80 |
| 38 | A8 | 88 | A | N1-C6-N6 | 5.05 | 121.63 | 118.60 |
| 80 | A6 | 65 | A | C8-N9-C4 | 5.05 | 107.82 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 80 | A6 | 1039 | A | O4'-C1'-N9 | 5.05 | 112.24 | 108.20 |
| 36 | A5 | 524 | U | C2-N3-C4 | -5.05 | 123.97 | 127.00 |
| 36 | A5 | 2731 | U | C5-C6-N1 | -5.05 | 120.17 | 122.70 |
| 36 | A5 | 2951 | G | C8-N9-C4 | 5.05 | 108.42 | 106.40 |
| 36 | A5 | 3195 | U | N1-C2-O2 | 5.05 | 126.34 | 122.80 |
| 1 | A2 | 312 | A | C8-N9-C4 | -5.05 | 103.78 | 105.80 |
| 1 | A2 | 819 | G | P-O3'-C3' | 5.05 | 125.76 | 119.70 |
| 1 | A2 | 972 | G | C5-N7-C8 | 5.05 | 106.83 | 104.30 |
| 36 | A1 | 68 | C | N3-C4-C5 | -5.05 | 119.88 | 121.90 |
| 36 | A1 | 545 | U | C5-C6-N1 | 5.05 | 125.22 | 122.70 |
| 36 | A1 | 2281 | A | N3-C4-C5 | 5.05 | 130.34 | 126.80 |
| 36 | A1 | 2829 | U | N1-C2-O2 | 5.05 | 126.34 | 122.80 |
| 38 | A4 | 26 | U | C5-C6-N1 | -5.05 | 120.17 | 122.70 |
| 80 | A6 | 359 | A | C8-N9-C1' | 5.05 | 136.79 | 127.70 |
| 37 | A7 | 41 | G | C5-C6-O6 | -5.05 | 125.57 | 128.60 |
| 38 | A8 | 17 | A | C6-C5-N7 | -5.05 | 128.76 | 132.30 |
| 36 | A1 | 1589 | A | O4'-C1'-N9 | -5.05 | 104.16 | 108.20 |
| 36 | A1 | 2169 | G | C5-N7-C8 | 5.05 | 106.83 | 104.30 |
| 36 | A1 | 2692 | A | N7-C8-N9 | 5.05 | 116.33 | 113.80 |
| 36 | A1 | 2899 | C | C5-C4-N4 | -5.05 | 116.67 | 120.20 |
| 38 | A4 | 29 | U | C5-C6-N1 | -5.05 | 120.17 | 122.70 |
| 80 | A6 | 1289 | U | N3-C4-O4 | 5.05 | 122.94 | 119.40 |
| 36 | A5 | 1192 | C | N3-C2-O2 | -5.05 | 118.36 | 121.90 |
| 36 | A5 | 1348 | U | C5-C6-N1 | 5.05 | 125.22 | 122.70 |
| 36 | A5 | 1726 | C | C6-N1-C2 | 5.05 | 122.32 | 120.30 |
| 36 | A5 | 2263 | C | N3-C2-O2 | -5.05 | 118.36 | 121.90 |
| 36 | A5 | 2541 | U | N1-C2-O2 | 5.05 | 126.33 | 122.80 |
| 36 | A5 | 2696 | A | C5-C6-N6 | 5.05 | 127.74 | 123.70 |
| 36 | A5 | 2931 | C | N1-C2-O2 | -5.05 | 115.87 | 118.90 |
| 80 | A6 | 970 | A | C4-C5-C6 | -5.05 | 114.48 | 117.00 |
| 36 | A5 | 1338 | C | N1-C2-O2 | -5.05 | 115.87 | 118.90 |
| 36 | A5 | 2944 | U | N1-C2-O2 | 5.05 | 126.33 | 122.80 |
| 33 | Af | 138 | ARG | NE-CZ-NH2 | -5.05 | 117.78 | 120.30 |
| 36 | A1 | 696 | C | N3-C4-N4 | -5.05 | 114.47 | 118.00 |
| 36 | A1 | 938 | C | N1-C2-N3 | 5.05 | 122.73 | 119.20 |
| 36 | A1 | 2573 | G | N7-C8-N9 | 5.05 | 115.62 | 113.10 |
| 36 | A1 | 2718 | U | N3-C2-O2 | -5.05 | 118.67 | 122.20 |
| 36 | A1 | 3174 | A | N7-C8-N9 | 5.05 | 116.32 | 113.80 |
| 37 | A3 | 101 | G | N9-C4-C5 | -5.05 | 103.38 | 105.40 |
| 80 | A6 | 101 | U | N3-C4-O4 | -5.05 | 115.87 | 119.40 |
| 36 | A5 | 41 | G | N1-C2-N2 | 5.05 | 120.74 | 116.20 |
| 36 | A5 | 1015 | U | C2-N3-C4 | 5.05 | 130.03 | 127.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 1480 | G | N3-C4-N9 | 5.05 | 129.03 | 126.00 |
| 37 | A7 | 14 | U | C2-N3-C4 | -5.05 | 123.97 | 127.00 |
| 47 | DI | 69 | ARG | NE-CZ-NH2 | 5.05 | 122.82 | 120.30 |
| 1 | A2 | 1148 | C | N1-C2-O2 | 5.04 | 121.93 | 118.90 |
| 1 | A2 | 1600 | A | N1-C6-N6 | 5.04 | 121.63 | 118.60 |
| 36 | A1 | 722 | G | C8-N9-C4 | -5.04 | 104.38 | 106.40 |
| 36 | A1 | 2892 | A | C4-C5-N7 | -5.04 | 108.18 | 110.70 |
| 80 | A6 | 102 | U | C2-N3-C4 | -5.04 | 123.97 | 127.00 |
| 36 | A5 | 367 | A | C6-N1-C2 | 5.04 | 121.63 | 118.60 |
| 36 | A5 | 2353 | G | C4-C5-N7 | 5.04 | 112.82 | 110.80 |
| 36 | A5 | 2701 | U | N3-C4-O4 | 5.04 | 122.93 | 119.40 |
| 1 | A2 | 440 | U | N3-C4-O4 | -5.04 | 115.87 | 119.40 |
| 36 | A1 | 584 | G | C4-C5-N7 | -5.04 | 108.78 | 110.80 |
| 80 | A6 | 1573 | A | C5-C6-N1 | 5.04 | 120.22 | 117.70 |
| 36 | A5 | 1303 | A | N7-C8-N9 | -5.04 | 111.28 | 113.80 |
| 36 | A5 | 2110 | G | C4-C5-N7 | 5.04 | 112.82 | 110.80 |
| 36 | A5 | 2407 | C | N3-C4-N4 | 5.04 | 121.53 | 118.00 |
| 37 | A7 | 20 | A | N1-C6-N6 | 5.04 | 121.63 | 118.60 |
| 37 | A7 | 83 | U | C5-C4-O4 | 5.04 | 128.93 | 125.90 |
| 1 | A2 | 6 | G | N1-C2-N2 | -5.04 | 111.66 | 116.20 |
| 1 | A2 | 192 | U | C6-N1-C2 | -5.04 | 117.97 | 121.00 |
| 36 | A1 | 342 | A | C5-C6-N1 | -5.04 | 115.18 | 117.70 |
| 36 | A1 | 1317 | A | C2-N3-C4 | 5.04 | 113.12 | 110.60 |
| 36 | A1 | 1839 | A | N1-C2-N3 | 5.04 | 131.82 | 129.30 |
| 36 | A1 | 2273 | G | C6-C5-N7 | 5.04 | 133.43 | 130.40 |
| 36 | A1 | 2408 | U | N3-C4-O4 | 5.04 | 122.93 | 119.40 |
| 36 | A1 | 2804 | A | C8-N9-C4 | -5.04 | 103.78 | 105.80 |
| 36 | A1 | 3256 | G | C6-C5-N7 | 5.04 | 133.43 | 130.40 |
| 80 | A6 | 305 | C | N3-C4-C5 | -5.04 | 119.88 | 121.90 |
| 80 | A6 | 310 | C | C5-C6-N1 | -5.04 | 118.48 | 121.00 |
| 36 | A5 | 1887 | A | C6-C5-N7 | -5.04 | 128.77 | 132.30 |
| 36 | A5 | 3189 | G | C8-N9-C4 | 5.04 | 108.42 | 106.40 |
| 73 | Dj | 5 | THR | C-N-CD | 5.04 | 138.99 | 128.40 |
| 1 | A2 | 1722 | A | N1-C6-N6 | -5.04 | 115.58 | 118.60 |
| 6 | AE | 164 | LEU | CA-CB-CG | 5.04 | 126.89 | 115.30 |
| 36 | A1 | 1510 | G | N9-C4-C5 | -5.04 | 103.38 | 105.40 |
| 36 | A1 | 2247 | G | N3-C2-N2 | -5.04 | 116.37 | 119.90 |
| 36 | A1 | 3372 | A | C6-N1-C2 | -5.04 | 115.58 | 118.60 |
| 36 | A5 | 2965 | U | C5-C6-N1 | -5.04 | 120.18 | 122.70 |
| 36 | A1 | 218 | G | C8-N9-C4 | -5.04 | 104.39 | 106.40 |
| 36 | A1 | 577 | C | N1-C2-O2 | -5.04 | 115.88 | 118.90 |
| 36 | A1 | 800 | G | C6-N1-C2 | 5.04 | 128.12 | 125.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 935 | U | C2-N3-C4 | -5.04 | 123.98 | 127.00 |
| 36 | A1 | 1216 | C | C6-N1-C1' | 5.04 | 126.85 | 120.80 |
| 36 | A1 | 2211 | U | C5-C6-N1 | 5.04 | 125.22 | 122.70 |
| 36 | A1 | 2795 | U | N3-C2-O2 | -5.04 | 118.67 | 122.20 |
| 36 | A1 | 2823 | G | C6-C5-N7 | 5.04 | 133.42 | 130.40 |
| 37 | A3 | 33 | U | N3-C2-O2 | -5.04 | 118.67 | 122.20 |
| 80 | A6 | 234 | G | N3-C4-C5 | -5.04 | 126.08 | 128.60 |
| 80 | A6 | 605 | A | N7-C8-N9 | -5.04 | 111.28 | 113.80 |
| 36 | A5 | 356 | C | C6-N1-C2 | 5.04 | 122.32 | 120.30 |
| 36 | A5 | 1902 | G | N9-C4-C5 | -5.04 | 103.39 | 105.40 |
| 36 | A5 | 2167 | A | N3-C4-C5 | -5.04 | 123.27 | 126.80 |
| 36 | A5 | 2531 | C | N3-C2-O2 | -5.04 | 118.37 | 121.90 |
| 37 | A7 | 88 | G | N9-C4-C5 | 5.04 | 107.42 | 105.40 |
| 55 | DR | 97 | ARG | NE-CZ-NH1 | -5.04 | 117.78 | 120.30 |
| 1 | A2 | 270 | C | C2-N1-C1' | 5.04 | 124.34 | 118.80 |
| 1 | A2 | 802 | G | N3-C4-C5 | -5.04 | 126.08 | 128.60 |
| 36 | A1 | 868 | C | C5-C4-N4 | 5.04 | 123.73 | 120.20 |
| 36 | A1 | 2395 | G | N1-C6-O6 | -5.04 | 116.88 | 119.90 |
| 80 | A6 | 20 | G | N3-C4-C5 | 5.04 | 131.12 | 128.60 |
| 80 | A6 | 363 | G | C4-C5-N7 | 5.04 | 112.81 | 110.80 |
| 36 | A5 | 587 | U | C6-N1-C2 | 5.04 | 124.02 | 121.00 |
| 36 | A5 | 998 | A | C4-C5-N7 | -5.04 | 108.18 | 110.70 |
| 36 | A5 | 2215 | A | N1-C6-N6 | 5.04 | 121.62 | 118.60 |
| 36 | A5 | 2284 | C | C2-N1-C1' | 5.04 | 124.34 | 118.80 |
| 36 | A5 | 2606 | G | N1-C2-N2 | -5.04 | 111.67 | 116.20 |
| 36 | A5 | 2774 | C | N3-C4-N4 | 5.04 | 121.53 | 118.00 |
| 36 | A5 | 2935 | U | N1-C2-O2 | 5.04 | 126.33 | 122.80 |
| 36 | A5 | 3145 | C | C5-C4-N4 | -5.04 | 116.67 | 120.20 |
| 1 | A2 | 345 | U | N1-C2-N3 | 5.04 | 117.92 | 114.90 |
| 1 | A2 | 498 | G | C4-N9-C1' | 5.04 | 133.05 | 126.50 |
| 36 | A1 | 2360 | C | N1-C2-N3 | 5.04 | 122.72 | 119.20 |
| 36 | A1 | 2551 | U | N3-C2-O2 | -5.04 | 118.68 | 122.20 |
| 36 | A1 | 2811 | A | C6-N1-C2 | -5.04 | 115.58 | 118.60 |
| 36 | A1 | 2878 | G | C6-N1-C2 | -5.04 | 122.08 | 125.10 |
| 37 | A3 | 14 | U | N3-C2-O2 | 5.04 | 125.72 | 122.20 |
| 80 | A6 | 101 | U | C5-C4-O4 | 5.04 | 128.92 | 125.90 |
| 80 | A6 | 342 | C | C6-N1-C2 | 5.04 | 122.31 | 120.30 |
| 80 | A6 | 394 | C | N3-C4-C5 | -5.04 | 119.89 | 121.90 |
| 80 | A6 | 583 | C | C2-N1-C1' | 5.04 | 124.34 | 118.80 |
| 36 | A5 | 1178 | G | N3-C2-N2 | -5.04 | 116.38 | 119.90 |
| 36 | A5 | 1314 | C | C4-C5-C6 | 5.04 | 119.92 | 117.40 |
| 36 | A5 | 1704 | A | C2-N3-C4 | -5.04 | 108.08 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 36 | A5 | 1832 | C | N3-C4-C5 | 5.04 | 123.92 | 121.90 |
| 36 | A5 | 2271 | A | C5-N7-C8 | 5.04 | 106.42 | 103.90 |
| 36 | A5 | 2280 | A | N3-C4-C5 | 5.04 | 130.32 | 126.80 |
| 36 | A5 | 3351 | U | N1-C2-O2 | 5.04 | 126.33 | 122.80 |
| 1 | A2 | 1220 | C | C6-N1-C2 | 5.03 | 122.31 | 120.30 |
| 36 | A1 | 271 | C | N1-C2-O2 | 5.03 | 121.92 | 118.90 |
| 36 | A1 | 1170 | A | N1-C6-N6 | 5.03 | 121.62 | 118.60 |
| 36 | A1 | 2174 | G | C6-C5-N7 | -5.03 | 127.38 | 130.40 |
| 36 | A1 | 2621 | G | C4-C5-N7 | -5.03 | 108.79 | 110.80 |
| 36 | A1 | 2788 | C | N3-C2-O2 | 5.03 | 125.42 | 121.90 |
| 38 | A4 | 15 | G | C5-N7-C8 | 5.03 | 106.82 | 104.30 |
| 36 | A5 | 282 | G | P-O3'-C3' | 5.03 | 125.74 | 119.70 |
| 36 | A5 | 982 | C | C4-C5-C6 | -5.03 | 114.88 | 117.40 |
| 36 | A5 | 2317 | A | C6-C5-N7 | -5.03 | 128.78 | 132.30 |
| 36 | A5 | 2430 | A | C4-C5-C6 | 5.03 | 119.52 | 117.00 |
| 36 | A5 | 2674 | A | N7-C8-N9 | -5.03 | 111.28 | 113.80 |
| 36 | A5 | 2958 | A | C4-N9-C1' | -5.03 | 117.24 | 126.30 |
| 36 | A5 | 3028 | G | N9-C4-C5 | -5.03 | 103.39 | 105.40 |
| 36 | A5 | 2280 | A | C8-N9-C4 | 5.03 | 107.81 | 105.80 |
| 11 | AJ | 175 | ARG | NE-CZ-NH1 | 5.03 | 122.81 | 120.30 |
| 36 | A1 | 28 | C | C2-N3-C4 | -5.03 | 117.39 | 119.90 |
| 36 | A1 | 2170 | U | N1-C2-N3 | 5.03 | 117.92 | 114.90 |
| 37 | A3 | 80 | G | N3-C4-C5 | -5.03 | 126.08 | 128.60 |
| 38 | A4 | 55 | U | C6-N1-C2 | -5.03 | 117.98 | 121.00 |
| 38 | A4 | 149 | A | N1-C6-N6 | -5.03 | 115.58 | 118.60 |
| 36 | A5 | 2623 | G | N3-C4-N9 | 5.03 | 129.02 | 126.00 |
| 36 | A5 | 2821 | C | N1-C2-O2 | -5.03 | 115.88 | 118.90 |
| 36 | A5 | 3191 | G | C5-N7-C8 | 5.03 | 106.81 | 104.30 |
| 37 | A7 | 26 | C | N1-C2-N3 | 5.03 | 122.72 | 119.20 |
| 54 | DQ | 3 | ILE | CB-CA-C | -5.03 | 101.54 | 111.60 |
| 1 | A2 | 1051 | G | C4-N9-C1' | 5.03 | 133.04 | 126.50 |
| 1 | A2 | 1679 | G | N3-C2-N2 | 5.03 | 123.42 | 119.90 |
| 36 | A1 | 304 | G | C4-C5-N7 | -5.03 | 108.79 | 110.80 |
| 36 | A1 | 1520 | G | C4-C5-N7 | -5.03 | 108.79 | 110.80 |
| 36 | A1 | 1807 | G | C4-N9-C1' | 5.03 | 133.04 | 126.50 |
| 36 | A1 | 2380 | U | N1-C2-O2 | -5.03 | 119.28 | 122.80 |
| 36 | A5 | 940 | G | C5-C6-N1 | 5.03 | 114.02 | 111.50 |
| 36 | A5 | 1040 | A | C2-N3-C4 | -5.03 | 108.08 | 110.60 |
| 36 | A5 | 3209 | A | O4'-C1'-N9 | 5.03 | 112.22 | 108.20 |
| 36 | A1 | 1178 | G | N1-C6-O6 | -5.03 | 116.88 | 119.90 |
| 36 | A1 | 1357 | G | N1-C6-O6 | 5.03 | 122.92 | 119.90 |
| 36 | A1 | 2965 | U | C2-N3-C4 | -5.03 | 123.98 | 127.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 38 | A4 | 140 | G | C4-C5-N7 | -5.03 | 108.79 | 110.80 |
| 80 | A6 | 512 | A | C3'-C2'-C1' | -5.03 | 97.48 | 101.50 |
| 36 | A5 | 16 | A | C5-C6-N1 | 5.03 | 120.21 | 117.70 |
| 36 | A5 | 584 | G | N1-C6-O6 | -5.03 | 116.88 | 119.90 |
| 36 | A5 | 1660 | C | N1-C2-N3 | 5.03 | 122.72 | 119.20 |
| 36 | A5 | 2337 | C | C5-C6-N1 | -5.03 | 118.49 | 121.00 |
| 36 | A5 | 3212 | C | N1-C2-N3 | 5.03 | 122.72 | 119.20 |
| 1 | A2 | 555 | A | N3-C4-C5 | -5.03 | 123.28 | 126.80 |
| 1 | A2 | 914 | G | C4-N9-C1' | 5.03 | 133.03 | 126.50 |
| 25 | AX | 111 | GLY | N-CA-C | -5.03 | 100.54 | 113.10 |
| 36 | A1 | 425 | G | N1-C2-N2 | -5.03 | 111.68 | 116.20 |
| 36 | A1 | 2383 | C | C6-N1-C2 | 5.03 | 122.31 | 120.30 |
| 36 | A1 | 2752 | U | C5-C6-N1 | -5.03 | 120.19 | 122.70 |
| 41 | BC | 246 | ARG | CG-CD-NE | -5.03 | 101.25 | 111.80 |
| 64 | Ba | 12 | ARG | NE-CZ-NH1 | 5.03 | 122.81 | 120.30 |
| 80 | A6 | 1269 | U | C6-N1-C2 | -5.03 | 117.98 | 121.00 |
| 80 | A6 | 1428 | G | N9-C4-C5 | 5.03 | 107.41 | 105.40 |
| 36 | A5 | 98 | G | C5-C6-O6 | -5.03 | 125.58 | 128.60 |
| 36 | A5 | 1906 | G | C5-C6-O6 | -5.03 | 125.58 | 128.60 |
| 36 | A5 | 2742 | C | C2-N3-C4 | -5.03 | 117.39 | 119.90 |
| 36 | A5 | 2813 | A | C5-C6-N6 | 5.03 | 127.72 | 123.70 |
| 36 | A5 | 2945 | G | C5-C6-O6 | -5.03 | 125.58 | 128.60 |
| 36 | A5 | 3049 | A | N1-C6-N6 | 5.03 | 121.61 | 118.60 |
| 36 | A5 | 3246 | G | C5-C6-O6 | -5.03 | 125.58 | 128.60 |
| 37 | A7 | 96 | U | N3-C4-C5 | 5.03 | 117.62 | 114.60 |
| 1 | A2 | 404 | G | N1-C6-O6 | 5.02 | 122.91 | 119.90 |
| 36 | A1 | 411 | U | C5-C6-N1 | -5.02 | 120.19 | 122.70 |
| 36 | A1 | 808 | A | C6-C5-N7 | 5.02 | 135.82 | 132.30 |
| 36 | A1 | 1493 | G | N3-C4-N9 | -5.02 | 122.99 | 126.00 |
| 36 | A1 | 1899 | G | N3-C2-N2 | 5.02 | 123.42 | 119.90 |
| 36 | A1 | 2154 | U | C2-N1-C1' | 5.02 | 123.73 | 117.70 |
| 80 | A6 | 96 | G | C2-N3-C4 | -5.02 | 109.39 | 111.90 |
| 36 | A5 | 949 | C | N1-C2-N3 | 5.02 | 122.72 | 119.20 |
| 36 | A5 | 1481 | A | C4-C5-C6 | 5.02 | 119.51 | 117.00 |
| 36 | A5 | 2647 | A | N1-C2-N3 | 5.02 | 131.81 | 129.30 |
| 38 | A8 | 79 | A | N1-C6-N6 | 5.02 | 121.61 | 118.60 |
| 1 | A2 | 1568 | C | P-O3'-C3' | 5.02 | 125.73 | 119.70 |
| 1 | A2 | 1629 | G | N1-C2-N2 | -5.02 | 111.68 | 116.20 |
| 36 | A1 | 869 | G | N3-C4-N9 | 5.02 | 129.01 | 126.00 |
| 36 | A1 | 995 | U | C5-C6-N1 | 5.02 | 125.21 | 122.70 |
| 36 | A1 | 1372 | C | C5-C6-N1 | -5.02 | 118.49 | 121.00 |
| 36 | A1 | 2249 | G | C6-N1-C2 | -5.02 | 122.09 | 125.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 36 | A1 | 2541 | U | N1-C2-O2 | 5.02 | 126.31 | 122.80 |
| 36 | A1 | 2924 | U | N3-C4-O4 | -5.02 | 115.88 | 119.40 |
| 36 | A1 | 3212 | C | C2-N3-C4 | -5.02 | 117.39 | 119.90 |
| 36 | A1 | 3218 | A | C2-N3-C4 | -5.02 | 108.09 | 110.60 |
| 49 | BL | 76 | THR | N-CA-CB | 5.02 | 119.84 | 110.30 |
| 80 | A6 | 531 | C | C6-N1-C2 | -5.02 | 118.29 | 120.30 |
| 80 | A6 | 972 | G | N7-C8-N9 | -5.02 | 110.59 | 113.10 |
| 36 | A5 | 191 | U | C2-N1-C1' | -5.02 | 111.67 | 117.70 |
| 36 | A5 | 391 | A | C8-N9-C4 | 5.02 | 107.81 | 105.80 |
| 36 | A5 | 2306 | C | C5-C6-N1 | 5.02 | 123.51 | 121.00 |
| 36 | A1 | 1306 | G | N3-C2-N2 | -5.02 | 116.39 | 119.90 |
| 36 | A1 | 2314 | U | N3-C4-O4 | 5.02 | 122.92 | 119.40 |
| 36 | A5 | 530 | G | N9-C4-C5 | 5.02 | 107.41 | 105.40 |
| 1 | A2 | 1600 | A | C3'-C2'-C1' | -5.02 | 97.48 | 101.50 |
| 1 | A2 | 1791 | A | C5-C6-N1 | 5.02 | 120.21 | 117.70 |
| 36 | A1 | 406 | G | C6-N1-C2 | 5.02 | 128.11 | 125.10 |
| 36 | A1 | 2204 | C | C6-N1-C2 | -5.02 | 118.29 | 120.30 |
| 36 | A1 | 2642 | A | N3-C4-N9 | -5.02 | 123.38 | 127.40 |
| 36 | A1 | 2770 | G | C5-N7-C8 | -5.02 | 101.79 | 104.30 |
| 36 | A1 | 2904 | U | N3-C4-C5 | 5.02 | 117.61 | 114.60 |
| 36 | A1 | 3098 | G | N3-C2-N2 | 5.02 | 123.41 | 119.90 |
| 36 | A5 | 609 | G | C8-N9-C4 | -5.02 | 104.39 | 106.40 |
| 36 | A5 | 840 | C | C4-C5-C6 | 5.02 | 119.91 | 117.40 |
| 36 | A5 | 2353 | G | N3-C4-C5 | -5.02 | 126.09 | 128.60 |
| 36 | A5 | 3048 | A | C5-C6-N6 | -5.02 | 119.69 | 123.70 |
| 59 | DV | 87 | ARG | NE-CZ-NH2 | -5.02 | 117.79 | 120.30 |
| 1 | A2 | 1441 | C | C5-C6-N1 | -5.02 | 118.49 | 121.00 |
| 36 | A1 | 357 | A | C5-C6-N1 | 5.02 | 120.21 | 117.70 |
| 36 | A1 | 2316 | G | N1-C6-O6 | 5.02 | 122.91 | 119.90 |
| 36 | A1 | 2381 | G | C8-N9-C4 | 5.02 | 108.41 | 106.40 |
| 80 | A6 | 805 | U | N3-C4-C5 | -5.02 | 111.59 | 114.60 |
| 36 | A5 | 432 | G | N1-C2-N2 | -5.02 | 111.68 | 116.20 |
| 36 | A5 | 1004 | U | C5-C4-O4 | 5.02 | 128.91 | 125.90 |
| 36 | A5 | 2179 | C | N3-C2-O2 | 5.02 | 125.41 | 121.90 |
| 36 | A5 | 2343 | C | N1-C2-O2 | -5.02 | 115.89 | 118.90 |
| 36 | A5 | 2393 | G | N7-C8-N9 | -5.02 | 110.59 | 113.10 |
| 36 | A5 | 2878 | G | C5-C6-N1 | 5.02 | 114.01 | 111.50 |
| 36 | A5 | 3266 | G | N3-C4-N9 | -5.02 | 122.99 | 126.00 |
| 38 | A8 | 40 | A | N7-C8-N9 | 5.02 | 116.31 | 113.80 |
| 33 | Af | 106 | TYR | N-CA-C | -5.02 | 97.46 | 111.00 |
| 36 | A1 | 634 | C | N3-C4-N4 | -5.02 | 114.49 | 118.00 |
| 36 | A1 | 1501 | U | C5-C6-N1 | 5.02 | 125.21 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A1 | 3088 | G | C5-N7-C8 | 5.02 | 106.81 | 104.30 |
| 80 | A6 | 1550 | A | C4-C5-N7 | 5.02 | 113.21 | 110.70 |
| 36 | A5 | 1932 | A | N1-C2-N3 | 5.02 | 131.81 | 129.30 |
| 36 | A5 | 2323 | G | C5-C6-O6 | 5.02 | 131.61 | 128.60 |
| 36 | A5 | 2972 | G | N1-C2-N2 | -5.02 | 111.69 | 116.20 |
| 36 | A1 | 1366 | A | C2-N3-C4 | 5.01 | 113.11 | 110.60 |
| 36 | A1 | 1382 | G | N1-C6-O6 | 5.01 | 122.91 | 119.90 |
| 36 | A1 | 1855 | U | C2-N1-C1' | 5.01 | 123.72 | 117.70 |
| 36 | A1 | 2117 | A | C4-C5-N7 | -5.01 | 108.19 | 110.70 |
| 36 | A1 | 2350 | C | N3-C2-O2 | -5.01 | 118.39 | 121.90 |
| 62 | BY | 112 | ASP | CB-CG-OD1 | 5.01 | 122.81 | 118.30 |
| 36 | A5 | 916 | G | C6-N1-C2 | 5.01 | 128.11 | 125.10 |
| 36 | A5 | 1463 | U | C5-C4-O4 | -5.01 | 122.89 | 125.90 |
| 36 | A5 | 1872 | C | C2-N3-C4 | -5.01 | 117.39 | 119.90 |
| 36 | A5 | 2379 | U | C2-N3-C4 | -5.01 | 123.99 | 127.00 |
| 36 | A5 | 2808 | A | C8-N9-C1' | -5.01 | 118.67 | 127.70 |
| 36 | A5 | 3241 | G | C6-C5-N7 | -5.01 | 127.39 | 130.40 |
| 38 | A8 | 4 | C | C6-N1-C2 | -5.01 | 118.29 | 120.30 |
| 38 | A8 | 99 | C | C2-N3-C4 | -5.01 | 117.39 | 119.90 |
| 48 | DJ | 92 | ARG | NE-CZ-NH1 | 5.01 | 122.81 | 120.30 |
| 36 | A5 | 2349 | U | N3-C4-O4 | -5.01 | 115.89 | 119.40 |
| 36 | A5 | 2369 | G | N3-C4-N9 | 5.01 | 129.01 | 126.00 |
| 1 | A2 | 613 | G | N3-C2-N2 | 5.01 | 123.41 | 119.90 |
| 1 | A2 | 1324 | G | N3-C4-C5 | 5.01 | 131.11 | 128.60 |
| 1 | A2 | 1780 | G | N1-C6-O6 | 5.01 | 122.91 | 119.90 |
| 36 | A1 | 582 | G | N1-C2-N2 | 5.01 | 120.71 | 116.20 |
| 36 | A1 | 1100 | U | N1-C2-N3 | 5.01 | 117.91 | 114.90 |
| 36 | A1 | 1157 | G | C5-C6-O6 | 5.01 | 131.61 | 128.60 |
| 36 | A1 | 2904 | U | C4-C5-C6 | -5.01 | 116.69 | 119.70 |
| 80 | A6 | 381 | C | N3-C4-N4 | -5.01 | 114.49 | 118.00 |
| 80 | A6 | 1200 | G | N3-C4-N9 | -5.01 | 122.99 | 126.00 |
| 80 | A6 | 1747 | G | C2-N3-C4 | -5.01 | 109.39 | 111.90 |
| 36 | A5 | 1078 | U | N3-C2-O2 | 5.01 | 125.71 | 122.20 |
| 36 | A5 | 2847 | A | C5-C6-N6 | 5.01 | 127.71 | 123.70 |
| 1 | A2 | 158 | U | P-O3'-C3' | 5.01 | 125.71 | 119.70 |
| 36 | A1 | 375 | A | C4-C5-N7 | 5.01 | 113.20 | 110.70 |
| 36 | A1 | 431 | U | C5-C6-N1 | -5.01 | 120.20 | 122.70 |
| 36 | A1 | 678 | G | C2-N3-C4 | 5.01 | 114.41 | 111.90 |
| 36 | A1 | 2117 | A | N9-C4-C5 | 5.01 | 107.80 | 105.80 |
| 13 | CL | 128 | CYS | N-CA-C | 5.01 | 124.52 | 111.00 |
| 36 | A5 | 820 | A | N1-C2-N3 | 5.01 | 131.80 | 129.30 |
| 36 | A5 | 880 | G | C8-N9-C4 | 5.01 | 108.40 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 36 | A5 | 914 | A | C2-N3-C4 | -5.01 | 108.09 | 110.60 |
| 36 | A5 | 1347 | U | C2-N1-C1' | -5.01 | 111.69 | 117.70 |
| 1 | A2 | 324 | U | N1-C2-N3 | 5.01 | 117.91 | 114.90 |
| 36 | A1 | 1377 | G | N3-C2-N2 | 5.01 | 123.41 | 119.90 |
| 36 | A1 | 2276 | G | N1-C2-N3 | -5.01 | 120.89 | 123.90 |
| 36 | A1 | 2411 | U | N3-C4-C5 | 5.01 | 117.61 | 114.60 |
| 36 | A1 | 3362 | A | C6-N1-C2 | -5.01 | 115.59 | 118.60 |
| 1 | A2 | 902 | G | N1-C6-O6 | 5.01 | 122.90 | 119.90 |
| 36 | A1 | 34 | A | C4-C5-N7 | 5.01 | 113.20 | 110.70 |
| 36 | A1 | 189 | G | N3-C2-N2 | 5.01 | 123.41 | 119.90 |
| 36 | A1 | 571 | U | C5-C6-N1 | -5.01 | 120.20 | 122.70 |
| 36 | A1 | 637 | C | P-O3'-C3' | 5.01 | 125.71 | 119.70 |
| 36 | A1 | 2409 | G | N1-C2-N2 | -5.01 | 111.69 | 116.20 |
| 36 | A1 | 2504 | U | C2-N1-C1' | 5.01 | 123.71 | 117.70 |
| 36 | A1 | 3172 | A | N7-C8-N9 | -5.01 | 111.30 | 113.80 |
| 36 | A1 | 3361 | G | N3-C2-N2 | 5.01 | 123.41 | 119.90 |
| 37 | A3 | 15 | C | N1-C2-O2 | -5.01 | 115.90 | 118.90 |
| 38 | A4 | 105 | A | C6-N1-C2 | 5.01 | 121.60 | 118.60 |
| 39 | BA | 44 | ILE | CB-CA-C | -5.01 | 101.59 | 111.60 |
| 47 | BI | 21 | ARG | NE-CZ-NH1 | -5.01 | 117.80 | 120.30 |
| 80 | A6 | 980 | G | C8-N9-C4 | 5.01 | 108.40 | 106.40 |
| 80 | A6 | 1329 | A | C4-C5-N7 | 5.01 | 113.20 | 110.70 |
| 36 | A5 | 126 | U | C2-N3-C4 | -5.01 | 124.00 | 127.00 |
| 36 | A5 | 270 | U | N1-C2-O2 | 5.01 | 126.30 | 122.80 |
| 36 | A5 | 628 | A | C5-C6-N1 | 5.01 | 120.20 | 117.70 |
| 36 | A5 | 2352 | A | C4-C5-C6 | 5.01 | 119.50 | 117.00 |
| 36 | A5 | 2361 | A | N1-C6-N6 | -5.01 | 115.60 | 118.60 |
| 36 | A5 | 2375 | G | N3-C2-N2 | 5.01 | 123.40 | 119.90 |
| 36 | A5 | 3094 | A | N7-C8-N9 | -5.01 | 111.30 | 113.80 |
| 36 | A5 | 3183 | A | N1-C6-N6 | 5.01 | 121.60 | 118.60 |
| 38 | A8 | 76 | C | C2-N1-C1' | -5.01 | 113.29 | 118.80 |
| 1 | A2 | 1215 | C | N3-C2-O2 | -5.00 | 118.40 | 121.90 |
| 17 | AP | 42 | ARG | NE-CZ-NH1 | 5.00 | 122.80 | 120.30 |
| 36 | A1 | 817 | A | C4-C5-C6 | 5.00 | 119.50 | 117.00 |
| 1 | A2 | 431 | C | N3-C2-O2 | -5.00 | 118.40 | 121.90 |
| 1 | A2 | 1633 | A | C8-N9-C4 | -5.00 | 103.80 | 105.80 |
| 36 | A1 | 2152 | A | C6-C5-N7 | 5.00 | 135.80 | 132.30 |
| 36 | A1 | 2294 | U | N1-C2-N3 | 5.00 | 117.90 | 114.90 |
| 36 | A1 | 2376 | G | C5-C6-O6 | -5.00 | 125.60 | 128.60 |
| 36 | A1 | 3188 | G | C4-N9-C1' | 5.00 | 133.01 | 126.50 |
| 37 | A3 | 2 | G | N1-C6-O6 | -5.00 | 116.90 | 119.90 |
| 37 | A3 | 37 | G | C5-C6-O6 | -5.00 | 125.60 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 80 | A6 | 1481 | C | N3-C2-O2 | -5.00 | 118.40 | 121.90 |
| 80 | A6 | 1666 | U | N1-C2-N3 | 5.00 | 117.90 | 114.90 |
| 36 | A5 | 2994 | A | N1-C2-N3 | 5.00 | 131.80 | 129.30 |
| 1 | A2 | 1258 | U | N1-C2-O2 | 5.00 | 126.30 | 122.80 |
| 1 | A2 | 1432 | U | C2-N1-C1' | -5.00 | 111.70 | 117.70 |
| 36 | A1 | 225 | C | N3-C4-N4 | 5.00 | 121.50 | 118.00 |
| 36 | A1 | 633 | C | C6-N1-C2 | 5.00 | 122.30 | 120.30 |
| 36 | A1 | 1523 | U | C2-N3-C4 | -5.00 | 124.00 | 127.00 |
| 36 | A1 | 1668 | G | N1-C2-N3 | 5.00 | 126.90 | 123.90 |
| 36 | A1 | 2168 | A | N9-C4-C5 | -5.00 | 103.80 | 105.80 |
| 36 | A1 | 2736 | A | N1-C2-N3 | 5.00 | 131.80 | 129.30 |
| 36 | A1 | 3015 | G | C2-N3-C4 | 5.00 | 114.40 | 111.90 |
| 36 | A5 | 509 | U | N3-C4-O4 | -5.00 | 115.90 | 119.40 |

There are no chirality outliers.

All (67) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 36 | A1 | 1329 | U | Sidechain |
| 36 | A1 | 406 | G | Sidechain |
| 36 | A1 | 835 | G | Sidechain |
| 36 | A5 | 2898 | G | Sidechain |
| 3 | AB | 131 | ASP | Peptide |
| 9 | AH | 131 | PHE | Peptide |
| 13 | AL | 127 | GLN | Peptide |
| 16 | AO | 124 | ASP | Peptide |
| 19 | AR | 22 | PRO | Peptide |
| 19 | AR | 85 | VAL | Peptide |
| 27 | AZ | 54 | VAL | Peptide |
| 27 | AZ | 93 | SER | Peptide |
| 27 | AZ | 96 | SER | Peptide |
| 29 | Ab | 42 | ASN | Peptide |
| 33 | Af | 105 | TYR | Peptide |
| 33 | Af | 138 | ARG | Peptide |
| 35 | Ah | 134 | ASP | Sidechain |
| 40 | BB | 172 | ALA | Peptide |
| 41 | BC | 318 | LEU | Peptide |
| 43 | BE | 129 | GLU | Peptide |
| 43 | BE | 51 | ARG | Peptide |
| 44 | BF | 157 | ASN | Peptide |
| 45 | BG | 158 | ASP | Peptide |
| 45 | BG | 30 | THR | Peptide |

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| Mol | Chain | Res | Type | Group |
|------------|--------------|------------|-------------|--------------|
| 45 | BG | 74 | THR | Peptide |
| 46 | BH | 21 | LYS | Peptide |
| 48 | BJ | 8 | PRO | Peptide |
| 52 | BO | 110[A] | PRO | Peptide |
| 52 | BO | 110[B] | PRO | Peptide |
| 57 | BT | 16 | GLN | Peptide |
| 65 | Bb | 19 | ASN | Peptide |
| 65 | Bb | 20 | GLY | Peptide |
| 67 | Bd | 110 | GLU | Peptide |
| 78 | Bo | 93 | LEU | Peptide |
| 2 | CA | 165 | ARG | Peptide |
| 5 | CD | 203 | PRO | Peptide |
| 7 | CF | 44 | ASN | Peptide |
| 7 | CF | 99 | MET | Peptide |
| 11 | CJ | 168 | ARG | Peptide |
| 11 | CJ | 88 | GLU | Peptide |
| 11 | CJ | 89 | ASP | Peptide |
| 16 | CO | 131 | GLY | Peptide |
| 17 | CP | 52 | LYS | Peptide |
| 18 | CQ | 41 | PRO | Peptide |
| 22 | CU | 70 | THR | Peptide |
| 25 | CX | 44 | GLY | Peptide |
| 27 | CZ | 85 | LYS | Peptide |
| 27 | CZ | 87 | GLY | Peptide |
| 33 | Cf | 102 | VAL | Peptide |
| 33 | Cf | 129 | GLY | Peptide |
| 39 | DA | 143 | GLU | Peptide |
| 39 | DA | 211 | HIS | Peptide |
| 41 | DC | 91 | GLY | Peptide |
| 42 | DD | 271 | LYS | Peptide |
| 43 | DE | 129 | GLU | Peptide |
| 44 | DF | 192 | GLY | Peptide |
| 44 | DF | 226 | GLY | Peptide |
| 52 | DO | 110[A] | PRO | Peptide |
| 52 | DO | 68[B] | ARG | Peptide |
| 56 | DS | 133 | ALA | Peptide |
| 59 | DV | 41 | GLY | Peptide |
| 62 | DY | 111 | LEU | Peptide |
| 63 | DZ | 101 | PHE | Peptide |
| 64 | Da | 26 | ARG | Peptide |
| 64 | Da | 66 | ALA | Peptide |
| 64 | Da | 75 | LEU | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 65 | Db | 19 | ASN | Peptide |

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 2 | AA | 204/252 (81%) | 143 (70%) | 35 (17%) | 26 (13%) | 0 | 1 |
| 2 | CA | 204/252 (81%) | 146 (72%) | 33 (16%) | 25 (12%) | 0 | 1 |
| 3 | AB | 212/255 (83%) | 133 (63%) | 41 (19%) | 38 (18%) | 0 | 0 |
| 3 | CB | 214/255 (84%) | 174 (81%) | 25 (12%) | 15 (7%) | 1 | 6 |
| 4 | AC | 215/254 (85%) | 187 (87%) | 16 (7%) | 12 (6%) | 2 | 10 |
| 4 | CC | 215/254 (85%) | 188 (87%) | 14 (6%) | 13 (6%) | 1 | 9 |
| 5 | AD | 221/240 (92%) | 180 (81%) | 28 (13%) | 13 (6%) | 1 | 9 |
| 5 | CD | 221/240 (92%) | 177 (80%) | 23 (10%) | 21 (10%) | 0 | 3 |
| 6 | AE | 258/261 (99%) | 201 (78%) | 36 (14%) | 21 (8%) | 1 | 4 |
| 6 | CE | 258/261 (99%) | 219 (85%) | 19 (7%) | 20 (8%) | 1 | 4 |
| 7 | AF | 204/225 (91%) | 154 (76%) | 31 (15%) | 19 (9%) | 0 | 3 |
| 7 | CF | 204/225 (91%) | 155 (76%) | 32 (16%) | 17 (8%) | 1 | 4 |
| 8 | AG | 224/236 (95%) | 190 (85%) | 22 (10%) | 12 (5%) | 2 | 11 |
| 8 | CG | 216/236 (92%) | 183 (85%) | 21 (10%) | 12 (6%) | 2 | 10 |
| 9 | AH | 182/190 (96%) | 127 (70%) | 28 (15%) | 27 (15%) | 0 | 1 |
| 9 | CH | 184/190 (97%) | 143 (78%) | 23 (12%) | 18 (10%) | 0 | 2 |
| 10 | AI | 184/200 (92%) | 155 (84%) | 14 (8%) | 15 (8%) | 1 | 4 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 10 | CI | 184/200 (92%) | 160 (87%) | 17 (9%) | 7 (4%) | 3 | 18 |
| 11 | AJ | 183/197 (93%) | 152 (83%) | 19 (10%) | 12 (7%) | 1 | 6 |
| 11 | CJ | 183/197 (93%) | 152 (83%) | 17 (9%) | 14 (8%) | 1 | 5 |
| 12 | AK | 94/105 (90%) | 66 (70%) | 18 (19%) | 10 (11%) | 0 | 2 |
| 12 | CK | 92/105 (88%) | 59 (64%) | 15 (16%) | 18 (20%) | 0 | 0 |
| 13 | AL | 153/156 (98%) | 125 (82%) | 19 (12%) | 9 (6%) | 1 | 9 |
| 13 | CL | 144/156 (92%) | 118 (82%) | 15 (10%) | 11 (8%) | 1 | 5 |
| 14 | AM | 122/143 (85%) | 66 (54%) | 23 (19%) | 33 (27%) | 0 | 0 |
| 14 | CM | 122/143 (85%) | 60 (49%) | 31 (25%) | 31 (25%) | 0 | 0 |
| 15 | AN | 148/151 (98%) | 125 (84%) | 15 (10%) | 8 (5%) | 2 | 11 |
| 15 | CN | 148/151 (98%) | 129 (87%) | 10 (7%) | 9 (6%) | 1 | 8 |
| 16 | AO | 125/137 (91%) | 94 (75%) | 16 (13%) | 15 (12%) | 0 | 1 |
| 16 | CO | 126/137 (92%) | 101 (80%) | 20 (16%) | 5 (4%) | 3 | 17 |
| 17 | AP | 122/142 (86%) | 92 (75%) | 15 (12%) | 15 (12%) | 0 | 1 |
| 17 | CP | 133/142 (94%) | 91 (68%) | 20 (15%) | 22 (16%) | 0 | 0 |
| 18 | AQ | 139/143 (97%) | 114 (82%) | 14 (10%) | 11 (8%) | 1 | 4 |
| 18 | CQ | 140/143 (98%) | 122 (87%) | 10 (7%) | 8 (6%) | 1 | 10 |
| 19 | AR | 116/136 (85%) | 87 (75%) | 17 (15%) | 12 (10%) | 0 | 2 |
| 19 | CR | 113/136 (83%) | 92 (81%) | 12 (11%) | 9 (8%) | 1 | 4 |
| 20 | AS | 143/146 (98%) | 110 (77%) | 19 (13%) | 14 (10%) | 0 | 2 |
| 20 | CS | 143/146 (98%) | 111 (78%) | 25 (18%) | 7 (5%) | 2 | 13 |
| 21 | AT | 141/144 (98%) | 111 (79%) | 18 (13%) | 12 (8%) | 1 | 4 |
| 21 | CT | 141/144 (98%) | 125 (89%) | 9 (6%) | 7 (5%) | 2 | 12 |
| 22 | AU | 105/121 (87%) | 87 (83%) | 13 (12%) | 5 (5%) | 2 | 13 |
| 22 | CU | 108/121 (89%) | 81 (75%) | 12 (11%) | 15 (14%) | 0 | 1 |
| 23 | AV | 85/87 (98%) | 64 (75%) | 11 (13%) | 10 (12%) | 0 | 1 |
| 23 | CV | 85/87 (98%) | 71 (84%) | 7 (8%) | 7 (8%) | 1 | 4 |
| 24 | AW | 127/130 (98%) | 114 (90%) | 10 (8%) | 3 (2%) | 6 | 29 |
| 24 | CW | 127/130 (98%) | 115 (91%) | 12 (9%) | 0 | 100 | 100 |
| 25 | AX | 142/145 (98%) | 111 (78%) | 13 (9%) | 18 (13%) | 0 | 1 |
| 25 | CX | 142/145 (98%) | 127 (89%) | 13 (9%) | 2 (1%) | 11 | 43 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 26 | AY | 132/135 (98%) | 106 (80%) | 13 (10%) | 13 (10%) | 0 | 2 |
| 26 | CY | 132/135 (98%) | 100 (76%) | 17 (13%) | 15 (11%) | 0 | 2 |
| 27 | AZ | 68/108 (63%) | 46 (68%) | 11 (16%) | 11 (16%) | 0 | 1 |
| 27 | CZ | 67/108 (62%) | 50 (75%) | 10 (15%) | 7 (10%) | 0 | 2 |
| 28 | Aa | 95/119 (80%) | 57 (60%) | 21 (22%) | 17 (18%) | 0 | 0 |
| 28 | Ca | 95/119 (80%) | 67 (70%) | 20 (21%) | 8 (8%) | 1 | 4 |
| 29 | Ab | 79/82 (96%) | 62 (78%) | 13 (16%) | 4 (5%) | 2 | 12 |
| 29 | Cb | 79/82 (96%) | 62 (78%) | 9 (11%) | 8 (10%) | 0 | 2 |
| 30 | Ac | 61/67 (91%) | 47 (77%) | 9 (15%) | 5 (8%) | 1 | 4 |
| 30 | Cc | 61/67 (91%) | 41 (67%) | 17 (28%) | 3 (5%) | 2 | 13 |
| 31 | Ad | 51/56 (91%) | 43 (84%) | 6 (12%) | 2 (4%) | 3 | 17 |
| 31 | Cd | 51/56 (91%) | 45 (88%) | 2 (4%) | 4 (8%) | 1 | 4 |
| 32 | Ae | 58/63 (92%) | 49 (84%) | 7 (12%) | 2 (3%) | 3 | 20 |
| 32 | Ce | 60/63 (95%) | 45 (75%) | 9 (15%) | 6 (10%) | 0 | 2 |
| 33 | Af | 50/152 (33%) | 30 (60%) | 9 (18%) | 11 (22%) | 0 | 0 |
| 33 | Cf | 50/152 (33%) | 26 (52%) | 13 (26%) | 11 (22%) | 0 | 0 |
| 34 | Ag | 316/319 (99%) | 273 (86%) | 30 (10%) | 13 (4%) | 3 | 16 |
| 34 | Cg | 316/319 (99%) | 262 (83%) | 38 (12%) | 16 (5%) | 2 | 12 |
| 35 | Ah | 120/273 (44%) | 92 (77%) | 17 (14%) | 11 (9%) | 1 | 3 |
| 39 | BA | 250/254 (98%) | 230 (92%) | 14 (6%) | 6 (2%) | 6 | 29 |
| 39 | DA | 250/254 (98%) | 213 (85%) | 30 (12%) | 7 (3%) | 5 | 25 |
| 40 | BB | 384/387 (99%) | 333 (87%) | 37 (10%) | 14 (4%) | 3 | 19 |
| 40 | DB | 384/387 (99%) | 341 (89%) | 34 (9%) | 9 (2%) | 6 | 30 |
| 41 | BC | 359/362 (99%) | 304 (85%) | 34 (10%) | 21 (6%) | 1 | 10 |
| 41 | DC | 359/362 (99%) | 306 (85%) | 32 (9%) | 21 (6%) | 1 | 10 |
| 42 | BD | 294/297 (99%) | 242 (82%) | 31 (10%) | 21 (7%) | 1 | 5 |
| 42 | DD | 292/297 (98%) | 267 (91%) | 19 (6%) | 6 (2%) | 7 | 33 |
| 43 | BE | 152/176 (86%) | 137 (90%) | 11 (7%) | 4 (3%) | 5 | 27 |
| 43 | DE | 153/176 (87%) | 134 (88%) | 15 (10%) | 4 (3%) | 5 | 27 |
| 44 | BF | 220/244 (90%) | 200 (91%) | 11 (5%) | 9 (4%) | 3 | 16 |
| 44 | DF | 221/244 (91%) | 201 (91%) | 15 (7%) | 5 (2%) | 6 | 30 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|----------|-------------|----|
| 45 | BG | 231/256 (90%) | 186 (80%) | 26 (11%) | 19 (8%) | 1 | 4 |
| 45 | DG | 229/256 (90%) | 180 (79%) | 28 (12%) | 21 (9%) | 1 | 3 |
| 46 | BH | 189/191 (99%) | 166 (88%) | 17 (9%) | 6 (3%) | 4 | 22 |
| 46 | DH | 189/191 (99%) | 172 (91%) | 13 (7%) | 4 (2%) | 7 | 33 |
| 47 | BI | 207/221 (94%) | 181 (87%) | 19 (9%) | 7 (3%) | 3 | 20 |
| 47 | DI | 209/221 (95%) | 175 (84%) | 22 (10%) | 12 (6%) | 1 | 10 |
| 48 | BJ | 167/174 (96%) | 120 (72%) | 26 (16%) | 21 (13%) | 0 | 1 |
| 48 | DJ | 167/174 (96%) | 135 (81%) | 19 (11%) | 13 (8%) | 1 | 4 |
| 49 | BL | 191/199 (96%) | 161 (84%) | 18 (9%) | 12 (6%) | 1 | 7 |
| 49 | DL | 192/199 (96%) | 161 (84%) | 20 (10%) | 11 (6%) | 1 | 10 |
| 50 | BM | 134/138 (97%) | 117 (87%) | 8 (6%) | 9 (7%) | 1 | 6 |
| 50 | DM | 135/138 (98%) | 124 (92%) | 10 (7%) | 1 (1%) | 22 | 60 |
| 51 | BN | 201/204 (98%) | 184 (92%) | 10 (5%) | 7 (4%) | 3 | 20 |
| 51 | DN | 201/204 (98%) | 182 (90%) | 13 (6%) | 6 (3%) | 4 | 24 |
| 52 | BO | 353/219 (161%) | 332 (94%) | 14 (4%) | 7 (2%) | 7 | 34 |
| 52 | DO | 352/219 (161%) | 324 (92%) | 18 (5%) | 10 (3%) | 5 | 25 |
| 53 | BP | 181/184 (98%) | 155 (86%) | 17 (9%) | 9 (5%) | 2 | 12 |
| 53 | DP | 153/184 (83%) | 142 (93%) | 9 (6%) | 2 (1%) | 12 | 45 |
| 54 | BQ | 183/186 (98%) | 162 (88%) | 17 (9%) | 4 (2%) | 6 | 31 |
| 54 | DQ | 183/186 (98%) | 168 (92%) | 9 (5%) | 6 (3%) | 4 | 21 |
| 55 | BR | 186/189 (98%) | 170 (91%) | 12 (6%) | 4 (2%) | 6 | 31 |
| 55 | DR | 186/189 (98%) | 167 (90%) | 16 (9%) | 3 (2%) | 9 | 40 |
| 56 | BS | 170/172 (99%) | 154 (91%) | 12 (7%) | 4 (2%) | 6 | 29 |
| 56 | DS | 170/172 (99%) | 163 (96%) | 6 (4%) | 1 (1%) | 25 | 64 |
| 57 | BT | 157/160 (98%) | 140 (89%) | 10 (6%) | 7 (4%) | 2 | 14 |
| 57 | DT | 157/160 (98%) | 146 (93%) | 9 (6%) | 2 (1%) | 12 | 45 |
| 58 | BU | 98/121 (81%) | 75 (76%) | 14 (14%) | 9 (9%) | 1 | 3 |
| 58 | DU | 96/121 (79%) | 80 (83%) | 13 (14%) | 3 (3%) | 4 | 23 |
| 59 | BV | 134/137 (98%) | 124 (92%) | 9 (7%) | 1 (1%) | 22 | 60 |
| 59 | DV | 134/137 (98%) | 124 (92%) | 8 (6%) | 2 (2%) | 10 | 42 |
| 60 | BW | 96/155 (62%) | 69 (72%) | 16 (17%) | 11 (12%) | 0 | 2 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 60 | DW | 133/155 (86%) | 106 (80%) | 19 (14%) | 8 (6%) | 1 | 9 |
| 61 | BX | 119/142 (84%) | 106 (89%) | 11 (9%) | 2 (2%) | 9 | 39 |
| 61 | DX | 118/142 (83%) | 103 (87%) | 7 (6%) | 8 (7%) | 1 | 6 |
| 62 | BY | 124/127 (98%) | 107 (86%) | 15 (12%) | 2 (2%) | 9 | 40 |
| 62 | DY | 124/127 (98%) | 107 (86%) | 12 (10%) | 5 (4%) | 3 | 17 |
| 63 | BZ | 133/136 (98%) | 114 (86%) | 9 (7%) | 10 (8%) | 1 | 5 |
| 63 | DZ | 133/136 (98%) | 107 (80%) | 13 (10%) | 13 (10%) | 0 | 2 |
| 64 | Ba | 146/149 (98%) | 120 (82%) | 15 (10%) | 11 (8%) | 1 | 5 |
| 64 | Da | 146/149 (98%) | 123 (84%) | 18 (12%) | 5 (3%) | 3 | 20 |
| 65 | Bb | 56/59 (95%) | 44 (79%) | 9 (16%) | 3 (5%) | 2 | 11 |
| 65 | Db | 56/59 (95%) | 44 (79%) | 7 (12%) | 5 (9%) | 1 | 3 |
| 66 | Bc | 95/105 (90%) | 86 (90%) | 8 (8%) | 1 (1%) | 14 | 50 |
| 66 | Dc | 98/105 (93%) | 87 (89%) | 8 (8%) | 3 (3%) | 4 | 23 |
| 67 | Bd | 107/113 (95%) | 94 (88%) | 8 (8%) | 5 (5%) | 2 | 14 |
| 67 | Dd | 107/113 (95%) | 88 (82%) | 13 (12%) | 6 (6%) | 2 | 10 |
| 68 | Be | 125/130 (96%) | 111 (89%) | 10 (8%) | 4 (3%) | 4 | 22 |
| 68 | De | 125/130 (96%) | 110 (88%) | 9 (7%) | 6 (5%) | 2 | 13 |
| 69 | Bf | 104/107 (97%) | 100 (96%) | 2 (2%) | 2 (2%) | 8 | 36 |
| 69 | Df | 104/107 (97%) | 96 (92%) | 5 (5%) | 3 (3%) | 4 | 24 |
| 70 | Bg | 110/121 (91%) | 97 (88%) | 9 (8%) | 4 (4%) | 3 | 19 |
| 70 | Dg | 110/121 (91%) | 93 (84%) | 13 (12%) | 4 (4%) | 3 | 19 |
| 71 | Bh | 117/120 (98%) | 99 (85%) | 10 (8%) | 8 (7%) | 1 | 6 |
| 71 | Dh | 117/120 (98%) | 99 (85%) | 14 (12%) | 4 (3%) | 3 | 20 |
| 72 | Bi | 97/100 (97%) | 75 (77%) | 11 (11%) | 11 (11%) | 0 | 2 |
| 72 | Di | 97/100 (97%) | 77 (79%) | 13 (13%) | 7 (7%) | 1 | 5 |
| 73 | Bj | 85/88 (97%) | 70 (82%) | 12 (14%) | 3 (4%) | 3 | 20 |
| 73 | Dj | 85/88 (97%) | 75 (88%) | 8 (9%) | 2 (2%) | 6 | 29 |
| 74 | Bk | 75/78 (96%) | 66 (88%) | 8 (11%) | 1 (1%) | 12 | 45 |
| 74 | Dk | 75/78 (96%) | 61 (81%) | 10 (13%) | 4 (5%) | 2 | 11 |
| 75 | Bl | 48/51 (94%) | 44 (92%) | 4 (8%) | 0 | 100 | 100 |
| 75 | Dl | 48/51 (94%) | 41 (85%) | 6 (12%) | 1 (2%) | 7 | 33 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|------------|-----------|-------------|-----|
| 76 | Bm | 50/128 (39%) | 45 (90%) | 3 (6%) | 2 (4%) | 3 | 17 |
| 76 | Dm | 50/128 (39%) | 48 (96%) | 1 (2%) | 1 (2%) | 7 | 34 |
| 77 | Bn | 23/25 (92%) | 20 (87%) | 3 (13%) | 0 | 100 | 100 |
| 77 | Dn | 23/25 (92%) | 22 (96%) | 0 | 1 (4%) | 2 | 15 |
| 78 | Bo | 103/106 (97%) | 86 (84%) | 13 (13%) | 4 (4%) | 3 | 17 |
| 78 | Do | 103/106 (97%) | 90 (87%) | 11 (11%) | 2 (2%) | 8 | 36 |
| 79 | Bp | 89/92 (97%) | 77 (86%) | 9 (10%) | 3 (3%) | 3 | 20 |
| 79 | Dp | 89/92 (97%) | 81 (91%) | 8 (9%) | 0 | 100 | 100 |
| 81 | Ch | 61/273 (22%) | 38 (62%) | 9 (15%) | 14 (23%) | 0 | 0 |
| 83 | Dq | 117/312 (38%) | 93 (80%) | 18 (15%) | 6 (5%) | 2 | 12 |
| All | All | 22511/24658 (91%) | 18787 (84%) | 2329 (10%) | 1395 (6%) | 1 | 8 |

All (1395) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AA | 4 | PRO |
| 2 | AA | 29 | VAL |
| 2 | AA | 30 | GLN |
| 2 | AA | 39 | ASN |
| 2 | AA | 66 | ALA |
| 2 | AA | 95 | ALA |
| 2 | AA | 111 | ILE |
| 2 | AA | 191 | ARG |
| 2 | AA | 203 | PHE |
| 2 | AA | 205 | ARG |
| 3 | AB | 21 | VAL |
| 3 | AB | 26 | ARG |
| 3 | AB | 49 | ASN |
| 3 | AB | 58 | SER |
| 3 | AB | 60 | ALA |
| 3 | AB | 63 | GLY |
| 3 | AB | 113 | MET |
| 3 | AB | 116 | LYS |
| 3 | AB | 176 | VAL |
| 3 | AB | 177 | GLN |
| 3 | AB | 179 | SER |
| 3 | AB | 182 | ALA |
| 3 | AB | 206 | PRO |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 3 | AB | 221 | PRO |
| 4 | AC | 146 | THR |
| 4 | AC | 148 | LEU |
| 5 | AD | 4 | LEU |
| 5 | AD | 62 | ASN |
| 5 | AD | 65 | ARG |
| 5 | AD | 93 | ASP |
| 5 | AD | 211 | PRO |
| 5 | AD | 212 | LYS |
| 5 | AD | 216 | PRO |
| 5 | AD | 220 | PRO |
| 6 | AE | 104 | ASP |
| 6 | AE | 142 | HIS |
| 6 | AE | 153 | ASN |
| 6 | AE | 164 | LEU |
| 6 | AE | 260 | GLY |
| 7 | AF | 26 | ALA |
| 7 | AF | 39 | GLU |
| 7 | AF | 43 | PHE |
| 7 | AF | 63 | GLN |
| 7 | AF | 101 | GLY |
| 7 | AF | 153 | GLY |
| 7 | AF | 206 | SER |
| 8 | AG | 20 | ASP |
| 8 | AG | 25 | ARG |
| 8 | AG | 154 | ARG |
| 8 | AG | 173 | PRO |
| 8 | AG | 174 | LYS |
| 9 | AH | 31 | SER |
| 9 | AH | 36 | ALA |
| 9 | AH | 64 | VAL |
| 9 | AH | 67 | LEU |
| 9 | AH | 98 | ILE |
| 9 | AH | 105 | THR |
| 9 | AH | 111 | LYS |
| 9 | AH | 112 | ARG |
| 9 | AH | 131 | PHE |
| 9 | AH | 133 | THR |
| 9 | AH | 134 | GLU |
| 9 | AH | 155 | ASP |
| 10 | AI | 13 | ALA |
| 10 | AI | 22 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 10 | AI | 147 | ALA |
| 10 | AI | 149 | SER |
| 11 | AJ | 98 | ALA |
| 11 | AJ | 100 | LYS |
| 11 | AJ | 118 | LEU |
| 11 | AJ | 121 | SER |
| 11 | AJ | 164 | PHE |
| 12 | AK | 60 | SER |
| 12 | AK | 81 | ASN |
| 12 | AK | 87 | VAL |
| 12 | AK | 88 | PRO |
| 12 | AK | 93 | GLN |
| 13 | AL | 7 | VAL |
| 13 | AL | 29 | LYS |
| 13 | AL | 133 | LYS |
| 14 | AM | 21 | GLU |
| 14 | AM | 25 | GLU |
| 14 | AM | 45 | LEU |
| 14 | AM | 55 | GLY |
| 14 | AM | 83 | GLU |
| 14 | AM | 87 | PRO |
| 14 | AM | 89 | ILE |
| 14 | AM | 90 | LYS |
| 14 | AM | 93 | ASP |
| 14 | AM | 126 | TRP |
| 15 | AN | 19 | SER |
| 15 | AN | 22 | ALA |
| 16 | AO | 38 | THR |
| 16 | AO | 39 | ILE |
| 16 | AO | 124 | ASP |
| 16 | AO | 125 | SER |
| 16 | AO | 126 | THR |
| 17 | AP | 29 | SER |
| 17 | AP | 54 | ALA |
| 17 | AP | 125 | PRO |
| 17 | AP | 126 | VAL |
| 18 | AQ | 41 | PRO |
| 18 | AQ | 58 | ASP |
| 18 | AQ | 59 | LYS |
| 18 | AQ | 114 | ARG |
| 18 | AQ | 116 | LEU |
| 18 | AQ | 138 | PHE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 19 | AR | 6 | THR |
| 19 | AR | 26 | LEU |
| 19 | AR | 85 | VAL |
| 19 | AR | 86 | PRO |
| 19 | AR | 88 | VAL |
| 19 | AR | 96 | SER |
| 19 | AR | 124 | VAL |
| 20 | AS | 14 | ILE |
| 20 | AS | 25 | ASN |
| 20 | AS | 28 | ILE |
| 20 | AS | 60 | GLU |
| 20 | AS | 91 | ASP |
| 20 | AS | 92 | ILE |
| 21 | AT | 31 | PRO |
| 21 | AT | 53 | TRP |
| 21 | AT | 69 | LYS |
| 22 | AU | 118 | VAL |
| 23 | AV | 4 | ASP |
| 23 | AV | 7 | GLN |
| 23 | AV | 11 | LEU |
| 25 | AX | 3 | LYS |
| 25 | AX | 41 | SER |
| 25 | AX | 96 | VAL |
| 25 | AX | 114 | LYS |
| 25 | AX | 128 | SER |
| 25 | AX | 131 | SER |
| 25 | AX | 137 | LYS |
| 25 | AX | 138 | GLU |
| 25 | AX | 144 | ARG |
| 26 | AY | 32 | ARG |
| 26 | AY | 36 | SER |
| 26 | AY | 78 | SER |
| 27 | AZ | 38 | HIS |
| 27 | AZ | 39 | ALA |
| 27 | AZ | 43 | ASP |
| 27 | AZ | 44 | GLN |
| 27 | AZ | 54 | VAL |
| 27 | AZ | 71 | ILE |
| 27 | AZ | 88 | ILE |
| 28 | Aa | 19 | LYS |
| 28 | Aa | 45 | VAL |
| 28 | Aa | 46 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 28 | Aa | 62 | TYR |
| 28 | Aa | 65 | PRO |
| 28 | Aa | 82 | ARG |
| 28 | Aa | 84 | VAL |
| 28 | Aa | 85 | ARG |
| 29 | Ab | 38 | PRO |
| 29 | Ab | 62 | ILE |
| 30 | Ac | 36 | THR |
| 30 | Ac | 51 | ASN |
| 31 | Ad | 8 | PHE |
| 32 | Ae | 47 | VAL |
| 33 | Af | 102 | VAL |
| 33 | Af | 103 | LEU |
| 33 | Af | 106 | TYR |
| 33 | Af | 111 | GLU |
| 33 | Af | 128 | ALA |
| 33 | Af | 148 | TYR |
| 34 | Ag | 51 | ASP |
| 34 | Ag | 160 | GLU |
| 34 | Ag | 318 | ALA |
| 35 | Ah | 47 | ALA |
| 35 | Ah | 52 | PRO |
| 35 | Ah | 85 | SER |
| 35 | Ah | 87 | THR |
| 39 | BA | 144 | ASN |
| 40 | BB | 3 | HIS |
| 40 | BB | 5 | LYS |
| 40 | BB | 140 | ASP |
| 40 | BB | 174 | LYS |
| 40 | BB | 300 | ARG |
| 40 | BB | 347 | SER |
| 40 | BB | 351 | LEU |
| 40 | BB | 385 | LYS |
| 41 | BC | 4 | PRO |
| 41 | BC | 268 | ALA |
| 41 | BC | 269 | SER |
| 41 | BC | 283 | THR |
| 41 | BC | 292 | SER |
| 41 | BC | 320 | ASN |
| 41 | BC | 338 | LYS |
| 41 | BC | 361 | HIS |
| 42 | BD | 20 | PHE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 42 | BD | 58 | LYS |
| 42 | BD | 124 | GLU |
| 42 | BD | 125 | VAL |
| 42 | BD | 210 | GLU |
| 42 | BD | 233 | ALA |
| 42 | BD | 234 | ASP |
| 42 | BD | 258 | LYS |
| 42 | BD | 276 | LYS |
| 42 | BD | 293 | LEU |
| 42 | BD | 295 | GLY |
| 43 | BE | 6 | ALA |
| 44 | BF | 25 | GLN |
| 44 | BF | 26 | VAL |
| 44 | BF | 216 | VAL |
| 45 | BG | 25 | PRO |
| 45 | BG | 31 | PRO |
| 45 | BG | 36 | ILE |
| 45 | BG | 37 | GLY |
| 45 | BG | 156 | ASP |
| 46 | BH | 50 | ASN |
| 46 | BH | 109 | ALA |
| 47 | BI | 113 | GLN |
| 47 | BI | 207 | GLU |
| 47 | BI | 218 | ALA |
| 47 | BI | 219 | ALA |
| 48 | BJ | 8 | PRO |
| 48 | BJ | 11 | ASP |
| 48 | BJ | 12 | LEU |
| 48 | BJ | 74 | PRO |
| 48 | BJ | 94 | ARG |
| 48 | BJ | 165 | GLN |
| 49 | BL | 5 | LYS |
| 49 | BL | 47 | ALA |
| 49 | BL | 50 | PRO |
| 49 | BL | 129 | ASN |
| 49 | BL | 131 | LYS |
| 49 | BL | 193 | ALA |
| 50 | BM | 8 | LYS |
| 50 | BM | 9 | ALA |
| 50 | BM | 135 | LEU |
| 50 | BM | 136 | ALA |
| 51 | BN | 74 | PRO |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 51 | BN | 75 | VAL |
| 52 | BO | 3[B] | SER |
| 52 | BO | 111[A] | PRO |
| 52 | BO | 111[B] | PRO |
| 53 | BP | 157 | VAL |
| 54 | BQ | 99 | THR |
| 55 | BR | 5 | ARG |
| 55 | BR | 47 | ASN |
| 56 | BS | 167 | ARG |
| 57 | BT | 124 | VAL |
| 57 | BT | 159 | PHE |
| 58 | BU | 107 | PHE |
| 60 | BW | 26 | SER |
| 60 | BW | 81 | PRO |
| 60 | BW | 86 | SER |
| 60 | BW | 97 | LYS |
| 61 | BX | 44 | PRO |
| 62 | BY | 84 | LYS |
| 63 | BZ | 17 | ARG |
| 63 | BZ | 59 | ALA |
| 63 | BZ | 125 | GLY |
| 63 | BZ | 128 | GLN |
| 63 | BZ | 129 | TRP |
| 64 | Ba | 66 | ALA |
| 64 | Ba | 76 | ASP |
| 66 | Bc | 100 | ILE |
| 67 | Bd | 5 | LYS |
| 67 | Bd | 6 | ASP |
| 67 | Bd | 7 | VAL |
| 67 | Bd | 83 | GLU |
| 67 | Bd | 84 | ASP |
| 68 | Be | 12 | LYS |
| 68 | Be | 27 | ARG |
| 68 | Be | 123 | LYS |
| 71 | Bh | 97 | ALA |
| 71 | Bh | 119 | LYS |
| 72 | Bi | 13 | LYS |
| 72 | Bi | 33 | ALA |
| 73 | Bj | 85 | LYS |
| 76 | Bm | 78 | ILE |
| 78 | Bo | 94 | GLY |
| 78 | Bo | 100 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | CA | 4 | PRO |
| 2 | CA | 8 | ASP |
| 2 | CA | 22 | THR |
| 2 | CA | 23 | HIS |
| 2 | CA | 44 | GLY |
| 2 | CA | 163 | ASN |
| 2 | CA | 164 | ASN |
| 2 | CA | 185 | ARG |
| 2 | CA | 187 | ALA |
| 2 | CA | 189 | VAL |
| 2 | CA | 203 | PHE |
| 2 | CA | 206 | ASP |
| 3 | CB | 26 | ARG |
| 3 | CB | 62 | LYS |
| 3 | CB | 81 | PHE |
| 3 | CB | 82 | ARG |
| 3 | CB | 147 | ALA |
| 3 | CB | 179 | SER |
| 3 | CB | 206 | PRO |
| 3 | CB | 210 | ILE |
| 3 | CB | 223 | PHE |
| 4 | CC | 91 | ARG |
| 4 | CC | 92 | ALA |
| 4 | CC | 107 | SER |
| 4 | CC | 248 | SER |
| 5 | CD | 4 | LEU |
| 5 | CD | 44 | THR |
| 5 | CD | 61 | GLU |
| 5 | CD | 91 | VAL |
| 5 | CD | 113 | LEU |
| 5 | CD | 115 | ILE |
| 5 | CD | 211 | PRO |
| 5 | CD | 212 | LYS |
| 5 | CD | 216 | PRO |
| 5 | CD | 217 | ILE |
| 5 | CD | 219 | ALA |
| 5 | CD | 220 | PRO |
| 6 | CE | 24 | SER |
| 6 | CE | 95 | THR |
| 6 | CE | 163 | ASP |
| 6 | CE | 164 | LEU |
| 6 | CE | 196 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 7 | CF | 28 | PRO |
| 7 | CF | 39 | GLU |
| 7 | CF | 54 | LYS |
| 7 | CF | 58 | LEU |
| 7 | CF | 125 | THR |
| 7 | CF | 153 | GLY |
| 7 | CF | 184 | PHE |
| 8 | CG | 153 | VAL |
| 8 | CG | 173 | PRO |
| 8 | CG | 174 | LYS |
| 9 | CH | 10 | SER |
| 9 | CH | 11 | GLN |
| 9 | CH | 31 | SER |
| 9 | CH | 64 | VAL |
| 9 | CH | 67 | LEU |
| 9 | CH | 74 | GLN |
| 9 | CH | 110 | GLN |
| 9 | CH | 116 | ARG |
| 9 | CH | 131 | PHE |
| 9 | CH | 163 | ASP |
| 9 | CH | 185 | ILE |
| 10 | CI | 116 | HIS |
| 11 | CJ | 118 | LEU |
| 11 | CJ | 121 | SER |
| 11 | CJ | 168 | ARG |
| 12 | CK | 23 | ALA |
| 12 | CK | 79 | TYR |
| 12 | CK | 82 | LEU |
| 12 | CK | 83 | PRO |
| 12 | CK | 88 | PRO |
| 12 | CK | 92 | ILE |
| 12 | CK | 97 | PRO |
| 14 | CM | 21 | GLU |
| 14 | CM | 66 | VAL |
| 14 | CM | 83 | GLU |
| 14 | CM | 84 | ASN |
| 14 | CM | 85 | LYS |
| 14 | CM | 87 | PRO |
| 14 | CM | 89 | ILE |
| 14 | CM | 91 | VAL |
| 14 | CM | 93 | ASP |
| 14 | CM | 109 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 15 | CN | 19 | SER |
| 15 | CN | 66 | ILE |
| 15 | CN | 87 | ASP |
| 16 | CO | 50 | ALA |
| 16 | CO | 126 | THR |
| 17 | CP | 9 | LYS |
| 17 | CP | 11 | VAL |
| 17 | CP | 51 | SER |
| 17 | CP | 52 | LYS |
| 17 | CP | 68 | PRO |
| 17 | CP | 125 | PRO |
| 17 | CP | 126 | VAL |
| 17 | CP | 127 | ARG |
| 17 | CP | 135 | THR |
| 18 | CQ | 42 | GLU |
| 18 | CQ | 115 | THR |
| 18 | CQ | 116 | LEU |
| 19 | CR | 88 | VAL |
| 19 | CR | 96 | SER |
| 19 | CR | 98 | GLY |
| 19 | CR | 104 | ASN |
| 19 | CR | 116 | LYS |
| 20 | CS | 91 | ASP |
| 20 | CS | 92 | ILE |
| 21 | CT | 29 | GLU |
| 21 | CT | 33 | TYR |
| 21 | CT | 34 | VAL |
| 22 | CU | 15 | GLN |
| 22 | CU | 17 | GLN |
| 22 | CU | 18 | GLN |
| 22 | CU | 49 | ASN |
| 22 | CU | 52 | LYS |
| 22 | CU | 96 | PRO |
| 22 | CU | 97 | VAL |
| 23 | CV | 78 | LEU |
| 25 | CX | 131 | SER |
| 26 | CY | 12 | VAL |
| 26 | CY | 30 | PRO |
| 26 | CY | 33 | ALA |
| 26 | CY | 35 | VAL |
| 26 | CY | 52 | LYS |
| 26 | CY | 68 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 26 | CY | 121 | THR |
| 26 | CY | 123 | LYS |
| 27 | CZ | 44 | GLN |
| 27 | CZ | 85 | LYS |
| 27 | CZ | 104 | ALA |
| 28 | Ca | 28 | LYS |
| 28 | Ca | 46 | GLU |
| 28 | Ca | 47 | ALA |
| 28 | Ca | 63 | ALA |
| 29 | Cb | 20 | LYS |
| 29 | Cb | 38 | PRO |
| 29 | Cb | 60 | SER |
| 29 | Cb | 62 | ILE |
| 31 | Cd | 6 | VAL |
| 31 | Cd | 19 | ARG |
| 32 | Ce | 45 | VAL |
| 32 | Ce | 60 | PRO |
| 33 | Cf | 102 | VAL |
| 33 | Cf | 103 | LEU |
| 33 | Cf | 106 | TYR |
| 33 | Cf | 136 | LYS |
| 33 | Cf | 148 | TYR |
| 34 | Cg | 4 | ASN |
| 34 | Cg | 160 | GLU |
| 34 | Cg | 163 | ASP |
| 34 | Cg | 165 | ASP |
| 34 | Cg | 318 | ALA |
| 81 | Ch | 42 | ALA |
| 81 | Ch | 50 | ASN |
| 81 | Ch | 66 | ALA |
| 81 | Ch | 69 | ARG |
| 39 | DA | 96 | LEU |
| 40 | DB | 129 | ALA |
| 40 | DB | 140 | ASP |
| 40 | DB | 347 | SER |
| 41 | DC | 14 | GLU |
| 41 | DC | 15 | ALA |
| 41 | DC | 90 | PHE |
| 41 | DC | 145 | ILE |
| 41 | DC | 302 | ALA |
| 41 | DC | 311 | HIS |
| 41 | DC | 329 | PRO |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 41 | DC | 330 | TYR |
| 41 | DC | 361 | HIS |
| 42 | DD | 215 | ASP |
| 42 | DD | 260 | PHE |
| 43 | DE | 97 | ASN |
| 43 | DE | 98 | VAL |
| 44 | DF | 158 | LYS |
| 45 | DG | 25 | PRO |
| 45 | DG | 26 | LEU |
| 45 | DG | 34 | PHE |
| 45 | DG | 122 | LYS |
| 47 | DI | 25 | ALA |
| 47 | DI | 82 | ARG |
| 47 | DI | 170 | LYS |
| 47 | DI | 175 | ASN |
| 47 | DI | 187 | ALA |
| 48 | DJ | 8 | PRO |
| 48 | DJ | 10 | ARG |
| 48 | DJ | 12 | LEU |
| 48 | DJ | 94 | ARG |
| 48 | DJ | 95 | ASN |
| 48 | DJ | 108 | GLU |
| 48 | DJ | 115 | LYS |
| 48 | DJ | 167 | TYR |
| 49 | DL | 47 | ALA |
| 49 | DL | 129 | ASN |
| 49 | DL | 134 | GLU |
| 49 | DL | 150 | PRO |
| 50 | DM | 136 | ALA |
| 51 | DN | 49 | ARG |
| 51 | DN | 146 | ALA |
| 51 | DN | 147 | ARG |
| 52 | DO | 110[A] | PRO |
| 52 | DO | 110[B] | PRO |
| 52 | DO | 111[A] | PRO |
| 52 | DO | 111[B] | PRO |
| 52 | DO | 180[A] | SER |
| 52 | DO | 180[B] | SER |
| 52 | DO | 181[A] | ALA |
| 52 | DO | 181[B] | ALA |
| 54 | DQ | 41 | ASP |
| 54 | DQ | 99 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 55 | DR | 35 | ALA |
| 56 | DS | 2 | ALA |
| 57 | DT | 136 | ARG |
| 59 | DV | 42 | SER |
| 60 | DW | 26 | SER |
| 60 | DW | 71 | ARG |
| 60 | DW | 76 | VAL |
| 61 | DX | 24 | LEU |
| 61 | DX | 25 | LYS |
| 61 | DX | 40 | LEU |
| 61 | DX | 44 | PRO |
| 61 | DX | 45 | LYS |
| 62 | DY | 77 | LYS |
| 62 | DY | 83 | ASP |
| 62 | DY | 84 | LYS |
| 62 | DY | 125 | LYS |
| 62 | DY | 126 | LEU |
| 63 | DZ | 5 | LEU |
| 63 | DZ | 125 | GLY |
| 63 | DZ | 129 | TRP |
| 64 | Da | 76 | ASP |
| 65 | Db | 21 | ILE |
| 65 | Db | 23 | LYS |
| 65 | Db | 25 | LYS |
| 65 | Db | 39 | PHE |
| 66 | Dc | 100 | ILE |
| 66 | Dc | 104 | LEU |
| 67 | Dd | 7 | VAL |
| 67 | Dd | 45 | GLY |
| 67 | Dd | 84 | ASP |
| 68 | De | 4 | LEU |
| 68 | De | 5 | PRO |
| 68 | De | 27 | ARG |
| 69 | Df | 88 | ASN |
| 70 | Dg | 10 | ARG |
| 70 | Dg | 100 | ILE |
| 71 | Dh | 40 | SER |
| 71 | Dh | 82 | ALA |
| 72 | Di | 33 | ALA |
| 72 | Di | 63 | ASN |
| 72 | Di | 64 | SER |
| 72 | Di | 98 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 73 | Dj | 87 | SER |
| 74 | Dk | 17 | ARG |
| 74 | Dk | 18 | ALA |
| 75 | Dl | 3 | ALA |
| 78 | Do | 78 | LYS |
| 2 | AA | 5 | ALA |
| 2 | AA | 49 | ASN |
| 2 | AA | 81 | PHE |
| 2 | AA | 94 | GLY |
| 2 | AA | 190 | ASP |
| 2 | AA | 194 | PRO |
| 2 | AA | 196 | SER |
| 3 | AB | 23 | PRO |
| 3 | AB | 55 | LYS |
| 3 | AB | 72 | ASP |
| 3 | AB | 79 | HIS |
| 3 | AB | 82 | ARG |
| 3 | AB | 93 | GLY |
| 3 | AB | 108 | ASP |
| 3 | AB | 148 | ASN |
| 3 | AB | 181 | LEU |
| 3 | AB | 207 | LEU |
| 4 | AC | 35 | TRP |
| 4 | AC | 203 | LYS |
| 4 | AC | 248 | SER |
| 5 | AD | 44 | THR |
| 5 | AD | 218 | LEU |
| 6 | AE | 12 | LEU |
| 6 | AE | 152 | PRO |
| 6 | AE | 157 | ASN |
| 6 | AE | 195 | ILE |
| 6 | AE | 245 | LYS |
| 7 | AF | 35 | GLN |
| 7 | AF | 45 | LYS |
| 7 | AF | 58 | LEU |
| 7 | AF | 127 | GLN |
| 7 | AF | 150 | GLY |
| 7 | AF | 223 | SER |
| 8 | AG | 24 | ILE |
| 8 | AG | 146 | GLY |
| 8 | AG | 152 | ASP |
| 8 | AG | 153 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 9 | AH | 32 | PRO |
| 9 | AH | 104 | ARG |
| 9 | AH | 156 | SER |
| 9 | AH | 186 | PRO |
| 10 | AI | 40 | ALA |
| 10 | AI | 105 | ASP |
| 10 | AI | 120 | THR |
| 10 | AI | 199 | LYS |
| 11 | AJ | 134 | ILE |
| 11 | AJ | 167 | ALA |
| 11 | AJ | 171 | ARG |
| 12 | AK | 30 | ALA |
| 12 | AK | 64 | TYR |
| 12 | AK | 82 | LEU |
| 14 | AM | 54 | ARG |
| 14 | AM | 63 | VAL |
| 14 | AM | 66 | VAL |
| 14 | AM | 84 | ASN |
| 14 | AM | 91 | VAL |
| 14 | AM | 113 | ARG |
| 14 | AM | 128 | ALA |
| 15 | AN | 13 | SER |
| 15 | AN | 27 | LYS |
| 15 | AN | 28 | LEU |
| 15 | AN | 68 | GLY |
| 16 | AO | 40 | ALA |
| 16 | AO | 42 | VAL |
| 16 | AO | 46 | MET |
| 16 | AO | 50 | ALA |
| 16 | AO | 51 | ASP |
| 16 | AO | 114 | ARG |
| 17 | AP | 48 | GLY |
| 17 | AP | 51 | SER |
| 17 | AP | 101 | ALA |
| 18 | AQ | 40 | GLU |
| 18 | AQ | 113 | ASP |
| 19 | AR | 25 | THR |
| 20 | AS | 59 | GLY |
| 20 | AS | 61 | LEU |
| 20 | AS | 142 | GLY |
| 21 | AT | 11 | ALA |
| 21 | AT | 28 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 21 | AT | 50 | ALA |
| 22 | AU | 17 | GLN |
| 23 | AV | 12 | TYR |
| 24 | AW | 66 | ASN |
| 25 | AX | 8 | GLY |
| 25 | AX | 97 | ASP |
| 26 | AY | 5 | VAL |
| 26 | AY | 11 | LYS |
| 27 | AZ | 73 | GLY |
| 28 | Aa | 36 | ILE |
| 28 | Aa | 63 | ALA |
| 28 | Aa | 75 | VAL |
| 28 | Aa | 86 | VAL |
| 29 | Ab | 63 | LEU |
| 30 | Ac | 35 | ASP |
| 30 | Ac | 61 | ARG |
| 31 | Ad | 34 | TYR |
| 33 | Af | 118 | ARG |
| 33 | Af | 127 | GLY |
| 34 | Ag | 3 | SER |
| 34 | Ag | 28 | GLY |
| 34 | Ag | 161 | LYS |
| 34 | Ag | 217 | ASP |
| 35 | Ah | 46 | LYS |
| 35 | Ah | 82 | THR |
| 35 | Ah | 89 | ARG |
| 35 | Ah | 140 | ASP |
| 39 | BA | 13 | GLY |
| 39 | BA | 70 | ARG |
| 40 | BB | 136 | LYS |
| 40 | BB | 138 | ALA |
| 41 | BC | 15 | ALA |
| 41 | BC | 107 | ARG |
| 41 | BC | 182 | LEU |
| 41 | BC | 232 | SER |
| 41 | BC | 311 | HIS |
| 41 | BC | 317 | PRO |
| 42 | BD | 137 | ASP |
| 42 | BD | 188 | GLU |
| 42 | BD | 209 | GLU |
| 42 | BD | 215 | ASP |
| 42 | BD | 292 | ALA |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 43 | BE | 97 | ASN |
| 43 | BE | 98 | VAL |
| 44 | BF | 24 | GLU |
| 44 | BF | 175 | LYS |
| 45 | BG | 39 | ALA |
| 45 | BG | 115 | ALA |
| 45 | BG | 159 | PRO |
| 45 | BG | 254 | ASP |
| 47 | BI | 194 | GLY |
| 48 | BJ | 9 | MET |
| 48 | BJ | 73 | GLY |
| 48 | BJ | 86 | VAL |
| 48 | BJ | 115 | LYS |
| 48 | BJ | 167 | TYR |
| 49 | BL | 136 | GLU |
| 49 | BL | 141 | ALA |
| 50 | BM | 10 | SER |
| 51 | BN | 144 | ARG |
| 51 | BN | 184 | LYS |
| 52 | BO | 17[A] | GLY |
| 52 | BO | 17[B] | GLY |
| 53 | BP | 164 | LYS |
| 53 | BP | 182 | ILE |
| 54 | BQ | 98 | LYS |
| 54 | BQ | 183 | GLY |
| 56 | BS | 2 | ALA |
| 56 | BS | 12 | ARG |
| 56 | BS | 13 | ARG |
| 57 | BT | 125 | ALA |
| 58 | BU | 11 | ILE |
| 58 | BU | 50 | LEU |
| 58 | BU | 51 | GLY |
| 58 | BU | 91 | ASP |
| 59 | BV | 82 | ALA |
| 61 | BX | 45 | LYS |
| 62 | BY | 92 | GLY |
| 64 | Ba | 47 | LYS |
| 64 | Ba | 57 | GLY |
| 64 | Ba | 121 | VAL |
| 70 | Bg | 74 | ARG |
| 70 | Bg | 77 | GLY |
| 71 | Bh | 90 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 71 | Bh | 95 | PHE |
| 71 | Bh | 96 | GLU |
| 72 | Bi | 28 | TYR |
| 72 | Bi | 49 | GLY |
| 72 | Bi | 50 | LEU |
| 73 | Bj | 65 | ARG |
| 79 | Bp | 60 | CYS |
| 2 | CA | 29 | VAL |
| 2 | CA | 30 | GLN |
| 2 | CA | 95 | ALA |
| 2 | CA | 103 | THR |
| 2 | CA | 111 | ILE |
| 2 | CA | 158 | VAL |
| 2 | CA | 186 | GLY |
| 2 | CA | 191 | ARG |
| 2 | CA | 194 | PRO |
| 3 | CB | 93 | GLY |
| 3 | CB | 154 | SER |
| 3 | CB | 209 | ASN |
| 3 | CB | 224 | ASP |
| 4 | CC | 93 | GLY |
| 4 | CC | 106 | ASP |
| 4 | CC | 153 | SER |
| 4 | CC | 163 | GLY |
| 4 | CC | 164 | SER |
| 5 | CD | 45 | LYS |
| 5 | CD | 221 | SER |
| 6 | CE | 12 | LEU |
| 6 | CE | 104 | ASP |
| 7 | CF | 35 | GLN |
| 7 | CF | 36 | ALA |
| 7 | CF | 55 | ASP |
| 7 | CF | 100 | ASN |
| 7 | CF | 204 | GLY |
| 8 | CG | 25 | ARG |
| 8 | CG | 68 | LEU |
| 8 | CG | 152 | ASP |
| 8 | CG | 154 | ARG |
| 9 | CH | 87 | ASP |
| 9 | CH | 112 | ARG |
| 10 | CI | 62 | THR |
| 10 | CI | 115 | ALA |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 11 | CJ | 105 | LEU |
| 11 | CJ | 110 | GLN |
| 11 | CJ | 134 | ILE |
| 11 | CJ | 147 | MET |
| 11 | CJ | 169 | PRO |
| 12 | CK | 9 | ASN |
| 12 | CK | 32 | HIS |
| 12 | CK | 35 | ILE |
| 12 | CK | 81 | ASN |
| 12 | CK | 94 | GLU |
| 13 | CL | 114 | ALA |
| 13 | CL | 133 | LYS |
| 13 | CL | 144 | ALA |
| 14 | CM | 22 | VAL |
| 14 | CM | 58 | LEU |
| 14 | CM | 63 | VAL |
| 14 | CM | 103 | LEU |
| 14 | CM | 119 | SER |
| 14 | CM | 131 | ASP |
| 15 | CN | 60 | VAL |
| 15 | CN | 139 | TRP |
| 15 | CN | 140 | LYS |
| 17 | CP | 6 | ASN |
| 17 | CP | 10 | ARG |
| 17 | CP | 14 | THR |
| 17 | CP | 17 | TYR |
| 17 | CP | 131 | ALA |
| 17 | CP | 132 | GLY |
| 18 | CQ | 39 | VAL |
| 18 | CQ | 142 | TYR |
| 19 | CR | 63 | LYS |
| 19 | CR | 99 | VAL |
| 20 | CS | 60 | GLU |
| 20 | CS | 61 | LEU |
| 21 | CT | 26 | GLY |
| 22 | CU | 16 | GLN |
| 22 | CU | 100 | VAL |
| 23 | CV | 4 | ASP |
| 23 | CV | 43 | GLY |
| 23 | CV | 44 | ARG |
| 26 | CY | 34 | ASN |
| 26 | CY | 58 | PHE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 27 | CZ | 38 | HIS |
| 28 | Ca | 62 | TYR |
| 29 | Cb | 57 | GLU |
| 30 | Cc | 61 | ARG |
| 30 | Cc | 62 | GLU |
| 32 | Ce | 47 | VAL |
| 32 | Ce | 51 | ASN |
| 32 | Ce | 61 | SER |
| 33 | Cf | 112 | GLY |
| 33 | Cf | 124 | PRO |
| 33 | Cf | 131 | PHE |
| 33 | Cf | 145 | HIS |
| 34 | Cg | 97 | GLY |
| 34 | Cg | 149 | ASP |
| 34 | Cg | 282 | SER |
| 81 | Ch | 46 | LYS |
| 81 | Ch | 47 | ALA |
| 81 | Ch | 48 | ARG |
| 81 | Ch | 63 | ASP |
| 81 | Ch | 65 | THR |
| 81 | Ch | 72 | ARG |
| 39 | DA | 24 | GLN |
| 39 | DA | 194 | ASN |
| 40 | DB | 235 | THR |
| 40 | DB | 293 | ASN |
| 41 | DC | 71 | VAL |
| 41 | DC | 190 | GLY |
| 41 | DC | 272 | VAL |
| 41 | DC | 345 | GLU |
| 41 | DC | 353 | ALA |
| 42 | DD | 125 | VAL |
| 42 | DD | 178 | ASN |
| 45 | DG | 81 | THR |
| 45 | DG | 121 | SER |
| 45 | DG | 188 | THR |
| 45 | DG | 203 | VAL |
| 45 | DG | 223 | ALA |
| 45 | DG | 240 | ASN |
| 46 | DH | 144 | ILE |
| 46 | DH | 189 | GLU |
| 47 | DI | 220 | GLN |
| 48 | DJ | 55 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 49 | DL | 135 | ALA |
| 49 | DL | 141 | ALA |
| 51 | DN | 184 | LYS |
| 53 | DP | 66 | SER |
| 53 | DP | 67 | ILE |
| 54 | DQ | 91 | ALA |
| 54 | DQ | 167 | SER |
| 58 | DU | 49 | ASN |
| 58 | DU | 91 | ASP |
| 59 | DV | 41 | GLY |
| 60 | DW | 63 | ILE |
| 60 | DW | 77 | LYS |
| 63 | DZ | 17 | ARG |
| 63 | DZ | 93 | LYS |
| 63 | DZ | 130 | PHE |
| 63 | DZ | 134 | LEU |
| 64 | Da | 24 | LYS |
| 66 | Dc | 10 | ILE |
| 67 | Dd | 83 | GLU |
| 68 | De | 6 | HIS |
| 68 | De | 12 | LYS |
| 68 | De | 124 | GLY |
| 69 | Df | 91 | ALA |
| 71 | Dh | 119 | LYS |
| 77 | Dn | 23 | ARG |
| 83 | Dq | 47 | GLY |
| 83 | Dq | 198 | PRO |
| 2 | AA | 27 | ARG |
| 2 | AA | 103 | THR |
| 3 | AB | 35 | PRO |
| 3 | AB | 38 | PHE |
| 3 | AB | 62 | LYS |
| 3 | AB | 209 | ASN |
| 4 | AC | 106 | ASP |
| 4 | AC | 150 | GLN |
| 4 | AC | 235 | LEU |
| 5 | AD | 54 | ARG |
| 6 | AE | 200 | ARG |
| 7 | AF | 33 | VAL |
| 7 | AF | 156 | ARG |
| 9 | AH | 5 | GLN |
| 9 | AH | 29 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 9 | AH | 74 | GLN |
| 9 | AH | 75 | THR |
| 9 | AH | 110 | GLN |
| 10 | AI | 41 | LYS |
| 10 | AI | 136 | SER |
| 10 | AI | 153 | GLU |
| 11 | AJ | 163 | PRO |
| 13 | AL | 4 | GLU |
| 13 | AL | 55 | ASP |
| 13 | AL | 146 | ALA |
| 13 | AL | 153 | PHE |
| 13 | AL | 154 | ALA |
| 14 | AM | 22 | VAL |
| 14 | AM | 81 | ASP |
| 14 | AM | 82 | PRO |
| 14 | AM | 85 | LYS |
| 14 | AM | 112 | ALA |
| 14 | AM | 135 | MET |
| 16 | AO | 18 | ARG |
| 16 | AO | 123 | SER |
| 17 | AP | 11 | VAL |
| 17 | AP | 22 | LEU |
| 17 | AP | 52 | LYS |
| 19 | AR | 83 | GLN |
| 19 | AR | 115 | LEU |
| 20 | AS | 10 | SER |
| 20 | AS | 80 | LYS |
| 20 | AS | 83 | ALA |
| 21 | AT | 25 | GLN |
| 22 | AU | 55 | PRO |
| 23 | AV | 2 | GLU |
| 23 | AV | 10 | GLU |
| 23 | AV | 15 | ARG |
| 25 | AX | 37 | ALA |
| 25 | AX | 40 | SER |
| 25 | AX | 89 | ASN |
| 26 | AY | 34 | ASN |
| 26 | AY | 51 | GLU |
| 26 | AY | 53 | ASP |
| 27 | AZ | 41 | ILE |
| 27 | AZ | 55 | PRO |
| 27 | AZ | 97 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 28 | Aa | 66 | LYS |
| 33 | Af | 138 | ARG |
| 34 | Ag | 15 | GLY |
| 34 | Ag | 96 | THR |
| 34 | Ag | 98 | GLU |
| 39 | BA | 250 | GLN |
| 40 | BB | 4 | ARG |
| 41 | BC | 14 | GLU |
| 41 | BC | 16 | THR |
| 42 | BD | 112 | LYS |
| 45 | BG | 78 | PHE |
| 45 | BG | 122 | LYS |
| 46 | BH | 42 | ASP |
| 47 | BI | 195 | ALA |
| 48 | BJ | 140 | ARG |
| 48 | BJ | 169 | ALA |
| 48 | BJ | 173 | ASP |
| 49 | BL | 134 | GLU |
| 49 | BL | 166 | ALA |
| 50 | BM | 28 | SER |
| 50 | BM | 95 | ALA |
| 51 | BN | 145 | ASP |
| 53 | BP | 160 | ALA |
| 55 | BR | 53 | LYS |
| 55 | BR | 64 | ARG |
| 57 | BT | 114 | ALA |
| 58 | BU | 10 | LYS |
| 58 | BU | 44 | GLU |
| 60 | BW | 17 | ARG |
| 60 | BW | 77 | LYS |
| 63 | BZ | 16 | GLY |
| 63 | BZ | 35 | SER |
| 63 | BZ | 102 | GLU |
| 64 | Ba | 93 | SER |
| 70 | Bg | 46 | ASP |
| 70 | Bg | 98 | GLN |
| 71 | Bh | 4 | VAL |
| 71 | Bh | 91 | ALA |
| 72 | Bi | 34 | SER |
| 72 | Bi | 95 | ALA |
| 72 | Bi | 98 | ARG |
| 78 | Bo | 34 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 79 | Bp | 58 | SER |
| 4 | CC | 238 | SER |
| 5 | CD | 179 | GLN |
| 5 | CD | 180 | GLY |
| 6 | CE | 57 | ASN |
| 6 | CE | 94 | ALA |
| 6 | CE | 168 | LYS |
| 6 | CE | 171 | ASP |
| 7 | CF | 43 | PHE |
| 8 | CG | 142 | ARG |
| 8 | CG | 165 | GLY |
| 9 | CH | 133 | THR |
| 10 | CI | 101 | ILE |
| 10 | CI | 136 | SER |
| 10 | CI | 137 | LYS |
| 11 | CJ | 162 | SER |
| 13 | CL | 6 | THR |
| 13 | CL | 121 | ASP |
| 13 | CL | 132 | SER |
| 14 | CM | 25 | GLU |
| 14 | CM | 26 | ASP |
| 14 | CM | 82 | PRO |
| 14 | CM | 135 | MET |
| 15 | CN | 22 | ALA |
| 16 | CO | 114 | ARG |
| 17 | CP | 69 | GLU |
| 19 | CR | 86 | PRO |
| 20 | CS | 33 | THR |
| 22 | CU | 13 | GLU |
| 22 | CU | 51 | VAL |
| 22 | CU | 53 | LYS |
| 22 | CU | 119 | ALA |
| 26 | CY | 11 | LYS |
| 26 | CY | 51 | GLU |
| 26 | CY | 132 | ARG |
| 31 | Cd | 11 | PRO |
| 34 | Cg | 39 | ASP |
| 34 | Cg | 161 | LYS |
| 34 | Cg | 297 | ASP |
| 81 | Ch | 84 | LYS |
| 39 | DA | 56 | ALA |
| 39 | DA | 144 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 39 | DA | 249 | SER |
| 40 | DB | 138 | ALA |
| 40 | DB | 155 | ALA |
| 41 | DC | 146 | PRO |
| 42 | DD | 270 | LYS |
| 43 | DE | 10 | TYR |
| 43 | DE | 32 | ALA |
| 45 | DG | 39 | ALA |
| 45 | DG | 123 | GLN |
| 45 | DG | 133 | LYS |
| 45 | DG | 237 | ILE |
| 47 | DI | 83 | ASP |
| 47 | DI | 101 | LYS |
| 47 | DI | 174 | THR |
| 47 | DI | 176 | LEU |
| 49 | DL | 101 | ARG |
| 49 | DL | 140 | SER |
| 51 | DN | 181 | ASN |
| 52 | DO | 12[A] | LYS |
| 52 | DO | 12[B] | LYS |
| 58 | DU | 48 | GLY |
| 60 | DW | 74 | LYS |
| 60 | DW | 134 | GLN |
| 61 | DX | 38 | LEU |
| 61 | DX | 47 | ALA |
| 61 | DX | 55 | ASN |
| 63 | DZ | 16 | GLY |
| 64 | Da | 47 | LYS |
| 67 | Dd | 5 | LYS |
| 67 | Dd | 86 | LYS |
| 70 | Dg | 79 | SER |
| 72 | Di | 34 | SER |
| 83 | Dq | 33 | VAL |
| 2 | AA | 33 | GLN |
| 2 | AA | 158 | VAL |
| 2 | AA | 164 | ASN |
| 2 | AA | 185 | ARG |
| 2 | AA | 189 | VAL |
| 3 | AB | 54 | LEU |
| 3 | AB | 61 | LEU |
| 3 | AB | 81 | PHE |
| 3 | AB | 112 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 3 | AB | 154 | SER |
| 3 | AB | 215 | VAL |
| 4 | AC | 39 | THR |
| 5 | AD | 217 | ILE |
| 6 | AE | 77 | ARG |
| 6 | AE | 80 | THR |
| 6 | AE | 163 | ASP |
| 6 | AE | 188 | ASN |
| 6 | AE | 193 | GLY |
| 7 | AF | 51 | VAL |
| 7 | AF | 79 | ASN |
| 8 | AG | 69 | LEU |
| 9 | AH | 13 | PRO |
| 9 | AH | 84 | LYS |
| 9 | AH | 132 | PRO |
| 10 | AI | 59 | ARG |
| 10 | AI | 152 | ILE |
| 12 | AK | 94 | GLU |
| 13 | AL | 145 | ALA |
| 14 | AM | 39 | ASP |
| 14 | AM | 68 | GLU |
| 14 | AM | 106 | ILE |
| 14 | AM | 107 | ASP |
| 14 | AM | 108 | ARG |
| 14 | AM | 129 | GLU |
| 14 | AM | 130 | THR |
| 15 | AN | 138 | ASN |
| 16 | AO | 69 | ALA |
| 18 | AQ | 142 | TYR |
| 19 | AR | 23 | LYS |
| 19 | AR | 72 | LYS |
| 21 | AT | 7 | ARG |
| 21 | AT | 23 | GLN |
| 21 | AT | 39 | THR |
| 23 | AV | 44 | ARG |
| 25 | AX | 92 | CYS |
| 25 | AX | 109 | ARG |
| 25 | AX | 112 | LYS |
| 26 | AY | 60 | PHE |
| 28 | Aa | 64 | LEU |
| 30 | Ac | 6 | PRO |
| 32 | Ae | 50 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 33 | Af | 145 | HIS |
| 34 | Ag | 136 | ILE |
| 34 | Ag | 163 | ASP |
| 34 | Ag | 237 | GLN |
| 40 | BB | 386 | ASP |
| 41 | BC | 146 | PRO |
| 41 | BC | 233 | LEU |
| 42 | BD | 6 | ASP |
| 42 | BD | 252 | ALA |
| 42 | BD | 253 | PHE |
| 43 | BE | 95 | GLY |
| 44 | BF | 160 | ARG |
| 45 | BG | 157 | VAL |
| 45 | BG | 253 | SER |
| 46 | BH | 13 | PRO |
| 47 | BI | 24 | ARG |
| 48 | BJ | 95 | ASN |
| 48 | BJ | 108 | GLU |
| 48 | BJ | 114 | ILE |
| 48 | BJ | 117 | ASP |
| 51 | BN | 94 | TYR |
| 51 | BN | 149 | ASN |
| 53 | BP | 158 | ALA |
| 53 | BP | 161 | ALA |
| 53 | BP | 163 | LYS |
| 54 | BQ | 162 | ALA |
| 57 | BT | 12 | ARG |
| 58 | BU | 31 | ALA |
| 58 | BU | 49 | ASN |
| 60 | BW | 64 | THR |
| 63 | BZ | 103 | GLN |
| 64 | Ba | 96 | LYS |
| 65 | Bb | 32 | LEU |
| 68 | Be | 40 | SER |
| 71 | Bh | 27 | GLU |
| 73 | Bj | 25 | ARG |
| 74 | Bk | 33 | LYS |
| 78 | Bo | 15 | LYS |
| 79 | Bp | 51 | ALA |
| 2 | CA | 10 | THR |
| 4 | CC | 40 | LYS |
| 4 | CC | 150 | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 4 | CC | 235 | LEU |
| 5 | CD | 111 | ASN |
| 5 | CD | 144 | ALA |
| 6 | CE | 189 | LEU |
| 6 | CE | 245 | LYS |
| 7 | CF | 29 | ILE |
| 7 | CF | 101 | GLY |
| 7 | CF | 151 | GLY |
| 8 | CG | 2 | LYS |
| 8 | CG | 70 | PRO |
| 9 | CH | 66 | SER |
| 11 | CJ | 65 | LYS |
| 11 | CJ | 126 | ARG |
| 12 | CK | 30 | ALA |
| 12 | CK | 95 | ARG |
| 13 | CL | 7 | VAL |
| 13 | CL | 55 | ASP |
| 13 | CL | 61 | THR |
| 13 | CL | 129 | ARG |
| 14 | CM | 45 | LEU |
| 14 | CM | 64 | SER |
| 14 | CM | 81 | ASP |
| 14 | CM | 106 | ILE |
| 14 | CM | 118 | ALA |
| 14 | CM | 128 | ALA |
| 14 | CM | 129 | GLU |
| 16 | CO | 124 | ASP |
| 17 | CP | 7 | ALA |
| 17 | CP | 48 | GLY |
| 17 | CP | 75 | PRO |
| 20 | CS | 145 | ARG |
| 21 | CT | 25 | GLN |
| 21 | CT | 66 | TYR |
| 22 | CU | 19 | ILE |
| 23 | CV | 10 | GLU |
| 25 | CX | 101 | GLU |
| 26 | CY | 53 | ASP |
| 27 | CZ | 103 | ARG |
| 28 | Ca | 15 | ARG |
| 28 | Ca | 35 | ALA |
| 28 | Ca | 59 | TYR |
| 29 | Cb | 58 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 32 | Ce | 54 | ARG |
| 33 | Cf | 138 | ARG |
| 34 | Cg | 298 | GLY |
| 81 | Ch | 43 | ASP |
| 81 | Ch | 64 | LYS |
| 39 | DA | 143 | GLU |
| 40 | DB | 333 | LYS |
| 41 | DC | 233 | LEU |
| 41 | DC | 306 | THR |
| 41 | DC | 331 | ALA |
| 41 | DC | 342 | LYS |
| 42 | DD | 124 | GLU |
| 44 | DF | 191 | VAL |
| 45 | DG | 206 | GLU |
| 46 | DH | 167 | VAL |
| 47 | DI | 207 | GLU |
| 49 | DL | 60 | ALA |
| 49 | DL | 76 | THR |
| 51 | DN | 48 | ALA |
| 55 | DR | 147 | ALA |
| 60 | DW | 25 | ASP |
| 63 | DZ | 34 | LYS |
| 63 | DZ | 36 | HIS |
| 64 | Da | 121 | VAL |
| 70 | Dg | 99 | LYS |
| 73 | Dj | 85 | LYS |
| 74 | Dk | 8 | ILE |
| 83 | Dq | 102 | SER |
| 3 | AB | 64 | ARG |
| 4 | AC | 36 | VAL |
| 5 | AD | 59 | LEU |
| 6 | AE | 233 | LYS |
| 7 | AF | 21 | THR |
| 7 | AF | 64 | VAL |
| 9 | AH | 73 | VAL |
| 9 | AH | 185 | ILE |
| 11 | AJ | 162 | SER |
| 14 | AM | 101 | ALA |
| 17 | AP | 38 | PRO |
| 21 | AT | 29 | GLU |
| 22 | AU | 49 | ASN |
| 23 | AV | 46 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | AV | 49 | GLU |
| 24 | AW | 67 | GLY |
| 24 | AW | 83 | ILE |
| 25 | AX | 70 | LYS |
| 26 | AY | 6 | THR |
| 26 | AY | 47 | VAL |
| 29 | Ab | 51 | GLN |
| 35 | Ah | 53 | ARG |
| 35 | Ah | 102 | THR |
| 39 | BA | 35 | ALA |
| 39 | BA | 251 | LYS |
| 41 | BC | 5 | GLN |
| 44 | BF | 178 | ILE |
| 45 | BG | 47 | SER |
| 46 | BH | 2 | LYS |
| 46 | BH | 107 | ASP |
| 48 | BJ | 24 | GLY |
| 48 | BJ | 111 | ASP |
| 48 | BJ | 172 | LEU |
| 49 | BL | 130 | GLY |
| 49 | BL | 133 | PRO |
| 50 | BM | 6 | ILE |
| 50 | BM | 36 | VAL |
| 52 | BO | 187[A] | GLU |
| 52 | BO | 187[B] | GLU |
| 57 | BT | 18 | ASP |
| 60 | BW | 80 | ARG |
| 60 | BW | 89 | LEU |
| 64 | Ba | 56 | VAL |
| 64 | Ba | 117 | ARG |
| 65 | Bb | 53 | ALA |
| 69 | Bf | 59 | VAL |
| 72 | Bi | 3 | VAL |
| 76 | Bm | 79 | GLU |
| 3 | CB | 63 | GLY |
| 6 | CE | 90 | ILE |
| 6 | CE | 205 | PHE |
| 9 | CH | 12 | ALA |
| 9 | CH | 13 | PRO |
| 10 | CI | 78 | ILE |
| 11 | CJ | 115 | LYS |
| 11 | CJ | 119 | ALA |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 11 | CJ | 150 | LEU |
| 12 | CK | 10 | LYS |
| 14 | CM | 59 | LEU |
| 14 | CM | 107 | ASP |
| 14 | CM | 127 | GLY |
| 15 | CN | 43 | LYS |
| 15 | CN | 137 | PRO |
| 17 | CP | 49 | MET |
| 17 | CP | 130 | ARG |
| 17 | CP | 136 | SER |
| 20 | CS | 14 | ILE |
| 21 | CT | 28 | LEU |
| 27 | CZ | 54 | VAL |
| 27 | CZ | 70 | LYS |
| 29 | Cb | 21 | LEU |
| 29 | Cb | 63 | LEU |
| 30 | Cc | 37 | SER |
| 31 | Cd | 7 | TRP |
| 33 | Cf | 146 | SER |
| 34 | Cg | 217 | ASP |
| 34 | Cg | 228 | LYS |
| 81 | Ch | 51 | ARG |
| 41 | DC | 5 | GLN |
| 44 | DF | 229 | PHE |
| 45 | DG | 69 | LEU |
| 45 | DG | 120 | LYS |
| 45 | DG | 124 | ASP |
| 46 | DH | 110 | LYS |
| 48 | DJ | 111 | ASP |
| 48 | DJ | 153 | LYS |
| 49 | DL | 121 | SER |
| 54 | DQ | 98 | LYS |
| 55 | DR | 183 | ALA |
| 57 | DT | 20 | ARG |
| 63 | DZ | 7 | ALA |
| 64 | Da | 129 | PHE |
| 65 | Db | 24 | PRO |
| 72 | Di | 9 | ILE |
| 74 | Dk | 19 | ASP |
| 76 | Dm | 78 | ILE |
| 83 | Dq | 197 | PHE |
| 2 | AA | 139 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 3 | AB | 78 | ASP |
| 3 | AB | 210 | ILE |
| 6 | AE | 3 | ARG |
| 6 | AE | 53 | LYS |
| 8 | AG | 132 | ARG |
| 9 | AH | 11 | GLN |
| 10 | AI | 10 | LYS |
| 10 | AI | 186 | GLY |
| 11 | AJ | 132 | ARG |
| 15 | AN | 60 | VAL |
| 17 | AP | 10 | ARG |
| 17 | AP | 23 | GLU |
| 17 | AP | 69 | GLU |
| 17 | AP | 130 | ARG |
| 20 | AS | 7 | GLU |
| 20 | AS | 34 | THR |
| 22 | AU | 117 | VAL |
| 26 | AY | 58 | PHE |
| 26 | AY | 77 | ASN |
| 28 | Aa | 10 | ARG |
| 35 | Ah | 88 | ARG |
| 40 | BB | 155 | ALA |
| 40 | BB | 317 | ILE |
| 41 | BC | 72 | ALA |
| 42 | BD | 259 | LYS |
| 44 | BF | 164 | SER |
| 45 | BG | 75 | ILE |
| 53 | BP | 162 | GLU |
| 60 | BW | 67 | VAL |
| 60 | BW | 76 | VAL |
| 64 | Ba | 91 | LEU |
| 65 | Bb | 21 | ILE |
| 69 | Bf | 91 | ALA |
| 72 | Bi | 21 | THR |
| 72 | Bi | 94 | ILE |
| 2 | CA | 109 | ASN |
| 2 | CA | 139 | VAL |
| 3 | CB | 21 | VAL |
| 6 | CE | 194 | THR |
| 12 | CK | 3 | MET |
| 12 | CK | 24 | LYS |
| 12 | CK | 31 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 13 | CL | 146 | ALA |
| 14 | CM | 115 | VAL |
| 18 | CQ | 40 | GLU |
| 19 | CR | 120 | SER |
| 23 | CV | 6 | GLY |
| 34 | Cg | 153 | GLN |
| 40 | DB | 187 | SER |
| 41 | DC | 328 | ASN |
| 44 | DF | 157 | ASN |
| 45 | DG | 202 | GLU |
| 47 | DI | 204 | GLY |
| 48 | DJ | 114 | ILE |
| 63 | DZ | 29 | HIS |
| 71 | Dh | 83 | LYS |
| 6 | AE | 234 | PRO |
| 11 | AJ | 117 | GLY |
| 16 | AO | 48 | VAL |
| 18 | AQ | 97 | VAL |
| 64 | Ba | 29 | PRO |
| 5 | CD | 203 | PRO |
| 8 | CG | 69 | LEU |
| 9 | CH | 32 | PRO |
| 18 | CQ | 97 | VAL |
| 44 | DF | 178 | ILE |
| 45 | DG | 190 | VAL |
| 83 | Dq | 196 | VAL |
| 2 | AA | 117 | GLU |
| 14 | AM | 40 | GLY |
| 28 | Aa | 50 | VAL |
| 28 | Aa | 59 | TYR |
| 44 | BF | 91 | GLY |
| 45 | BG | 158 | ASP |
| 5 | CD | 43 | PRO |
| 22 | CU | 118 | VAL |
| 23 | CV | 77 | GLY |
| 63 | DZ | 103 | GLN |
| 72 | Di | 3 | VAL |
| 78 | Do | 31 | GLY |
| 3 | AB | 197 | ILE |
| 4 | AC | 145 | GLY |
| 18 | AQ | 29 | ILE |
| 21 | AT | 100 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33 | Af | 147 | VAL |
| 45 | BG | 116 | VAL |
| 45 | BG | 119 | GLY |
| 45 | BG | 135 | GLY |
| 63 | BZ | 36 | HIS |
| 2 | CA | 94 | GLY |
| 6 | CE | 150 | PRO |
| 6 | CE | 195 | ILE |
| 7 | CF | 152 | GLY |
| 16 | CO | 131 | GLY |
| 34 | Cg | 15 | GLY |
| 45 | DG | 73 | PRO |
| 48 | DJ | 118 | PRO |
| 54 | DQ | 42 | ALA |
| 6 | AE | 45 | ILE |
| 8 | AG | 70 | PRO |
| 12 | AK | 89 | GLY |
| 14 | AM | 117 | GLY |
| 41 | BC | 131 | VAL |
| 53 | BP | 84 | PRO |
| 5 | CD | 163 | PRO |
| 6 | CE | 260 | GLY |
| 18 | CQ | 4 | VAL |
| 26 | CY | 29 | HIS |
| 69 | Df | 59 | VAL |
| 4 | AC | 163 | GLY |
| 57 | BT | 123 | GLY |
| 6 | CE | 30 | ARG |

5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|---------------|-----------|----------|-------------|
| 2 | AA | 164/210 (78%) | 122 (74%) | 42 (26%) | 0 3 |
| 2 | CA | 165/210 (79%) | 131 (79%) | 34 (21%) | 1 6 |
| 3 | AB | 191/224 (85%) | 137 (72%) | 54 (28%) | 0 2 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|---|
| 3 | CB | 192/224 (86%) | 148 (77%) | 44 (23%) | 1 | 4 |
| 4 | AC | 176/205 (86%) | 130 (74%) | 46 (26%) | 0 | 2 |
| 4 | CC | 176/205 (86%) | 133 (76%) | 43 (24%) | 0 | 3 |
| 5 | AD | 182/195 (93%) | 138 (76%) | 44 (24%) | 0 | 3 |
| 5 | CD | 182/195 (93%) | 140 (77%) | 42 (23%) | 1 | 4 |
| 6 | AE | 221/222 (100%) | 166 (75%) | 55 (25%) | 0 | 3 |
| 6 | CE | 221/222 (100%) | 178 (80%) | 43 (20%) | 1 | 7 |
| 7 | AF | 173/191 (91%) | 137 (79%) | 36 (21%) | 1 | 5 |
| 7 | CF | 173/191 (91%) | 132 (76%) | 41 (24%) | 1 | 3 |
| 8 | AG | 188/201 (94%) | 149 (79%) | 39 (21%) | 1 | 6 |
| 8 | CG | 187/201 (93%) | 143 (76%) | 44 (24%) | 1 | 3 |
| 9 | AH | 165/170 (97%) | 124 (75%) | 41 (25%) | 0 | 3 |
| 9 | CH | 165/170 (97%) | 127 (77%) | 38 (23%) | 1 | 4 |
| 10 | AI | 150/161 (93%) | 118 (79%) | 32 (21%) | 1 | 5 |
| 10 | CI | 150/161 (93%) | 117 (78%) | 33 (22%) | 1 | 4 |
| 11 | AJ | 158/166 (95%) | 117 (74%) | 41 (26%) | 0 | 2 |
| 11 | CJ | 158/166 (95%) | 124 (78%) | 34 (22%) | 1 | 5 |
| 12 | AK | 77/98 (79%) | 58 (75%) | 19 (25%) | 0 | 3 |
| 12 | CK | 73/98 (74%) | 56 (77%) | 17 (23%) | 1 | 4 |
| 13 | AL | 129/137 (94%) | 105 (81%) | 24 (19%) | 1 | 8 |
| 13 | CL | 129/137 (94%) | 100 (78%) | 29 (22%) | 1 | 4 |
| 14 | AM | 88/119 (74%) | 55 (62%) | 33 (38%) | 0 | 0 |
| 14 | CM | 88/119 (74%) | 55 (62%) | 33 (38%) | 0 | 0 |
| 15 | AN | 127/128 (99%) | 91 (72%) | 36 (28%) | 0 | 2 |
| 15 | CN | 127/128 (99%) | 103 (81%) | 24 (19%) | 1 | 8 |
| 16 | AO | 81/105 (77%) | 57 (70%) | 24 (30%) | 0 | 1 |
| 16 | CO | 97/105 (92%) | 71 (73%) | 26 (27%) | 0 | 2 |
| 17 | AP | 101/118 (86%) | 82 (81%) | 19 (19%) | 1 | 8 |
| 17 | CP | 103/118 (87%) | 81 (79%) | 22 (21%) | 1 | 5 |
| 18 | AQ | 117/119 (98%) | 84 (72%) | 33 (28%) | 0 | 2 |
| 18 | CQ | 118/119 (99%) | 92 (78%) | 26 (22%) | 1 | 4 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 19 | AR | 94/124 (76%) | 70 (74%) | 24 (26%) | 0 | 3 |
| 19 | CR | 92/124 (74%) | 74 (80%) | 18 (20%) | 1 | 7 |
| 20 | AS | 128/129 (99%) | 87 (68%) | 41 (32%) | 0 | 1 |
| 20 | CS | 128/129 (99%) | 98 (77%) | 30 (23%) | 1 | 4 |
| 21 | AT | 115/116 (99%) | 84 (73%) | 31 (27%) | 0 | 2 |
| 21 | CT | 115/116 (99%) | 88 (76%) | 27 (24%) | 1 | 3 |
| 22 | AU | 100/114 (88%) | 71 (71%) | 29 (29%) | 0 | 2 |
| 22 | CU | 103/114 (90%) | 69 (67%) | 34 (33%) | 0 | 1 |
| 23 | AV | 74/74 (100%) | 56 (76%) | 18 (24%) | 0 | 3 |
| 23 | CV | 74/74 (100%) | 57 (77%) | 17 (23%) | 1 | 4 |
| 24 | AW | 110/111 (99%) | 84 (76%) | 26 (24%) | 1 | 3 |
| 24 | CW | 110/111 (99%) | 96 (87%) | 14 (13%) | 4 | 19 |
| 25 | AX | 119/120 (99%) | 97 (82%) | 22 (18%) | 1 | 8 |
| 25 | CX | 119/120 (99%) | 101 (85%) | 18 (15%) | 3 | 14 |
| 26 | AY | 112/113 (99%) | 84 (75%) | 28 (25%) | 0 | 3 |
| 26 | CY | 112/113 (99%) | 90 (80%) | 22 (20%) | 1 | 7 |
| 27 | AZ | 61/89 (68%) | 43 (70%) | 18 (30%) | 0 | 1 |
| 27 | CZ | 61/89 (68%) | 44 (72%) | 17 (28%) | 0 | 2 |
| 28 | Aa | 83/101 (82%) | 65 (78%) | 18 (22%) | 1 | 5 |
| 28 | Ca | 83/101 (82%) | 68 (82%) | 15 (18%) | 1 | 9 |
| 29 | Ab | 70/71 (99%) | 62 (89%) | 8 (11%) | 5 | 24 |
| 29 | Cb | 70/71 (99%) | 57 (81%) | 13 (19%) | 1 | 8 |
| 30 | Ac | 56/60 (93%) | 38 (68%) | 18 (32%) | 0 | 1 |
| 30 | Cc | 56/60 (93%) | 38 (68%) | 18 (32%) | 0 | 1 |
| 31 | Ad | 47/49 (96%) | 38 (81%) | 9 (19%) | 1 | 8 |
| 31 | Cd | 47/49 (96%) | 36 (77%) | 11 (23%) | 1 | 4 |
| 32 | Ae | 51/54 (94%) | 43 (84%) | 8 (16%) | 2 | 13 |
| 32 | Ce | 53/54 (98%) | 37 (70%) | 16 (30%) | 0 | 1 |
| 33 | Af | 43/112 (38%) | 32 (74%) | 11 (26%) | 0 | 3 |
| 33 | Cf | 43/112 (38%) | 32 (74%) | 11 (26%) | 0 | 3 |
| 34 | Ag | 259/262 (99%) | 222 (86%) | 37 (14%) | 3 | 15 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 34 | Cg | 260/262 (99%) | 226 (87%) | 34 (13%) | 4 | 18 |
| 35 | Ah | 97/195 (50%) | 74 (76%) | 23 (24%) | 1 | 3 |
| 39 | BA | 193/196 (98%) | 160 (83%) | 33 (17%) | 2 | 10 |
| 39 | DA | 192/196 (98%) | 154 (80%) | 38 (20%) | 1 | 7 |
| 40 | BB | 321/323 (99%) | 240 (75%) | 81 (25%) | 0 | 3 |
| 40 | DB | 321/323 (99%) | 251 (78%) | 70 (22%) | 1 | 5 |
| 41 | BC | 288/289 (100%) | 227 (79%) | 61 (21%) | 1 | 5 |
| 41 | DC | 288/289 (100%) | 222 (77%) | 66 (23%) | 1 | 4 |
| 42 | BD | 244/245 (100%) | 189 (78%) | 55 (22%) | 1 | 4 |
| 42 | DD | 243/245 (99%) | 195 (80%) | 48 (20%) | 1 | 7 |
| 43 | BE | 134/153 (88%) | 116 (87%) | 18 (13%) | 4 | 17 |
| 43 | DE | 135/153 (88%) | 115 (85%) | 20 (15%) | 3 | 14 |
| 44 | BF | 186/205 (91%) | 165 (89%) | 21 (11%) | 6 | 24 |
| 44 | DF | 187/205 (91%) | 158 (84%) | 29 (16%) | 2 | 13 |
| 45 | BG | 187/208 (90%) | 151 (81%) | 36 (19%) | 1 | 8 |
| 45 | DG | 177/208 (85%) | 138 (78%) | 39 (22%) | 1 | 4 |
| 46 | BH | 171/171 (100%) | 131 (77%) | 40 (23%) | 1 | 4 |
| 46 | DH | 171/171 (100%) | 132 (77%) | 39 (23%) | 1 | 4 |
| 47 | BI | 177/187 (95%) | 143 (81%) | 34 (19%) | 1 | 8 |
| 47 | DI | 179/187 (96%) | 142 (79%) | 37 (21%) | 1 | 6 |
| 48 | BJ | 147/150 (98%) | 111 (76%) | 36 (24%) | 0 | 3 |
| 48 | DJ | 147/150 (98%) | 114 (78%) | 33 (22%) | 1 | 4 |
| 49 | BL | 154/159 (97%) | 123 (80%) | 31 (20%) | 1 | 6 |
| 49 | DL | 154/159 (97%) | 124 (80%) | 30 (20%) | 1 | 7 |
| 50 | BM | 107/109 (98%) | 84 (78%) | 23 (22%) | 1 | 5 |
| 50 | DM | 108/109 (99%) | 84 (78%) | 24 (22%) | 1 | 4 |
| 51 | BN | 175/176 (99%) | 146 (83%) | 29 (17%) | 2 | 11 |
| 51 | DN | 175/176 (99%) | 142 (81%) | 33 (19%) | 1 | 8 |
| 52 | BO | 323/179 (180%) | 276 (85%) | 47 (15%) | 3 | 15 |
| 52 | DO | 323/179 (180%) | 267 (83%) | 56 (17%) | 2 | 10 |
| 53 | BP | 140/146 (96%) | 109 (78%) | 31 (22%) | 1 | 4 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 53 | DP | 125/146 (86%) | 103 (82%) | 22 (18%) | 2 | 10 |
| 54 | BQ | 150/151 (99%) | 126 (84%) | 24 (16%) | 2 | 12 |
| 54 | DQ | 150/151 (99%) | 124 (83%) | 26 (17%) | 2 | 10 |
| 55 | BR | 153/154 (99%) | 116 (76%) | 37 (24%) | 0 | 3 |
| 55 | DR | 153/154 (99%) | 121 (79%) | 32 (21%) | 1 | 5 |
| 56 | BS | 156/156 (100%) | 127 (81%) | 29 (19%) | 1 | 8 |
| 56 | DS | 156/156 (100%) | 123 (79%) | 33 (21%) | 1 | 5 |
| 57 | BT | 136/137 (99%) | 103 (76%) | 33 (24%) | 0 | 3 |
| 57 | DT | 136/137 (99%) | 109 (80%) | 27 (20%) | 1 | 7 |
| 58 | BU | 87/107 (81%) | 73 (84%) | 14 (16%) | 2 | 12 |
| 58 | DU | 85/107 (79%) | 62 (73%) | 23 (27%) | 0 | 2 |
| 59 | BV | 104/105 (99%) | 88 (85%) | 16 (15%) | 2 | 13 |
| 59 | DV | 104/105 (99%) | 96 (92%) | 8 (8%) | 13 | 42 |
| 60 | BW | 57/129 (44%) | 49 (86%) | 8 (14%) | 3 | 16 |
| 60 | DW | 100/129 (78%) | 85 (85%) | 15 (15%) | 3 | 14 |
| 61 | BX | 104/118 (88%) | 78 (75%) | 26 (25%) | 0 | 3 |
| 61 | DX | 104/118 (88%) | 81 (78%) | 23 (22%) | 1 | 4 |
| 62 | BY | 109/110 (99%) | 87 (80%) | 22 (20%) | 1 | 6 |
| 62 | DY | 109/110 (99%) | 85 (78%) | 24 (22%) | 1 | 4 |
| 63 | BZ | 115/116 (99%) | 88 (76%) | 27 (24%) | 1 | 3 |
| 63 | DZ | 115/116 (99%) | 89 (77%) | 26 (23%) | 1 | 4 |
| 64 | Ba | 118/119 (99%) | 97 (82%) | 21 (18%) | 2 | 9 |
| 64 | Da | 118/119 (99%) | 95 (80%) | 23 (20%) | 1 | 7 |
| 65 | Bb | 46/47 (98%) | 36 (78%) | 10 (22%) | 1 | 5 |
| 65 | Db | 46/47 (98%) | 35 (76%) | 11 (24%) | 0 | 3 |
| 66 | Bc | 81/88 (92%) | 63 (78%) | 18 (22%) | 1 | 4 |
| 66 | Dc | 84/88 (96%) | 68 (81%) | 16 (19%) | 1 | 8 |
| 67 | Bd | 92/97 (95%) | 73 (79%) | 19 (21%) | 1 | 6 |
| 67 | Dd | 94/97 (97%) | 73 (78%) | 21 (22%) | 1 | 4 |
| 68 | Be | 109/111 (98%) | 87 (80%) | 22 (20%) | 1 | 6 |
| 68 | De | 109/111 (98%) | 89 (82%) | 20 (18%) | 1 | 9 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|------------|-------------|----|
| 69 | Bf | 90/91 (99%) | 77 (86%) | 13 (14%) | 3 | 15 |
| 69 | Df | 90/91 (99%) | 79 (88%) | 11 (12%) | 5 | 21 |
| 70 | Bg | 95/103 (92%) | 70 (74%) | 25 (26%) | 0 | 2 |
| 70 | Dg | 95/103 (92%) | 71 (75%) | 24 (25%) | 0 | 3 |
| 71 | Bh | 104/105 (99%) | 79 (76%) | 25 (24%) | 0 | 3 |
| 71 | Dh | 103/105 (98%) | 77 (75%) | 26 (25%) | 0 | 3 |
| 72 | Bi | 81/82 (99%) | 58 (72%) | 23 (28%) | 0 | 2 |
| 72 | Di | 80/82 (98%) | 51 (64%) | 29 (36%) | 0 | 1 |
| 73 | Bj | 70/71 (99%) | 56 (80%) | 14 (20%) | 1 | 7 |
| 73 | Dj | 70/71 (99%) | 53 (76%) | 17 (24%) | 0 | 3 |
| 74 | Bk | 68/69 (99%) | 48 (71%) | 20 (29%) | 0 | 1 |
| 74 | Dk | 67/69 (97%) | 53 (79%) | 14 (21%) | 1 | 5 |
| 75 | Bl | 45/46 (98%) | 36 (80%) | 9 (20%) | 1 | 7 |
| 75 | Dl | 45/46 (98%) | 34 (76%) | 11 (24%) | 0 | 3 |
| 76 | Bm | 47/116 (40%) | 37 (79%) | 10 (21%) | 1 | 5 |
| 76 | Dm | 47/116 (40%) | 34 (72%) | 13 (28%) | 0 | 2 |
| 77 | Bn | 23/23 (100%) | 15 (65%) | 8 (35%) | 0 | 1 |
| 77 | Dn | 23/23 (100%) | 16 (70%) | 7 (30%) | 0 | 1 |
| 78 | Bo | 90/91 (99%) | 68 (76%) | 22 (24%) | 0 | 3 |
| 78 | Do | 90/91 (99%) | 74 (82%) | 16 (18%) | 2 | 9 |
| 79 | Bp | 71/72 (99%) | 56 (79%) | 15 (21%) | 1 | 5 |
| 79 | Dp | 71/72 (99%) | 61 (86%) | 10 (14%) | 3 | 16 |
| 81 | Ch | 54/199 (27%) | 38 (70%) | 16 (30%) | 0 | 1 |
| 83 | Dq | 105/233 (45%) | 76 (72%) | 29 (28%) | 0 | 2 |
| All | All | 19013/20583 (92%) | 14917 (78%) | 4096 (22%) | 1 | 5 |

All (4096) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AA | 7 | PHE |
| 2 | AA | 10 | THR |
| 2 | AA | 24 | LEU |
| 2 | AA | 27 | ARG |
| 2 | AA | 29 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | AA | 33 | GLN |
| 2 | AA | 34 | GLU |
| 2 | AA | 37 | VAL |
| 2 | AA | 43 | ASP |
| 2 | AA | 45 | VAL |
| 2 | AA | 47 | VAL |
| 2 | AA | 50 | VAL |
| 2 | AA | 57 | LEU |
| 2 | AA | 59 | LEU |
| 2 | AA | 62 | ARG |
| 2 | AA | 76 | ILE |
| 2 | AA | 79 | ARG |
| 2 | AA | 84 | ARG |
| 2 | AA | 87 | LEU |
| 2 | AA | 88 | LYS |
| 2 | AA | 96 | THR |
| 2 | AA | 101 | ARG |
| 2 | AA | 103 | THR |
| 2 | AA | 110 | TYR |
| 2 | AA | 111 | ILE |
| 2 | AA | 114 | SER |
| 2 | AA | 117 | GLU |
| 2 | AA | 119 | ARG |
| 2 | AA | 123 | VAL |
| 2 | AA | 131 | GLN |
| 2 | AA | 135 | GLU |
| 2 | AA | 140 | ASN |
| 2 | AA | 154 | GLU |
| 2 | AA | 157 | ASP |
| 2 | AA | 162 | CYS |
| 2 | AA | 168 | HIS |
| 2 | AA | 172 | LEU |
| 2 | AA | 177 | LEU |
| 2 | AA | 184 | LEU |
| 2 | AA | 185 | ARG |
| 2 | AA | 196 | SER |
| 2 | AA | 197 | ILE |
| 3 | AB | 21 | VAL |
| 3 | AB | 22 | ASP |
| 3 | AB | 36 | SER |
| 3 | AB | 38 | PHE |
| 3 | AB | 47 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 3 | AB | 54 | LEU |
| 3 | AB | 55 | LYS |
| 3 | AB | 58 | SER |
| 3 | AB | 61 | LEU |
| 3 | AB | 65 | VAL |
| 3 | AB | 68 | VAL |
| 3 | AB | 70 | LEU |
| 3 | AB | 73 | LEU |
| 3 | AB | 77 | GLU |
| 3 | AB | 78 | ASP |
| 3 | AB | 80 | SER |
| 3 | AB | 81 | PHE |
| 3 | AB | 83 | LYS |
| 3 | AB | 85 | LYS |
| 3 | AB | 89 | ASP |
| 3 | AB | 94 | LYS |
| 3 | AB | 96 | LEU |
| 3 | AB | 97 | LEU |
| 3 | AB | 105 | PHE |
| 3 | AB | 108 | ASP |
| 3 | AB | 109 | LYS |
| 3 | AB | 110 | LEU |
| 3 | AB | 115 | ARG |
| 3 | AB | 117 | TRP |
| 3 | AB | 124 | ASN |
| 3 | AB | 131 | ASP |
| 3 | AB | 135 | LEU |
| 3 | AB | 146 | GLN |
| 3 | AB | 148 | ASN |
| 3 | AB | 149 | GLN |
| 3 | AB | 154 | SER |
| 3 | AB | 166 | LYS |
| 3 | AB | 170 | GLU |
| 3 | AB | 177 | GLN |
| 3 | AB | 179 | SER |
| 3 | AB | 180 | THR |
| 3 | AB | 181 | LEU |
| 3 | AB | 183 | GLN |
| 3 | AB | 184 | LEU |
| 3 | AB | 193 | ILE |
| 3 | AB | 202 | LYS |
| 3 | AB | 214 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 3 | AB | 215 | VAL |
| 3 | AB | 218 | LEU |
| 3 | AB | 219 | LYS |
| 3 | AB | 220 | GLN |
| 3 | AB | 223 | PHE |
| 3 | AB | 225 | VAL |
| 3 | AB | 228 | LEU |
| 4 | AC | 41 | LEU |
| 4 | AC | 50 | ILE |
| 4 | AC | 53 | ILE |
| 4 | AC | 58 | LEU |
| 4 | AC | 64 | LYS |
| 4 | AC | 70 | ASP |
| 4 | AC | 71 | THR |
| 4 | AC | 72 | LEU |
| 4 | AC | 73 | LEU |
| 4 | AC | 76 | LEU |
| 4 | AC | 77 | GLN |
| 4 | AC | 80 | VAL |
| 4 | AC | 87 | GLN |
| 4 | AC | 89 | GLN |
| 4 | AC | 90 | THR |
| 4 | AC | 95 | ARG |
| 4 | AC | 96 | THR |
| 4 | AC | 97 | ARG |
| 4 | AC | 106 | ASP |
| 4 | AC | 111 | VAL |
| 4 | AC | 117 | THR |
| 4 | AC | 119 | LYS |
| 4 | AC | 130 | ILE |
| 4 | AC | 134 | LEU |
| 4 | AC | 137 | ILE |
| 4 | AC | 139 | ILE |
| 4 | AC | 140 | ARG |
| 4 | AC | 141 | ARG |
| 4 | AC | 146 | THR |
| 4 | AC | 148 | LEU |
| 4 | AC | 159 | THR |
| 4 | AC | 166 | THR |
| 4 | AC | 174 | ARG |
| 4 | AC | 185 | LYS |
| 4 | AC | 187 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 4 | AC | 201 | ASN |
| 4 | AC | 206 | THR |
| 4 | AC | 208 | GLU |
| 4 | AC | 221 | THR |
| 4 | AC | 222 | TYR |
| 4 | AC | 224 | PHE |
| 4 | AC | 226 | THR |
| 4 | AC | 237 | VAL |
| 4 | AC | 240 | LEU |
| 4 | AC | 245 | ASP |
| 4 | AC | 246 | GLU |
| 5 | AD | 4 | LEU |
| 5 | AD | 5 | ILE |
| 5 | AD | 7 | LYS |
| 5 | AD | 21 | LEU |
| 5 | AD | 23 | GLU |
| 5 | AD | 29 | LEU |
| 5 | AD | 37 | VAL |
| 5 | AD | 39 | VAL |
| 5 | AD | 53 | THR |
| 5 | AD | 57 | ASP |
| 5 | AD | 65 | ARG |
| 5 | AD | 66 | ILE |
| 5 | AD | 81 | PRO |
| 5 | AD | 84 | ILE |
| 5 | AD | 89 | GLU |
| 5 | AD | 90 | ARG |
| 5 | AD | 92 | GLN |
| 5 | AD | 93 | ASP |
| 5 | AD | 94 | ARG |
| 5 | AD | 96 | LEU |
| 5 | AD | 105 | MET |
| 5 | AD | 117 | ARG |
| 5 | AD | 127 | MET |
| 5 | AD | 129 | SER |
| 5 | AD | 134 | CYS |
| 5 | AD | 141 | LYS |
| 5 | AD | 142 | LEU |
| 5 | AD | 146 | ARG |
| 5 | AD | 151 | LYS |
| 5 | AD | 158 | ILE |
| 5 | AD | 170 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 5 | AD | 172 | THR |
| 5 | AD | 176 | LEU |
| 5 | AD | 178 | ARG |
| 5 | AD | 181 | VAL |
| 5 | AD | 182 | LEU |
| 5 | AD | 187 | LYS |
| 5 | AD | 190 | ARG |
| 5 | AD | 204 | ASP |
| 5 | AD | 210 | GLU |
| 5 | AD | 215 | GLU |
| 5 | AD | 220 | PRO |
| 5 | AD | 221 | SER |
| 5 | AD | 222 | VAL |
| 6 | AE | 7 | LYS |
| 6 | AE | 9 | LEU |
| 6 | AE | 12 | LEU |
| 6 | AE | 23 | LEU |
| 6 | AE | 26 | CYS |
| 6 | AE | 38 | LEU |
| 6 | AE | 39 | ARG |
| 6 | AE | 45 | ILE |
| 6 | AE | 48 | LEU |
| 6 | AE | 56 | LEU |
| 6 | AE | 59 | ARG |
| 6 | AE | 62 | LYS |
| 6 | AE | 67 | GLN |
| 6 | AE | 68 | ARG |
| 6 | AE | 70 | VAL |
| 6 | AE | 72 | VAL |
| 6 | AE | 77 | ARG |
| 6 | AE | 92 | LEU |
| 6 | AE | 95 | THR |
| 6 | AE | 105 | VAL |
| 6 | AE | 116 | ASP |
| 6 | AE | 117 | GLU |
| 6 | AE | 123 | LEU |
| 6 | AE | 126 | VAL |
| 6 | AE | 129 | VAL |
| 6 | AE | 131 | LEU |
| 6 | AE | 133 | LYS |
| 6 | AE | 146 | THR |
| 6 | AE | 153 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 6 | AE | 155 | LYS |
| 6 | AE | 158 | ASP |
| 6 | AE | 164 | LEU |
| 6 | AE | 166 | SER |
| 6 | AE | 176 | ASP |
| 6 | AE | 180 | LEU |
| 6 | AE | 182 | TYR |
| 6 | AE | 187 | ARG |
| 6 | AE | 192 | ILE |
| 6 | AE | 197 | HIS |
| 6 | AE | 198 | LYS |
| 6 | AE | 206 | ASP |
| 6 | AE | 211 | LYS |
| 6 | AE | 215 | ASP |
| 6 | AE | 220 | THR |
| 6 | AE | 222 | LEU |
| 6 | AE | 226 | PHE |
| 6 | AE | 227 | VAL |
| 6 | AE | 237 | SER |
| 6 | AE | 240 | LYS |
| 6 | AE | 242 | LYS |
| 6 | AE | 246 | LEU |
| 6 | AE | 248 | ILE |
| 6 | AE | 258 | GLN |
| 6 | AE | 259 | GLN |
| 6 | AE | 261 | LEU |
| 7 | AF | 21 | THR |
| 7 | AF | 23 | VAL |
| 7 | AF | 24 | VAL |
| 7 | AF | 25 | LEU |
| 7 | AF | 27 | THR |
| 7 | AF | 32 | GLU |
| 7 | AF | 41 | LYS |
| 7 | AF | 42 | LEU |
| 7 | AF | 43 | PHE |
| 7 | AF | 45 | LYS |
| 7 | AF | 53 | VAL |
| 7 | AF | 63 | GLN |
| 7 | AF | 65 | ARG |
| 7 | AF | 68 | ILE |
| 7 | AF | 70 | VAL |
| 7 | AF | 76 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 7 | AF | 79 | ASN |
| 7 | AF | 84 | LYS |
| 7 | AF | 89 | ILE |
| 7 | AF | 93 | LEU |
| 7 | AF | 94 | THR |
| 7 | AF | 117 | THR |
| 7 | AF | 119 | ASP |
| 7 | AF | 130 | ILE |
| 7 | AF | 146 | THR |
| 7 | AF | 147 | THR |
| 7 | AF | 156 | ARG |
| 7 | AF | 157 | ARG |
| 7 | AF | 160 | VAL |
| 7 | AF | 162 | VAL |
| 7 | AF | 163 | SER |
| 7 | AF | 193 | THR |
| 7 | AF | 203 | LYS |
| 7 | AF | 206 | SER |
| 7 | AF | 216 | GLU |
| 7 | AF | 225 | ARG |
| 8 | AG | 21 | GLU |
| 8 | AG | 25 | ARG |
| 8 | AG | 45 | PHE |
| 8 | AG | 58 | LYS |
| 8 | AG | 59 | GLN |
| 8 | AG | 69 | LEU |
| 8 | AG | 70 | PRO |
| 8 | AG | 71 | THR |
| 8 | AG | 76 | LEU |
| 8 | AG | 78 | THR |
| 8 | AG | 79 | LYS |
| 8 | AG | 82 | SER |
| 8 | AG | 98 | ARG |
| 8 | AG | 105 | ASP |
| 8 | AG | 109 | LEU |
| 8 | AG | 115 | LYS |
| 8 | AG | 120 | GLU |
| 8 | AG | 124 | LEU |
| 8 | AG | 126 | ASP |
| 8 | AG | 127 | THR |
| 8 | AG | 129 | VAL |
| 8 | AG | 132 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 8 | AG | 133 | LEU |
| 8 | AG | 137 | ARG |
| 8 | AG | 143 | LYS |
| 8 | AG | 150 | GLU |
| 8 | AG | 151 | ASP |
| 8 | AG | 154 | ARG |
| 8 | AG | 155 | ASP |
| 8 | AG | 162 | VAL |
| 8 | AG | 170 | THR |
| 8 | AG | 175 | ILE |
| 8 | AG | 176 | GLN |
| 8 | AG | 177 | ARG |
| 8 | AG | 179 | VAL |
| 8 | AG | 211 | LEU |
| 8 | AG | 212 | LEU |
| 8 | AG | 217 | SER |
| 8 | AG | 223 | LYS |
| 9 | AH | 9 | LEU |
| 9 | AH | 25 | VAL |
| 9 | AH | 37 | GLU |
| 9 | AH | 38 | LEU |
| 9 | AH | 42 | GLN |
| 9 | AH | 46 | ILE |
| 9 | AH | 50 | ASP |
| 9 | AH | 51 | VAL |
| 9 | AH | 60 | ILE |
| 9 | AH | 66 | SER |
| 9 | AH | 67 | LEU |
| 9 | AH | 70 | PHE |
| 9 | AH | 71 | HIS |
| 9 | AH | 74 | GLN |
| 9 | AH | 75 | THR |
| 9 | AH | 77 | LEU |
| 9 | AH | 78 | THR |
| 9 | AH | 79 | ARG |
| 9 | AH | 80 | GLU |
| 9 | AH | 85 | PHE |
| 9 | AH | 87 | ASP |
| 9 | AH | 97 | ARG |
| 9 | AH | 103 | SER |
| 9 | AH | 105 | THR |
| 9 | AH | 109 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 9 | AH | 110 | GLN |
| 9 | AH | 114 | ARG |
| 9 | AH | 116 | ARG |
| 9 | AH | 117 | THR |
| 9 | AH | 126 | LEU |
| 9 | AH | 131 | PHE |
| 9 | AH | 143 | LEU |
| 9 | AH | 144 | VAL |
| 9 | AH | 148 | LYS |
| 9 | AH | 154 | LEU |
| 9 | AH | 162 | ILE |
| 9 | AH | 167 | GLU |
| 9 | AH | 181 | ILE |
| 9 | AH | 184 | GLU |
| 9 | AH | 185 | ILE |
| 9 | AH | 187 | SER |
| 10 | AI | 6 | ASP |
| 10 | AI | 7 | SER |
| 10 | AI | 8 | ARG |
| 10 | AI | 14 | THR |
| 10 | AI | 20 | GLN |
| 10 | AI | 21 | PHE |
| 10 | AI | 26 | LYS |
| 10 | AI | 28 | GLU |
| 10 | AI | 29 | LEU |
| 10 | AI | 36 | THR |
| 10 | AI | 46 | VAL |
| 10 | AI | 49 | ARG |
| 10 | AI | 58 | LEU |
| 10 | AI | 76 | THR |
| 10 | AI | 103 | GLN |
| 10 | AI | 107 | THR |
| 10 | AI | 120 | THR |
| 10 | AI | 121 | LEU |
| 10 | AI | 123 | LYS |
| 10 | AI | 135 | LYS |
| 10 | AI | 137 | LYS |
| 10 | AI | 138 | ASN |
| 10 | AI | 140 | GLU |
| 10 | AI | 142 | LYS |
| 10 | AI | 151 | LYS |
| 10 | AI | 152 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 10 | AI | 154 | SER |
| 10 | AI | 155 | SER |
| 10 | AI | 164 | ARG |
| 10 | AI | 184 | LEU |
| 10 | AI | 196 | LEU |
| 10 | AI | 199 | LYS |
| 11 | AJ | 3 | ARG |
| 11 | AJ | 6 | ARG |
| 11 | AJ | 7 | THR |
| 11 | AJ | 13 | SER |
| 11 | AJ | 14 | THR |
| 11 | AJ | 22 | SER |
| 11 | AJ | 28 | LEU |
| 11 | AJ | 39 | LYS |
| 11 | AJ | 46 | SER |
| 11 | AJ | 49 | LEU |
| 11 | AJ | 54 | ARG |
| 11 | AJ | 60 | LEU |
| 11 | AJ | 78 | ARG |
| 11 | AJ | 79 | ARG |
| 11 | AJ | 82 | ARG |
| 11 | AJ | 88 | GLU |
| 11 | AJ | 89 | ASP |
| 11 | AJ | 92 | LYS |
| 11 | AJ | 93 | LEU |
| 11 | AJ | 94 | ASP |
| 11 | AJ | 96 | VAL |
| 11 | AJ | 97 | LEU |
| 11 | AJ | 99 | LEU |
| 11 | AJ | 101 | VAL |
| 11 | AJ | 105 | LEU |
| 11 | AJ | 109 | LEU |
| 11 | AJ | 110 | GLN |
| 11 | AJ | 111 | THR |
| 11 | AJ | 120 | LYS |
| 11 | AJ | 130 | THR |
| 11 | AJ | 133 | HIS |
| 11 | AJ | 134 | ILE |
| 11 | AJ | 138 | LYS |
| 11 | AJ | 149 | ARG |
| 11 | AJ | 151 | ASP |
| 11 | AJ | 161 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 11 | AJ | 171 | ARG |
| 11 | AJ | 172 | VAL |
| 11 | AJ | 174 | ARG |
| 11 | AJ | 175 | ARG |
| 11 | AJ | 182 | GLU |
| 12 | AK | 1 | MET |
| 12 | AK | 7 | ASP |
| 12 | AK | 8 | ARG |
| 12 | AK | 13 | GLN |
| 12 | AK | 20 | VAL |
| 12 | AK | 27 | PHE |
| 12 | AK | 29 | GLN |
| 12 | AK | 31 | LYS |
| 12 | AK | 32 | HIS |
| 12 | AK | 46 | LEU |
| 12 | AK | 49 | LEU |
| 12 | AK | 50 | THR |
| 12 | AK | 55 | VAL |
| 12 | AK | 56 | LYS |
| 12 | AK | 71 | GLU |
| 12 | AK | 76 | LEU |
| 12 | AK | 78 | GLU |
| 12 | AK | 80 | LEU |
| 12 | AK | 82 | LEU |
| 13 | AL | 3 | THR |
| 13 | AL | 7 | VAL |
| 13 | AL | 21 | ASN |
| 13 | AL | 27 | THR |
| 13 | AL | 29 | LYS |
| 13 | AL | 30 | ARG |
| 13 | AL | 40 | LEU |
| 13 | AL | 43 | LYS |
| 13 | AL | 44 | THR |
| 13 | AL | 54 | ILE |
| 13 | AL | 56 | LYS |
| 13 | AL | 67 | ARG |
| 13 | AL | 69 | LYS |
| 13 | AL | 74 | THR |
| 13 | AL | 79 | LYS |
| 13 | AL | 80 | MET |
| 13 | AL | 83 | THR |
| 13 | AL | 99 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 13 | AL | 109 | VAL |
| 13 | AL | 123 | VAL |
| 13 | AL | 131 | ILE |
| 13 | AL | 136 | ARG |
| 13 | AL | 140 | VAL |
| 13 | AL | 141 | LYS |
| 14 | AM | 25 | GLU |
| 14 | AM | 28 | LEU |
| 14 | AM | 33 | ARG |
| 14 | AM | 36 | LEU |
| 14 | AM | 43 | ARG |
| 14 | AM | 45 | LEU |
| 14 | AM | 50 | LYS |
| 14 | AM | 53 | THR |
| 14 | AM | 58 | LEU |
| 14 | AM | 59 | LEU |
| 14 | AM | 61 | VAL |
| 14 | AM | 62 | LEU |
| 14 | AM | 63 | VAL |
| 14 | AM | 71 | ILE |
| 14 | AM | 74 | LEU |
| 14 | AM | 75 | VAL |
| 14 | AM | 83 | GLU |
| 14 | AM | 85 | LYS |
| 14 | AM | 88 | LEU |
| 14 | AM | 89 | ILE |
| 14 | AM | 97 | LEU |
| 14 | AM | 103 | LEU |
| 14 | AM | 116 | VAL |
| 14 | AM | 119 | SER |
| 14 | AM | 121 | VAL |
| 14 | AM | 125 | ASN |
| 14 | AM | 126 | TRP |
| 14 | AM | 129 | GLU |
| 14 | AM | 132 | GLU |
| 14 | AM | 135 | MET |
| 14 | AM | 138 | GLU |
| 14 | AM | 139 | HIS |
| 14 | AM | 140 | PHE |
| 15 | AN | 3 | ARG |
| 15 | AN | 4 | MET |
| 15 | AN | 9 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 15 | AN | 12 | SER |
| 15 | AN | 16 | ILE |
| 15 | AN | 21 | ASN |
| 15 | AN | 27 | LYS |
| 15 | AN | 33 | VAL |
| 15 | AN | 36 | GLN |
| 15 | AN | 39 | LYS |
| 15 | AN | 42 | ARG |
| 15 | AN | 45 | LEU |
| 15 | AN | 50 | ILE |
| 15 | AN | 56 | ASP |
| 15 | AN | 58 | HIS |
| 15 | AN | 60 | VAL |
| 15 | AN | 64 | ARG |
| 15 | AN | 66 | ILE |
| 15 | AN | 67 | THR |
| 15 | AN | 76 | LYS |
| 15 | AN | 77 | SER |
| 15 | AN | 83 | GLU |
| 15 | AN | 84 | ILE |
| 15 | AN | 88 | LEU |
| 15 | AN | 94 | LYS |
| 15 | AN | 97 | SER |
| 15 | AN | 102 | LEU |
| 15 | AN | 105 | ASN |
| 15 | AN | 109 | LYS |
| 15 | AN | 114 | ARG |
| 15 | AN | 115 | LEU |
| 15 | AN | 125 | LEU |
| 15 | AN | 145 | THR |
| 15 | AN | 149 | LEU |
| 15 | AN | 150 | VAL |
| 15 | AN | 151 | ASN |
| 16 | AO | 13 | VAL |
| 16 | AO | 14 | PHE |
| 16 | AO | 16 | VAL |
| 16 | AO | 20 | TYR |
| 16 | AO | 24 | ASN |
| 16 | AO | 26 | THR |
| 16 | AO | 29 | HIS |
| 16 | AO | 31 | THR |
| 16 | AO | 39 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 16 | AO | 42 | VAL |
| 16 | AO | 43 | THR |
| 16 | AO | 51 | ASP |
| 16 | AO | 92 | LYS |
| 16 | AO | 99 | GLN |
| 16 | AO | 102 | LEU |
| 16 | AO | 103 | ARG |
| 16 | AO | 107 | ARG |
| 16 | AO | 108 | SER |
| 16 | AO | 118 | VAL |
| 16 | AO | 123 | SER |
| 16 | AO | 124 | ASP |
| 16 | AO | 125 | SER |
| 16 | AO | 133 | ARG |
| 16 | AO | 137 | LEU |
| 17 | AP | 14 | THR |
| 17 | AP | 22 | LEU |
| 17 | AP | 24 | LYS |
| 17 | AP | 26 | LEU |
| 17 | AP | 31 | GLU |
| 17 | AP | 35 | LYS |
| 17 | AP | 40 | ARG |
| 17 | AP | 44 | ARG |
| 17 | AP | 47 | ARG |
| 17 | AP | 50 | THR |
| 17 | AP | 52 | LYS |
| 17 | AP | 69 | GLU |
| 17 | AP | 86 | VAL |
| 17 | AP | 92 | SER |
| 17 | AP | 100 | LYS |
| 17 | AP | 110 | GLU |
| 17 | AP | 121 | ILE |
| 17 | AP | 125 | PRO |
| 17 | AP | 130 | ARG |
| 18 | AQ | 4 | VAL |
| 18 | AQ | 14 | LYS |
| 18 | AQ | 17 | THR |
| 18 | AQ | 23 | LYS |
| 18 | AQ | 26 | LYS |
| 18 | AQ | 28 | LEU |
| 18 | AQ | 36 | ILE |
| 18 | AQ | 44 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 18 | AQ | 45 | ARG |
| 18 | AQ | 52 | LEU |
| 18 | AQ | 53 | LEU |
| 18 | AQ | 54 | LEU |
| 18 | AQ | 57 | LEU |
| 18 | AQ | 59 | LYS |
| 18 | AQ | 63 | ILE |
| 18 | AQ | 66 | ARG |
| 18 | AQ | 68 | ARG |
| 18 | AQ | 69 | VAL |
| 18 | AQ | 76 | SER |
| 18 | AQ | 90 | VAL |
| 18 | AQ | 94 | GLN |
| 18 | AQ | 98 | ASP |
| 18 | AQ | 101 | SER |
| 18 | AQ | 106 | LYS |
| 18 | AQ | 115 | THR |
| 18 | AQ | 118 | ILE |
| 18 | AQ | 123 | ARG |
| 18 | AQ | 127 | LYS |
| 18 | AQ | 128 | LYS |
| 18 | AQ | 136 | SER |
| 18 | AQ | 137 | ARG |
| 18 | AQ | 138 | PHE |
| 18 | AQ | 141 | SER |
| 19 | AR | 5 | ARG |
| 19 | AR | 25 | THR |
| 19 | AR | 26 | LEU |
| 19 | AR | 29 | GLN |
| 19 | AR | 30 | THR |
| 19 | AR | 34 | LEU |
| 19 | AR | 36 | ASP |
| 19 | AR | 38 | ILE |
| 19 | AR | 44 | LYS |
| 19 | AR | 46 | LEU |
| 19 | AR | 49 | LYS |
| 19 | AR | 54 | THR |
| 19 | AR | 69 | ILE |
| 19 | AR | 72 | LYS |
| 19 | AR | 73 | LEU |
| 19 | AR | 78 | ARG |
| 19 | AR | 83 | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 19 | AR | 84 | TYR |
| 19 | AR | 87 | GLU |
| 19 | AR | 105 | GLN |
| 19 | AR | 107 | SER |
| 19 | AR | 113 | LEU |
| 19 | AR | 115 | LEU |
| 19 | AR | 119 | LEU |
| 20 | AS | 3 | LEU |
| 20 | AS | 5 | VAL |
| 20 | AS | 8 | GLN |
| 20 | AS | 11 | PHE |
| 20 | AS | 12 | GLN |
| 20 | AS | 13 | HIS |
| 20 | AS | 14 | ILE |
| 20 | AS | 15 | LEU |
| 20 | AS | 17 | LEU |
| 20 | AS | 20 | THR |
| 20 | AS | 21 | ASN |
| 20 | AS | 26 | ILE |
| 20 | AS | 28 | ILE |
| 20 | AS | 34 | THR |
| 20 | AS | 38 | VAL |
| 20 | AS | 40 | ARG |
| 20 | AS | 46 | VAL |
| 20 | AS | 53 | ASP |
| 20 | AS | 54 | LEU |
| 20 | AS | 57 | ARG |
| 20 | AS | 60 | GLU |
| 20 | AS | 61 | LEU |
| 20 | AS | 71 | GLN |
| 20 | AS | 74 | GLN |
| 20 | AS | 77 | THR |
| 20 | AS | 80 | LYS |
| 20 | AS | 81 | ILE |
| 20 | AS | 86 | LEU |
| 20 | AS | 89 | GLN |
| 20 | AS | 92 | ILE |
| 20 | AS | 93 | THR |
| 20 | AS | 107 | SER |
| 20 | AS | 108 | LYS |
| 20 | AS | 110 | ARG |
| 20 | AS | 116 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 20 | AS | 119 | ILE |
| 20 | AS | 132 | ARG |
| 20 | AS | 136 | GLN |
| 20 | AS | 138 | THR |
| 20 | AS | 140 | THR |
| 20 | AS | 143 | ARG |
| 21 | AT | 4 | VAL |
| 21 | AT | 6 | VAL |
| 21 | AT | 13 | ASP |
| 21 | AT | 18 | TYR |
| 21 | AT | 22 | LEU |
| 21 | AT | 25 | GLN |
| 21 | AT | 28 | LEU |
| 21 | AT | 30 | VAL |
| 21 | AT | 33 | TYR |
| 21 | AT | 34 | VAL |
| 21 | AT | 35 | ASP |
| 21 | AT | 36 | ILE |
| 21 | AT | 37 | VAL |
| 21 | AT | 57 | ARG |
| 21 | AT | 63 | ARG |
| 21 | AT | 67 | MET |
| 21 | AT | 68 | ARG |
| 21 | AT | 84 | LYS |
| 21 | AT | 86 | ARG |
| 21 | AT | 88 | VAL |
| 21 | AT | 89 | ARG |
| 21 | AT | 92 | LYS |
| 21 | AT | 94 | ILE |
| 21 | AT | 103 | LYS |
| 21 | AT | 111 | ILE |
| 21 | AT | 126 | GLU |
| 21 | AT | 130 | ARG |
| 21 | AT | 131 | ASP |
| 21 | AT | 132 | LEU |
| 21 | AT | 134 | ARG |
| 21 | AT | 144 | GLU |
| 22 | AU | 15 | GLN |
| 22 | AU | 17 | GLN |
| 22 | AU | 18 | GLN |
| 22 | AU | 20 | ILE |
| 22 | AU | 22 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 22 | AU | 23 | ARG |
| 22 | AU | 27 | THR |
| 22 | AU | 30 | LYS |
| 22 | AU | 31 | VAL |
| 22 | AU | 34 | LEU |
| 22 | AU | 35 | GLU |
| 22 | AU | 42 | VAL |
| 22 | AU | 47 | GLN |
| 22 | AU | 48 | HIS |
| 22 | AU | 51 | VAL |
| 22 | AU | 57 | ARG |
| 22 | AU | 58 | LEU |
| 22 | AU | 60 | THR |
| 22 | AU | 61 | LYS |
| 22 | AU | 66 | SER |
| 22 | AU | 74 | GLU |
| 22 | AU | 76 | SER |
| 22 | AU | 81 | THR |
| 22 | AU | 88 | LYS |
| 22 | AU | 89 | ARG |
| 22 | AU | 99 | ILE |
| 22 | AU | 103 | ILE |
| 22 | AU | 108 | ILE |
| 22 | AU | 121 | ASN |
| 23 | AV | 1 | MET |
| 23 | AV | 2 | GLU |
| 23 | AV | 3 | ASN |
| 23 | AV | 5 | LYS |
| 23 | AV | 7 | GLN |
| 23 | AV | 11 | LEU |
| 23 | AV | 25 | LYS |
| 23 | AV | 41 | GLU |
| 23 | AV | 49 | GLU |
| 23 | AV | 50 | TYR |
| 23 | AV | 52 | THR |
| 23 | AV | 60 | ARG |
| 23 | AV | 62 | ARG |
| 23 | AV | 68 | SER |
| 23 | AV | 69 | LEU |
| 23 | AV | 74 | GLN |
| 23 | AV | 76 | ASP |
| 23 | AV | 80 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 24 | AW | 3 | ARG |
| 24 | AW | 6 | VAL |
| 24 | AW | 7 | LEU |
| 24 | AW | 23 | ARG |
| 24 | AW | 24 | GLN |
| 24 | AW | 25 | VAL |
| 24 | AW | 27 | ILE |
| 24 | AW | 30 | SER |
| 24 | AW | 43 | LYS |
| 24 | AW | 53 | ILE |
| 24 | AW | 56 | HIS |
| 24 | AW | 65 | LEU |
| 24 | AW | 66 | ASN |
| 24 | AW | 69 | LEU |
| 24 | AW | 74 | VAL |
| 24 | AW | 76 | SER |
| 24 | AW | 83 | ILE |
| 24 | AW | 87 | GLU |
| 24 | AW | 93 | LEU |
| 24 | AW | 98 | GLN |
| 24 | AW | 103 | ILE |
| 24 | AW | 104 | LEU |
| 24 | AW | 105 | THR |
| 24 | AW | 114 | GLU |
| 24 | AW | 121 | VAL |
| 24 | AW | 129 | VAL |
| 25 | AX | 7 | ARG |
| 25 | AX | 9 | LEU |
| 25 | AX | 14 | LYS |
| 25 | AX | 18 | HIS |
| 25 | AX | 19 | ARG |
| 25 | AX | 28 | ASN |
| 25 | AX | 40 | SER |
| 25 | AX | 60 | GLU |
| 25 | AX | 82 | LYS |
| 25 | AX | 84 | THR |
| 25 | AX | 103 | LEU |
| 25 | AX | 107 | PHE |
| 25 | AX | 109 | ARG |
| 25 | AX | 110 | LYS |
| 25 | AX | 114 | LYS |
| 25 | AX | 117 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | AX | 131 | SER |
| 25 | AX | 133 | LEU |
| 25 | AX | 137 | LYS |
| 25 | AX | 138 | GLU |
| 25 | AX | 140 | LYS |
| 25 | AX | 144 | ARG |
| 26 | AY | 17 | LEU |
| 26 | AY | 29 | HIS |
| 26 | AY | 32 | ARG |
| 26 | AY | 34 | ASN |
| 26 | AY | 44 | LEU |
| 26 | AY | 46 | GLU |
| 26 | AY | 47 | VAL |
| 26 | AY | 49 | LYS |
| 26 | AY | 51 | GLU |
| 26 | AY | 52 | LYS |
| 26 | AY | 57 | VAL |
| 26 | AY | 61 | ARG |
| 26 | AY | 62 | THR |
| 26 | AY | 75 | VAL |
| 26 | AY | 84 | LYS |
| 26 | AY | 88 | THR |
| 26 | AY | 93 | ARG |
| 26 | AY | 96 | LEU |
| 26 | AY | 99 | LYS |
| 26 | AY | 102 | LYS |
| 26 | AY | 105 | ARG |
| 26 | AY | 112 | LYS |
| 26 | AY | 123 | LYS |
| 26 | AY | 124 | ARG |
| 26 | AY | 127 | LYS |
| 26 | AY | 128 | LYS |
| 26 | AY | 129 | VAL |
| 26 | AY | 135 | ASP |
| 27 | AZ | 38 | HIS |
| 27 | AZ | 42 | LEU |
| 27 | AZ | 49 | ARG |
| 27 | AZ | 50 | ILE |
| 27 | AZ | 58 | ARG |
| 27 | AZ | 59 | TYR |
| 27 | AZ | 69 | LEU |
| 27 | AZ | 71 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 27 | AZ | 75 | LEU |
| 27 | AZ | 77 | ARG |
| 27 | AZ | 80 | LEU |
| 27 | AZ | 85 | LYS |
| 27 | AZ | 92 | ILE |
| 27 | AZ | 93 | SER |
| 27 | AZ | 95 | HIS |
| 27 | AZ | 96 | SER |
| 27 | AZ | 100 | ILE |
| 27 | AZ | 105 | THR |
| 28 | Aa | 12 | LYS |
| 28 | Aa | 36 | ILE |
| 28 | Aa | 41 | ILE |
| 28 | Aa | 44 | ILE |
| 28 | Aa | 45 | VAL |
| 28 | Aa | 53 | LEU |
| 28 | Aa | 58 | VAL |
| 28 | Aa | 61 | GLU |
| 28 | Aa | 64 | LEU |
| 28 | Aa | 66 | LYS |
| 28 | Aa | 67 | THR |
| 28 | Aa | 69 | ASN |
| 28 | Aa | 70 | LYS |
| 28 | Aa | 82 | ARG |
| 28 | Aa | 83 | ILE |
| 28 | Aa | 85 | ARG |
| 28 | Aa | 86 | VAL |
| 28 | Aa | 90 | GLU |
| 29 | Ab | 3 | LEU |
| 29 | Ab | 4 | VAL |
| 29 | Ab | 20 | LYS |
| 29 | Ab | 29 | ARG |
| 29 | Ab | 33 | LEU |
| 29 | Ab | 34 | ASP |
| 29 | Ab | 41 | LEU |
| 29 | Ab | 67 | THR |
| 30 | Ac | 5 | THR |
| 30 | Ac | 13 | ILE |
| 30 | Ac | 14 | LYS |
| 30 | Ac | 15 | VAL |
| 30 | Ac | 19 | THR |
| 30 | Ac | 32 | PHE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 30 | Ac | 33 | LEU |
| 30 | Ac | 34 | GLU |
| 30 | Ac | 38 | ARG |
| 30 | Ac | 39 | THR |
| 30 | Ac | 49 | ARG |
| 30 | Ac | 52 | ASP |
| 30 | Ac | 57 | MET |
| 30 | Ac | 58 | GLU |
| 30 | Ac | 59 | SER |
| 30 | Ac | 62 | GLU |
| 30 | Ac | 64 | ARG |
| 30 | Ac | 65 | ARG |
| 31 | Ad | 6 | VAL |
| 31 | Ad | 8 | PHE |
| 31 | Ad | 22 | ARG |
| 31 | Ad | 25 | SER |
| 31 | Ad | 30 | LEU |
| 31 | Ad | 32 | ARG |
| 31 | Ad | 36 | LEU |
| 31 | Ad | 39 | CYS |
| 31 | Ad | 48 | ASN |
| 32 | Ae | 20 | LYS |
| 32 | Ae | 25 | GLU |
| 32 | Ae | 26 | LYS |
| 32 | Ae | 28 | LYS |
| 32 | Ae | 29 | LYS |
| 32 | Ae | 42 | ARG |
| 32 | Ae | 48 | THR |
| 32 | Ae | 50 | VAL |
| 33 | Af | 102 | VAL |
| 33 | Af | 108 | VAL |
| 33 | Af | 120 | GLU |
| 33 | Af | 121 | CYS |
| 33 | Af | 125 | THR |
| 33 | Af | 130 | VAL |
| 33 | Af | 137 | ASP |
| 33 | Af | 140 | TYR |
| 33 | Af | 146 | SER |
| 33 | Af | 147 | VAL |
| 33 | Af | 151 | ASN |
| 34 | Ag | 6 | VAL |
| 34 | Ag | 7 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 34 | Ag | 8 | VAL |
| 34 | Ag | 46 | LYS |
| 34 | Ag | 48 | THR |
| 34 | Ag | 51 | ASP |
| 34 | Ag | 52 | GLN |
| 34 | Ag | 59 | ARG |
| 34 | Ag | 71 | CYS |
| 34 | Ag | 76 | ASP |
| 34 | Ag | 87 | LYS |
| 34 | Ag | 88 | THR |
| 34 | Ag | 94 | VAL |
| 34 | Ag | 96 | THR |
| 34 | Ag | 112 | SER |
| 34 | Ag | 117 | LYS |
| 34 | Ag | 118 | LYS |
| 34 | Ag | 129 | LYS |
| 34 | Ag | 134 | TRP |
| 34 | Ag | 136 | ILE |
| 34 | Ag | 137 | LYS |
| 34 | Ag | 141 | LEU |
| 34 | Ag | 149 | ASP |
| 34 | Ag | 153 | GLN |
| 34 | Ag | 165 | ASP |
| 34 | Ag | 166 | SER |
| 34 | Ag | 188 | ILE |
| 34 | Ag | 199 | ILE |
| 34 | Ag | 207 | ASP |
| 34 | Ag | 221 | MET |
| 34 | Ag | 238 | ASP |
| 34 | Ag | 250 | TYR |
| 34 | Ag | 266 | ASP |
| 34 | Ag | 268 | GLN |
| 34 | Ag | 292 | LEU |
| 34 | Ag | 300 | THR |
| 34 | Ag | 317 | THR |
| 35 | Ah | 28 | SER |
| 35 | Ah | 34 | LYS |
| 35 | Ah | 46 | LYS |
| 35 | Ah | 51 | ARG |
| 35 | Ah | 61 | ILE |
| 35 | Ah | 64 | LYS |
| 35 | Ah | 65 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 35 | Ah | 68 | ARG |
| 35 | Ah | 75 | ASP |
| 35 | Ah | 78 | ASP |
| 35 | Ah | 82 | THR |
| 35 | Ah | 84 | LYS |
| 35 | Ah | 88 | ARG |
| 35 | Ah | 89 | ARG |
| 35 | Ah | 94 | HIS |
| 35 | Ah | 96 | ARG |
| 35 | Ah | 97 | THR |
| 35 | Ah | 100 | THR |
| 35 | Ah | 102 | THR |
| 35 | Ah | 105 | LYS |
| 35 | Ah | 112 | ASP |
| 35 | Ah | 130 | GLU |
| 35 | Ah | 139 | GLU |
| 39 | BA | 10 | LYS |
| 39 | BA | 18 | SER |
| 39 | BA | 20 | THR |
| 39 | BA | 30 | ARG |
| 39 | BA | 32 | LEU |
| 39 | BA | 44 | ILE |
| 39 | BA | 45 | VAL |
| 39 | BA | 48 | ILE |
| 39 | BA | 62 | VAL |
| 39 | BA | 70 | ARG |
| 39 | BA | 72 | ARG |
| 39 | BA | 74 | GLU |
| 39 | BA | 88 | ILE |
| 39 | BA | 95 | SER |
| 39 | BA | 101 | VAL |
| 39 | BA | 104 | LEU |
| 39 | BA | 116 | VAL |
| 39 | BA | 157 | VAL |
| 39 | BA | 165 | VAL |
| 39 | BA | 177 | LYS |
| 39 | BA | 179 | LEU |
| 39 | BA | 180 | LEU |
| 39 | BA | 181 | LYS |
| 39 | BA | 190 | ARG |
| 39 | BA | 191 | LEU |
| 39 | BA | 202 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 39 | BA | 204 | MET |
| 39 | BA | 207 | VAL |
| 39 | BA | 219 | ILE |
| 39 | BA | 225 | ILE |
| 39 | BA | 227 | ARG |
| 39 | BA | 230 | VAL |
| 39 | BA | 247 | ARG |
| 40 | BB | 2 | SER |
| 40 | BB | 7 | GLU |
| 40 | BB | 10 | ARG |
| 40 | BB | 17 | LEU |
| 40 | BB | 19 | ARG |
| 40 | BB | 20 | LYS |
| 40 | BB | 25 | ILE |
| 40 | BB | 30 | LYS |
| 40 | BB | 37 | ARG |
| 40 | BB | 39 | LYS |
| 40 | BB | 47 | LEU |
| 40 | BB | 50 | LYS |
| 40 | BB | 56 | ILE |
| 40 | BB | 73 | VAL |
| 40 | BB | 79 | VAL |
| 40 | BB | 84 | VAL |
| 40 | BB | 85 | VAL |
| 40 | BB | 90 | VAL |
| 40 | BB | 100 | ARG |
| 40 | BB | 103 | THR |
| 40 | BB | 105 | VAL |
| 40 | BB | 110 | LEU |
| 40 | BB | 111 | SER |
| 40 | BB | 114 | VAL |
| 40 | BB | 116 | ARG |
| 40 | BB | 121 | ASN |
| 40 | BB | 134 | SER |
| 40 | BB | 139 | GLN |
| 40 | BB | 146 | ARG |
| 40 | BB | 148 | LEU |
| 40 | BB | 150 | ARG |
| 40 | BB | 153 | LYS |
| 40 | BB | 156 | SER |
| 40 | BB | 162 | VAL |
| 40 | BB | 166 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 40 | BB | 167 | ARG |
| 40 | BB | 169 | THR |
| 40 | BB | 173 | GLN |
| 40 | BB | 183 | LEU |
| 40 | BB | 187 | SER |
| 40 | BB | 188 | ILE |
| 40 | BB | 192 | VAL |
| 40 | BB | 196 | ARG |
| 40 | BB | 200 | GLU |
| 40 | BB | 202 | THR |
| 40 | BB | 205 | VAL |
| 40 | BB | 206 | ASP |
| 40 | BB | 210 | GLU |
| 40 | BB | 221 | THR |
| 40 | BB | 229 | VAL |
| 40 | BB | 232 | ARG |
| 40 | BB | 235 | THR |
| 40 | BB | 238 | LEU |
| 40 | BB | 241 | LYS |
| 40 | BB | 242 | THR |
| 40 | BB | 244 | ARG |
| 40 | BB | 264 | VAL |
| 40 | BB | 281 | LYS |
| 40 | BB | 300 | ARG |
| 40 | BB | 301 | THR |
| 40 | BB | 305 | ILE |
| 40 | BB | 308 | MET |
| 40 | BB | 319 | ASN |
| 40 | BB | 320 | ASP |
| 40 | BB | 324 | VAL |
| 40 | BB | 325 | LYS |
| 40 | BB | 328 | ILE |
| 40 | BB | 332 | ARG |
| 40 | BB | 338 | LEU |
| 40 | BB | 341 | SER |
| 40 | BB | 344 | THR |
| 40 | BB | 347 | SER |
| 40 | BB | 349 | LYS |
| 40 | BB | 352 | GLU |
| 40 | BB | 355 | SER |
| 40 | BB | 361 | THR |
| 40 | BB | 364 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 40 | BB | 372 | THR |
| 40 | BB | 380 | MET |
| 40 | BB | 385 | LYS |
| 40 | BB | 387 | LEU |
| 41 | BC | 4 | PRO |
| 41 | BC | 22 | LEU |
| 41 | BC | 25 | VAL |
| 41 | BC | 40 | THR |
| 41 | BC | 47 | ARG |
| 41 | BC | 53 | SER |
| 41 | BC | 60 | THR |
| 41 | BC | 71 | VAL |
| 41 | BC | 73 | ARG |
| 41 | BC | 74 | ILE |
| 41 | BC | 93 | MET |
| 41 | BC | 99 | MET |
| 41 | BC | 122 | THR |
| 41 | BC | 124 | SER |
| 41 | BC | 133 | SER |
| 41 | BC | 136 | LEU |
| 41 | BC | 138 | ARG |
| 41 | BC | 144 | LYS |
| 41 | BC | 148 | ILE |
| 41 | BC | 150 | LEU |
| 41 | BC | 152 | VAL |
| 41 | BC | 156 | LEU |
| 41 | BC | 170 | LYS |
| 41 | BC | 172 | VAL |
| 41 | BC | 177 | ASP |
| 41 | BC | 179 | LEU |
| 41 | BC | 185 | LYS |
| 41 | BC | 187 | LEU |
| 41 | BC | 188 | ARG |
| 41 | BC | 193 | LYS |
| 41 | BC | 200 | THR |
| 41 | BC | 203 | ARG |
| 41 | BC | 206 | LEU |
| 41 | BC | 220 | ARG |
| 41 | BC | 222 | VAL |
| 41 | BC | 230 | VAL |
| 41 | BC | 233 | LEU |
| 41 | BC | 246 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 41 | BC | 258 | LEU |
| 41 | BC | 259 | ASP |
| 41 | BC | 267 | VAL |
| 41 | BC | 283 | THR |
| 41 | BC | 287 | THR |
| 41 | BC | 289 | ILE |
| 41 | BC | 295 | ILE |
| 41 | BC | 306 | THR |
| 41 | BC | 307 | GLN |
| 41 | BC | 313 | LEU |
| 41 | BC | 319 | LYS |
| 41 | BC | 323 | VAL |
| 41 | BC | 332 | LYS |
| 41 | BC | 333 | VAL |
| 41 | BC | 339 | LEU |
| 41 | BC | 343 | LYS |
| 41 | BC | 345 | GLU |
| 41 | BC | 346 | LYS |
| 41 | BC | 349 | THR |
| 41 | BC | 350 | LYS |
| 41 | BC | 354 | VAL |
| 41 | BC | 356 | THR |
| 41 | BC | 358 | THR |
| 42 | BD | 4 | GLN |
| 42 | BD | 5 | LYS |
| 42 | BD | 8 | LYS |
| 42 | BD | 9 | SER |
| 42 | BD | 10 | SER |
| 42 | BD | 15 | ARG |
| 42 | BD | 22 | ARG |
| 42 | BD | 23 | ARG |
| 42 | BD | 35 | ARG |
| 42 | BD | 41 | LYS |
| 42 | BD | 50 | ARG |
| 42 | BD | 64 | ILE |
| 42 | BD | 68 | THR |
| 42 | BD | 69 | ILE |
| 42 | BD | 81 | HIS |
| 42 | BD | 85 | ARG |
| 42 | BD | 89 | THR |
| 42 | BD | 92 | LEU |
| 42 | BD | 93 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 42 | BD | 95 | TRP |
| 42 | BD | 105 | ILE |
| 42 | BD | 109 | THR |
| 42 | BD | 115 | LEU |
| 42 | BD | 118 | THR |
| 42 | BD | 123 | GLU |
| 42 | BD | 131 | LEU |
| 42 | BD | 135 | VAL |
| 42 | BD | 137 | ASP |
| 42 | BD | 140 | ARG |
| 42 | BD | 144 | VAL |
| 42 | BD | 146 | LEU |
| 42 | BD | 148 | ILE |
| 42 | BD | 151 | GLN |
| 42 | BD | 152 | ARG |
| 42 | BD | 154 | THR |
| 42 | BD | 155 | THR |
| 42 | BD | 163 | LEU |
| 42 | BD | 177 | GLU |
| 42 | BD | 185 | PHE |
| 42 | BD | 187 | THR |
| 42 | BD | 188 | GLU |
| 42 | BD | 196 | ARG |
| 42 | BD | 211 | LEU |
| 42 | BD | 222 | LEU |
| 42 | BD | 231 | ILE |
| 42 | BD | 232 | ASP |
| 42 | BD | 254 | LYS |
| 42 | BD | 257 | GLU |
| 42 | BD | 259 | LYS |
| 42 | BD | 263 | GLU |
| 42 | BD | 264 | GLN |
| 42 | BD | 273 | ARG |
| 42 | BD | 277 | LEU |
| 42 | BD | 280 | GLU |
| 42 | BD | 293 | LEU |
| 43 | BE | 5 | LYS |
| 43 | BE | 15 | VAL |
| 43 | BE | 18 | LEU |
| 43 | BE | 21 | THR |
| 43 | BE | 52 | VAL |
| 43 | BE | 64 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 43 | BE | 65 | ILE |
| 43 | BE | 78 | ARG |
| 43 | BE | 79 | VAL |
| 43 | BE | 84 | VAL |
| 43 | BE | 89 | THR |
| 43 | BE | 93 | VAL |
| 43 | BE | 94 | GLU |
| 43 | BE | 108 | LYS |
| 43 | BE | 129 | GLU |
| 43 | BE | 134 | ARG |
| 43 | BE | 152 | THR |
| 43 | BE | 175 | LYS |
| 44 | BF | 24 | GLU |
| 44 | BF | 25 | GLN |
| 44 | BF | 38 | LYS |
| 44 | BF | 56 | GLU |
| 44 | BF | 77 | VAL |
| 44 | BF | 82 | LYS |
| 44 | BF | 92 | ILE |
| 44 | BF | 93 | ASN |
| 44 | BF | 98 | LYS |
| 44 | BF | 110 | ARG |
| 44 | BF | 121 | LYS |
| 44 | BF | 124 | LEU |
| 44 | BF | 143 | THR |
| 44 | BF | 151 | ARG |
| 44 | BF | 179 | LEU |
| 44 | BF | 184 | LEU |
| 44 | BF | 208 | SER |
| 44 | BF | 216 | VAL |
| 44 | BF | 229 | PHE |
| 44 | BF | 239 | LEU |
| 44 | BF | 244 | ASN |
| 45 | BG | 26 | LEU |
| 45 | BG | 27 | THR |
| 45 | BG | 36 | ILE |
| 45 | BG | 41 | GLN |
| 45 | BG | 47 | SER |
| 45 | BG | 50 | VAL |
| 45 | BG | 61 | GLN |
| 45 | BG | 63 | LYS |
| 45 | BG | 74 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 45 | BG | 79 | GLN |
| 45 | BG | 81 | THR |
| 45 | BG | 82 | LEU |
| 45 | BG | 84 | ARG |
| 45 | BG | 90 | THR |
| 45 | BG | 92 | LYS |
| 45 | BG | 110 | THR |
| 45 | BG | 118 | GLU |
| 45 | BG | 132 | VAL |
| 45 | BG | 136 | LEU |
| 45 | BG | 150 | LEU |
| 45 | BG | 156 | ASP |
| 45 | BG | 160 | ILE |
| 45 | BG | 163 | VAL |
| 45 | BG | 169 | LEU |
| 45 | BG | 181 | LYS |
| 45 | BG | 185 | ARG |
| 45 | BG | 203 | VAL |
| 45 | BG | 204 | ARG |
| 45 | BG | 214 | LEU |
| 45 | BG | 216 | SER |
| 45 | BG | 238 | LEU |
| 45 | BG | 241 | LYS |
| 45 | BG | 246 | MET |
| 45 | BG | 248 | LYS |
| 45 | BG | 251 | LYS |
| 45 | BG | 254 | ASP |
| 46 | BH | 4 | ILE |
| 46 | BH | 5 | GLN |
| 46 | BH | 9 | GLN |
| 46 | BH | 18 | VAL |
| 46 | BH | 20 | ILE |
| 46 | BH | 22 | SER |
| 46 | BH | 24 | ILE |
| 46 | BH | 33 | THR |
| 46 | BH | 36 | LYS |
| 46 | BH | 41 | ILE |
| 46 | BH | 48 | VAL |
| 46 | BH | 49 | ASN |
| 46 | BH | 52 | LEU |
| 46 | BH | 62 | ARG |
| 46 | BH | 68 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 46 | BH | 69 | ARG |
| 46 | BH | 70 | THR |
| 46 | BH | 80 | THR |
| 46 | BH | 82 | VAL |
| 46 | BH | 91 | ARG |
| 46 | BH | 123 | ILE |
| 46 | BH | 132 | VAL |
| 46 | BH | 135 | GLU |
| 46 | BH | 137 | SER |
| 46 | BH | 138 | THR |
| 46 | BH | 139 | ASN |
| 46 | BH | 147 | SER |
| 46 | BH | 151 | VAL |
| 46 | BH | 152 | GLU |
| 46 | BH | 157 | ASN |
| 46 | BH | 161 | LEU |
| 46 | BH | 162 | GLN |
| 46 | BH | 164 | ILE |
| 46 | BH | 168 | ARG |
| 46 | BH | 172 | ILE |
| 46 | BH | 173 | ARG |
| 46 | BH | 177 | ASP |
| 46 | BH | 189 | GLU |
| 46 | BH | 190 | ASP |
| 46 | BH | 191 | LEU |
| 47 | BI | 3 | ARG |
| 47 | BI | 19 | LYS |
| 47 | BI | 24 | ARG |
| 47 | BI | 26 | VAL |
| 47 | BI | 30 | LYS |
| 47 | BI | 32 | ARG |
| 47 | BI | 33 | ILE |
| 47 | BI | 36 | LEU |
| 47 | BI | 40 | LYS |
| 47 | BI | 42 | THR |
| 47 | BI | 48 | LEU |
| 47 | BI | 52 | LEU |
| 47 | BI | 57 | LEU |
| 47 | BI | 63 | GLU |
| 47 | BI | 77 | THR |
| 47 | BI | 78 | THR |
| 47 | BI | 87 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 47 | BI | 90 | ARG |
| 47 | BI | 99 | ILE |
| 47 | BI | 116 | ARG |
| 47 | BI | 128 | ARG |
| 47 | BI | 129 | VAL |
| 47 | BI | 130 | ASP |
| 47 | BI | 139 | ARG |
| 47 | BI | 140 | THR |
| 47 | BI | 156 | ARG |
| 47 | BI | 163 | GLN |
| 47 | BI | 165 | ILE |
| 47 | BI | 174 | THR |
| 47 | BI | 185 | ARG |
| 47 | BI | 191 | LYS |
| 47 | BI | 197 | VAL |
| 47 | BI | 203 | LYS |
| 47 | BI | 207 | GLU |
| 48 | BJ | 6 | GLN |
| 48 | BJ | 7 | ASN |
| 48 | BJ | 9 | MET |
| 48 | BJ | 10 | ARG |
| 48 | BJ | 12 | LEU |
| 48 | BJ | 13 | LYS |
| 48 | BJ | 16 | LYS |
| 48 | BJ | 19 | LEU |
| 48 | BJ | 26 | SER |
| 48 | BJ | 31 | THR |
| 48 | BJ | 34 | SER |
| 48 | BJ | 44 | THR |
| 48 | BJ | 46 | VAL |
| 48 | BJ | 55 | ARG |
| 48 | BJ | 65 | ILE |
| 48 | BJ | 70 | THR |
| 48 | BJ | 80 | LEU |
| 48 | BJ | 82 | ARG |
| 48 | BJ | 84 | LEU |
| 48 | BJ | 94 | ARG |
| 48 | BJ | 106 | ILE |
| 48 | BJ | 107 | ASP |
| 48 | BJ | 112 | LEU |
| 48 | BJ | 115 | LYS |
| 48 | BJ | 119 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 48 | BJ | 120 | ILE |
| 48 | BJ | 122 | ILE |
| 48 | BJ | 130 | VAL |
| 48 | BJ | 134 | PRO |
| 48 | BJ | 138 | VAL |
| 48 | BJ | 140 | ARG |
| 48 | BJ | 142 | LYS |
| 48 | BJ | 158 | ASP |
| 48 | BJ | 161 | SER |
| 48 | BJ | 166 | LYS |
| 48 | BJ | 172 | LEU |
| 49 | BL | 5 | LYS |
| 49 | BL | 13 | HIS |
| 49 | BL | 15 | ARG |
| 49 | BL | 23 | LYS |
| 49 | BL | 46 | ILE |
| 49 | BL | 51 | LEU |
| 49 | BL | 54 | LEU |
| 49 | BL | 55 | ARG |
| 49 | BL | 58 | VAL |
| 49 | BL | 59 | ARG |
| 49 | BL | 63 | VAL |
| 49 | BL | 67 | ARG |
| 49 | BL | 69 | VAL |
| 49 | BL | 85 | LEU |
| 49 | BL | 91 | ARG |
| 49 | BL | 100 | ARG |
| 49 | BL | 107 | GLU |
| 49 | BL | 114 | GLN |
| 49 | BL | 115 | ARG |
| 49 | BL | 124 | ILE |
| 49 | BL | 131 | LYS |
| 49 | BL | 136 | GLU |
| 49 | BL | 140 | SER |
| 49 | BL | 147 | ILE |
| 49 | BL | 164 | GLU |
| 49 | BL | 168 | ARG |
| 49 | BL | 171 | ARG |
| 49 | BL | 180 | ARG |
| 49 | BL | 182 | ILE |
| 49 | BL | 190 | LYS |
| 49 | BL | 194 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 50 | BM | 5 | SER |
| 50 | BM | 8 | LYS |
| 50 | BM | 13 | ARG |
| 50 | BM | 20 | VAL |
| 50 | BM | 25 | LYS |
| 50 | BM | 27 | GLN |
| 50 | BM | 50 | LYS |
| 50 | BM | 53 | VAL |
| 50 | BM | 58 | ILE |
| 50 | BM | 64 | VAL |
| 50 | BM | 66 | THR |
| 50 | BM | 72 | LEU |
| 50 | BM | 82 | SER |
| 50 | BM | 90 | VAL |
| 50 | BM | 92 | GLU |
| 50 | BM | 102 | LYS |
| 50 | BM | 106 | ARG |
| 50 | BM | 108 | ARG |
| 50 | BM | 113 | THR |
| 50 | BM | 125 | LYS |
| 50 | BM | 126 | GLN |
| 50 | BM | 130 | THR |
| 50 | BM | 135 | LEU |
| 51 | BN | 10 | LEU |
| 51 | BN | 15 | GLN |
| 51 | BN | 18 | VAL |
| 51 | BN | 19 | LEU |
| 51 | BN | 20 | ARG |
| 51 | BN | 22 | LEU |
| 51 | BN | 27 | VAL |
| 51 | BN | 38 | ARG |
| 51 | BN | 49 | ARG |
| 51 | BN | 50 | ARG |
| 51 | BN | 68 | ARG |
| 51 | BN | 80 | THR |
| 51 | BN | 85 | THR |
| 51 | BN | 89 | VAL |
| 51 | BN | 92 | LEU |
| 51 | BN | 96 | ARG |
| 51 | BN | 97 | SER |
| 51 | BN | 98 | LEU |
| 51 | BN | 105 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 51 | BN | 109 | ARG |
| 51 | BN | 117 | ASN |
| 51 | BN | 131 | GLU |
| 51 | BN | 133 | ILE |
| 51 | BN | 151 | ILE |
| 51 | BN | 155 | VAL |
| 51 | BN | 182 | ASN |
| 51 | BN | 183 | THR |
| 51 | BN | 190 | THR |
| 51 | BN | 198 | SER |
| 52 | BO | 3[B] | SER |
| 52 | BO | 12[A] | LYS |
| 52 | BO | 12[B] | LYS |
| 52 | BO | 16[B] | LEU |
| 52 | BO | 22[A] | VAL |
| 52 | BO | 22[B] | THR |
| 52 | BO | 25[A] | LYS |
| 52 | BO | 25[B] | LYS |
| 52 | BO | 34[A] | VAL |
| 52 | BO | 34[B] | VAL |
| 52 | BO | 58[A] | LEU |
| 52 | BO | 58[B] | LEU |
| 52 | BO | 59[A] | ARG |
| 52 | BO | 59[B] | ARG |
| 52 | BO | 67[A] | THR |
| 52 | BO | 67[B] | THR |
| 52 | BO | 78[A] | ARG |
| 52 | BO | 78[B] | ARG |
| 52 | BO | 80[B] | LEU |
| 52 | BO | 84[A] | LEU |
| 52 | BO | 85[A] | ARG |
| 52 | BO | 85[B] | ARG |
| 52 | BO | 106[A] | GLU |
| 52 | BO | 106[B] | GLU |
| 52 | BO | 110[A] | PRO |
| 52 | BO | 110[B] | PRO |
| 52 | BO | 116[A] | LYS |
| 52 | BO | 116[B] | LYS |
| 52 | BO | 117[A] | ARG |
| 52 | BO | 117[B] | ARG |
| 52 | BO | 122[A] | GLN |
| 52 | BO | 122[B] | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 52 | BO | 124[A] | LEU |
| 52 | BO | 124[B] | LEU |
| 52 | BO | 126[A] | VAL |
| 52 | BO | 126[B] | VAL |
| 52 | BO | 128[A] | ARG |
| 52 | BO | 128[B] | ARG |
| 52 | BO | 142[A] | SER |
| 52 | BO | 142[B] | SER |
| 52 | BO | 143[A] | THR |
| 52 | BO | 143[B] | THR |
| 52 | BO | 163[B] | ARG |
| 52 | BO | 175[A] | THR |
| 52 | BO | 175[B] | THR |
| 52 | BO | 182[A] | ASN |
| 52 | BO | 186[B] | SER |
| 53 | BP | 3 | ARG |
| 53 | BP | 9 | THR |
| 53 | BP | 23 | ARG |
| 53 | BP | 24 | VAL |
| 53 | BP | 29 | THR |
| 53 | BP | 32 | THR |
| 53 | BP | 36 | ILE |
| 53 | BP | 52 | LEU |
| 53 | BP | 53 | ASP |
| 53 | BP | 56 | ARG |
| 53 | BP | 67 | ILE |
| 53 | BP | 69 | ARG |
| 53 | BP | 70 | THR |
| 53 | BP | 78 | VAL |
| 53 | BP | 94 | LEU |
| 53 | BP | 111 | LYS |
| 53 | BP | 112 | LEU |
| 53 | BP | 114 | VAL |
| 53 | BP | 120 | ASN |
| 53 | BP | 123 | PRO |
| 53 | BP | 126 | ARG |
| 53 | BP | 127 | ARG |
| 53 | BP | 136 | ILE |
| 53 | BP | 142 | SER |
| 53 | BP | 144 | SER |
| 53 | BP | 153 | LYS |
| 53 | BP | 166 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 53 | BP | 171 | ARG |
| 53 | BP | 173 | ARG |
| 53 | BP | 180 | LYS |
| 53 | BP | 181 | ARG |
| 54 | BQ | 3 | ILE |
| 54 | BQ | 17 | THR |
| 54 | BQ | 24 | VAL |
| 54 | BQ | 26 | LEU |
| 54 | BQ | 32 | LEU |
| 54 | BQ | 34 | THR |
| 54 | BQ | 41 | ASP |
| 54 | BQ | 46 | LYS |
| 54 | BQ | 49 | LEU |
| 54 | BQ | 57 | ILE |
| 54 | BQ | 64 | VAL |
| 54 | BQ | 69 | ARG |
| 54 | BQ | 74 | GLU |
| 54 | BQ | 81 | VAL |
| 54 | BQ | 86 | THR |
| 54 | BQ | 88 | THR |
| 54 | BQ | 93 | ILE |
| 54 | BQ | 98 | LYS |
| 54 | BQ | 113 | LYS |
| 54 | BQ | 135 | GLN |
| 54 | BQ | 138 | LEU |
| 54 | BQ | 150 | VAL |
| 54 | BQ | 168 | THR |
| 54 | BQ | 180 | ARG |
| 55 | BR | 5 | ARG |
| 55 | BR | 8 | LYS |
| 55 | BR | 10 | LEU |
| 55 | BR | 20 | ARG |
| 55 | BR | 22 | VAL |
| 55 | BR | 25 | ASP |
| 55 | BR | 29 | THR |
| 55 | BR | 30 | SER |
| 55 | BR | 41 | ILE |
| 55 | BR | 43 | LYS |
| 55 | BR | 49 | THR |
| 55 | BR | 52 | LYS |
| 55 | BR | 60 | LYS |
| 55 | BR | 71 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 55 | BR | 74 | ARG |
| 55 | BR | 81 | ARG |
| 55 | BR | 86 | GLU |
| 55 | BR | 91 | SER |
| 55 | BR | 98 | ARG |
| 55 | BR | 99 | LEU |
| 55 | BR | 100 | ARG |
| 55 | BR | 103 | ARG |
| 55 | BR | 104 | ARG |
| 55 | BR | 106 | LEU |
| 55 | BR | 108 | LYS |
| 55 | BR | 115 | ILE |
| 55 | BR | 116 | ASP |
| 55 | BR | 128 | LYS |
| 55 | BR | 135 | LYS |
| 55 | BR | 138 | LEU |
| 55 | BR | 144 | GLN |
| 55 | BR | 153 | LYS |
| 55 | BR | 164 | LEU |
| 55 | BR | 165 | LYS |
| 55 | BR | 175 | GLN |
| 55 | BR | 177 | VAL |
| 55 | BR | 182 | ASP |
| 56 | BS | 1 | MET |
| 56 | BS | 12 | ARG |
| 56 | BS | 13 | ARG |
| 56 | BS | 17 | GLU |
| 56 | BS | 40 | ARG |
| 56 | BS | 45 | LEU |
| 56 | BS | 51 | VAL |
| 56 | BS | 58 | ILE |
| 56 | BS | 61 | ILE |
| 56 | BS | 71 | LYS |
| 56 | BS | 80 | ARG |
| 56 | BS | 87 | THR |
| 56 | BS | 97 | VAL |
| 56 | BS | 100 | VAL |
| 56 | BS | 105 | THR |
| 56 | BS | 115 | ARG |
| 56 | BS | 117 | ARG |
| 56 | BS | 130 | GLU |
| 56 | BS | 132 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 56 | BS | 137 | ARG |
| 56 | BS | 138 | GLN |
| 56 | BS | 142 | GLN |
| 56 | BS | 155 | ARG |
| 56 | BS | 160 | THR |
| 56 | BS | 162 | THR |
| 56 | BS | 166 | LYS |
| 56 | BS | 167 | ARG |
| 56 | BS | 169 | SER |
| 56 | BS | 172 | TYR |
| 57 | BT | 4 | SER |
| 57 | BT | 9 | SER |
| 57 | BT | 12 | ARG |
| 57 | BT | 25 | VAL |
| 57 | BT | 26 | HIS |
| 57 | BT | 27 | LEU |
| 57 | BT | 28 | SER |
| 57 | BT | 32 | LYS |
| 57 | BT | 55 | LYS |
| 57 | BT | 75 | ILE |
| 57 | BT | 78 | LYS |
| 57 | BT | 79 | MET |
| 57 | BT | 80 | VAL |
| 57 | BT | 83 | ARG |
| 57 | BT | 88 | ARG |
| 57 | BT | 89 | LEU |
| 57 | BT | 96 | ILE |
| 57 | BT | 102 | ARG |
| 57 | BT | 103 | GLN |
| 57 | BT | 104 | GLU |
| 57 | BT | 118 | GLU |
| 57 | BT | 124 | VAL |
| 57 | BT | 126 | VAL |
| 57 | BT | 127 | GLN |
| 57 | BT | 128 | LEU |
| 57 | BT | 139 | ARG |
| 57 | BT | 143 | THR |
| 57 | BT | 144 | GLU |
| 57 | BT | 146 | ASN |
| 57 | BT | 149 | GLN |
| 57 | BT | 158 | THR |
| 57 | BT | 159 | PHE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 57 | BT | 160 | ILE |
| 58 | BU | 10 | LYS |
| 58 | BU | 27 | VAL |
| 58 | BU | 29 | ASP |
| 58 | BU | 38 | ILE |
| 58 | BU | 39 | ASP |
| 58 | BU | 43 | VAL |
| 58 | BU | 49 | ASN |
| 58 | BU | 52 | ASN |
| 58 | BU | 61 | THR |
| 58 | BU | 66 | VAL |
| 58 | BU | 82 | LYS |
| 58 | BU | 88 | GLN |
| 58 | BU | 93 | ILE |
| 58 | BU | 100 | THR |
| 59 | BV | 13 | ILE |
| 59 | BV | 32 | ARG |
| 59 | BV | 33 | ASN |
| 59 | BV | 45 | ARG |
| 59 | BV | 48 | ARG |
| 59 | BV | 63 | LYS |
| 59 | BV | 64 | LYS |
| 59 | BV | 69 | LEU |
| 59 | BV | 73 | VAL |
| 59 | BV | 74 | MET |
| 59 | BV | 83 | LYS |
| 59 | BV | 84 | SER |
| 59 | BV | 102 | ILE |
| 59 | BV | 115 | THR |
| 59 | BV | 120 | LYS |
| 59 | BV | 125 | LEU |
| 60 | BW | 4 | GLU |
| 60 | BW | 5 | ILE |
| 60 | BW | 19 | THR |
| 60 | BW | 25 | ASP |
| 60 | BW | 34 | SER |
| 60 | BW | 39 | LEU |
| 60 | BW | 54 | LEU |
| 60 | BW | 63 | ILE |
| 61 | BX | 27 | ARG |
| 61 | BX | 34 | LEU |
| 61 | BX | 36 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 61 | BX | 37 | THR |
| 61 | BX | 38 | LEU |
| 61 | BX | 39 | LYS |
| 61 | BX | 40 | LEU |
| 61 | BX | 45 | LYS |
| 61 | BX | 48 | SER |
| 61 | BX | 63 | ILE |
| 61 | BX | 71 | THR |
| 61 | BX | 73 | MET |
| 61 | BX | 75 | LYS |
| 61 | BX | 85 | GLN |
| 61 | BX | 86 | VAL |
| 61 | BX | 92 | LYS |
| 61 | BX | 105 | VAL |
| 61 | BX | 108 | LEU |
| 61 | BX | 109 | LYS |
| 61 | BX | 115 | ARG |
| 61 | BX | 125 | ARG |
| 61 | BX | 127 | THR |
| 61 | BX | 133 | LEU |
| 61 | BX | 135 | ILE |
| 61 | BX | 139 | ILE |
| 61 | BX | 142 | ILE |
| 62 | BY | 3 | LYS |
| 62 | BY | 8 | VAL |
| 62 | BY | 13 | ARG |
| 62 | BY | 17 | LYS |
| 62 | BY | 37 | LYS |
| 62 | BY | 40 | ARG |
| 62 | BY | 45 | ILE |
| 62 | BY | 50 | ILE |
| 62 | BY | 51 | ARG |
| 62 | BY | 56 | VAL |
| 62 | BY | 57 | LEU |
| 62 | BY | 74 | TYR |
| 62 | BY | 76 | LEU |
| 62 | BY | 80 | VAL |
| 62 | BY | 90 | VAL |
| 62 | BY | 94 | SER |
| 62 | BY | 95 | VAL |
| 62 | BY | 97 | ILE |
| 62 | BY | 105 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 62 | BY | 115 | ARG |
| 62 | BY | 122 | LYS |
| 62 | BY | 125 | LYS |
| 63 | BZ | 14 | VAL |
| 63 | BZ | 15 | ARG |
| 63 | BZ | 17 | ARG |
| 63 | BZ | 24 | VAL |
| 63 | BZ | 34 | LYS |
| 63 | BZ | 43 | VAL |
| 63 | BZ | 46 | ILE |
| 63 | BZ | 53 | VAL |
| 63 | BZ | 54 | THR |
| 63 | BZ | 64 | LYS |
| 63 | BZ | 72 | ILE |
| 63 | BZ | 75 | VAL |
| 63 | BZ | 80 | LEU |
| 63 | BZ | 81 | LEU |
| 63 | BZ | 83 | THR |
| 63 | BZ | 86 | THR |
| 63 | BZ | 87 | LEU |
| 63 | BZ | 90 | GLU |
| 63 | BZ | 92 | PHE |
| 63 | BZ | 97 | SER |
| 63 | BZ | 99 | GLU |
| 63 | BZ | 102 | GLU |
| 63 | BZ | 103 | GLN |
| 63 | BZ | 109 | GLU |
| 63 | BZ | 121 | ARG |
| 63 | BZ | 127 | ASN |
| 63 | BZ | 134 | LEU |
| 64 | Ba | 6 | THR |
| 64 | Ba | 7 | LYS |
| 64 | Ba | 8 | THR |
| 64 | Ba | 10 | LYS |
| 64 | Ba | 12 | ARG |
| 64 | Ba | 16 | SER |
| 64 | Ba | 29 | PRO |
| 64 | Ba | 42 | ARG |
| 64 | Ba | 47 | LYS |
| 64 | Ba | 60 | TYR |
| 64 | Ba | 76 | ASP |
| 64 | Ba | 78 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 64 | Ba | 84 | GLU |
| 64 | Ba | 91 | LEU |
| 64 | Ba | 92 | LYS |
| 64 | Ba | 96 | LYS |
| 64 | Ba | 115 | LYS |
| 64 | Ba | 120 | ASN |
| 64 | Ba | 130 | VAL |
| 64 | Ba | 133 | LEU |
| 64 | Ba | 139 | ARG |
| 65 | Bb | 14 | ARG |
| 65 | Bb | 22 | LYS |
| 65 | Bb | 23 | LYS |
| 65 | Bb | 25 | LYS |
| 65 | Bb | 28 | LYS |
| 65 | Bb | 33 | LYS |
| 65 | Bb | 35 | VAL |
| 65 | Bb | 38 | LYS |
| 65 | Bb | 50 | THR |
| 65 | Bb | 59 | LYS |
| 66 | Bc | 16 | LEU |
| 66 | Bc | 30 | THR |
| 66 | Bc | 32 | LYS |
| 66 | Bc | 34 | LEU |
| 66 | Bc | 36 | GLN |
| 66 | Bc | 40 | LYS |
| 66 | Bc | 48 | THR |
| 66 | Bc | 52 | ARG |
| 66 | Bc | 54 | SER |
| 66 | Bc | 61 | MET |
| 66 | Bc | 79 | THR |
| 66 | Bc | 83 | LYS |
| 66 | Bc | 87 | VAL |
| 66 | Bc | 93 | LEU |
| 66 | Bc | 97 | ASP |
| 66 | Bc | 99 | ASP |
| 66 | Bc | 100 | ILE |
| 66 | Bc | 103 | THR |
| 67 | Bd | 6 | ASP |
| 67 | Bd | 8 | VAL |
| 67 | Bd | 13 | THR |
| 67 | Bd | 16 | LEU |
| 67 | Bd | 26 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 67 | Bd | 28 | ARG |
| 67 | Bd | 31 | ARG |
| 67 | Bd | 46 | THR |
| 67 | Bd | 47 | ASP |
| 67 | Bd | 53 | PRO |
| 67 | Bd | 55 | LEU |
| 67 | Bd | 64 | VAL |
| 67 | Bd | 68 | GLU |
| 67 | Bd | 79 | ARG |
| 67 | Bd | 82 | GLU |
| 67 | Bd | 86 | LYS |
| 67 | Bd | 94 | GLU |
| 67 | Bd | 102 | LYS |
| 67 | Bd | 106 | THR |
| 68 | Be | 4 | LEU |
| 68 | Be | 18 | LYS |
| 68 | Be | 19 | ARG |
| 68 | Be | 27 | ARG |
| 68 | Be | 33 | ARG |
| 68 | Be | 51 | SER |
| 68 | Be | 54 | LYS |
| 68 | Be | 61 | LYS |
| 68 | Be | 62 | LYS |
| 68 | Be | 73 | THR |
| 68 | Be | 75 | LEU |
| 68 | Be | 76 | VAL |
| 68 | Be | 82 | LEU |
| 68 | Be | 84 | THR |
| 68 | Be | 85 | LEU |
| 68 | Be | 87 | MET |
| 68 | Be | 103 | LYS |
| 68 | Be | 106 | VAL |
| 68 | Be | 109 | LEU |
| 68 | Be | 125 | ARG |
| 68 | Be | 126 | LEU |
| 68 | Be | 128 | LEU |
| 69 | Bf | 10 | LYS |
| 69 | Bf | 15 | SER |
| 69 | Bf | 20 | LYS |
| 69 | Bf | 28 | SER |
| 69 | Bf | 31 | LYS |
| 69 | Bf | 49 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 69 | Bf | 59 | VAL |
| 69 | Bf | 60 | ARG |
| 69 | Bf | 70 | LYS |
| 69 | Bf | 80 | VAL |
| 69 | Bf | 92 | LYS |
| 69 | Bf | 98 | VAL |
| 69 | Bf | 106 | ASN |
| 70 | Bg | 3 | GLN |
| 70 | Bg | 5 | VAL |
| 70 | Bg | 8 | ARG |
| 70 | Bg | 20 | ILE |
| 70 | Bg | 21 | LYS |
| 70 | Bg | 23 | VAL |
| 70 | Bg | 24 | LYS |
| 70 | Bg | 29 | ILE |
| 70 | Bg | 33 | GLN |
| 70 | Bg | 38 | LEU |
| 70 | Bg | 44 | CYS |
| 70 | Bg | 51 | LEU |
| 70 | Bg | 52 | GLN |
| 70 | Bg | 56 | THR |
| 70 | Bg | 58 | ARG |
| 70 | Bg | 65 | VAL |
| 70 | Bg | 71 | THR |
| 70 | Bg | 72 | VAL |
| 70 | Bg | 74 | ARG |
| 70 | Bg | 86 | LYS |
| 70 | Bg | 88 | ARG |
| 70 | Bg | 95 | ILE |
| 70 | Bg | 99 | LYS |
| 70 | Bg | 102 | LYS |
| 70 | Bg | 104 | VAL |
| 71 | Bh | 15 | GLU |
| 71 | Bh | 20 | GLN |
| 71 | Bh | 21 | LEU |
| 71 | Bh | 27 | GLU |
| 71 | Bh | 28 | LEU |
| 71 | Bh | 38 | ARG |
| 71 | Bh | 44 | ILE |
| 71 | Bh | 45 | LYS |
| 71 | Bh | 46 | THR |
| 71 | Bh | 48 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 71 | Bh | 49 | LYS |
| 71 | Bh | 50 | SER |
| 71 | Bh | 71 | LYS |
| 71 | Bh | 73 | LYS |
| 71 | Bh | 74 | LYS |
| 71 | Bh | 81 | ARG |
| 71 | Bh | 85 | THR |
| 71 | Bh | 89 | ARG |
| 71 | Bh | 100 | VAL |
| 71 | Bh | 101 | THR |
| 71 | Bh | 104 | GLN |
| 71 | Bh | 105 | ARG |
| 71 | Bh | 107 | LYS |
| 71 | Bh | 115 | LYS |
| 71 | Bh | 119 | LYS |
| 72 | Bi | 11 | LEU |
| 72 | Bi | 17 | VAL |
| 72 | Bi | 18 | THR |
| 72 | Bi | 21 | THR |
| 72 | Bi | 25 | LYS |
| 72 | Bi | 26 | ILE |
| 72 | Bi | 29 | LYS |
| 72 | Bi | 34 | SER |
| 72 | Bi | 36 | ARG |
| 72 | Bi | 42 | SER |
| 72 | Bi | 45 | ARG |
| 72 | Bi | 57 | LEU |
| 72 | Bi | 58 | ILE |
| 72 | Bi | 60 | LEU |
| 72 | Bi | 62 | ARG |
| 72 | Bi | 64 | SER |
| 72 | Bi | 68 | ARG |
| 72 | Bi | 70 | ARG |
| 72 | Bi | 76 | ARG |
| 72 | Bi | 81 | THR |
| 72 | Bi | 88 | GLU |
| 72 | Bi | 90 | MET |
| 72 | Bi | 99 | ARG |
| 73 | Bj | 3 | LYS |
| 73 | Bj | 5 | THR |
| 73 | Bj | 17 | THR |
| 73 | Bj | 24 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 73 | Bj | 25 | ARG |
| 73 | Bj | 33 | THR |
| 73 | Bj | 36 | SER |
| 73 | Bj | 37 | CYS |
| 73 | Bj | 59 | THR |
| 73 | Bj | 67 | LEU |
| 73 | Bj | 75 | LYS |
| 73 | Bj | 80 | THR |
| 73 | Bj | 82 | SER |
| 73 | Bj | 84 | SER |
| 74 | Bk | 3 | ARG |
| 74 | Bk | 5 | ILE |
| 74 | Bk | 6 | THR |
| 74 | Bk | 8 | ILE |
| 74 | Bk | 12 | LEU |
| 74 | Bk | 19 | ASP |
| 74 | Bk | 24 | THR |
| 74 | Bk | 31 | LEU |
| 74 | Bk | 32 | ASN |
| 74 | Bk | 41 | THR |
| 74 | Bk | 45 | VAL |
| 74 | Bk | 46 | ARG |
| 74 | Bk | 48 | SER |
| 74 | Bk | 50 | SER |
| 74 | Bk | 53 | THR |
| 74 | Bk | 64 | LYS |
| 74 | Bk | 65 | LEU |
| 74 | Bk | 67 | GLN |
| 74 | Bk | 72 | THR |
| 74 | Bk | 77 | ARG |
| 75 | Bl | 5 | LYS |
| 75 | Bl | 6 | SER |
| 75 | Bl | 21 | ARG |
| 75 | Bl | 23 | LEU |
| 75 | Bl | 27 | ILE |
| 75 | Bl | 34 | THR |
| 75 | Bl | 36 | ARG |
| 75 | Bl | 45 | ARG |
| 75 | Bl | 51 | ILE |
| 76 | Bm | 77 | ILE |
| 76 | Bm | 78 | ILE |
| 76 | Bm | 79 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 76 | Bm | 83 | LYS |
| 76 | Bm | 85 | LEU |
| 76 | Bm | 108 | THR |
| 76 | Bm | 112 | LYS |
| 76 | Bm | 113 | ARG |
| 76 | Bm | 114 | LYS |
| 76 | Bm | 127 | LEU |
| 77 | Bn | 4 | LYS |
| 77 | Bn | 6 | ARG |
| 77 | Bn | 9 | ARG |
| 77 | Bn | 10 | THR |
| 77 | Bn | 11 | ARG |
| 77 | Bn | 16 | LYS |
| 77 | Bn | 19 | LYS |
| 77 | Bn | 21 | ARG |
| 78 | Bo | 2 | VAL |
| 78 | Bo | 3 | ASN |
| 78 | Bo | 8 | ARG |
| 78 | Bo | 17 | CYS |
| 78 | Bo | 26 | THR |
| 78 | Bo | 29 | LYS |
| 78 | Bo | 34 | SER |
| 78 | Bo | 35 | LEU |
| 78 | Bo | 47 | GLN |
| 78 | Bo | 60 | LYS |
| 78 | Bo | 66 | LYS |
| 78 | Bo | 72 | LEU |
| 78 | Bo | 76 | LYS |
| 78 | Bo | 79 | THR |
| 78 | Bo | 80 | ARG |
| 78 | Bo | 83 | LEU |
| 78 | Bo | 84 | THR |
| 78 | Bo | 93 | LEU |
| 78 | Bo | 99 | GLN |
| 78 | Bo | 100 | LYS |
| 78 | Bo | 104 | LEU |
| 78 | Bo | 105 | GLN |
| 79 | Bp | 5 | THR |
| 79 | Bp | 6 | LYS |
| 79 | Bp | 11 | THR |
| 79 | Bp | 24 | ARG |
| 79 | Bp | 32 | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 79 | Bp | 45 | LYS |
| 79 | Bp | 48 | LYS |
| 79 | Bp | 49 | ARG |
| 79 | Bp | 56 | THR |
| 79 | Bp | 59 | CYS |
| 79 | Bp | 60 | CYS |
| 79 | Bp | 73 | THR |
| 79 | Bp | 78 | THR |
| 79 | Bp | 84 | ARG |
| 79 | Bp | 91 | GLU |
| 2 | CA | 6 | THR |
| 2 | CA | 9 | LEU |
| 2 | CA | 12 | GLU |
| 2 | CA | 21 | ASN |
| 2 | CA | 29 | VAL |
| 2 | CA | 30 | GLN |
| 2 | CA | 31 | VAL |
| 2 | CA | 41 | ARG |
| 2 | CA | 45 | VAL |
| 2 | CA | 49 | ASN |
| 2 | CA | 50 | VAL |
| 2 | CA | 57 | LEU |
| 2 | CA | 59 | LEU |
| 2 | CA | 62 | ARG |
| 2 | CA | 76 | ILE |
| 2 | CA | 88 | LYS |
| 2 | CA | 96 | THR |
| 2 | CA | 103 | THR |
| 2 | CA | 110 | TYR |
| 2 | CA | 124 | THR |
| 2 | CA | 131 | GLN |
| 2 | CA | 139 | VAL |
| 2 | CA | 146 | LEU |
| 2 | CA | 151 | SER |
| 2 | CA | 154 | GLU |
| 2 | CA | 167 | LYS |
| 2 | CA | 172 | LEU |
| 2 | CA | 180 | GLU |
| 2 | CA | 183 | ARG |
| 2 | CA | 185 | ARG |
| 2 | CA | 188 | LEU |
| 2 | CA | 189 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | CA | 196 | SER |
| 2 | CA | 198 | MET |
| 3 | CB | 21 | VAL |
| 3 | CB | 22 | ASP |
| 3 | CB | 33 | LYS |
| 3 | CB | 36 | SER |
| 3 | CB | 37 | THR |
| 3 | CB | 40 | ASN |
| 3 | CB | 47 | LEU |
| 3 | CB | 51 | SER |
| 3 | CB | 55 | LYS |
| 3 | CB | 61 | LEU |
| 3 | CB | 62 | LYS |
| 3 | CB | 65 | VAL |
| 3 | CB | 70 | LEU |
| 3 | CB | 73 | LEU |
| 3 | CB | 81 | PHE |
| 3 | CB | 83 | LYS |
| 3 | CB | 85 | LYS |
| 3 | CB | 89 | ASP |
| 3 | CB | 90 | GLU |
| 3 | CB | 105 | PHE |
| 3 | CB | 106 | THR |
| 3 | CB | 108 | ASP |
| 3 | CB | 116 | LYS |
| 3 | CB | 125 | VAL |
| 3 | CB | 126 | THR |
| 3 | CB | 129 | THR |
| 3 | CB | 137 | ILE |
| 3 | CB | 154 | SER |
| 3 | CB | 159 | SER |
| 3 | CB | 170 | GLU |
| 3 | CB | 173 | THR |
| 3 | CB | 177 | GLN |
| 3 | CB | 180 | THR |
| 3 | CB | 181 | LEU |
| 3 | CB | 184 | LEU |
| 3 | CB | 203 | ASP |
| 3 | CB | 204 | ILE |
| 3 | CB | 212 | VAL |
| 3 | CB | 213 | ARG |
| 3 | CB | 214 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 3 | CB | 215 | VAL |
| 3 | CB | 219 | LYS |
| 3 | CB | 222 | LYS |
| 3 | CB | 234 | GLU |
| 4 | CC | 41 | LEU |
| 4 | CC | 50 | ILE |
| 4 | CC | 53 | ILE |
| 4 | CC | 54 | GLU |
| 4 | CC | 55 | GLU |
| 4 | CC | 58 | LEU |
| 4 | CC | 69 | ILE |
| 4 | CC | 71 | THR |
| 4 | CC | 72 | LEU |
| 4 | CC | 73 | LEU |
| 4 | CC | 76 | LEU |
| 4 | CC | 77 | GLN |
| 4 | CC | 81 | MET |
| 4 | CC | 83 | ILE |
| 4 | CC | 89 | GLN |
| 4 | CC | 90 | THR |
| 4 | CC | 91 | ARG |
| 4 | CC | 94 | GLN |
| 4 | CC | 95 | ARG |
| 4 | CC | 97 | ARG |
| 4 | CC | 106 | ASP |
| 4 | CC | 111 | VAL |
| 4 | CC | 130 | ILE |
| 4 | CC | 139 | ILE |
| 4 | CC | 140 | ARG |
| 4 | CC | 141 | ARG |
| 4 | CC | 146 | THR |
| 4 | CC | 148 | LEU |
| 4 | CC | 150 | GLN |
| 4 | CC | 159 | THR |
| 4 | CC | 164 | SER |
| 4 | CC | 170 | ILE |
| 4 | CC | 185 | LYS |
| 4 | CC | 194 | GLU |
| 4 | CC | 206 | THR |
| 4 | CC | 207 | LEU |
| 4 | CC | 218 | ILE |
| 4 | CC | 225 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 4 | CC | 229 | LEU |
| 4 | CC | 233 | GLN |
| 4 | CC | 240 | LEU |
| 4 | CC | 245 | ASP |
| 4 | CC | 248 | SER |
| 5 | CD | 4 | LEU |
| 5 | CD | 5 | ILE |
| 5 | CD | 7 | LYS |
| 5 | CD | 9 | ARG |
| 5 | CD | 10 | LYS |
| 5 | CD | 11 | LEU |
| 5 | CD | 21 | LEU |
| 5 | CD | 37 | VAL |
| 5 | CD | 39 | VAL |
| 5 | CD | 40 | ARG |
| 5 | CD | 41 | VAL |
| 5 | CD | 45 | LYS |
| 5 | CD | 53 | THR |
| 5 | CD | 55 | THR |
| 5 | CD | 59 | LEU |
| 5 | CD | 65 | ARG |
| 5 | CD | 66 | ILE |
| 5 | CD | 67 | ASN |
| 5 | CD | 69 | LEU |
| 5 | CD | 76 | ARG |
| 5 | CD | 84 | ILE |
| 5 | CD | 93 | ASP |
| 5 | CD | 94 | ARG |
| 5 | CD | 115 | ILE |
| 5 | CD | 116 | ARG |
| 5 | CD | 117 | ARG |
| 5 | CD | 127 | MET |
| 5 | CD | 142 | LEU |
| 5 | CD | 143 | ARG |
| 5 | CD | 146 | ARG |
| 5 | CD | 150 | MET |
| 5 | CD | 158 | ILE |
| 5 | CD | 162 | GLN |
| 5 | CD | 170 | THR |
| 5 | CD | 172 | THR |
| 5 | CD | 178 | ARG |
| 5 | CD | 202 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 5 | CD | 204 | ASP |
| 5 | CD | 208 | ILE |
| 5 | CD | 212 | LYS |
| 5 | CD | 213 | GLU |
| 5 | CD | 223 | LYS |
| 6 | CE | 6 | LYS |
| 6 | CE | 7 | LYS |
| 6 | CE | 9 | LEU |
| 6 | CE | 12 | LEU |
| 6 | CE | 23 | LEU |
| 6 | CE | 38 | LEU |
| 6 | CE | 39 | ARG |
| 6 | CE | 42 | LEU |
| 6 | CE | 48 | LEU |
| 6 | CE | 49 | ARG |
| 6 | CE | 50 | ASN |
| 6 | CE | 51 | ARG |
| 6 | CE | 67 | GLN |
| 6 | CE | 70 | VAL |
| 6 | CE | 71 | LYS |
| 6 | CE | 95 | THR |
| 6 | CE | 97 | GLU |
| 6 | CE | 102 | VAL |
| 6 | CE | 105 | VAL |
| 6 | CE | 106 | LYS |
| 6 | CE | 113 | ARG |
| 6 | CE | 116 | ASP |
| 6 | CE | 123 | LEU |
| 6 | CE | 131 | LEU |
| 6 | CE | 147 | ILE |
| 6 | CE | 148 | ARG |
| 6 | CE | 160 | VAL |
| 6 | CE | 176 | ASP |
| 6 | CE | 180 | LEU |
| 6 | CE | 181 | VAL |
| 6 | CE | 182 | TYR |
| 6 | CE | 184 | THR |
| 6 | CE | 187 | ARG |
| 6 | CE | 219 | VAL |
| 6 | CE | 221 | ARG |
| 6 | CE | 222 | LEU |
| 6 | CE | 223 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 6 | CE | 227 | VAL |
| 6 | CE | 236 | ILE |
| 6 | CE | 237 | SER |
| 6 | CE | 245 | LYS |
| 6 | CE | 246 | LEU |
| 6 | CE | 261 | LEU |
| 7 | CF | 23 | VAL |
| 7 | CF | 25 | LEU |
| 7 | CF | 27 | THR |
| 7 | CF | 32 | GLU |
| 7 | CF | 33 | VAL |
| 7 | CF | 38 | THR |
| 7 | CF | 39 | GLU |
| 7 | CF | 41 | LYS |
| 7 | CF | 50 | GLU |
| 7 | CF | 63 | GLN |
| 7 | CF | 64 | VAL |
| 7 | CF | 65 | ARG |
| 7 | CF | 68 | ILE |
| 7 | CF | 70 | VAL |
| 7 | CF | 76 | ARG |
| 7 | CF | 84 | LYS |
| 7 | CF | 89 | ILE |
| 7 | CF | 92 | ARG |
| 7 | CF | 93 | LEU |
| 7 | CF | 94 | THR |
| 7 | CF | 109 | LYS |
| 7 | CF | 112 | ARG |
| 7 | CF | 114 | ILE |
| 7 | CF | 125 | THR |
| 7 | CF | 128 | ASN |
| 7 | CF | 147 | THR |
| 7 | CF | 148 | ARG |
| 7 | CF | 156 | ARG |
| 7 | CF | 157 | ARG |
| 7 | CF | 162 | VAL |
| 7 | CF | 167 | ARG |
| 7 | CF | 170 | GLN |
| 7 | CF | 187 | ILE |
| 7 | CF | 190 | ILE |
| 7 | CF | 194 | LEU |
| 7 | CF | 203 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 7 | CF | 208 | SER |
| 7 | CF | 212 | LYS |
| 7 | CF | 213 | LYS |
| 7 | CF | 216 | GLU |
| 7 | CF | 225 | ARG |
| 8 | CG | 6 | SER |
| 8 | CG | 12 | SER |
| 8 | CG | 17 | GLU |
| 8 | CG | 20 | ASP |
| 8 | CG | 21 | GLU |
| 8 | CG | 25 | ARG |
| 8 | CG | 30 | LYS |
| 8 | CG | 31 | ARG |
| 8 | CG | 44 | GLU |
| 8 | CG | 46 | LYS |
| 8 | CG | 51 | LYS |
| 8 | CG | 71 | THR |
| 8 | CG | 73 | ILE |
| 8 | CG | 76 | LEU |
| 8 | CG | 78 | THR |
| 8 | CG | 79 | LYS |
| 8 | CG | 81 | VAL |
| 8 | CG | 89 | ASP |
| 8 | CG | 93 | LYS |
| 8 | CG | 108 | VAL |
| 8 | CG | 109 | LEU |
| 8 | CG | 111 | LEU |
| 8 | CG | 115 | LYS |
| 8 | CG | 120 | GLU |
| 8 | CG | 121 | LEU |
| 8 | CG | 122 | GLU |
| 8 | CG | 126 | ASP |
| 8 | CG | 127 | THR |
| 8 | CG | 128 | THR |
| 8 | CG | 132 | ARG |
| 8 | CG | 137 | ARG |
| 8 | CG | 143 | LYS |
| 8 | CG | 150 | GLU |
| 8 | CG | 151 | ASP |
| 8 | CG | 153 | VAL |
| 8 | CG | 155 | ASP |
| 8 | CG | 168 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 8 | CG | 169 | TYR |
| 8 | CG | 170 | THR |
| 8 | CG | 176 | GLN |
| 8 | CG | 179 | VAL |
| 8 | CG | 193 | LEU |
| 8 | CG | 212 | LEU |
| 8 | CG | 215 | ARG |
| 9 | CH | 11 | GLN |
| 9 | CH | 14 | THR |
| 9 | CH | 24 | PHE |
| 9 | CH | 28 | GLU |
| 9 | CH | 33 | GLU |
| 9 | CH | 35 | LYS |
| 9 | CH | 39 | ARG |
| 9 | CH | 41 | LEU |
| 9 | CH | 42 | GLN |
| 9 | CH | 49 | ILE |
| 9 | CH | 51 | VAL |
| 9 | CH | 67 | LEU |
| 9 | CH | 77 | LEU |
| 9 | CH | 78 | THR |
| 9 | CH | 79 | ARG |
| 9 | CH | 81 | LEU |
| 9 | CH | 86 | GLN |
| 9 | CH | 87 | ASP |
| 9 | CH | 97 | ARG |
| 9 | CH | 105 | THR |
| 9 | CH | 106 | SER |
| 9 | CH | 108 | GLN |
| 9 | CH | 110 | GLN |
| 9 | CH | 114 | ARG |
| 9 | CH | 116 | ARG |
| 9 | CH | 117 | THR |
| 9 | CH | 118 | LEU |
| 9 | CH | 122 | HIS |
| 9 | CH | 126 | LEU |
| 9 | CH | 134 | GLU |
| 9 | CH | 135 | ILE |
| 9 | CH | 136 | VAL |
| 9 | CH | 143 | LEU |
| 9 | CH | 144 | VAL |
| 9 | CH | 181 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 9 | CH | 182 | VAL |
| 9 | CH | 185 | ILE |
| 9 | CH | 187 | SER |
| 10 | CI | 5 | ARG |
| 10 | CI | 18 | ARG |
| 10 | CI | 25 | ARG |
| 10 | CI | 29 | LEU |
| 10 | CI | 36 | THR |
| 10 | CI | 46 | VAL |
| 10 | CI | 47 | ARG |
| 10 | CI | 58 | LEU |
| 10 | CI | 59 | ARG |
| 10 | CI | 60 | ILE |
| 10 | CI | 61 | GLU |
| 10 | CI | 62 | THR |
| 10 | CI | 64 | ASN |
| 10 | CI | 66 | SER |
| 10 | CI | 74 | LYS |
| 10 | CI | 76 | THR |
| 10 | CI | 77 | ARG |
| 10 | CI | 78 | ILE |
| 10 | CI | 82 | VAL |
| 10 | CI | 89 | GLU |
| 10 | CI | 110 | ARG |
| 10 | CI | 111 | GLN |
| 10 | CI | 120 | THR |
| 10 | CI | 138 | ASN |
| 10 | CI | 141 | ARG |
| 10 | CI | 151 | LYS |
| 10 | CI | 152 | ILE |
| 10 | CI | 153 | GLU |
| 10 | CI | 155 | SER |
| 10 | CI | 158 | SER |
| 10 | CI | 183 | ILE |
| 10 | CI | 184 | LEU |
| 10 | CI | 199 | LYS |
| 11 | CJ | 3 | ARG |
| 11 | CJ | 7 | THR |
| 11 | CJ | 22 | SER |
| 11 | CJ | 28 | LEU |
| 11 | CJ | 33 | GLU |
| 11 | CJ | 39 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 11 | CJ | 45 | ILE |
| 11 | CJ | 48 | GLN |
| 11 | CJ | 49 | LEU |
| 11 | CJ | 78 | ARG |
| 11 | CJ | 82 | ARG |
| 11 | CJ | 90 | LYS |
| 11 | CJ | 93 | LEU |
| 11 | CJ | 101 | VAL |
| 11 | CJ | 105 | LEU |
| 11 | CJ | 109 | LEU |
| 11 | CJ | 110 | GLN |
| 11 | CJ | 111 | THR |
| 11 | CJ | 115 | LYS |
| 11 | CJ | 120 | LYS |
| 11 | CJ | 130 | THR |
| 11 | CJ | 134 | ILE |
| 11 | CJ | 140 | ILE |
| 11 | CJ | 142 | ASN |
| 11 | CJ | 145 | SER |
| 11 | CJ | 149 | ARG |
| 11 | CJ | 151 | ASP |
| 11 | CJ | 161 | THR |
| 11 | CJ | 171 | ARG |
| 11 | CJ | 172 | VAL |
| 11 | CJ | 175 | ARG |
| 11 | CJ | 179 | ARG |
| 11 | CJ | 180 | LYS |
| 11 | CJ | 186 | GLU |
| 12 | CK | 3 | MET |
| 12 | CK | 5 | LYS |
| 12 | CK | 13 | GLN |
| 12 | CK | 15 | LEU |
| 12 | CK | 20 | VAL |
| 12 | CK | 21 | VAL |
| 12 | CK | 26 | ASP |
| 12 | CK | 27 | PHE |
| 12 | CK | 33 | GLU |
| 12 | CK | 36 | ASP |
| 12 | CK | 40 | LEU |
| 12 | CK | 55 | VAL |
| 12 | CK | 57 | THR |
| 12 | CK | 71 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 12 | CK | 74 | GLU |
| 12 | CK | 76 | LEU |
| 12 | CK | 77 | ARG |
| 13 | CL | 3 | THR |
| 13 | CL | 5 | LEU |
| 13 | CL | 10 | GLU |
| 13 | CL | 21 | ASN |
| 13 | CL | 26 | LYS |
| 13 | CL | 27 | THR |
| 13 | CL | 30 | ARG |
| 13 | CL | 31 | THR |
| 13 | CL | 32 | LYS |
| 13 | CL | 33 | ARG |
| 13 | CL | 40 | LEU |
| 13 | CL | 44 | THR |
| 13 | CL | 47 | THR |
| 13 | CL | 56 | LYS |
| 13 | CL | 60 | PHE |
| 13 | CL | 67 | ARG |
| 13 | CL | 72 | THR |
| 13 | CL | 74 | THR |
| 13 | CL | 80 | MET |
| 13 | CL | 83 | THR |
| 13 | CL | 96 | LYS |
| 13 | CL | 98 | ASN |
| 13 | CL | 109 | VAL |
| 13 | CL | 123 | VAL |
| 13 | CL | 128 | CYS |
| 13 | CL | 129 | ARG |
| 13 | CL | 131 | ILE |
| 13 | CL | 138 | ASN |
| 13 | CL | 140 | VAL |
| 14 | CM | 25 | GLU |
| 14 | CM | 28 | LEU |
| 14 | CM | 36 | LEU |
| 14 | CM | 39 | ASP |
| 14 | CM | 43 | ARG |
| 14 | CM | 52 | LEU |
| 14 | CM | 58 | LEU |
| 14 | CM | 59 | LEU |
| 14 | CM | 61 | VAL |
| 14 | CM | 62 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 14 | CM | 63 | VAL |
| 14 | CM | 65 | SER |
| 14 | CM | 66 | VAL |
| 14 | CM | 71 | ILE |
| 14 | CM | 74 | LEU |
| 14 | CM | 75 | VAL |
| 14 | CM | 83 | GLU |
| 14 | CM | 85 | LYS |
| 14 | CM | 88 | LEU |
| 14 | CM | 89 | ILE |
| 14 | CM | 91 | VAL |
| 14 | CM | 97 | LEU |
| 14 | CM | 103 | LEU |
| 14 | CM | 116 | VAL |
| 14 | CM | 121 | VAL |
| 14 | CM | 129 | GLU |
| 14 | CM | 132 | GLU |
| 14 | CM | 134 | SER |
| 14 | CM | 135 | MET |
| 14 | CM | 136 | ILE |
| 14 | CM | 138 | GLU |
| 14 | CM | 139 | HIS |
| 14 | CM | 140 | PHE |
| 15 | CN | 13 | SER |
| 15 | CN | 14 | SER |
| 15 | CN | 16 | ILE |
| 15 | CN | 20 | ARG |
| 15 | CN | 21 | ASN |
| 15 | CN | 27 | LYS |
| 15 | CN | 28 | LEU |
| 15 | CN | 39 | LYS |
| 15 | CN | 64 | ARG |
| 15 | CN | 66 | ILE |
| 15 | CN | 70 | LYS |
| 15 | CN | 76 | LYS |
| 15 | CN | 80 | LEU |
| 15 | CN | 84 | ILE |
| 15 | CN | 86 | GLU |
| 15 | CN | 87 | ASP |
| 15 | CN | 88 | LEU |
| 15 | CN | 104 | ARG |
| 15 | CN | 114 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 15 | CN | 115 | LEU |
| 15 | CN | 125 | LEU |
| 15 | CN | 127 | ARG |
| 15 | CN | 134 | VAL |
| 15 | CN | 138 | ASN |
| 16 | CO | 16 | VAL |
| 16 | CO | 18 | ARG |
| 16 | CO | 20 | TYR |
| 16 | CO | 26 | THR |
| 16 | CO | 28 | VAL |
| 16 | CO | 31 | THR |
| 16 | CO | 33 | LEU |
| 16 | CO | 34 | SER |
| 16 | CO | 51 | ASP |
| 16 | CO | 52 | ARG |
| 16 | CO | 62 | LEU |
| 16 | CO | 65 | GLN |
| 16 | CO | 71 | CYS |
| 16 | CO | 79 | VAL |
| 16 | CO | 81 | VAL |
| 16 | CO | 84 | ARG |
| 16 | CO | 92 | LYS |
| 16 | CO | 102 | LEU |
| 16 | CO | 103 | ARG |
| 16 | CO | 107 | ARG |
| 16 | CO | 114 | ARG |
| 16 | CO | 119 | THR |
| 16 | CO | 124 | ASP |
| 16 | CO | 125 | SER |
| 16 | CO | 127 | ARG |
| 16 | CO | 137 | LEU |
| 17 | CP | 12 | PHE |
| 17 | CP | 21 | ASP |
| 17 | CP | 22 | LEU |
| 17 | CP | 24 | LYS |
| 17 | CP | 27 | GLU |
| 17 | CP | 36 | LEU |
| 17 | CP | 43 | ARG |
| 17 | CP | 44 | ARG |
| 17 | CP | 61 | ARG |
| 17 | CP | 69 | GLU |
| 17 | CP | 71 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 17 | CP | 72 | LYS |
| 17 | CP | 77 | ARG |
| 17 | CP | 92 | SER |
| 17 | CP | 104 | GLN |
| 17 | CP | 107 | ILE |
| 17 | CP | 110 | GLU |
| 17 | CP | 121 | ILE |
| 17 | CP | 122 | THR |
| 17 | CP | 124 | THR |
| 17 | CP | 125 | PRO |
| 17 | CP | 127 | ARG |
| 18 | CQ | 17 | THR |
| 18 | CQ | 23 | LYS |
| 18 | CQ | 28 | LEU |
| 18 | CQ | 34 | SER |
| 18 | CQ | 37 | THR |
| 18 | CQ | 40 | GLU |
| 18 | CQ | 43 | ILE |
| 18 | CQ | 47 | LYS |
| 18 | CQ | 48 | VAL |
| 18 | CQ | 53 | LEU |
| 18 | CQ | 54 | LEU |
| 18 | CQ | 57 | LEU |
| 18 | CQ | 63 | ILE |
| 18 | CQ | 68 | ARG |
| 18 | CQ | 69 | VAL |
| 18 | CQ | 81 | ILE |
| 18 | CQ | 90 | VAL |
| 18 | CQ | 94 | GLN |
| 18 | CQ | 98 | ASP |
| 18 | CQ | 113 | ASP |
| 18 | CQ | 114 | ARG |
| 18 | CQ | 117 | LEU |
| 18 | CQ | 123 | ARG |
| 18 | CQ | 128 | LYS |
| 18 | CQ | 137 | ARG |
| 18 | CQ | 141 | SER |
| 19 | CR | 3 | ARG |
| 19 | CR | 8 | THR |
| 19 | CR | 19 | ARG |
| 19 | CR | 31 | ASN |
| 19 | CR | 34 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 19 | CR | 38 | ILE |
| 19 | CR | 46 | LEU |
| 19 | CR | 47 | ARG |
| 19 | CR | 54 | THR |
| 19 | CR | 66 | VAL |
| 19 | CR | 69 | ILE |
| 19 | CR | 78 | ARG |
| 19 | CR | 83 | GLN |
| 19 | CR | 85 | VAL |
| 19 | CR | 88 | VAL |
| 19 | CR | 89 | SER |
| 19 | CR | 104 | ASN |
| 19 | CR | 113 | LEU |
| 20 | CS | 2 | SER |
| 20 | CS | 3 | LEU |
| 20 | CS | 4 | VAL |
| 20 | CS | 5 | VAL |
| 20 | CS | 6 | GLN |
| 20 | CS | 10 | SER |
| 20 | CS | 13 | HIS |
| 20 | CS | 15 | LEU |
| 20 | CS | 17 | LEU |
| 20 | CS | 18 | LEU |
| 20 | CS | 26 | ILE |
| 20 | CS | 27 | LYS |
| 20 | CS | 28 | ILE |
| 20 | CS | 34 | THR |
| 20 | CS | 36 | LYS |
| 20 | CS | 38 | VAL |
| 20 | CS | 40 | ARG |
| 20 | CS | 55 | HIS |
| 20 | CS | 61 | LEU |
| 20 | CS | 63 | GLN |
| 20 | CS | 68 | ARG |
| 20 | CS | 85 | PHE |
| 20 | CS | 89 | GLN |
| 20 | CS | 94 | ASP |
| 20 | CS | 100 | THR |
| 20 | CS | 116 | LEU |
| 20 | CS | 119 | ILE |
| 20 | CS | 136 | GLN |
| 20 | CS | 138 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 20 | CS | 144 | ARG |
| 21 | CT | 6 | VAL |
| 21 | CT | 13 | ASP |
| 21 | CT | 22 | LEU |
| 21 | CT | 23 | GLN |
| 21 | CT | 27 | LYS |
| 21 | CT | 28 | LEU |
| 21 | CT | 30 | VAL |
| 21 | CT | 34 | VAL |
| 21 | CT | 36 | ILE |
| 21 | CT | 39 | THR |
| 21 | CT | 57 | ARG |
| 21 | CT | 68 | ARG |
| 21 | CT | 71 | VAL |
| 21 | CT | 75 | LYS |
| 21 | CT | 88 | VAL |
| 21 | CT | 89 | ARG |
| 21 | CT | 111 | ILE |
| 21 | CT | 123 | ARG |
| 21 | CT | 126 | GLU |
| 21 | CT | 131 | ASP |
| 21 | CT | 132 | LEU |
| 21 | CT | 135 | ILE |
| 21 | CT | 139 | THR |
| 21 | CT | 140 | LEU |
| 21 | CT | 141 | GLU |
| 21 | CT | 142 | GLU |
| 21 | CT | 144 | GLU |
| 22 | CU | 12 | GLN |
| 22 | CU | 15 | GLN |
| 22 | CU | 22 | ILE |
| 22 | CU | 23 | ARG |
| 22 | CU | 26 | LEU |
| 22 | CU | 27 | THR |
| 22 | CU | 30 | LYS |
| 22 | CU | 31 | VAL |
| 22 | CU | 39 | SER |
| 22 | CU | 44 | ASN |
| 22 | CU | 47 | GLN |
| 22 | CU | 51 | VAL |
| 22 | CU | 52 | LYS |
| 22 | CU | 57 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 22 | CU | 60 | THR |
| 22 | CU | 63 | LEU |
| 22 | CU | 70 | THR |
| 22 | CU | 72 | ASN |
| 22 | CU | 74 | GLU |
| 22 | CU | 77 | LYS |
| 22 | CU | 81 | THR |
| 22 | CU | 88 | LYS |
| 22 | CU | 89 | ARG |
| 22 | CU | 96 | PRO |
| 22 | CU | 99 | ILE |
| 22 | CU | 102 | ARG |
| 22 | CU | 103 | ILE |
| 22 | CU | 104 | THR |
| 22 | CU | 105 | GLN |
| 22 | CU | 108 | ILE |
| 22 | CU | 113 | ASP |
| 22 | CU | 115 | GLU |
| 22 | CU | 116 | VAL |
| 22 | CU | 118 | VAL |
| 23 | CV | 1 | MET |
| 23 | CV | 2 | GLU |
| 23 | CV | 5 | LYS |
| 23 | CV | 10 | GLU |
| 23 | CV | 11 | LEU |
| 23 | CV | 12 | TYR |
| 23 | CV | 25 | LYS |
| 23 | CV | 32 | VAL |
| 23 | CV | 38 | LYS |
| 23 | CV | 41 | GLU |
| 23 | CV | 52 | THR |
| 23 | CV | 62 | ARG |
| 23 | CV | 68 | SER |
| 23 | CV | 69 | LEU |
| 23 | CV | 78 | LEU |
| 23 | CV | 81 | ASN |
| 23 | CV | 86 | SER |
| 24 | CW | 7 | LEU |
| 24 | CW | 23 | ARG |
| 24 | CW | 25 | VAL |
| 24 | CW | 26 | LEU |
| 24 | CW | 43 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 24 | CW | 65 | LEU |
| 24 | CW | 68 | ARG |
| 24 | CW | 74 | VAL |
| 24 | CW | 88 | LYS |
| 24 | CW | 93 | LEU |
| 24 | CW | 98 | GLN |
| 24 | CW | 103 | ILE |
| 24 | CW | 117 | ARG |
| 24 | CW | 129 | VAL |
| 25 | CX | 9 | LEU |
| 25 | CX | 14 | LYS |
| 25 | CX | 17 | VAL |
| 25 | CX | 19 | ARG |
| 25 | CX | 20 | ARG |
| 25 | CX | 23 | ARG |
| 25 | CX | 31 | LYS |
| 25 | CX | 40 | SER |
| 25 | CX | 55 | GLU |
| 25 | CX | 73 | ARG |
| 25 | CX | 83 | VAL |
| 25 | CX | 84 | THR |
| 25 | CX | 96 | VAL |
| 25 | CX | 100 | ASP |
| 25 | CX | 103 | LEU |
| 25 | CX | 107 | PHE |
| 25 | CX | 109 | ARG |
| 25 | CX | 133 | LEU |
| 26 | CY | 6 | THR |
| 26 | CY | 10 | ARG |
| 26 | CY | 13 | ILE |
| 26 | CY | 14 | SER |
| 26 | CY | 21 | LYS |
| 26 | CY | 26 | ASP |
| 26 | CY | 29 | HIS |
| 26 | CY | 36 | SER |
| 26 | CY | 37 | LYS |
| 26 | CY | 43 | LYS |
| 26 | CY | 44 | LEU |
| 26 | CY | 49 | LYS |
| 26 | CY | 51 | GLU |
| 26 | CY | 62 | THR |
| 26 | CY | 77 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 26 | CY | 78 | SER |
| 26 | CY | 83 | LYS |
| 26 | CY | 88 | THR |
| 26 | CY | 100 | VAL |
| 26 | CY | 105 | ARG |
| 26 | CY | 128 | LYS |
| 26 | CY | 135 | ASP |
| 27 | CZ | 37 | GLN |
| 27 | CZ | 41 | ILE |
| 27 | CZ | 43 | ASP |
| 27 | CZ | 45 | GLU |
| 27 | CZ | 46 | LYS |
| 27 | CZ | 51 | LEU |
| 27 | CZ | 53 | GLU |
| 27 | CZ | 57 | TYR |
| 27 | CZ | 60 | VAL |
| 27 | CZ | 70 | LYS |
| 27 | CZ | 71 | ILE |
| 27 | CZ | 81 | ARG |
| 27 | CZ | 86 | GLU |
| 27 | CZ | 93 | SER |
| 27 | CZ | 97 | LYS |
| 27 | CZ | 102 | THR |
| 27 | CZ | 105 | THR |
| 28 | Ca | 4 | LYS |
| 28 | Ca | 10 | ARG |
| 28 | Ca | 26 | CYS |
| 28 | Ca | 34 | LYS |
| 28 | Ca | 41 | ILE |
| 28 | Ca | 44 | ILE |
| 28 | Ca | 50 | VAL |
| 28 | Ca | 53 | LEU |
| 28 | Ca | 55 | GLU |
| 28 | Ca | 67 | THR |
| 28 | Ca | 76 | SER |
| 28 | Ca | 82 | ARG |
| 28 | Ca | 85 | ARG |
| 28 | Ca | 89 | ARG |
| 28 | Ca | 98 | PRO |
| 29 | Cb | 17 | ARG |
| 29 | Cb | 22 | LYS |
| 29 | Cb | 34 | ASP |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 29 | Cb | 41 | LEU |
| 29 | Cb | 43 | ILE |
| 29 | Cb | 44 | THR |
| 29 | Cb | 52 | THR |
| 29 | Cb | 55 | THR |
| 29 | Cb | 61 | THR |
| 29 | Cb | 72 | LYS |
| 29 | Cb | 77 | THR |
| 29 | Cb | 78 | SER |
| 29 | Cb | 81 | ARG |
| 30 | Cc | 5 | THR |
| 30 | Cc | 7 | VAL |
| 30 | Cc | 11 | LYS |
| 30 | Cc | 14 | LYS |
| 30 | Cc | 16 | LEU |
| 30 | Cc | 19 | THR |
| 30 | Cc | 22 | ARG |
| 30 | Cc | 30 | VAL |
| 30 | Cc | 32 | PHE |
| 30 | Cc | 33 | LEU |
| 30 | Cc | 35 | ASP |
| 30 | Cc | 36 | THR |
| 30 | Cc | 40 | ILE |
| 30 | Cc | 49 | ARG |
| 30 | Cc | 54 | LEU |
| 30 | Cc | 62 | GLU |
| 30 | Cc | 64 | ARG |
| 30 | Cc | 65 | ARG |
| 31 | Cd | 4 | GLU |
| 31 | Cd | 10 | HIS |
| 31 | Cd | 16 | LYS |
| 31 | Cd | 25 | SER |
| 31 | Cd | 30 | LEU |
| 31 | Cd | 32 | ARG |
| 31 | Cd | 36 | LEU |
| 31 | Cd | 40 | ARG |
| 31 | Cd | 53 | ASN |
| 31 | Cd | 54 | LYS |
| 31 | Cd | 56 | ARG |
| 32 | Ce | 4 | VAL |
| 32 | Ce | 13 | LYS |
| 32 | Ce | 23 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 32 | Ce | 26 | LYS |
| 32 | Ce | 28 | LYS |
| 32 | Ce | 29 | LYS |
| 32 | Ce | 36 | LYS |
| 32 | Ce | 39 | LEU |
| 32 | Ce | 41 | THR |
| 32 | Ce | 44 | PHE |
| 32 | Ce | 45 | VAL |
| 32 | Ce | 47 | VAL |
| 32 | Ce | 50 | VAL |
| 32 | Ce | 53 | LYS |
| 32 | Ce | 54 | ARG |
| 32 | Ce | 56 | MET |
| 33 | Cf | 102 | VAL |
| 33 | Cf | 106 | TYR |
| 33 | Cf | 107 | LYS |
| 33 | Cf | 108 | VAL |
| 33 | Cf | 113 | LYS |
| 33 | Cf | 115 | THR |
| 33 | Cf | 135 | HIS |
| 33 | Cf | 140 | TYR |
| 33 | Cf | 141 | CYS |
| 33 | Cf | 146 | SER |
| 33 | Cf | 151 | ASN |
| 34 | Cg | 22 | SER |
| 34 | Cg | 25 | THR |
| 34 | Cg | 29 | GLN |
| 34 | Cg | 40 | LYS |
| 34 | Cg | 52 | GLN |
| 34 | Cg | 59 | ARG |
| 34 | Cg | 65 | SER |
| 34 | Cg | 76 | ASP |
| 34 | Cg | 96 | THR |
| 34 | Cg | 136 | ILE |
| 34 | Cg | 145 | LEU |
| 34 | Cg | 153 | GLN |
| 34 | Cg | 168 | THR |
| 34 | Cg | 176 | LYS |
| 34 | Cg | 184 | ASN |
| 34 | Cg | 188 | ILE |
| 34 | Cg | 199 | ILE |
| 34 | Cg | 202 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 34 | Cg | 222 | LEU |
| 34 | Cg | 228 | LYS |
| 34 | Cg | 232 | TYR |
| 34 | Cg | 250 | TYR |
| 34 | Cg | 256 | THR |
| 34 | Cg | 264 | SER |
| 34 | Cg | 266 | ASP |
| 34 | Cg | 272 | ASP |
| 34 | Cg | 274 | LEU |
| 34 | Cg | 278 | PHE |
| 34 | Cg | 297 | ASP |
| 34 | Cg | 308 | ASN |
| 34 | Cg | 309 | VAL |
| 34 | Cg | 310 | ILE |
| 34 | Cg | 312 | VAL |
| 34 | Cg | 319 | ASN |
| 81 | Ch | 23 | LYS |
| 81 | Ch | 28 | SER |
| 81 | Ch | 34 | LYS |
| 81 | Ch | 43 | ASP |
| 81 | Ch | 45 | SER |
| 81 | Ch | 46 | LYS |
| 81 | Ch | 48 | ARG |
| 81 | Ch | 49 | LYS |
| 81 | Ch | 50 | ASN |
| 81 | Ch | 53 | ARG |
| 81 | Ch | 61 | ILE |
| 81 | Ch | 64 | LYS |
| 81 | Ch | 74 | LYS |
| 81 | Ch | 75 | ASP |
| 81 | Ch | 77 | THR |
| 81 | Ch | 82 | THR |
| 39 | DA | 15 | ILE |
| 39 | DA | 23 | ARG |
| 39 | DA | 32 | LEU |
| 39 | DA | 41 | ILE |
| 39 | DA | 44 | ILE |
| 39 | DA | 45 | VAL |
| 39 | DA | 46 | LYS |
| 39 | DA | 48 | ILE |
| 39 | DA | 61 | VAL |
| 39 | DA | 62 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 39 | DA | 71 | LEU |
| 39 | DA | 96 | LEU |
| 39 | DA | 101 | VAL |
| 39 | DA | 112 | ILE |
| 39 | DA | 113 | VAL |
| 39 | DA | 114 | SER |
| 39 | DA | 119 | LYS |
| 39 | DA | 134 | VAL |
| 39 | DA | 137 | ILE |
| 39 | DA | 142 | ASP |
| 39 | DA | 147 | ARG |
| 39 | DA | 155 | LYS |
| 39 | DA | 158 | ILE |
| 39 | DA | 169 | ILE |
| 39 | DA | 179 | LEU |
| 39 | DA | 180 | LEU |
| 39 | DA | 181 | LYS |
| 39 | DA | 193 | ARG |
| 39 | DA | 202 | VAL |
| 39 | DA | 207 | VAL |
| 39 | DA | 215 | ASN |
| 39 | DA | 224 | THR |
| 39 | DA | 226 | SER |
| 39 | DA | 227 | ARG |
| 39 | DA | 230 | VAL |
| 39 | DA | 241 | ARG |
| 39 | DA | 243 | THR |
| 39 | DA | 246 | LEU |
| 40 | DB | 3 | HIS |
| 40 | DB | 4 | ARG |
| 40 | DB | 10 | ARG |
| 40 | DB | 17 | LEU |
| 40 | DB | 19 | ARG |
| 40 | DB | 20 | LYS |
| 40 | DB | 21 | ARG |
| 40 | DB | 24 | SER |
| 40 | DB | 30 | LYS |
| 40 | DB | 43 | LEU |
| 40 | DB | 47 | LEU |
| 40 | DB | 50 | LYS |
| 40 | DB | 56 | ILE |
| 40 | DB | 67 | PHE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 40 | DB | 70 | ARG |
| 40 | DB | 77 | THR |
| 40 | DB | 79 | VAL |
| 40 | DB | 81 | THR |
| 40 | DB | 84 | VAL |
| 40 | DB | 85 | VAL |
| 40 | DB | 89 | VAL |
| 40 | DB | 100 | ARG |
| 40 | DB | 103 | THR |
| 40 | DB | 114 | VAL |
| 40 | DB | 116 | ARG |
| 40 | DB | 139 | GLN |
| 40 | DB | 146 | ARG |
| 40 | DB | 148 | LEU |
| 40 | DB | 150 | ARG |
| 40 | DB | 153 | LYS |
| 40 | DB | 157 | VAL |
| 40 | DB | 169 | THR |
| 40 | DB | 175 | LYS |
| 40 | DB | 183 | LEU |
| 40 | DB | 187 | SER |
| 40 | DB | 188 | ILE |
| 40 | DB | 192 | VAL |
| 40 | DB | 196 | ARG |
| 40 | DB | 202 | THR |
| 40 | DB | 205 | VAL |
| 40 | DB | 213 | GLU |
| 40 | DB | 221 | THR |
| 40 | DB | 229 | VAL |
| 40 | DB | 232 | ARG |
| 40 | DB | 235 | THR |
| 40 | DB | 236 | LYS |
| 40 | DB | 238 | LEU |
| 40 | DB | 242 | THR |
| 40 | DB | 248 | LYS |
| 40 | DB | 252 | ILE |
| 40 | DB | 284 | ARG |
| 40 | DB | 291 | GLU |
| 40 | DB | 297 | SER |
| 40 | DB | 301 | THR |
| 40 | DB | 304 | THR |
| 40 | DB | 308 | MET |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 40 | DB | 322 | ILE |
| 40 | DB | 324 | VAL |
| 40 | DB | 328 | ILE |
| 40 | DB | 332 | ARG |
| 40 | DB | 338 | LEU |
| 40 | DB | 340 | LYS |
| 40 | DB | 346 | THR |
| 40 | DB | 347 | SER |
| 40 | DB | 355 | SER |
| 40 | DB | 361 | THR |
| 40 | DB | 367 | LYS |
| 40 | DB | 369 | ARG |
| 40 | DB | 380 | MET |
| 40 | DB | 382 | THR |
| 41 | DC | 2 | SER |
| 41 | DC | 7 | THR |
| 41 | DC | 16 | THR |
| 41 | DC | 18 | ASN |
| 41 | DC | 25 | VAL |
| 41 | DC | 27 | SER |
| 41 | DC | 52 | VAL |
| 41 | DC | 53 | SER |
| 41 | DC | 55 | LYS |
| 41 | DC | 71 | VAL |
| 41 | DC | 85 | SER |
| 41 | DC | 93 | MET |
| 41 | DC | 99 | MET |
| 41 | DC | 112 | LYS |
| 41 | DC | 120 | TYR |
| 41 | DC | 122 | THR |
| 41 | DC | 136 | LEU |
| 41 | DC | 138 | ARG |
| 41 | DC | 144 | LYS |
| 41 | DC | 145 | ILE |
| 41 | DC | 150 | LEU |
| 41 | DC | 153 | SER |
| 41 | DC | 156 | LEU |
| 41 | DC | 158 | SER |
| 41 | DC | 160 | GLN |
| 41 | DC | 161 | LYS |
| 41 | DC | 170 | LYS |
| 41 | DC | 176 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 41 | DC | 177 | ASP |
| 41 | DC | 179 | LEU |
| 41 | DC | 182 | LEU |
| 41 | DC | 186 | LYS |
| 41 | DC | 187 | LEU |
| 41 | DC | 198 | ARG |
| 41 | DC | 203 | ARG |
| 41 | DC | 206 | LEU |
| 41 | DC | 220 | ARG |
| 41 | DC | 222 | VAL |
| 41 | DC | 230 | VAL |
| 41 | DC | 246 | ARG |
| 41 | DC | 258 | LEU |
| 41 | DC | 259 | ASP |
| 41 | DC | 265 | GLU |
| 41 | DC | 267 | VAL |
| 41 | DC | 283 | THR |
| 41 | DC | 287 | THR |
| 41 | DC | 289 | ILE |
| 41 | DC | 290 | ILE |
| 41 | DC | 300 | ARG |
| 41 | DC | 307 | GLN |
| 41 | DC | 313 | LEU |
| 41 | DC | 319 | LYS |
| 41 | DC | 323 | VAL |
| 41 | DC | 327 | LEU |
| 41 | DC | 333 | VAL |
| 41 | DC | 339 | LEU |
| 41 | DC | 342 | LYS |
| 41 | DC | 345 | GLU |
| 41 | DC | 349 | THR |
| 41 | DC | 354 | VAL |
| 41 | DC | 356 | THR |
| 41 | DC | 357 | GLU |
| 41 | DC | 358 | THR |
| 41 | DC | 359 | LEU |
| 41 | DC | 360 | LYS |
| 41 | DC | 362 | ASP |
| 42 | DD | 4 | GLN |
| 42 | DD | 5 | LYS |
| 42 | DD | 13 | SER |
| 42 | DD | 34 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 42 | DD | 35 | ARG |
| 42 | DD | 41 | LYS |
| 42 | DD | 51 | LEU |
| 42 | DD | 65 | ILE |
| 42 | DD | 68 | THR |
| 42 | DD | 70 | THR |
| 42 | DD | 74 | VAL |
| 42 | DD | 81 | HIS |
| 42 | DD | 89 | THR |
| 42 | DD | 93 | THR |
| 42 | DD | 110 | LEU |
| 42 | DD | 112 | LYS |
| 42 | DD | 113 | LEU |
| 42 | DD | 118 | THR |
| 42 | DD | 124 | GLU |
| 42 | DD | 130 | GLU |
| 42 | DD | 131 | LEU |
| 42 | DD | 133 | GLU |
| 42 | DD | 136 | GLU |
| 42 | DD | 146 | LEU |
| 42 | DD | 148 | ILE |
| 42 | DD | 152 | ARG |
| 42 | DD | 155 | THR |
| 42 | DD | 164 | LYS |
| 42 | DD | 185 | PHE |
| 42 | DD | 186 | GLU |
| 42 | DD | 189 | GLU |
| 42 | DD | 190 | ILE |
| 42 | DD | 191 | ASP |
| 42 | DD | 194 | LEU |
| 42 | DD | 205 | SER |
| 42 | DD | 211 | LEU |
| 42 | DD | 218 | ARG |
| 42 | DD | 227 | LEU |
| 42 | DD | 232 | ASP |
| 42 | DD | 251 | PRO |
| 42 | DD | 254 | LYS |
| 42 | DD | 258 | LYS |
| 42 | DD | 259 | LYS |
| 42 | DD | 262 | LYS |
| 42 | DD | 268 | GLU |
| 42 | DD | 273 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 42 | DD | 275 | THR |
| 42 | DD | 282 | ARG |
| 43 | DE | 5 | LYS |
| 43 | DE | 8 | LYS |
| 43 | DE | 20 | LYS |
| 43 | DE | 21 | THR |
| 43 | DE | 46 | ARG |
| 43 | DE | 50 | LYS |
| 43 | DE | 64 | LEU |
| 43 | DE | 65 | ILE |
| 43 | DE | 76 | LEU |
| 43 | DE | 78 | ARG |
| 43 | DE | 79 | VAL |
| 43 | DE | 89 | THR |
| 43 | DE | 93 | VAL |
| 43 | DE | 98 | VAL |
| 43 | DE | 99 | GLU |
| 43 | DE | 109 | GLU |
| 43 | DE | 143 | LYS |
| 43 | DE | 152 | THR |
| 43 | DE | 155 | LEU |
| 43 | DE | 162 | SER |
| 44 | DF | 22 | THR |
| 44 | DF | 24 | GLU |
| 44 | DF | 26 | VAL |
| 44 | DF | 39 | GLU |
| 44 | DF | 41 | ARG |
| 44 | DF | 45 | LEU |
| 44 | DF | 53 | LYS |
| 44 | DF | 54 | GLU |
| 44 | DF | 56 | GLU |
| 44 | DF | 60 | ARG |
| 44 | DF | 83 | LEU |
| 44 | DF | 88 | ARG |
| 44 | DF | 98 | LYS |
| 44 | DF | 101 | LYS |
| 44 | DF | 121 | LYS |
| 44 | DF | 124 | LEU |
| 44 | DF | 130 | ILE |
| 44 | DF | 156 | ILE |
| 44 | DF | 158 | LYS |
| 44 | DF | 159 | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 44 | DF | 173 | LEU |
| 44 | DF | 175 | LYS |
| 44 | DF | 179 | LEU |
| 44 | DF | 184 | LEU |
| 44 | DF | 196 | LYS |
| 44 | DF | 206 | LYS |
| 44 | DF | 219 | LYS |
| 44 | DF | 229 | PHE |
| 44 | DF | 239 | LEU |
| 45 | DG | 26 | LEU |
| 45 | DG | 41 | GLN |
| 45 | DG | 50 | VAL |
| 45 | DG | 68 | ARG |
| 45 | DG | 70 | LYS |
| 45 | DG | 74 | THR |
| 45 | DG | 79 | GLN |
| 45 | DG | 81 | THR |
| 45 | DG | 85 | ASN |
| 45 | DG | 89 | GLU |
| 45 | DG | 92 | LYS |
| 45 | DG | 95 | ASN |
| 45 | DG | 110 | THR |
| 45 | DG | 126 | SER |
| 45 | DG | 128 | LYS |
| 45 | DG | 136 | LEU |
| 45 | DG | 145 | ASN |
| 45 | DG | 146 | LYS |
| 45 | DG | 149 | LYS |
| 45 | DG | 150 | LEU |
| 45 | DG | 153 | ILE |
| 45 | DG | 160 | ILE |
| 45 | DG | 169 | LEU |
| 45 | DG | 172 | LYS |
| 45 | DG | 173 | MET |
| 45 | DG | 183 | LYS |
| 45 | DG | 185 | ARG |
| 45 | DG | 189 | LEU |
| 45 | DG | 208 | GLU |
| 45 | DG | 213 | LYS |
| 45 | DG | 214 | LEU |
| 45 | DG | 216 | SER |
| 45 | DG | 217 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 45 | DG | 219 | ASP |
| 45 | DG | 222 | PHE |
| 45 | DG | 230 | LYS |
| 45 | DG | 241 | LYS |
| 45 | DG | 245 | LYS |
| 45 | DG | 248 | LYS |
| 46 | DH | 4 | ILE |
| 46 | DH | 5 | GLN |
| 46 | DH | 6 | THR |
| 46 | DH | 18 | VAL |
| 46 | DH | 19 | SER |
| 46 | DH | 20 | ILE |
| 46 | DH | 31 | ARG |
| 46 | DH | 33 | THR |
| 46 | DH | 43 | VAL |
| 46 | DH | 44 | THR |
| 46 | DH | 52 | LEU |
| 46 | DH | 55 | VAL |
| 46 | DH | 62 | ARG |
| 46 | DH | 63 | LYS |
| 46 | DH | 68 | LEU |
| 46 | DH | 69 | ARG |
| 46 | DH | 70 | THR |
| 46 | DH | 80 | THR |
| 46 | DH | 82 | VAL |
| 46 | DH | 92 | TYR |
| 46 | DH | 106 | LYS |
| 46 | DH | 121 | LYS |
| 46 | DH | 123 | ILE |
| 46 | DH | 129 | ARG |
| 46 | DH | 130 | ASP |
| 46 | DH | 132 | VAL |
| 46 | DH | 133 | THR |
| 46 | DH | 134 | ILE |
| 46 | DH | 138 | THR |
| 46 | DH | 144 | ILE |
| 46 | DH | 151 | VAL |
| 46 | DH | 157 | ASN |
| 46 | DH | 161 | LEU |
| 46 | DH | 162 | GLN |
| 46 | DH | 164 | ILE |
| 46 | DH | 169 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 46 | DH | 177 | ASP |
| 46 | DH | 179 | ILE |
| 46 | DH | 191 | LEU |
| 47 | DI | 4 | ARG |
| 47 | DI | 24 | ARG |
| 47 | DI | 26 | VAL |
| 47 | DI | 36 | LEU |
| 47 | DI | 42 | THR |
| 47 | DI | 52 | LEU |
| 47 | DI | 57 | LEU |
| 47 | DI | 58 | GLU |
| 47 | DI | 63 | GLU |
| 47 | DI | 71 | CYS |
| 47 | DI | 74 | LYS |
| 47 | DI | 76 | MET |
| 47 | DI | 78 | THR |
| 47 | DI | 83 | ASP |
| 47 | DI | 87 | LEU |
| 47 | DI | 91 | VAL |
| 47 | DI | 99 | ILE |
| 47 | DI | 129 | VAL |
| 47 | DI | 139 | ARG |
| 47 | DI | 140 | THR |
| 47 | DI | 143 | SER |
| 47 | DI | 144 | ASN |
| 47 | DI | 145 | LYS |
| 47 | DI | 153 | ARG |
| 47 | DI | 163 | GLN |
| 47 | DI | 167 | LEU |
| 47 | DI | 169 | LYS |
| 47 | DI | 174 | THR |
| 47 | DI | 177 | ASP |
| 47 | DI | 178 | ARG |
| 47 | DI | 185 | ARG |
| 47 | DI | 200 | LEU |
| 47 | DI | 206 | LEU |
| 47 | DI | 211 | ARG |
| 47 | DI | 212 | GLU |
| 47 | DI | 215 | GLU |
| 47 | DI | 217 | PHE |
| 48 | DJ | 10 | ARG |
| 48 | DJ | 12 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 48 | DJ | 13 | LYS |
| 48 | DJ | 16 | LYS |
| 48 | DJ | 22 | SER |
| 48 | DJ | 29 | ARG |
| 48 | DJ | 30 | LEU |
| 48 | DJ | 31 | THR |
| 48 | DJ | 34 | SER |
| 48 | DJ | 35 | LYS |
| 48 | DJ | 44 | THR |
| 48 | DJ | 46 | VAL |
| 48 | DJ | 80 | LEU |
| 48 | DJ | 87 | LYS |
| 48 | DJ | 92 | ARG |
| 48 | DJ | 94 | ARG |
| 48 | DJ | 106 | ILE |
| 48 | DJ | 107 | ASP |
| 48 | DJ | 112 | LEU |
| 48 | DJ | 114 | ILE |
| 48 | DJ | 129 | VAL |
| 48 | DJ | 130 | VAL |
| 48 | DJ | 132 | ASN |
| 48 | DJ | 137 | ARG |
| 48 | DJ | 138 | VAL |
| 48 | DJ | 140 | ARG |
| 48 | DJ | 142 | LYS |
| 48 | DJ | 147 | THR |
| 48 | DJ | 158 | ASP |
| 48 | DJ | 159 | THR |
| 48 | DJ | 160 | VAL |
| 48 | DJ | 161 | SER |
| 48 | DJ | 165 | GLN |
| 49 | DL | 45 | LYS |
| 49 | DL | 46 | ILE |
| 49 | DL | 54 | LEU |
| 49 | DL | 55 | ARG |
| 49 | DL | 59 | ARG |
| 49 | DL | 63 | VAL |
| 49 | DL | 67 | ARG |
| 49 | DL | 68 | LYS |
| 49 | DL | 69 | VAL |
| 49 | DL | 73 | ARG |
| 49 | DL | 85 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 49 | DL | 100 | ARG |
| 49 | DL | 107 | GLU |
| 49 | DL | 114 | GLN |
| 49 | DL | 115 | ARG |
| 49 | DL | 118 | GLU |
| 49 | DL | 121 | SER |
| 49 | DL | 123 | ILE |
| 49 | DL | 124 | ILE |
| 49 | DL | 128 | ARG |
| 49 | DL | 131 | LYS |
| 49 | DL | 152 | THR |
| 49 | DL | 154 | VAL |
| 49 | DL | 157 | ARG |
| 49 | DL | 164 | GLU |
| 49 | DL | 171 | ARG |
| 49 | DL | 175 | SER |
| 49 | DL | 184 | GLU |
| 49 | DL | 189 | GLU |
| 49 | DL | 194 | GLU |
| 50 | DM | 3 | THR |
| 50 | DM | 10 | SER |
| 50 | DM | 13 | ARG |
| 50 | DM | 20 | VAL |
| 50 | DM | 24 | LYS |
| 50 | DM | 42 | LYS |
| 50 | DM | 53 | VAL |
| 50 | DM | 62 | GLN |
| 50 | DM | 63 | VAL |
| 50 | DM | 64 | VAL |
| 50 | DM | 72 | LEU |
| 50 | DM | 74 | ARG |
| 50 | DM | 80 | THR |
| 50 | DM | 82 | SER |
| 50 | DM | 92 | GLU |
| 50 | DM | 106 | ARG |
| 50 | DM | 107 | GLU |
| 50 | DM | 124 | ARG |
| 50 | DM | 126 | GLN |
| 50 | DM | 128 | ARG |
| 50 | DM | 130 | THR |
| 50 | DM | 132 | LYS |
| 50 | DM | 133 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 50 | DM | 135 | LEU |
| 51 | DN | 5 | LYS |
| 51 | DN | 7 | LEU |
| 51 | DN | 8 | GLU |
| 51 | DN | 10 | LEU |
| 51 | DN | 12 | ARG |
| 51 | DN | 15 | GLN |
| 51 | DN | 18 | VAL |
| 51 | DN | 22 | LEU |
| 51 | DN | 24 | ARG |
| 51 | DN | 41 | ARG |
| 51 | DN | 49 | ARG |
| 51 | DN | 54 | LYS |
| 51 | DN | 68 | ARG |
| 51 | DN | 80 | THR |
| 51 | DN | 85 | THR |
| 51 | DN | 92 | LEU |
| 51 | DN | 93 | LYS |
| 51 | DN | 96 | ARG |
| 51 | DN | 97 | SER |
| 51 | DN | 104 | GLU |
| 51 | DN | 105 | ARG |
| 51 | DN | 109 | ARG |
| 51 | DN | 117 | ASN |
| 51 | DN | 134 | LEU |
| 51 | DN | 138 | GLN |
| 51 | DN | 153 | ASP |
| 51 | DN | 155 | VAL |
| 51 | DN | 159 | ARG |
| 51 | DN | 170 | LYS |
| 51 | DN | 184 | LYS |
| 51 | DN | 190 | THR |
| 51 | DN | 196 | THR |
| 51 | DN | 204 | LYS |
| 52 | DO | 3[A] | VAL |
| 52 | DO | 3[B] | SER |
| 52 | DO | 12[A] | LYS |
| 52 | DO | 12[B] | LYS |
| 52 | DO | 16[B] | LEU |
| 52 | DO | 22[B] | THR |
| 52 | DO | 27[B] | VAL |
| 52 | DO | 34[A] | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 52 | DO | 34[B] | VAL |
| 52 | DO | 41[A] | LEU |
| 52 | DO | 41[B] | LEU |
| 52 | DO | 58[A] | LEU |
| 52 | DO | 58[B] | LEU |
| 52 | DO | 59[A] | ARG |
| 52 | DO | 59[B] | ARG |
| 52 | DO | 67[A] | THR |
| 52 | DO | 67[B] | THR |
| 52 | DO | 74[A] | ARG |
| 52 | DO | 74[B] | ARG |
| 52 | DO | 78[A] | ARG |
| 52 | DO | 78[B] | ARG |
| 52 | DO | 80[B] | LEU |
| 52 | DO | 85[A] | ARG |
| 52 | DO | 85[B] | ARG |
| 52 | DO | 100[A] | GLU |
| 52 | DO | 100[B] | GLU |
| 52 | DO | 106[A] | GLU |
| 52 | DO | 106[B] | GLU |
| 52 | DO | 108[A] | ILE |
| 52 | DO | 108[B] | ILE |
| 52 | DO | 117[A] | ARG |
| 52 | DO | 117[B] | ARG |
| 52 | DO | 124[A] | LEU |
| 52 | DO | 124[B] | LEU |
| 52 | DO | 126[A] | VAL |
| 52 | DO | 126[B] | VAL |
| 52 | DO | 128[A] | ARG |
| 52 | DO | 128[B] | ARG |
| 52 | DO | 129[A] | LEU |
| 52 | DO | 129[B] | LEU |
| 52 | DO | 130[A] | LYS |
| 52 | DO | 130[B] | LYS |
| 52 | DO | 144[A] | SER |
| 52 | DO | 144[B] | SER |
| 52 | DO | 160[A] | ARG |
| 52 | DO | 160[B] | ARG |
| 52 | DO | 163[B] | ARG |
| 52 | DO | 166[A] | GLU |
| 52 | DO | 166[B] | GLU |
| 52 | DO | 171[A] | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 52 | DO | 171[B] | LYS |
| 52 | DO | 175[A] | THR |
| 52 | DO | 175[B] | THR |
| 52 | DO | 182[A] | ASN |
| 52 | DO | 184[A] | THR |
| 52 | DO | 197[A] | LEU |
| 53 | DP | 9 | THR |
| 53 | DP | 24 | VAL |
| 53 | DP | 29 | THR |
| 53 | DP | 31 | GLU |
| 53 | DP | 32 | THR |
| 53 | DP | 41 | LEU |
| 53 | DP | 52 | LEU |
| 53 | DP | 56 | ARG |
| 53 | DP | 69 | ARG |
| 53 | DP | 74 | LYS |
| 53 | DP | 78 | VAL |
| 53 | DP | 79 | THR |
| 53 | DP | 80 | LYS |
| 53 | DP | 89 | LYS |
| 53 | DP | 94 | LEU |
| 53 | DP | 103 | GLU |
| 53 | DP | 112 | LEU |
| 53 | DP | 114 | VAL |
| 53 | DP | 119 | VAL |
| 53 | DP | 126 | ARG |
| 53 | DP | 128 | ARG |
| 53 | DP | 138 | LYS |
| 54 | DQ | 3 | ILE |
| 54 | DQ | 7 | SER |
| 54 | DQ | 17 | THR |
| 54 | DQ | 24 | VAL |
| 54 | DQ | 26 | LEU |
| 54 | DQ | 31 | LYS |
| 54 | DQ | 32 | LEU |
| 54 | DQ | 34 | THR |
| 54 | DQ | 49 | LEU |
| 54 | DQ | 57 | ILE |
| 54 | DQ | 64 | VAL |
| 54 | DQ | 80 | THR |
| 54 | DQ | 81 | VAL |
| 54 | DQ | 86 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 54 | DQ | 93 | ILE |
| 54 | DQ | 98 | LYS |
| 54 | DQ | 100 | THR |
| 54 | DQ | 105 | ARG |
| 54 | DQ | 113 | LYS |
| 54 | DQ | 135 | GLN |
| 54 | DQ | 138 | LEU |
| 54 | DQ | 147 | ARG |
| 54 | DQ | 161 | LYS |
| 54 | DQ | 165 | ILE |
| 54 | DQ | 166 | LEU |
| 54 | DQ | 170 | ARG |
| 55 | DR | 5 | ARG |
| 55 | DR | 7 | GLN |
| 55 | DR | 10 | LEU |
| 55 | DR | 17 | VAL |
| 55 | DR | 20 | ARG |
| 55 | DR | 27 | ASN |
| 55 | DR | 29 | THR |
| 55 | DR | 36 | ASN |
| 55 | DR | 39 | ASN |
| 55 | DR | 43 | LYS |
| 55 | DR | 49 | THR |
| 55 | DR | 55 | VAL |
| 55 | DR | 56 | THR |
| 55 | DR | 63 | THR |
| 55 | DR | 70 | LYS |
| 55 | DR | 71 | ARG |
| 55 | DR | 74 | ARG |
| 55 | DR | 98 | ARG |
| 55 | DR | 99 | LEU |
| 55 | DR | 105 | LEU |
| 55 | DR | 106 | LEU |
| 55 | DR | 114 | LYS |
| 55 | DR | 126 | GLU |
| 55 | DR | 138 | LEU |
| 55 | DR | 152 | GLU |
| 55 | DR | 153 | LYS |
| 55 | DR | 158 | GLU |
| 55 | DR | 162 | ARG |
| 55 | DR | 164 | LEU |
| 55 | DR | 167 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 55 | DR | 173 | ARG |
| 55 | DR | 180 | LYS |
| 56 | DS | 1 | MET |
| 56 | DS | 13 | ARG |
| 56 | DS | 15 | PRO |
| 56 | DS | 17 | GLU |
| 56 | DS | 21 | GLU |
| 56 | DS | 23 | LYS |
| 56 | DS | 40 | ARG |
| 56 | DS | 50 | LYS |
| 56 | DS | 51 | VAL |
| 56 | DS | 52 | LYS |
| 56 | DS | 61 | ILE |
| 56 | DS | 71 | LYS |
| 56 | DS | 74 | ASN |
| 56 | DS | 80 | ARG |
| 56 | DS | 87 | THR |
| 56 | DS | 96 | ASP |
| 56 | DS | 97 | VAL |
| 56 | DS | 100 | VAL |
| 56 | DS | 104 | GLU |
| 56 | DS | 105 | THR |
| 56 | DS | 115 | ARG |
| 56 | DS | 117 | ARG |
| 56 | DS | 130 | GLU |
| 56 | DS | 136 | LYS |
| 56 | DS | 146 | LYS |
| 56 | DS | 148 | LEU |
| 56 | DS | 149 | LYS |
| 56 | DS | 155 | ARG |
| 56 | DS | 161 | LYS |
| 56 | DS | 162 | THR |
| 56 | DS | 166 | LYS |
| 56 | DS | 169 | SER |
| 56 | DS | 172 | TYR |
| 57 | DT | 17 | ARG |
| 57 | DT | 25 | VAL |
| 57 | DT | 26 | HIS |
| 57 | DT | 27 | LEU |
| 57 | DT | 35 | LYS |
| 57 | DT | 36 | VAL |
| 57 | DT | 47 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 57 | DT | 55 | LYS |
| 57 | DT | 68 | THR |
| 57 | DT | 71 | SER |
| 57 | DT | 78 | LYS |
| 57 | DT | 80 | VAL |
| 57 | DT | 83 | ARG |
| 57 | DT | 88 | ARG |
| 57 | DT | 89 | LEU |
| 57 | DT | 96 | ILE |
| 57 | DT | 102 | ARG |
| 57 | DT | 104 | GLU |
| 57 | DT | 118 | GLU |
| 57 | DT | 126 | VAL |
| 57 | DT | 131 | GLN |
| 57 | DT | 135 | PRO |
| 57 | DT | 139 | ARG |
| 57 | DT | 143 | THR |
| 57 | DT | 149 | GLN |
| 57 | DT | 150 | THR |
| 57 | DT | 160 | ILE |
| 58 | DU | 13 | LYS |
| 58 | DU | 14 | THR |
| 58 | DU | 16 | THR |
| 58 | DU | 21 | SER |
| 58 | DU | 23 | THR |
| 58 | DU | 27 | VAL |
| 58 | DU | 28 | PHE |
| 58 | DU | 37 | LEU |
| 58 | DU | 39 | ASP |
| 58 | DU | 43 | VAL |
| 58 | DU | 50 | LEU |
| 58 | DU | 52 | ASN |
| 58 | DU | 54 | VAL |
| 58 | DU | 55 | THR |
| 58 | DU | 58 | GLU |
| 58 | DU | 61 | THR |
| 58 | DU | 62 | VAL |
| 58 | DU | 63 | VAL |
| 58 | DU | 68 | THR |
| 58 | DU | 90 | ARG |
| 58 | DU | 98 | THR |
| 58 | DU | 100 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 58 | DU | 105 | LEU |
| 59 | DV | 13 | ILE |
| 59 | DV | 14 | SER |
| 59 | DV | 48 | ARG |
| 59 | DV | 70 | ARG |
| 59 | DV | 88 | ARG |
| 59 | DV | 91 | VAL |
| 59 | DV | 110 | LYS |
| 59 | DV | 115 | THR |
| 60 | DW | 1 | MET |
| 60 | DW | 5 | ILE |
| 60 | DW | 25 | ASP |
| 60 | DW | 47 | ARG |
| 60 | DW | 56 | ARG |
| 60 | DW | 57 | LYS |
| 60 | DW | 63 | ILE |
| 60 | DW | 95 | SER |
| 60 | DW | 97 | LYS |
| 60 | DW | 100 | VAL |
| 60 | DW | 105 | ARG |
| 60 | DW | 107 | GLU |
| 60 | DW | 126 | GLU |
| 60 | DW | 127 | LYS |
| 60 | DW | 135 | SER |
| 61 | DX | 24 | LEU |
| 61 | DX | 27 | ARG |
| 61 | DX | 34 | LEU |
| 61 | DX | 37 | THR |
| 61 | DX | 38 | LEU |
| 61 | DX | 40 | LEU |
| 61 | DX | 56 | ARG |
| 61 | DX | 57 | LEU |
| 61 | DX | 63 | ILE |
| 61 | DX | 70 | GLU |
| 61 | DX | 71 | THR |
| 61 | DX | 73 | MET |
| 61 | DX | 74 | LYS |
| 61 | DX | 86 | VAL |
| 61 | DX | 101 | GLU |
| 61 | DX | 108 | LEU |
| 61 | DX | 109 | LYS |
| 61 | DX | 115 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 61 | DX | 121 | LYS |
| 61 | DX | 125 | ARG |
| 61 | DX | 133 | LEU |
| 61 | DX | 135 | ILE |
| 61 | DX | 142 | ILE |
| 62 | DY | 12 | ARG |
| 62 | DY | 13 | ARG |
| 62 | DY | 14 | LYS |
| 62 | DY | 17 | LYS |
| 62 | DY | 37 | LYS |
| 62 | DY | 40 | ARG |
| 62 | DY | 43 | TYR |
| 62 | DY | 45 | ILE |
| 62 | DY | 50 | ILE |
| 62 | DY | 52 | ARG |
| 62 | DY | 57 | LEU |
| 62 | DY | 59 | VAL |
| 62 | DY | 66 | GLN |
| 62 | DY | 71 | SER |
| 62 | DY | 74 | TYR |
| 62 | DY | 76 | LEU |
| 62 | DY | 80 | VAL |
| 62 | DY | 83 | ASP |
| 62 | DY | 87 | LYS |
| 62 | DY | 94 | SER |
| 62 | DY | 95 | VAL |
| 62 | DY | 97 | ILE |
| 62 | DY | 103 | LYS |
| 62 | DY | 120 | GLN |
| 63 | DZ | 3 | LYS |
| 63 | DZ | 14 | VAL |
| 63 | DZ | 17 | ARG |
| 63 | DZ | 24 | VAL |
| 63 | DZ | 30 | ASP |
| 63 | DZ | 31 | GLU |
| 63 | DZ | 34 | LYS |
| 63 | DZ | 55 | LYS |
| 63 | DZ | 65 | ARG |
| 63 | DZ | 72 | ILE |
| 63 | DZ | 81 | LEU |
| 63 | DZ | 83 | THR |
| 63 | DZ | 86 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 63 | DZ | 89 | VAL |
| 63 | DZ | 93 | LYS |
| 63 | DZ | 95 | VAL |
| 63 | DZ | 99 | GLU |
| 63 | DZ | 100 | THR |
| 63 | DZ | 102 | GLU |
| 63 | DZ | 103 | GLN |
| 63 | DZ | 105 | SER |
| 63 | DZ | 121 | ARG |
| 63 | DZ | 126 | LYS |
| 63 | DZ | 127 | ASN |
| 63 | DZ | 134 | LEU |
| 63 | DZ | 135 | ARG |
| 64 | Da | 6 | THR |
| 64 | Da | 8 | THR |
| 64 | Da | 10 | LYS |
| 64 | Da | 12 | ARG |
| 64 | Da | 16 | SER |
| 64 | Da | 24 | LYS |
| 64 | Da | 34 | MET |
| 64 | Da | 42 | ARG |
| 64 | Da | 44 | ASN |
| 64 | Da | 47 | LYS |
| 64 | Da | 60 | TYR |
| 64 | Da | 78 | LEU |
| 64 | Da | 80 | THR |
| 64 | Da | 82 | ILE |
| 64 | Da | 85 | ASP |
| 64 | Da | 91 | LEU |
| 64 | Da | 97 | GLU |
| 64 | Da | 98 | THR |
| 64 | Da | 115 | LYS |
| 64 | Da | 128 | ARG |
| 64 | Da | 130 | VAL |
| 64 | Da | 132 | LYS |
| 64 | Da | 133 | LEU |
| 65 | Db | 14 | ARG |
| 65 | Db | 15 | LYS |
| 65 | Db | 21 | ILE |
| 65 | Db | 22 | LYS |
| 65 | Db | 26 | THR |
| 65 | Db | 33 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 65 | Db | 38 | LYS |
| 65 | Db | 50 | THR |
| 65 | Db | 52 | LYS |
| 65 | Db | 58 | LYS |
| 65 | Db | 59 | LYS |
| 66 | Dc | 8 | GLU |
| 66 | Dc | 9 | SER |
| 66 | Dc | 18 | ILE |
| 66 | Dc | 19 | LYS |
| 66 | Dc | 30 | THR |
| 66 | Dc | 33 | SER |
| 66 | Dc | 34 | LEU |
| 66 | Dc | 40 | LYS |
| 66 | Dc | 41 | LEU |
| 66 | Dc | 48 | THR |
| 66 | Dc | 61 | MET |
| 66 | Dc | 68 | TYR |
| 66 | Dc | 86 | ARG |
| 66 | Dc | 87 | VAL |
| 66 | Dc | 99 | ASP |
| 66 | Dc | 100 | ILE |
| 67 | Dd | 6 | ASP |
| 67 | Dd | 8 | VAL |
| 67 | Dd | 13 | THR |
| 67 | Dd | 16 | LEU |
| 67 | Dd | 26 | LYS |
| 67 | Dd | 31 | ARG |
| 67 | Dd | 34 | LYS |
| 67 | Dd | 44 | MET |
| 67 | Dd | 55 | LEU |
| 67 | Dd | 61 | LYS |
| 67 | Dd | 76 | SER |
| 67 | Dd | 82 | GLU |
| 67 | Dd | 89 | LEU |
| 67 | Dd | 90 | PHE |
| 67 | Dd | 96 | VAL |
| 67 | Dd | 100 | SER |
| 67 | Dd | 102 | LYS |
| 67 | Dd | 104 | LEU |
| 67 | Dd | 105 | GLN |
| 67 | Dd | 106 | THR |
| 67 | Dd | 110 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 68 | De | 4 | LEU |
| 68 | De | 14 | THR |
| 68 | De | 16 | LYS |
| 68 | De | 18 | LYS |
| 68 | De | 19 | ARG |
| 68 | De | 27 | ARG |
| 68 | De | 31 | ASN |
| 68 | De | 33 | ARG |
| 68 | De | 35 | GLN |
| 68 | De | 51 | SER |
| 68 | De | 61 | LYS |
| 68 | De | 73 | THR |
| 68 | De | 75 | LEU |
| 68 | De | 82 | LEU |
| 68 | De | 87 | MET |
| 68 | De | 91 | THR |
| 68 | De | 106 | VAL |
| 68 | De | 109 | LEU |
| 68 | De | 125 | ARG |
| 68 | De | 126 | LEU |
| 69 | Df | 4 | SER |
| 69 | Df | 10 | LYS |
| 69 | Df | 20 | LYS |
| 69 | Df | 28 | SER |
| 69 | Df | 31 | LYS |
| 69 | Df | 49 | ILE |
| 69 | Df | 70 | LYS |
| 69 | Df | 81 | VAL |
| 69 | Df | 84 | THR |
| 69 | Df | 98 | VAL |
| 69 | Df | 107 | ILE |
| 70 | Dg | 5 | VAL |
| 70 | Dg | 9 | ARG |
| 70 | Dg | 16 | ARG |
| 70 | Dg | 19 | LYS |
| 70 | Dg | 20 | ILE |
| 70 | Dg | 23 | VAL |
| 70 | Dg | 24 | LYS |
| 70 | Dg | 29 | ILE |
| 70 | Dg | 30 | LEU |
| 70 | Dg | 31 | ARG |
| 70 | Dg | 35 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 70 | Dg | 36 | LYS |
| 70 | Dg | 44 | CYS |
| 70 | Dg | 54 | ILE |
| 70 | Dg | 58 | ARG |
| 70 | Dg | 65 | VAL |
| 70 | Dg | 70 | LYS |
| 70 | Dg | 79 | SER |
| 70 | Dg | 85 | VAL |
| 70 | Dg | 86 | LYS |
| 70 | Dg | 88 | ARG |
| 70 | Dg | 90 | ILE |
| 70 | Dg | 98 | GLN |
| 70 | Dg | 104 | VAL |
| 71 | Dh | 15 | GLU |
| 71 | Dh | 20 | GLN |
| 71 | Dh | 21 | LEU |
| 71 | Dh | 27 | GLU |
| 71 | Dh | 28 | LEU |
| 71 | Dh | 38 | ARG |
| 71 | Dh | 40 | SER |
| 71 | Dh | 45 | LYS |
| 71 | Dh | 47 | VAL |
| 71 | Dh | 48 | ARG |
| 71 | Dh | 57 | VAL |
| 71 | Dh | 62 | GLN |
| 71 | Dh | 66 | VAL |
| 71 | Dh | 69 | LEU |
| 71 | Dh | 79 | ASP |
| 71 | Dh | 81 | ARG |
| 71 | Dh | 84 | LYS |
| 71 | Dh | 85 | THR |
| 71 | Dh | 86 | ARG |
| 71 | Dh | 89 | ARG |
| 71 | Dh | 90 | ARG |
| 71 | Dh | 98 | SER |
| 71 | Dh | 100 | VAL |
| 71 | Dh | 101 | THR |
| 71 | Dh | 107 | LYS |
| 71 | Dh | 119 | LYS |
| 72 | Di | 3 | VAL |
| 72 | Di | 7 | ILE |
| 72 | Di | 9 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 72 | Di | 11 | LEU |
| 72 | Di | 17 | VAL |
| 72 | Di | 18 | THR |
| 72 | Di | 21 | THR |
| 72 | Di | 26 | ILE |
| 72 | Di | 29 | LYS |
| 72 | Di | 34 | SER |
| 72 | Di | 36 | ARG |
| 72 | Di | 37 | THR |
| 72 | Di | 38 | LYS |
| 72 | Di | 43 | LEU |
| 72 | Di | 45 | ARG |
| 72 | Di | 57 | LEU |
| 72 | Di | 58 | ILE |
| 72 | Di | 60 | LEU |
| 72 | Di | 61 | ILE |
| 72 | Di | 66 | GLU |
| 72 | Di | 68 | ARG |
| 72 | Di | 74 | LYS |
| 72 | Di | 75 | LYS |
| 72 | Di | 76 | ARG |
| 72 | Di | 81 | THR |
| 72 | Di | 88 | GLU |
| 72 | Di | 90 | MET |
| 72 | Di | 94 | ILE |
| 72 | Di | 98 | ARG |
| 73 | Dj | 3 | LYS |
| 73 | Dj | 11 | ARG |
| 73 | Dj | 17 | THR |
| 73 | Dj | 25 | ARG |
| 73 | Dj | 33 | THR |
| 73 | Dj | 36 | SER |
| 73 | Dj | 44 | THR |
| 73 | Dj | 55 | ARG |
| 73 | Dj | 58 | THR |
| 73 | Dj | 59 | THR |
| 73 | Dj | 64 | MET |
| 73 | Dj | 65 | ARG |
| 73 | Dj | 67 | LEU |
| 73 | Dj | 68 | LYS |
| 73 | Dj | 75 | LYS |
| 73 | Dj | 80 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 73 | Dj | 84 | SER |
| 74 | Dk | 5 | ILE |
| 74 | Dk | 12 | LEU |
| 74 | Dk | 24 | THR |
| 74 | Dk | 31 | LEU |
| 74 | Dk | 39 | ARG |
| 74 | Dk | 41 | THR |
| 74 | Dk | 46 | ARG |
| 74 | Dk | 50 | SER |
| 74 | Dk | 53 | THR |
| 74 | Dk | 61 | LYS |
| 74 | Dk | 64 | LYS |
| 74 | Dk | 65 | LEU |
| 74 | Dk | 67 | GLN |
| 74 | Dk | 68 | SER |
| 75 | Dl | 11 | GLN |
| 75 | Dl | 15 | LYS |
| 75 | Dl | 17 | LYS |
| 75 | Dl | 21 | ARG |
| 75 | Dl | 23 | LEU |
| 75 | Dl | 27 | ILE |
| 75 | Dl | 29 | LEU |
| 75 | Dl | 41 | ARG |
| 75 | Dl | 45 | ARG |
| 75 | Dl | 47 | THR |
| 75 | Dl | 51 | ILE |
| 76 | Dm | 78 | ILE |
| 76 | Dm | 79 | GLU |
| 76 | Dm | 83 | LYS |
| 76 | Dm | 85 | LEU |
| 76 | Dm | 88 | LYS |
| 76 | Dm | 91 | CYS |
| 76 | Dm | 93 | LYS |
| 76 | Dm | 106 | ARG |
| 76 | Dm | 112 | LYS |
| 76 | Dm | 113 | ARG |
| 76 | Dm | 114 | LYS |
| 76 | Dm | 126 | LYS |
| 76 | Dm | 127 | LEU |
| 77 | Dn | 6 | ARG |
| 77 | Dn | 9 | ARG |
| 77 | Dn | 13 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 77 | Dn | 16 | LYS |
| 77 | Dn | 21 | ARG |
| 77 | Dn | 23 | ARG |
| 77 | Dn | 24 | SER |
| 78 | Do | 7 | THR |
| 78 | Do | 8 | ARG |
| 78 | Do | 18 | ARG |
| 78 | Do | 46 | LYS |
| 78 | Do | 47 | GLN |
| 78 | Do | 61 | LYS |
| 78 | Do | 63 | LYS |
| 78 | Do | 71 | ARG |
| 78 | Do | 78 | LYS |
| 78 | Do | 79 | THR |
| 78 | Do | 83 | LEU |
| 78 | Do | 84 | THR |
| 78 | Do | 89 | LYS |
| 78 | Do | 93 | LEU |
| 78 | Do | 104 | LEU |
| 78 | Do | 105 | GLN |
| 79 | Dp | 3 | LYS |
| 79 | Dp | 24 | ARG |
| 79 | Dp | 42 | CYS |
| 79 | Dp | 48 | LYS |
| 79 | Dp | 49 | ARG |
| 79 | Dp | 54 | ILE |
| 79 | Dp | 56 | THR |
| 79 | Dp | 79 | VAL |
| 79 | Dp | 89 | MET |
| 79 | Dp | 90 | VAL |
| 83 | Dq | 4 | ILE |
| 83 | Dq | 5 | ARG |
| 83 | Dq | 10 | GLU |
| 83 | Dq | 30 | VAL |
| 83 | Dq | 32 | ASN |
| 83 | Dq | 39 | HIS |
| 83 | Dq | 42 | ARG |
| 83 | Dq | 44 | GLU |
| 83 | Dq | 51 | VAL |
| 83 | Dq | 52 | LEU |
| 83 | Dq | 55 | LYS |
| 83 | Dq | 57 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 83 | Dq | 67 | LEU |
| 83 | Dq | 68 | SER |
| 83 | Dq | 70 | LEU |
| 83 | Dq | 72 | ASP |
| 83 | Dq | 74 | GLU |
| 83 | Dq | 75 | LYS |
| 83 | Dq | 76 | LEU |
| 83 | Dq | 79 | PHE |
| 83 | Dq | 80 | VAL |
| 83 | Dq | 81 | LYS |
| 83 | Dq | 84 | VAL |
| 83 | Dq | 91 | GLU |
| 83 | Dq | 93 | LEU |
| 83 | Dq | 96 | ILE |
| 83 | Dq | 97 | LYS |
| 83 | Dq | 185 | LEU |
| 83 | Dq | 196 | VAL |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | AA | 168 | HIS |
| 3 | AB | 101 | HIS |
| 3 | AB | 146 | GLN |
| 3 | AB | 149 | GLN |
| 3 | AB | 177 | GLN |
| 4 | AC | 82 | ASN |
| 4 | AC | 89 | GLN |
| 4 | AC | 94 | GLN |
| 5 | AD | 179 | GLN |
| 6 | AE | 98 | ASN |
| 7 | AF | 104 | ASN |
| 7 | AF | 128 | ASN |
| 7 | AF | 170 | GLN |
| 10 | AI | 64 | ASN |
| 10 | AI | 103 | GLN |
| 11 | AJ | 110 | GLN |
| 11 | AJ | 131 | GLN |
| 13 | AL | 110 | HIS |
| 14 | AM | 125 | ASN |
| 18 | AQ | 62 | ASN |
| 18 | AQ | 74 | HIS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 20 | AS | 89 | GLN |
| 21 | AT | 64 | HIS |
| 23 | AV | 74 | GLN |
| 24 | AW | 24 | GLN |
| 24 | AW | 80 | ASN |
| 27 | AZ | 95 | HIS |
| 31 | Ad | 48 | ASN |
| 31 | Ad | 53 | ASN |
| 35 | Ah | 108 | GLN |
| 39 | BA | 83 | HIS |
| 39 | BA | 132 | ASN |
| 39 | BA | 209 | HIS |
| 40 | BB | 3 | HIS |
| 41 | BC | 48 | GLN |
| 41 | BC | 114 | ASN |
| 41 | BC | 221 | ASN |
| 41 | BC | 311 | HIS |
| 42 | BD | 40 | HIS |
| 42 | BD | 63 | GLN |
| 43 | BE | 167 | ASN |
| 44 | BF | 225 | GLN |
| 44 | BF | 244 | ASN |
| 45 | BG | 38 | GLN |
| 45 | BG | 240 | ASN |
| 46 | BH | 50 | ASN |
| 47 | BI | 14 | ASN |
| 47 | BI | 144 | ASN |
| 48 | BJ | 109 | HIS |
| 51 | BN | 37 | HIS |
| 54 | BQ | 9 | GLN |
| 54 | BQ | 145 | ASN |
| 57 | BT | 16 | GLN |
| 57 | BT | 103 | GLN |
| 59 | BV | 33 | ASN |
| 59 | BV | 98 | ASN |
| 64 | Ba | 74 | ASN |
| 65 | Bb | 43 | HIS |
| 65 | Bb | 45 | HIS |
| 70 | Bg | 52 | GLN |
| 74 | Bk | 40 | GLN |
| 78 | Bo | 82 | GLN |
| 2 | CA | 23 | HIS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | CA | 49 | ASN |
| 3 | CB | 146 | GLN |
| 3 | CB | 153 | HIS |
| 4 | CC | 199 | GLN |
| 4 | CC | 250 | GLN |
| 6 | CE | 67 | GLN |
| 6 | CE | 142 | HIS |
| 6 | CE | 157 | ASN |
| 6 | CE | 216 | ASN |
| 7 | CF | 170 | GLN |
| 9 | CH | 89 | HIS |
| 9 | CH | 122 | HIS |
| 11 | CJ | 110 | GLN |
| 11 | CJ | 124 | HIS |
| 11 | CJ | 142 | ASN |
| 12 | CK | 29 | GLN |
| 12 | CK | 32 | HIS |
| 17 | CP | 103 | ASN |
| 18 | CQ | 77 | GLN |
| 18 | CQ | 83 | GLN |
| 19 | CR | 31 | ASN |
| 20 | CS | 90 | ASN |
| 21 | CT | 64 | HIS |
| 24 | CW | 12 | ASN |
| 26 | CY | 22 | GLN |
| 26 | CY | 34 | ASN |
| 29 | Cb | 19 | HIS |
| 32 | Ce | 17 | GLN |
| 34 | Cg | 182 | ASN |
| 34 | Cg | 184 | ASN |
| 39 | DA | 209 | HIS |
| 39 | DA | 215 | ASN |
| 41 | DC | 48 | GLN |
| 41 | DC | 114 | ASN |
| 41 | DC | 221 | ASN |
| 41 | DC | 291 | ASN |
| 42 | DD | 40 | HIS |
| 42 | DD | 63 | GLN |
| 42 | DD | 81 | HIS |
| 43 | DE | 167 | ASN |
| 44 | DF | 80 | GLN |
| 46 | DH | 102 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48 | DJ | 109 | HIS |
| 48 | DJ | 132 | ASN |
| 49 | DL | 19 | GLN |
| 50 | DM | 126 | GLN |
| 53 | DP | 55 | GLN |
| 54 | DQ | 9 | GLN |
| 57 | DT | 49 | GLN |
| 58 | DU | 40 | HIS |
| 59 | DV | 33 | ASN |
| 63 | DZ | 57 | HIS |
| 64 | Da | 44 | ASN |
| 69 | Df | 77 | ASN |
| 70 | Dg | 52 | GLN |
| 71 | Dh | 20 | GLN |
| 83 | Dq | 36 | GLN |

5.3.3 RNA [i](#)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------------|-------------------|-----------------|
| 1 | A2 | 1764/1800 (98%) | 545 (30%) | 86 (4%) |
| 36 | A1 | 3146/3396 (92%) | 738 (23%) | 127 (4%) |
| 36 | A5 | 3145/3396 (92%) | 731 (23%) | 129 (4%) |
| 37 | A3 | 120/121 (99%) | 22 (18%) | 3 (2%) |
| 37 | A7 | 120/121 (99%) | 18 (15%) | 0 |
| 38 | A4 | 157/158 (99%) | 38 (24%) | 5 (3%) |
| 38 | A8 | 157/158 (99%) | 32 (20%) | 3 (1%) |
| 80 | A6 | 1766/1800 (98%) | 499 (28%) | 60 (3%) |
| All | All | 10375/10950 (94%) | 2623 (25%) | 413 (3%) |

All (2623) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A2 | 2 | A |
| 1 | A2 | 4 | C |
| 1 | A2 | 8 | U |
| 1 | A2 | 16 | G |
| 1 | A2 | 20 | G |
| 1 | A2 | 25 | C |
| 1 | A2 | 26 | A |
| 1 | A2 | 27 | U |
| 1 | A2 | 34 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A2 | 39 | A |
| 1 | A2 | 41 | A |
| 1 | A2 | 42 | G |
| 1 | A2 | 45 | U |
| 1 | A2 | 46 | A |
| 1 | A2 | 47 | A |
| 1 | A2 | 50 | C |
| 1 | A2 | 57 | G |
| 1 | A2 | 60 | U |
| 1 | A2 | 67 | A |
| 1 | A2 | 68 | A |
| 1 | A2 | 69 | G |
| 1 | A2 | 72 | A |
| 1 | A2 | 73 | U |
| 1 | A2 | 74 | U |
| 1 | A2 | 75 | U |
| 1 | A2 | 76 | A |
| 1 | A2 | 77 | U |
| 1 | A2 | 78 | A |
| 1 | A2 | 97 | C |
| 1 | A2 | 100 | A |
| 1 | A2 | 101 | U |
| 1 | A2 | 104 | A |
| 1 | A2 | 114 | C |
| 1 | A2 | 126 | A |
| 1 | A2 | 127 | G |
| 1 | A2 | 131 | C |
| 1 | A2 | 132 | U |
| 1 | A2 | 133 | U |
| 1 | A2 | 134 | U |
| 1 | A2 | 135 | A |
| 1 | A2 | 136 | C |
| 1 | A2 | 137 | U |
| 1 | A2 | 138 | A |
| 1 | A2 | 139 | C |
| 1 | A2 | 140 | A |
| 1 | A2 | 141 | U |
| 1 | A2 | 144 | U |
| 1 | A2 | 145 | A |
| 1 | A2 | 146 | U |
| 1 | A2 | 153 | G |
| 1 | A2 | 158 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A2 | 159 | U |
| 1 | A2 | 175 | G |
| 1 | A2 | 178 | U |
| 1 | A2 | 179 | A |
| 1 | A2 | 185 | U |
| 1 | A2 | 186 | C |
| 1 | A2 | 187 | G |
| 1 | A2 | 188 | A |
| 1 | A2 | 189 | C |
| 1 | A2 | 190 | C |
| 1 | A2 | 191 | C |
| 1 | A2 | 192 | U |
| 1 | A2 | 193 | U |
| 1 | A2 | 194 | U |
| 1 | A2 | 195 | G |
| 1 | A2 | 196 | G |
| 1 | A2 | 197 | A |
| 1 | A2 | 198 | A |
| 1 | A2 | 199 | G |
| 1 | A2 | 200 | A |
| 1 | A2 | 215 | A |
| 1 | A2 | 218 | A |
| 1 | A2 | 219 | A |
| 1 | A2 | 223 | U |
| 1 | A2 | 225 | A |
| 1 | A2 | 226 | A |
| 1 | A2 | 227 | U |
| 1 | A2 | 228 | G |
| 1 | A2 | 229 | U |
| 1 | A2 | 233 | C |
| 1 | A2 | 234 | G |
| 1 | A2 | 235 | G |
| 1 | A2 | 236 | A |
| 1 | A2 | 238 | U |
| 1 | A2 | 239 | C |
| 1 | A2 | 240 | U |
| 1 | A2 | 241 | U |
| 1 | A2 | 242 | U |
| 1 | A2 | 249 | U |
| 1 | A2 | 250 | C |
| 1 | A2 | 261 | U |
| 1 | A2 | 262 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A2 | 265 | A |
| 1 | A2 | 266 | A |
| 1 | A2 | 271 | A |
| 1 | A2 | 272 | U |
| 1 | A2 | 274 | G |
| 1 | A2 | 275 | C |
| 1 | A2 | 276 | C |
| 1 | A2 | 277 | U |
| 1 | A2 | 278 | U |
| 1 | A2 | 279 | G |
| 1 | A2 | 280 | U |
| 1 | A2 | 281 | G |
| 1 | A2 | 288 | A |
| 1 | A2 | 290 | G |
| 1 | A2 | 299 | A |
| 1 | A2 | 301 | A |
| 1 | A2 | 306 | U |
| 1 | A2 | 308 | C |
| 1 | A2 | 309 | C |
| 1 | A2 | 314 | C |
| 1 | A2 | 316 | A |
| 1 | A2 | 319 | U |
| 1 | A2 | 320 | U |
| 1 | A2 | 321 | C |
| 1 | A2 | 322 | G |
| 1 | A2 | 337 | G |
| 1 | A2 | 338 | C |
| 1 | A2 | 341 | A |
| 1 | A2 | 348 | U |
| 1 | A2 | 352 | A |
| 1 | A2 | 359 | A |
| 1 | A2 | 360 | A |
| 1 | A2 | 361 | C |
| 1 | A2 | 399 | A |
| 1 | A2 | 400 | A |
| 1 | A2 | 401 | A |
| 1 | A2 | 402 | C |
| 1 | A2 | 403 | G |
| 1 | A2 | 404 | G |
| 1 | A2 | 411 | C |
| 1 | A2 | 416 | A |
| 1 | A2 | 418 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A2 | 423 | G |
| 1 | A2 | 424 | C |
| 1 | A2 | 425 | A |
| 1 | A2 | 426 | G |
| 1 | A2 | 428 | A |
| 1 | A2 | 434 | G |
| 1 | A2 | 439 | U |
| 1 | A2 | 444 | C |
| 1 | A2 | 445 | A |
| 1 | A2 | 446 | A |
| 1 | A2 | 448 | C |
| 1 | A2 | 467 | G |
| 1 | A2 | 468 | A |
| 1 | A2 | 470 | A |
| 1 | A2 | 475 | A |
| 1 | A2 | 477 | A |
| 1 | A2 | 484 | C |
| 1 | A2 | 485 | A |
| 1 | A2 | 486 | G |
| 1 | A2 | 487 | G |
| 1 | A2 | 488 | G |
| 1 | A2 | 493 | U |
| 1 | A2 | 494 | U |
| 1 | A2 | 495 | C |
| 1 | A2 | 496 | G |
| 1 | A2 | 497 | G |
| 1 | A2 | 498 | G |
| 1 | A2 | 499 | U |
| 1 | A2 | 500 | C |
| 1 | A2 | 502 | U |
| 1 | A2 | 503 | G |
| 1 | A2 | 504 | U |
| 1 | A2 | 505 | A |
| 1 | A2 | 506 | A |
| 1 | A2 | 507 | U |
| 1 | A2 | 508 | U |
| 1 | A2 | 510 | G |
| 1 | A2 | 511 | A |
| 1 | A2 | 512 | A |
| 1 | A2 | 513 | U |
| 1 | A2 | 515 | A |
| 1 | A2 | 516 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A2 | 519 | C |
| 1 | A2 | 525 | A |
| 1 | A2 | 527 | A |
| 1 | A2 | 532 | U |
| 1 | A2 | 538 | A |
| 1 | A2 | 539 | G |
| 1 | A2 | 540 | G |
| 1 | A2 | 541 | A |
| 1 | A2 | 542 | A |
| 1 | A2 | 543 | C |
| 1 | A2 | 544 | A |
| 1 | A2 | 545 | A |
| 1 | A2 | 548 | G |
| 1 | A2 | 555 | A |
| 1 | A2 | 556 | A |
| 1 | A2 | 557 | G |
| 1 | A2 | 558 | U |
| 1 | A2 | 559 | C |
| 1 | A2 | 565 | C |
| 1 | A2 | 570 | A |
| 1 | A2 | 575 | C |
| 1 | A2 | 579 | A |
| 1 | A2 | 580 | A |
| 1 | A2 | 582 | U |
| 1 | A2 | 583 | C |
| 1 | A2 | 585 | A |
| 1 | A2 | 594 | A |
| 1 | A2 | 595 | G |
| 1 | A2 | 597 | G |
| 1 | A2 | 605 | A |
| 1 | A2 | 607 | G |
| 1 | A2 | 611 | U |
| 1 | A2 | 619 | A |
| 1 | A2 | 620 | A |
| 1 | A2 | 622 | A |
| 1 | A2 | 623 | A |
| 1 | A2 | 624 | G |
| 1 | A2 | 630 | A |
| 1 | A2 | 639 | U |
| 1 | A2 | 640 | U |
| 1 | A2 | 650 | U |
| 1 | A2 | 653 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A2 | 655 | G |
| 1 | A2 | 656 | G |
| 1 | A2 | 657 | U |
| 1 | A2 | 658 | C |
| 1 | A2 | 677 | G |
| 1 | A2 | 679 | U |
| 1 | A2 | 680 | U |
| 1 | A2 | 684 | A |
| 1 | A2 | 685 | A |
| 1 | A2 | 686 | C |
| 1 | A2 | 692 | C |
| 1 | A2 | 694 | U |
| 1 | A2 | 696 | C |
| 1 | A2 | 697 | C |
| 1 | A2 | 699 | U |
| 1 | A2 | 700 | C |
| 1 | A2 | 701 | U |
| 1 | A2 | 702 | G |
| 1 | A2 | 703 | G |
| 1 | A2 | 704 | C |
| 1 | A2 | 705 | U |
| 1 | A2 | 706 | A |
| 1 | A2 | 707 | A |
| 1 | A2 | 709 | C |
| 1 | A2 | 710 | U |
| 1 | A2 | 712 | G |
| 1 | A2 | 713 | A |
| 1 | A2 | 714 | G |
| 1 | A2 | 717 | C |
| 1 | A2 | 718 | U |
| 1 | A2 | 719 | U |
| 1 | A2 | 720 | G |
| 1 | A2 | 721 | U |
| 1 | A2 | 722 | G |
| 1 | A2 | 723 | G |
| 1 | A2 | 725 | U |
| 1 | A2 | 727 | U |
| 1 | A2 | 728 | U |
| 1 | A2 | 729 | G |
| 1 | A2 | 730 | G |
| 1 | A2 | 731 | C |
| 1 | A2 | 732 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A2 | 733 | A |
| 1 | A2 | 734 | A |
| 1 | A2 | 735 | C |
| 1 | A2 | 736 | C |
| 1 | A2 | 737 | A |
| 1 | A2 | 738 | G |
| 1 | A2 | 742 | U |
| 1 | A2 | 743 | U |
| 1 | A2 | 745 | U |
| 1 | A2 | 754 | A |
| 1 | A2 | 755 | A |
| 1 | A2 | 756 | A |
| 1 | A2 | 758 | U |
| 1 | A2 | 765 | G |
| 1 | A2 | 766 | U |
| 1 | A2 | 771 | A |
| 1 | A2 | 774 | A |
| 1 | A2 | 775 | G |
| 1 | A2 | 778 | G |
| 1 | A2 | 779 | U |
| 1 | A2 | 780 | A |
| 1 | A2 | 781 | U |
| 1 | A2 | 782 | U |
| 1 | A2 | 783 | G |
| 1 | A2 | 784 | C |
| 1 | A2 | 785 | U |
| 1 | A2 | 787 | G |
| 1 | A2 | 789 | A |
| 1 | A2 | 793 | A |
| 1 | A2 | 794 | U |
| 1 | A2 | 795 | U |
| 1 | A2 | 806 | A |
| 1 | A2 | 811 | A |
| 1 | A2 | 812 | A |
| 1 | A2 | 813 | U |
| 1 | A2 | 815 | G |
| 1 | A2 | 816 | G |
| 1 | A2 | 818 | C |
| 1 | A2 | 819 | G |
| 1 | A2 | 820 | U |
| 1 | A2 | 821 | U |
| 1 | A2 | 823 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A2 | 824 | G |
| 1 | A2 | 829 | A |
| 1 | A2 | 830 | U |
| 1 | A2 | 831 | U |
| 1 | A2 | 832 | U |
| 1 | A2 | 833 | U |
| 1 | A2 | 837 | G |
| 1 | A2 | 838 | G |
| 1 | A2 | 840 | U |
| 1 | A2 | 846 | G |
| 1 | A2 | 848 | C |
| 1 | A2 | 849 | C |
| 1 | A2 | 854 | U |
| 1 | A2 | 862 | A |
| 1 | A2 | 863 | A |
| 1 | A2 | 864 | U |
| 1 | A2 | 873 | U |
| 1 | A2 | 876 | G |
| 1 | A2 | 892 | A |
| 1 | A2 | 896 | U |
| 1 | A2 | 898 | A |
| 1 | A2 | 912 | U |
| 1 | A2 | 913 | G |
| 1 | A2 | 914 | G |
| 1 | A2 | 921 | U |
| 1 | A2 | 928 | U |
| 1 | A2 | 933 | A |
| 1 | A2 | 935 | U |
| 1 | A2 | 942 | G |
| 1 | A2 | 944 | A |
| 1 | A2 | 951 | A |
| 1 | A2 | 959 | U |
| 1 | A2 | 960 | U |
| 1 | A2 | 961 | U |
| 1 | A2 | 966 | A |
| 1 | A2 | 968 | U |
| 1 | A2 | 982 | U |
| 1 | A2 | 988 | A |
| 1 | A2 | 992 | A |
| 1 | A2 | 993 | A |
| 1 | A2 | 995 | A |
| 1 | A2 | 997 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A2 | 1003 | A |
| 1 | A2 | 1004 | U |
| 1 | A2 | 1005 | A |
| 1 | A2 | 1020 | A |
| 1 | A2 | 1021 | C |
| 1 | A2 | 1026 | A |
| 1 | A2 | 1028 | C |
| 1 | A2 | 1031 | U |
| 1 | A2 | 1039 | A |
| 1 | A2 | 1040 | G |
| 1 | A2 | 1052 | U |
| 1 | A2 | 1053 | G |
| 1 | A2 | 1058 | U |
| 1 | A2 | 1059 | U |
| 1 | A2 | 1060 | U |
| 1 | A2 | 1061 | A |
| 1 | A2 | 1064 | G |
| 1 | A2 | 1073 | G |
| 1 | A2 | 1074 | G |
| 1 | A2 | 1079 | U |
| 1 | A2 | 1080 | U |
| 1 | A2 | 1082 | C |
| 1 | A2 | 1083 | G |
| 1 | A2 | 1084 | A |
| 1 | A2 | 1086 | A |
| 1 | A2 | 1087 | A |
| 1 | A2 | 1091 | A |
| 1 | A2 | 1092 | A |
| 1 | A2 | 1093 | A |
| 1 | A2 | 1096 | C |
| 1 | A2 | 1097 | U |
| 1 | A2 | 1100 | G |
| 1 | A2 | 1104 | U |
| 1 | A2 | 1111 | G |
| 1 | A2 | 1138 | A |
| 1 | A2 | 1139 | A |
| 1 | A2 | 1146 | G |
| 1 | A2 | 1149 | G |
| 1 | A2 | 1151 | A |
| 1 | A2 | 1152 | A |
| 1 | A2 | 1155 | G |
| 1 | A2 | 1157 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A2 | 1158 | C |
| 1 | A2 | 1160 | A |
| 1 | A2 | 1162 | C |
| 1 | A2 | 1167 | G |
| 1 | A2 | 1185 | U |
| 1 | A2 | 1188 | G |
| 1 | A2 | 1191 | U |
| 1 | A2 | 1194 | A |
| 1 | A2 | 1196 | A |
| 1 | A2 | 1197 | C |
| 1 | A2 | 1199 | G |
| 1 | A2 | 1200 | G |
| 1 | A2 | 1202 | A |
| 1 | A2 | 1207 | C |
| 1 | A2 | 1208 | A |
| 1 | A2 | 1217 | A |
| 1 | A2 | 1218 | G |
| 1 | A2 | 1219 | A |
| 1 | A2 | 1221 | A |
| 1 | A2 | 1226 | A |
| 1 | A2 | 1227 | A |
| 1 | A2 | 1228 | G |
| 1 | A2 | 1229 | G |
| 1 | A2 | 1235 | C |
| 1 | A2 | 1243 | G |
| 1 | A2 | 1244 | A |
| 1 | A2 | 1245 | G |
| 1 | A2 | 1250 | U |
| 1 | A2 | 1251 | U |
| 1 | A2 | 1257 | U |
| 1 | A2 | 1258 | U |
| 1 | A2 | 1260 | U |
| 1 | A2 | 1269 | U |
| 1 | A2 | 1286 | U |
| 1 | A2 | 1301 | U |
| 1 | A2 | 1314 | U |
| 1 | A2 | 1315 | U |
| 1 | A2 | 1321 | A |
| 1 | A2 | 1329 | A |
| 1 | A2 | 1337 | A |
| 1 | A2 | 1339 | C |
| 1 | A2 | 1340 | U |

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Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A2 | 1341 | A |
| 1 | A2 | 1344 | A |
| 1 | A2 | 1345 | A |
| 1 | A2 | 1349 | G |
| 1 | A2 | 1354 | G |
| 1 | A2 | 1361 | U |
| 1 | A2 | 1363 | U |
| 1 | A2 | 1364 | G |
| 1 | A2 | 1370 | U |
| 1 | A2 | 1371 | A |
| 1 | A2 | 1372 | U |
| 1 | A2 | 1379 | C |
| 1 | A2 | 1382 | A |
| 1 | A2 | 1383 | G |
| 1 | A2 | 1388 | A |
| 1 | A2 | 1390 | U |
| 1 | A2 | 1398 | U |
| 1 | A2 | 1399 | C |
| 1 | A2 | 1400 | A |
| 1 | A2 | 1412 | G |
| 1 | A2 | 1413 | U |
| 1 | A2 | 1414 | U |
| 1 | A2 | 1415 | U |
| 1 | A2 | 1420 | C |
| 1 | A2 | 1421 | A |
| 1 | A2 | 1427 | A |
| 1 | A2 | 1428 | G |
| 1 | A2 | 1429 | G |
| 1 | A2 | 1431 | C |
| 1 | A2 | 1445 | G |
| 1 | A2 | 1446 | A |
| 1 | A2 | 1448 | G |
| 1 | A2 | 1454 | G |
| 1 | A2 | 1457 | C |
| 1 | A2 | 1459 | C |
| 1 | A2 | 1461 | C |
| 1 | A2 | 1462 | G |
| 1 | A2 | 1471 | A |
| 1 | A2 | 1473 | U |
| 1 | A2 | 1474 | G |
| 1 | A2 | 1475 | A |
| 1 | A2 | 1478 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A2 | 1482 | C |
| 1 | A2 | 1486 | G |
| 1 | A2 | 1488 | G |
| 1 | A2 | 1489 | U |
| 1 | A2 | 1490 | C |
| 1 | A2 | 1491 | U |
| 1 | A2 | 1492 | A |
| 1 | A2 | 1493 | A |
| 1 | A2 | 1499 | G |
| 1 | A2 | 1500 | C |
| 1 | A2 | 1506 | G |
| 1 | A2 | 1514 | U |
| 1 | A2 | 1516 | A |
| 1 | A2 | 1518 | C |
| 1 | A2 | 1521 | G |
| 1 | A2 | 1523 | G |
| 1 | A2 | 1524 | A |
| 1 | A2 | 1535 | U |
| 1 | A2 | 1536 | G |
| 1 | A2 | 1537 | C |
| 1 | A2 | 1538 | U |
| 1 | A2 | 1539 | G |
| 1 | A2 | 1540 | G |
| 1 | A2 | 1557 | U |
| 1 | A2 | 1559 | A |
| 1 | A2 | 1569 | A |
| 1 | A2 | 1573 | A |
| 1 | A2 | 1574 | G |
| 1 | A2 | 1575 | G |
| 1 | A2 | 1584 | G |
| 1 | A2 | 1590 | G |
| 1 | A2 | 1601 | G |
| 1 | A2 | 1616 | G |
| 1 | A2 | 1619 | C |
| 1 | A2 | 1624 | C |
| 1 | A2 | 1625 | C |
| 1 | A2 | 1631 | A |
| 1 | A2 | 1635 | A |
| 1 | A2 | 1649 | G |
| 1 | A2 | 1657 | U |
| 1 | A2 | 1658 | G |
| 1 | A2 | 1663 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A2 | 1680 | G |
| 1 | A2 | 1682 | U |
| 1 | A2 | 1683 | C |
| 1 | A2 | 1684 | U |
| 1 | A2 | 1685 | G |
| 1 | A2 | 1686 | C |
| 1 | A2 | 1687 | U |
| 1 | A2 | 1693 | A |
| 1 | A2 | 1712 | A |
| 1 | A2 | 1713 | G |
| 1 | A2 | 1716 | C |
| 1 | A2 | 1717 | G |
| 1 | A2 | 1727 | G |
| 1 | A2 | 1729 | C |
| 1 | A2 | 1731 | A |
| 1 | A2 | 1759 | C |
| 1 | A2 | 1760 | G |
| 1 | A2 | 1761 | U |
| 1 | A2 | 1762 | A |
| 1 | A2 | 1766 | A |
| 1 | A2 | 1768 | G |
| 1 | A2 | 1769 | U |
| 1 | A2 | 1770 | U |
| 1 | A2 | 1780 | G |
| 1 | A2 | 1782 | A |
| 1 | A2 | 1783 | C |
| 1 | A2 | 1789 | G |
| 1 | A2 | 1792 | G |
| 1 | A2 | 1793 | G |
| 1 | A2 | 1794 | A |
| 1 | A2 | 1795 | U |
| 1 | A2 | 1796 | C |
| 36 | A1 | 13 | A |
| 36 | A1 | 14 | U |
| 36 | A1 | 16 | A |
| 36 | A1 | 26 | A |
| 36 | A1 | 40 | A |
| 36 | A1 | 42 | C |
| 36 | A1 | 43 | A |
| 36 | A1 | 49 | A |
| 36 | A1 | 59 | G |
| 36 | A1 | 60 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A1 | 65 | A |
| 36 | A1 | 66 | A |
| 36 | A1 | 68 | C |
| 36 | A1 | 74 | G |
| 36 | A1 | 75 | G |
| 36 | A1 | 76 | G |
| 36 | A1 | 83 | U |
| 36 | A1 | 92 | G |
| 36 | A1 | 93 | C |
| 36 | A1 | 99 | A |
| 36 | A1 | 109 | A |
| 36 | A1 | 110 | G |
| 36 | A1 | 113 | C |
| 36 | A1 | 121 | A |
| 36 | A1 | 122 | A |
| 36 | A1 | 133 | U |
| 36 | A1 | 135 | C |
| 36 | A1 | 136 | G |
| 36 | A1 | 147 | U |
| 36 | A1 | 154 | U |
| 36 | A1 | 156 | G |
| 36 | A1 | 157 | A |
| 36 | A1 | 161 | G |
| 36 | A1 | 166 | C |
| 36 | A1 | 169 | U |
| 36 | A1 | 170 | G |
| 36 | A1 | 173 | G |
| 36 | A1 | 182 | U |
| 36 | A1 | 187 | A |
| 36 | A1 | 190 | U |
| 36 | A1 | 191 | U |
| 36 | A1 | 192 | C |
| 36 | A1 | 210 | U |
| 36 | A1 | 214 | G |
| 36 | A1 | 218 | G |
| 36 | A1 | 219 | A |
| 36 | A1 | 224 | C |
| 36 | A1 | 234 | G |
| 36 | A1 | 235 | A |
| 36 | A1 | 238 | A |
| 36 | A1 | 240 | U |
| 36 | A1 | 241 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A1 | 243 | G |
| 36 | A1 | 244 | G |
| 36 | A1 | 245 | U |
| 36 | A1 | 249 | U |
| 36 | A1 | 250 | U |
| 36 | A1 | 251 | G |
| 36 | A1 | 252 | U |
| 36 | A1 | 263 | C |
| 36 | A1 | 265 | A |
| 36 | A1 | 269 | G |
| 36 | A1 | 282 | G |
| 36 | A1 | 283 | G |
| 36 | A1 | 286 | U |
| 36 | A1 | 295 | A |
| 36 | A1 | 296 | A |
| 36 | A1 | 298 | U |
| 36 | A1 | 301 | G |
| 36 | A1 | 305 | U |
| 36 | A1 | 307 | A |
| 36 | A1 | 318 | A |
| 36 | A1 | 323 | A |
| 36 | A1 | 329 | U |
| 36 | A1 | 338 | A |
| 36 | A1 | 339 | C |
| 36 | A1 | 349 | A |
| 36 | A1 | 350 | C |
| 36 | A1 | 351 | A |
| 36 | A1 | 352 | A |
| 36 | A1 | 370 | U |
| 36 | A1 | 373 | A |
| 36 | A1 | 376 | G |
| 36 | A1 | 395 | A |
| 36 | A1 | 397 | A |
| 36 | A1 | 398 | A |
| 36 | A1 | 399 | A |
| 36 | A1 | 401 | U |
| 36 | A1 | 402 | A |
| 36 | A1 | 403 | C |
| 36 | A1 | 421 | G |
| 36 | A1 | 422 | A |
| 36 | A1 | 439 | C |
| 36 | A1 | 440 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A1 | 495 | G |
| 36 | A1 | 517 | G |
| 36 | A1 | 520 | U |
| 36 | A1 | 521 | A |
| 36 | A1 | 531 | G |
| 36 | A1 | 535 | G |
| 36 | A1 | 544 | C |
| 36 | A1 | 546 | C |
| 36 | A1 | 547 | G |
| 36 | A1 | 548 | G |
| 36 | A1 | 549 | U |
| 36 | A1 | 550 | A |
| 36 | A1 | 551 | A |
| 36 | A1 | 552 | G |
| 36 | A1 | 555 | U |
| 36 | A1 | 556 | U |
| 36 | A1 | 557 | A |
| 36 | A1 | 558 | U |
| 36 | A1 | 559 | A |
| 36 | A1 | 578 | A |
| 36 | A1 | 579 | G |
| 36 | A1 | 585 | A |
| 36 | A1 | 592 | A |
| 36 | A1 | 600 | G |
| 36 | A1 | 601 | U |
| 36 | A1 | 603 | A |
| 36 | A1 | 604 | G |
| 36 | A1 | 609 | G |
| 36 | A1 | 611 | A |
| 36 | A1 | 619 | A |
| 36 | A1 | 620 | U |
| 36 | A1 | 621 | A |
| 36 | A1 | 622 | A |
| 36 | A1 | 625 | G |
| 36 | A1 | 636 | C |
| 36 | A1 | 637 | C |
| 36 | A1 | 638 | C |
| 36 | A1 | 649 | A |
| 36 | A1 | 656 | A |
| 36 | A1 | 660 | A |
| 36 | A1 | 677 | A |
| 36 | A1 | 681 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A1 | 683 | U |
| 36 | A1 | 691 | A |
| 36 | A1 | 705 | A |
| 36 | A1 | 708 | G |
| 36 | A1 | 712 | G |
| 36 | A1 | 715 | A |
| 36 | A1 | 716 | A |
| 36 | A1 | 719 | U |
| 36 | A1 | 720 | A |
| 36 | A1 | 725 | G |
| 36 | A1 | 726 | G |
| 36 | A1 | 733 | G |
| 36 | A1 | 758 | C |
| 36 | A1 | 764 | U |
| 36 | A1 | 765 | C |
| 36 | A1 | 766 | U |
| 36 | A1 | 767 | U |
| 36 | A1 | 768 | C |
| 36 | A1 | 776 | U |
| 36 | A1 | 777 | U |
| 36 | A1 | 781 | G |
| 36 | A1 | 785 | G |
| 36 | A1 | 786 | A |
| 36 | A1 | 801 | A |
| 36 | A1 | 806 | A |
| 36 | A1 | 807 | A |
| 36 | A1 | 817 | A |
| 36 | A1 | 830 | A |
| 36 | A1 | 849 | C |
| 36 | A1 | 861 | C |
| 36 | A1 | 871 | U |
| 36 | A1 | 874 | U |
| 36 | A1 | 879 | U |
| 36 | A1 | 883 | A |
| 36 | A1 | 896 | A |
| 36 | A1 | 907 | G |
| 36 | A1 | 908 | G |
| 36 | A1 | 914 | A |
| 36 | A1 | 916 | G |
| 36 | A1 | 917 | A |
| 36 | A1 | 921 | A |
| 36 | A1 | 923 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A1 | 924 | G |
| 36 | A1 | 925 | A |
| 36 | A1 | 937 | G |
| 36 | A1 | 944 | C |
| 36 | A1 | 947 | G |
| 36 | A1 | 959 | C |
| 36 | A1 | 960 | U |
| 36 | A1 | 974 | G |
| 36 | A1 | 979 | U |
| 36 | A1 | 980 | A |
| 36 | A1 | 981 | U |
| 36 | A1 | 982 | C |
| 36 | A1 | 989 | A |
| 36 | A1 | 994 | G |
| 36 | A1 | 1001 | G |
| 36 | A1 | 1002 | A |
| 36 | A1 | 1003 | A |
| 36 | A1 | 1006 | A |
| 36 | A1 | 1010 | G |
| 36 | A1 | 1014 | U |
| 36 | A1 | 1015 | U |
| 36 | A1 | 1016 | C |
| 36 | A1 | 1017 | C |
| 36 | A1 | 1018 | G |
| 36 | A1 | 1020 | G |
| 36 | A1 | 1021 | G |
| 36 | A1 | 1024 | G |
| 36 | A1 | 1025 | A |
| 36 | A1 | 1029 | G |
| 36 | A1 | 1032 | C |
| 36 | A1 | 1036 | A |
| 36 | A1 | 1037 | C |
| 36 | A1 | 1047 | A |
| 36 | A1 | 1049 | C |
| 36 | A1 | 1052 | U |
| 36 | A1 | 1057 | A |
| 36 | A1 | 1064 | A |
| 36 | A1 | 1065 | A |
| 36 | A1 | 1071 | U |
| 36 | A1 | 1072 | G |
| 36 | A1 | 1079 | A |
| 36 | A1 | 1081 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A1 | 1082 | U |
| 36 | A1 | 1083 | G |
| 36 | A1 | 1087 | G |
| 36 | A1 | 1093 | A |
| 36 | A1 | 1094 | U |
| 36 | A1 | 1095 | U |
| 36 | A1 | 1096 | U |
| 36 | A1 | 1097 | G |
| 36 | A1 | 1098 | A |
| 36 | A1 | 1103 | A |
| 36 | A1 | 1104 | G |
| 36 | A1 | 1117 | G |
| 36 | A1 | 1131 | G |
| 36 | A1 | 1153 | A |
| 36 | A1 | 1159 | A |
| 36 | A1 | 1180 | A |
| 36 | A1 | 1181 | U |
| 36 | A1 | 1182 | A |
| 36 | A1 | 1185 | C |
| 36 | A1 | 1191 | U |
| 36 | A1 | 1192 | C |
| 36 | A1 | 1201 | C |
| 36 | A1 | 1202 | A |
| 36 | A1 | 1209 | G |
| 36 | A1 | 1212 | A |
| 36 | A1 | 1213 | G |
| 36 | A1 | 1216 | C |
| 36 | A1 | 1218 | U |
| 36 | A1 | 1222 | G |
| 36 | A1 | 1225 | A |
| 36 | A1 | 1227 | C |
| 36 | A1 | 1232 | C |
| 36 | A1 | 1233 | G |
| 36 | A1 | 1234 | G |
| 36 | A1 | 1236 | G |
| 36 | A1 | 1237 | G |
| 36 | A1 | 1239 | C |
| 36 | A1 | 1241 | U |
| 36 | A1 | 1242 | G |
| 36 | A1 | 1243 | G |
| 36 | A1 | 1245 | A |
| 36 | A1 | 1246 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A1 | 1248 | C |
| 36 | A1 | 1249 | G |
| 36 | A1 | 1251 | A |
| 36 | A1 | 1258 | U |
| 36 | A1 | 1262 | G |
| 36 | A1 | 1263 | A |
| 36 | A1 | 1264 | G |
| 36 | A1 | 1265 | U |
| 36 | A1 | 1266 | G |
| 36 | A1 | 1267 | U |
| 36 | A1 | 1269 | U |
| 36 | A1 | 1270 | A |
| 36 | A1 | 1271 | A |
| 36 | A1 | 1272 | C |
| 36 | A1 | 1274 | A |
| 36 | A1 | 1277 | C |
| 36 | A1 | 1278 | A |
| 36 | A1 | 1279 | C |
| 36 | A1 | 1280 | C |
| 36 | A1 | 1281 | G |
| 36 | A1 | 1285 | G |
| 36 | A1 | 1287 | A |
| 36 | A1 | 1292 | C |
| 36 | A1 | 1307 | G |
| 36 | A1 | 1308 | A |
| 36 | A1 | 1309 | U |
| 36 | A1 | 1312 | C |
| 36 | A1 | 1313 | G |
| 36 | A1 | 1325 | U |
| 36 | A1 | 1329 | U |
| 36 | A1 | 1330 | A |
| 36 | A1 | 1345 | G |
| 36 | A1 | 1348 | U |
| 36 | A1 | 1349 | G |
| 36 | A1 | 1351 | U |
| 36 | A1 | 1352 | A |
| 36 | A1 | 1353 | U |
| 36 | A1 | 1355 | A |
| 36 | A1 | 1356 | U |
| 36 | A1 | 1357 | G |
| 36 | A1 | 1366 | A |
| 36 | A1 | 1386 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A1 | 1399 | A |
| 36 | A1 | 1400 | G |
| 36 | A1 | 1401 | A |
| 36 | A1 | 1414 | G |
| 36 | A1 | 1418 | A |
| 36 | A1 | 1419 | A |
| 36 | A1 | 1428 | A |
| 36 | A1 | 1434 | G |
| 36 | A1 | 1437 | C |
| 36 | A1 | 1440 | G |
| 36 | A1 | 1443 | G |
| 36 | A1 | 1446 | A |
| 36 | A1 | 1449 | A |
| 36 | A1 | 1450 | G |
| 36 | A1 | 1454 | A |
| 36 | A1 | 1478 | C |
| 36 | A1 | 1481 | A |
| 36 | A1 | 1482 | A |
| 36 | A1 | 1485 | G |
| 36 | A1 | 1488 | G |
| 36 | A1 | 1508 | C |
| 36 | A1 | 1526 | U |
| 36 | A1 | 1527 | C |
| 36 | A1 | 1528 | G |
| 36 | A1 | 1529 | A |
| 36 | A1 | 1549 | U |
| 36 | A1 | 1555 | U |
| 36 | A1 | 1556 | C |
| 36 | A1 | 1557 | A |
| 36 | A1 | 1558 | A |
| 36 | A1 | 1560 | G |
| 36 | A1 | 1561 | G |
| 36 | A1 | 1562 | C |
| 36 | A1 | 1563 | C |
| 36 | A1 | 1564 | U |
| 36 | A1 | 1566 | A |
| 36 | A1 | 1567 | U |
| 36 | A1 | 1568 | U |
| 36 | A1 | 1569 | U |
| 36 | A1 | 1570 | U |
| 36 | A1 | 1572 | U |
| 36 | A1 | 1575 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A1 | 1576 | G |
| 36 | A1 | 1577 | G |
| 36 | A1 | 1579 | C |
| 36 | A1 | 1581 | C |
| 36 | A1 | 1582 | C |
| 36 | A1 | 1583 | A |
| 36 | A1 | 1587 | A |
| 36 | A1 | 1589 | A |
| 36 | A1 | 1593 | A |
| 36 | A1 | 1607 | U |
| 36 | A1 | 1608 | C |
| 36 | A1 | 1620 | U |
| 36 | A1 | 1629 | U |
| 36 | A1 | 1643 | A |
| 36 | A1 | 1645 | U |
| 36 | A1 | 1655 | G |
| 36 | A1 | 1657 | C |
| 36 | A1 | 1683 | A |
| 36 | A1 | 1705 | U |
| 36 | A1 | 1716 | U |
| 36 | A1 | 1717 | U |
| 36 | A1 | 1724 | U |
| 36 | A1 | 1725 | C |
| 36 | A1 | 1736 | G |
| 36 | A1 | 1742 | U |
| 36 | A1 | 1746 | U |
| 36 | A1 | 1750 | A |
| 36 | A1 | 1751 | G |
| 36 | A1 | 1752 | A |
| 36 | A1 | 1760 | A |
| 36 | A1 | 1761 | C |
| 36 | A1 | 1762 | C |
| 36 | A1 | 1765 | U |
| 36 | A1 | 1766 | G |
| 36 | A1 | 1767 | C |
| 36 | A1 | 1770 | G |
| 36 | A1 | 1779 | C |
| 36 | A1 | 1780 | G |
| 36 | A1 | 1781 | C |
| 36 | A1 | 1797 | A |
| 36 | A1 | 1806 | A |
| 36 | A1 | 1807 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A1 | 1809 | A |
| 36 | A1 | 1810 | A |
| 36 | A1 | 1812 | G |
| 36 | A1 | 1814 | A |
| 36 | A1 | 1816 | A |
| 36 | A1 | 1817 | G |
| 36 | A1 | 1818 | U |
| 36 | A1 | 1819 | U |
| 36 | A1 | 1820 | U |
| 36 | A1 | 1821 | U |
| 36 | A1 | 1834 | U |
| 36 | A1 | 1835 | A |
| 36 | A1 | 1836 | C |
| 36 | A1 | 1839 | A |
| 36 | A1 | 1840 | U |
| 36 | A1 | 1841 | A |
| 36 | A1 | 1842 | A |
| 36 | A1 | 1845 | G |
| 36 | A1 | 1846 | C |
| 36 | A1 | 1849 | C |
| 36 | A1 | 1850 | A |
| 36 | A1 | 1855 | U |
| 36 | A1 | 1876 | U |
| 36 | A1 | 1879 | A |
| 36 | A1 | 1880 | U |
| 36 | A1 | 1886 | A |
| 36 | A1 | 1901 | A |
| 36 | A1 | 1905 | G |
| 36 | A1 | 1906 | G |
| 36 | A1 | 1951 | C |
| 36 | A1 | 1952 | G |
| 36 | A1 | 1953 | G |
| 36 | A1 | 1954 | G |
| 36 | A1 | 1955 | U |
| 36 | A1 | 2094 | C |
| 36 | A1 | 2101 | C |
| 36 | A1 | 2102 | U |
| 36 | A1 | 2112 | U |
| 36 | A1 | 2113 | A |
| 36 | A1 | 2114 | C |
| 36 | A1 | 2116 | G |
| 36 | A1 | 2121 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A1 | 2122 | G |
| 36 | A1 | 2130 | G |
| 36 | A1 | 2131 | A |
| 36 | A1 | 2140 | U |
| 36 | A1 | 2148 | U |
| 36 | A1 | 2158 | A |
| 36 | A1 | 2163 | C |
| 36 | A1 | 2169 | G |
| 36 | A1 | 2170 | U |
| 36 | A1 | 2187 | G |
| 36 | A1 | 2188 | A |
| 36 | A1 | 2193 | U |
| 36 | A1 | 2201 | G |
| 36 | A1 | 2205 | U |
| 36 | A1 | 2206 | G |
| 36 | A1 | 2208 | A |
| 36 | A1 | 2209 | U |
| 36 | A1 | 2210 | G |
| 36 | A1 | 2213 | A |
| 36 | A1 | 2223 | A |
| 36 | A1 | 2228 | A |
| 36 | A1 | 2244 | A |
| 36 | A1 | 2249 | G |
| 36 | A1 | 2250 | G |
| 36 | A1 | 2252 | A |
| 36 | A1 | 2253 | G |
| 36 | A1 | 2255 | A |
| 36 | A1 | 2256 | A |
| 36 | A1 | 2262 | A |
| 36 | A1 | 2263 | C |
| 36 | A1 | 2272 | G |
| 36 | A1 | 2273 | G |
| 36 | A1 | 2278 | C |
| 36 | A1 | 2281 | A |
| 36 | A1 | 2282 | U |
| 36 | A1 | 2283 | G |
| 36 | A1 | 2284 | C |
| 36 | A1 | 2288 | G |
| 36 | A1 | 2291 | A |
| 36 | A1 | 2293 | C |
| 36 | A1 | 2299 | A |
| 36 | A1 | 2304 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A1 | 2307 | G |
| 36 | A1 | 2310 | U |
| 36 | A1 | 2313 | A |
| 36 | A1 | 2314 | U |
| 36 | A1 | 2315 | G |
| 36 | A1 | 2319 | U |
| 36 | A1 | 2330 | C |
| 36 | A1 | 2336 | U |
| 36 | A1 | 2360 | C |
| 36 | A1 | 2374 | C |
| 36 | A1 | 2375 | G |
| 36 | A1 | 2378 | C |
| 36 | A1 | 2385 | G |
| 36 | A1 | 2388 | U |
| 36 | A1 | 2393 | G |
| 36 | A1 | 2397 | A |
| 36 | A1 | 2398 | A |
| 36 | A1 | 2401 | A |
| 36 | A1 | 2402 | A |
| 36 | A1 | 2403 | G |
| 36 | A1 | 2404 | A |
| 36 | A1 | 2405 | C |
| 36 | A1 | 2406 | C |
| 36 | A1 | 2411 | U |
| 36 | A1 | 2418 | G |
| 36 | A1 | 2419 | A |
| 36 | A1 | 2435 | G |
| 36 | A1 | 2437 | G |
| 36 | A1 | 2443 | A |
| 36 | A1 | 2444 | C |
| 36 | A1 | 2445 | A |
| 36 | A1 | 2502 | A |
| 36 | A1 | 2503 | G |
| 36 | A1 | 2504 | U |
| 36 | A1 | 2505 | U |
| 36 | A1 | 2507 | C |
| 36 | A1 | 2511 | A |
| 36 | A1 | 2513 | U |
| 36 | A1 | 2514 | U |
| 36 | A1 | 2515 | A |
| 36 | A1 | 2522 | G |
| 36 | A1 | 2523 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A1 | 2525 | G |
| 36 | A1 | 2526 | C |
| 36 | A1 | 2529 | A |
| 36 | A1 | 2531 | C |
| 36 | A1 | 2532 | U |
| 36 | A1 | 2533 | G |
| 36 | A1 | 2534 | G |
| 36 | A1 | 2537 | U |
| 36 | A1 | 2538 | U |
| 36 | A1 | 2539 | C |
| 36 | A1 | 2540 | A |
| 36 | A1 | 2541 | U |
| 36 | A1 | 2542 | U |
| 36 | A1 | 2543 | U |
| 36 | A1 | 2545 | C |
| 36 | A1 | 2547 | A |
| 36 | A1 | 2548 | C |
| 36 | A1 | 2549 | G |
| 36 | A1 | 2552 | C |
| 36 | A1 | 2553 | U |
| 36 | A1 | 2554 | A |
| 36 | A1 | 2555 | G |
| 36 | A1 | 2561 | A |
| 36 | A1 | 2568 | C |
| 36 | A1 | 2569 | A |
| 36 | A1 | 2570 | U |
| 36 | A1 | 2571 | U |
| 36 | A1 | 2572 | C |
| 36 | A1 | 2573 | G |
| 36 | A1 | 2576 | G |
| 36 | A1 | 2581 | U |
| 36 | A1 | 2582 | C |
| 36 | A1 | 2585 | G |
| 36 | A1 | 2586 | G |
| 36 | A1 | 2593 | A |
| 36 | A1 | 2594 | C |
| 36 | A1 | 2606 | G |
| 36 | A1 | 2607 | G |
| 36 | A1 | 2614 | G |
| 36 | A1 | 2626 | A |
| 36 | A1 | 2637 | A |
| 36 | A1 | 2652 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A1 | 2656 | A |
| 36 | A1 | 2672 | G |
| 36 | A1 | 2674 | A |
| 36 | A1 | 2677 | G |
| 36 | A1 | 2681 | U |
| 36 | A1 | 2689 | A |
| 36 | A1 | 2690 | G |
| 36 | A1 | 2691 | A |
| 36 | A1 | 2693 | C |
| 36 | A1 | 2694 | A |
| 36 | A1 | 2696 | A |
| 36 | A1 | 2699 | G |
| 36 | A1 | 2705 | A |
| 36 | A1 | 2709 | C |
| 36 | A1 | 2714 | G |
| 36 | A1 | 2728 | G |
| 36 | A1 | 2729 | U |
| 36 | A1 | 2752 | U |
| 36 | A1 | 2753 | G |
| 36 | A1 | 2762 | A |
| 36 | A1 | 2771 | U |
| 36 | A1 | 2772 | C |
| 36 | A1 | 2777 | G |
| 36 | A1 | 2778 | G |
| 36 | A1 | 2779 | A |
| 36 | A1 | 2796 | G |
| 36 | A1 | 2799 | A |
| 36 | A1 | 2800 | G |
| 36 | A1 | 2801 | A |
| 36 | A1 | 2810 | C |
| 36 | A1 | 2816 | G |
| 36 | A1 | 2817 | A |
| 36 | A1 | 2818 | U |
| 36 | A1 | 2819 | A |
| 36 | A1 | 2829 | U |
| 36 | A1 | 2842 | U |
| 36 | A1 | 2843 | U |
| 36 | A1 | 2845 | A |
| 36 | A1 | 2849 | C |
| 36 | A1 | 2860 | U |
| 36 | A1 | 2867 | C |
| 36 | A1 | 2871 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A1 | 2872 | A |
| 36 | A1 | 2873 | U |
| 36 | A1 | 2875 | U |
| 36 | A1 | 2878 | G |
| 36 | A1 | 2879 | C |
| 36 | A1 | 2882 | U |
| 36 | A1 | 2887 | A |
| 36 | A1 | 2889 | C |
| 36 | A1 | 2896 | A |
| 36 | A1 | 2897 | A |
| 36 | A1 | 2898 | G |
| 36 | A1 | 2899 | C |
| 36 | A1 | 2914 | G |
| 36 | A1 | 2923 | U |
| 36 | A1 | 2927 | C |
| 36 | A1 | 2935 | U |
| 36 | A1 | 2936 | A |
| 36 | A1 | 2937 | G |
| 36 | A1 | 2942 | C |
| 36 | A1 | 2945 | G |
| 36 | A1 | 2947 | G |
| 36 | A1 | 2957 | G |
| 36 | A1 | 2971 | A |
| 36 | A1 | 2983 | C |
| 36 | A1 | 2990 | G |
| 36 | A1 | 2992 | U |
| 36 | A1 | 2996 | U |
| 36 | A1 | 2997 | G |
| 36 | A1 | 3006 | A |
| 36 | A1 | 3012 | A |
| 36 | A1 | 3056 | U |
| 36 | A1 | 3057 | U |
| 36 | A1 | 3058 | U |
| 36 | A1 | 3059 | G |
| 36 | A1 | 3078 | U |
| 36 | A1 | 3079 | U |
| 36 | A1 | 3086 | A |
| 36 | A1 | 3087 | A |
| 36 | A1 | 3092 | C |
| 36 | A1 | 3113 | A |
| 36 | A1 | 3119 | U |
| 36 | A1 | 3122 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A1 | 3130 | A |
| 36 | A1 | 3131 | U |
| 36 | A1 | 3139 | A |
| 36 | A1 | 3142 | A |
| 36 | A1 | 3143 | C |
| 36 | A1 | 3151 | U |
| 36 | A1 | 3153 | U |
| 36 | A1 | 3154 | C |
| 36 | A1 | 3155 | U |
| 36 | A1 | 3156 | U |
| 36 | A1 | 3157 | U |
| 36 | A1 | 3164 | C |
| 36 | A1 | 3165 | A |
| 36 | A1 | 3168 | A |
| 36 | A1 | 3169 | U |
| 36 | A1 | 3170 | A |
| 36 | A1 | 3171 | U |
| 36 | A1 | 3173 | G |
| 36 | A1 | 3174 | A |
| 36 | A1 | 3176 | G |
| 36 | A1 | 3179 | U |
| 36 | A1 | 3181 | C |
| 36 | A1 | 3185 | U |
| 36 | A1 | 3187 | A |
| 36 | A1 | 3196 | U |
| 36 | A1 | 3197 | G |
| 36 | A1 | 3198 | U |
| 36 | A1 | 3199 | G |
| 36 | A1 | 3207 | U |
| 36 | A1 | 3209 | A |
| 36 | A1 | 3210 | A |
| 36 | A1 | 3217 | C |
| 36 | A1 | 3218 | A |
| 36 | A1 | 3219 | G |
| 36 | A1 | 3223 | A |
| 36 | A1 | 3228 | C |
| 36 | A1 | 3229 | G |
| 36 | A1 | 3235 | C |
| 36 | A1 | 3238 | G |
| 36 | A1 | 3239 | G |
| 36 | A1 | 3242 | G |
| 36 | A1 | 3243 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A1 | 3245 | A |
| 36 | A1 | 3246 | G |
| 36 | A1 | 3247 | G |
| 36 | A1 | 3253 | G |
| 36 | A1 | 3256 | G |
| 36 | A1 | 3259 | U |
| 36 | A1 | 3265 | C |
| 36 | A1 | 3269 | U |
| 36 | A1 | 3270 | U |
| 36 | A1 | 3272 | C |
| 36 | A1 | 3273 | A |
| 36 | A1 | 3276 | G |
| 36 | A1 | 3279 | A |
| 36 | A1 | 3281 | U |
| 36 | A1 | 3286 | G |
| 36 | A1 | 3287 | U |
| 36 | A1 | 3289 | G |
| 36 | A1 | 3294 | A |
| 36 | A1 | 3295 | A |
| 36 | A1 | 3303 | G |
| 36 | A1 | 3304 | U |
| 36 | A1 | 3307 | A |
| 36 | A1 | 3313 | U |
| 36 | A1 | 3316 | A |
| 36 | A1 | 3317 | U |
| 36 | A1 | 3318 | G |
| 36 | A1 | 3319 | U |
| 36 | A1 | 3320 | A |
| 36 | A1 | 3328 | G |
| 36 | A1 | 3330 | A |
| 36 | A1 | 3331 | U |
| 36 | A1 | 3332 | U |
| 36 | A1 | 3333 | G |
| 36 | A1 | 3335 | A |
| 36 | A1 | 3336 | A |
| 36 | A1 | 3341 | U |
| 36 | A1 | 3342 | A |
| 36 | A1 | 3345 | G |
| 36 | A1 | 3347 | A |
| 36 | A1 | 3348 | G |
| 36 | A1 | 3349 | C |
| 36 | A1 | 3350 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A1 | 3351 | U |
| 36 | A1 | 3352 | U |
| 36 | A1 | 3353 | G |
| 36 | A1 | 3354 | U |
| 36 | A1 | 3355 | U |
| 36 | A1 | 3356 | G |
| 36 | A1 | 3369 | G |
| 36 | A1 | 3375 | A |
| 36 | A1 | 3376 | A |
| 36 | A1 | 3378 | C |
| 36 | A1 | 3382 | U |
| 36 | A1 | 3383 | G |
| 36 | A1 | 3389 | U |
| 36 | A1 | 3396 | U |
| 37 | A3 | 7 | G |
| 37 | A3 | 13 | A |
| 37 | A3 | 14 | U |
| 37 | A3 | 21 | G |
| 37 | A3 | 22 | A |
| 37 | A3 | 26 | C |
| 37 | A3 | 42 | A |
| 37 | A3 | 45 | A |
| 37 | A3 | 51 | A |
| 37 | A3 | 53 | U |
| 37 | A3 | 54 | U |
| 37 | A3 | 65 | G |
| 37 | A3 | 73 | C |
| 37 | A3 | 74 | C |
| 37 | A3 | 76 | A |
| 37 | A3 | 91 | G |
| 37 | A3 | 95 | A |
| 37 | A3 | 102 | A |
| 37 | A3 | 103 | A |
| 37 | A3 | 110 | G |
| 37 | A3 | 112 | G |
| 37 | A3 | 115 | G |
| 38 | A4 | 34 | U |
| 38 | A4 | 35 | C |
| 38 | A4 | 47 | C |
| 38 | A4 | 48 | A |
| 38 | A4 | 51 | G |
| 38 | A4 | 52 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 38 | A4 | 53 | A |
| 38 | A4 | 59 | A |
| 38 | A4 | 62 | C |
| 38 | A4 | 63 | G |
| 38 | A4 | 77 | A |
| 38 | A4 | 79 | A |
| 38 | A4 | 80 | A |
| 38 | A4 | 81 | U |
| 38 | A4 | 82 | U |
| 38 | A4 | 83 | C |
| 38 | A4 | 84 | C |
| 38 | A4 | 85 | G |
| 38 | A4 | 86 | U |
| 38 | A4 | 87 | G |
| 38 | A4 | 90 | U |
| 38 | A4 | 92 | A |
| 38 | A4 | 93 | U |
| 38 | A4 | 95 | G |
| 38 | A4 | 104 | A |
| 38 | A4 | 106 | C |
| 38 | A4 | 111 | A |
| 38 | A4 | 113 | U |
| 38 | A4 | 125 | U |
| 38 | A4 | 126 | A |
| 38 | A4 | 127 | U |
| 38 | A4 | 128 | U |
| 38 | A4 | 138 | A |
| 38 | A4 | 151 | C |
| 38 | A4 | 152 | G |
| 38 | A4 | 155 | A |
| 38 | A4 | 157 | U |
| 38 | A4 | 158 | U |
| 80 | A6 | 2 | A |
| 80 | A6 | 4 | C |
| 80 | A6 | 13 | C |
| 80 | A6 | 17 | C |
| 80 | A6 | 24 | U |
| 80 | A6 | 25 | C |
| 80 | A6 | 26 | A |
| 80 | A6 | 27 | U |
| 80 | A6 | 34 | G |
| 80 | A6 | 42 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 80 | A6 | 47 | A |
| 80 | A6 | 57 | G |
| 80 | A6 | 60 | U |
| 80 | A6 | 67 | A |
| 80 | A6 | 68 | A |
| 80 | A6 | 69 | G |
| 80 | A6 | 72 | A |
| 80 | A6 | 73 | U |
| 80 | A6 | 74 | U |
| 80 | A6 | 75 | U |
| 80 | A6 | 76 | A |
| 80 | A6 | 77 | U |
| 80 | A6 | 101 | U |
| 80 | A6 | 104 | A |
| 80 | A6 | 111 | U |
| 80 | A6 | 114 | C |
| 80 | A6 | 115 | G |
| 80 | A6 | 132 | U |
| 80 | A6 | 137 | U |
| 80 | A6 | 138 | A |
| 80 | A6 | 140 | A |
| 80 | A6 | 141 | U |
| 80 | A6 | 144 | U |
| 80 | A6 | 145 | A |
| 80 | A6 | 146 | U |
| 80 | A6 | 153 | G |
| 80 | A6 | 158 | U |
| 80 | A6 | 159 | U |
| 80 | A6 | 161 | U |
| 80 | A6 | 166 | C |
| 80 | A6 | 175 | G |
| 80 | A6 | 178 | U |
| 80 | A6 | 179 | A |
| 80 | A6 | 182 | A |
| 80 | A6 | 184 | C |
| 80 | A6 | 185 | U |
| 80 | A6 | 187 | G |
| 80 | A6 | 188 | A |
| 80 | A6 | 190 | C |
| 80 | A6 | 191 | C |
| 80 | A6 | 192 | U |
| 80 | A6 | 193 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 80 | A6 | 194 | U |
| 80 | A6 | 195 | G |
| 80 | A6 | 196 | G |
| 80 | A6 | 197 | A |
| 80 | A6 | 198 | A |
| 80 | A6 | 199 | G |
| 80 | A6 | 200 | A |
| 80 | A6 | 215 | A |
| 80 | A6 | 216 | U |
| 80 | A6 | 217 | A |
| 80 | A6 | 218 | A |
| 80 | A6 | 219 | A |
| 80 | A6 | 220 | A |
| 80 | A6 | 221 | A |
| 80 | A6 | 222 | A |
| 80 | A6 | 226 | A |
| 80 | A6 | 227 | U |
| 80 | A6 | 228 | G |
| 80 | A6 | 229 | U |
| 80 | A6 | 230 | C |
| 80 | A6 | 231 | U |
| 80 | A6 | 232 | U |
| 80 | A6 | 233 | C |
| 80 | A6 | 234 | G |
| 80 | A6 | 235 | G |
| 80 | A6 | 238 | U |
| 80 | A6 | 240 | U |
| 80 | A6 | 241 | U |
| 80 | A6 | 249 | U |
| 80 | A6 | 250 | C |
| 80 | A6 | 260 | U |
| 80 | A6 | 261 | U |
| 80 | A6 | 262 | U |
| 80 | A6 | 265 | A |
| 80 | A6 | 268 | C |
| 80 | A6 | 271 | A |
| 80 | A6 | 272 | U |
| 80 | A6 | 273 | G |
| 80 | A6 | 275 | C |
| 80 | A6 | 277 | U |
| 80 | A6 | 278 | U |
| 80 | A6 | 280 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 80 | A6 | 281 | G |
| 80 | A6 | 283 | U |
| 80 | A6 | 287 | G |
| 80 | A6 | 299 | A |
| 80 | A6 | 301 | A |
| 80 | A6 | 308 | C |
| 80 | A6 | 314 | C |
| 80 | A6 | 316 | A |
| 80 | A6 | 319 | U |
| 80 | A6 | 320 | U |
| 80 | A6 | 321 | C |
| 80 | A6 | 322 | G |
| 80 | A6 | 323 | A |
| 80 | A6 | 325 | G |
| 80 | A6 | 337 | G |
| 80 | A6 | 338 | C |
| 80 | A6 | 341 | A |
| 80 | A6 | 352 | A |
| 80 | A6 | 359 | A |
| 80 | A6 | 360 | A |
| 80 | A6 | 361 | C |
| 80 | A6 | 381 | C |
| 80 | A6 | 393 | C |
| 80 | A6 | 396 | G |
| 80 | A6 | 400 | A |
| 80 | A6 | 401 | A |
| 80 | A6 | 402 | C |
| 80 | A6 | 404 | G |
| 80 | A6 | 416 | A |
| 80 | A6 | 418 | G |
| 80 | A6 | 424 | C |
| 80 | A6 | 425 | A |
| 80 | A6 | 426 | G |
| 80 | A6 | 434 | G |
| 80 | A6 | 439 | U |
| 80 | A6 | 444 | C |
| 80 | A6 | 446 | A |
| 80 | A6 | 448 | C |
| 80 | A6 | 454 | U |
| 80 | A6 | 464 | A |
| 80 | A6 | 468 | A |
| 80 | A6 | 469 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 80 | A6 | 470 | A |
| 80 | A6 | 475 | A |
| 80 | A6 | 477 | A |
| 80 | A6 | 480 | G |
| 80 | A6 | 484 | C |
| 80 | A6 | 486 | G |
| 80 | A6 | 487 | G |
| 80 | A6 | 488 | G |
| 80 | A6 | 489 | C |
| 80 | A6 | 490 | C |
| 80 | A6 | 492 | A |
| 80 | A6 | 493 | U |
| 80 | A6 | 494 | U |
| 80 | A6 | 495 | C |
| 80 | A6 | 496 | G |
| 80 | A6 | 497 | G |
| 80 | A6 | 500 | C |
| 80 | A6 | 501 | U |
| 80 | A6 | 503 | G |
| 80 | A6 | 504 | U |
| 80 | A6 | 505 | A |
| 80 | A6 | 506 | A |
| 80 | A6 | 508 | U |
| 80 | A6 | 510 | G |
| 80 | A6 | 511 | A |
| 80 | A6 | 512 | A |
| 80 | A6 | 513 | U |
| 80 | A6 | 515 | A |
| 80 | A6 | 519 | C |
| 80 | A6 | 527 | A |
| 80 | A6 | 532 | U |
| 80 | A6 | 535 | A |
| 80 | A6 | 538 | A |
| 80 | A6 | 539 | G |
| 80 | A6 | 540 | G |
| 80 | A6 | 541 | A |
| 80 | A6 | 542 | A |
| 80 | A6 | 543 | C |
| 80 | A6 | 544 | A |
| 80 | A6 | 548 | G |
| 80 | A6 | 555 | A |
| 80 | A6 | 556 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 80 | A6 | 557 | G |
| 80 | A6 | 558 | U |
| 80 | A6 | 559 | C |
| 80 | A6 | 565 | C |
| 80 | A6 | 566 | C |
| 80 | A6 | 570 | A |
| 80 | A6 | 574 | G |
| 80 | A6 | 578 | U |
| 80 | A6 | 579 | A |
| 80 | A6 | 580 | A |
| 80 | A6 | 582 | U |
| 80 | A6 | 594 | A |
| 80 | A6 | 595 | G |
| 80 | A6 | 597 | G |
| 80 | A6 | 609 | U |
| 80 | A6 | 610 | G |
| 80 | A6 | 617 | U |
| 80 | A6 | 619 | A |
| 80 | A6 | 620 | A |
| 80 | A6 | 621 | A |
| 80 | A6 | 622 | A |
| 80 | A6 | 623 | A |
| 80 | A6 | 630 | A |
| 80 | A6 | 637 | C |
| 80 | A6 | 639 | U |
| 80 | A6 | 640 | U |
| 80 | A6 | 645 | C |
| 80 | A6 | 648 | G |
| 80 | A6 | 651 | G |
| 80 | A6 | 652 | G |
| 80 | A6 | 653 | C |
| 80 | A6 | 654 | C |
| 80 | A6 | 655 | G |
| 80 | A6 | 658 | C |
| 80 | A6 | 676 | G |
| 80 | A6 | 678 | A |
| 80 | A6 | 679 | U |
| 80 | A6 | 680 | U |
| 80 | A6 | 681 | U |
| 80 | A6 | 682 | C |
| 80 | A6 | 683 | C |
| 80 | A6 | 684 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 80 | A6 | 688 | G |
| 80 | A6 | 691 | C |
| 80 | A6 | 695 | U |
| 80 | A6 | 696 | C |
| 80 | A6 | 697 | C |
| 80 | A6 | 698 | U |
| 80 | A6 | 706 | A |
| 80 | A6 | 710 | U |
| 80 | A6 | 711 | U |
| 80 | A6 | 714 | G |
| 80 | A6 | 718 | U |
| 80 | A6 | 719 | U |
| 80 | A6 | 720 | G |
| 80 | A6 | 721 | U |
| 80 | A6 | 722 | G |
| 80 | A6 | 723 | G |
| 80 | A6 | 726 | C |
| 80 | A6 | 730 | G |
| 80 | A6 | 733 | A |
| 80 | A6 | 734 | A |
| 80 | A6 | 735 | C |
| 80 | A6 | 742 | U |
| 80 | A6 | 747 | C |
| 80 | A6 | 751 | G |
| 80 | A6 | 753 | A |
| 80 | A6 | 754 | A |
| 80 | A6 | 755 | A |
| 80 | A6 | 756 | A |
| 80 | A6 | 765 | G |
| 80 | A6 | 766 | U |
| 80 | A6 | 774 | A |
| 80 | A6 | 775 | G |
| 80 | A6 | 780 | A |
| 80 | A6 | 781 | U |
| 80 | A6 | 782 | U |
| 80 | A6 | 783 | G |
| 80 | A6 | 787 | G |
| 80 | A6 | 789 | A |
| 80 | A6 | 792 | U |
| 80 | A6 | 793 | A |
| 80 | A6 | 794 | U |
| 80 | A6 | 806 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 80 | A6 | 811 | A |
| 80 | A6 | 812 | A |
| 80 | A6 | 815 | G |
| 80 | A6 | 821 | U |
| 80 | A6 | 823 | G |
| 80 | A6 | 825 | U |
| 80 | A6 | 826 | U |
| 80 | A6 | 829 | A |
| 80 | A6 | 830 | U |
| 80 | A6 | 831 | U |
| 80 | A6 | 832 | U |
| 80 | A6 | 834 | G |
| 80 | A6 | 835 | U |
| 80 | A6 | 841 | U |
| 80 | A6 | 850 | A |
| 80 | A6 | 856 | A |
| 80 | A6 | 863 | A |
| 80 | A6 | 876 | G |
| 80 | A6 | 886 | U |
| 80 | A6 | 898 | A |
| 80 | A6 | 913 | G |
| 80 | A6 | 914 | G |
| 80 | A6 | 916 | U |
| 80 | A6 | 926 | A |
| 80 | A6 | 928 | U |
| 80 | A6 | 933 | A |
| 80 | A6 | 935 | U |
| 80 | A6 | 942 | G |
| 80 | A6 | 949 | C |
| 80 | A6 | 959 | U |
| 80 | A6 | 960 | U |
| 80 | A6 | 966 | A |
| 80 | A6 | 967 | A |
| 80 | A6 | 968 | U |
| 80 | A6 | 969 | C |
| 80 | A6 | 970 | A |
| 80 | A6 | 971 | A |
| 80 | A6 | 976 | G |
| 80 | A6 | 991 | G |
| 80 | A6 | 992 | A |
| 80 | A6 | 993 | A |
| 80 | A6 | 997 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 80 | A6 | 1004 | U |
| 80 | A6 | 1005 | A |
| 80 | A6 | 1021 | C |
| 80 | A6 | 1026 | A |
| 80 | A6 | 1028 | C |
| 80 | A6 | 1031 | U |
| 80 | A6 | 1039 | A |
| 80 | A6 | 1040 | G |
| 80 | A6 | 1042 | G |
| 80 | A6 | 1052 | U |
| 80 | A6 | 1053 | G |
| 80 | A6 | 1057 | U |
| 80 | A6 | 1058 | U |
| 80 | A6 | 1059 | U |
| 80 | A6 | 1060 | U |
| 80 | A6 | 1061 | A |
| 80 | A6 | 1062 | A |
| 80 | A6 | 1063 | U |
| 80 | A6 | 1066 | C |
| 80 | A6 | 1067 | C |
| 80 | A6 | 1074 | G |
| 80 | A6 | 1082 | C |
| 80 | A6 | 1083 | G |
| 80 | A6 | 1091 | A |
| 80 | A6 | 1092 | A |
| 80 | A6 | 1096 | C |
| 80 | A6 | 1097 | U |
| 80 | A6 | 1098 | U |
| 80 | A6 | 1099 | U |
| 80 | A6 | 1100 | G |
| 80 | A6 | 1101 | G |
| 80 | A6 | 1109 | G |
| 80 | A6 | 1138 | A |
| 80 | A6 | 1139 | A |
| 80 | A6 | 1151 | A |
| 80 | A6 | 1154 | G |
| 80 | A6 | 1158 | C |
| 80 | A6 | 1159 | C |
| 80 | A6 | 1160 | A |
| 80 | A6 | 1162 | C |
| 80 | A6 | 1167 | G |
| 80 | A6 | 1185 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 80 | A6 | 1193 | A |
| 80 | A6 | 1194 | A |
| 80 | A6 | 1196 | A |
| 80 | A6 | 1197 | C |
| 80 | A6 | 1199 | G |
| 80 | A6 | 1200 | G |
| 80 | A6 | 1202 | A |
| 80 | A6 | 1203 | A |
| 80 | A6 | 1208 | A |
| 80 | A6 | 1217 | A |
| 80 | A6 | 1218 | G |
| 80 | A6 | 1220 | C |
| 80 | A6 | 1221 | A |
| 80 | A6 | 1225 | U |
| 80 | A6 | 1226 | A |
| 80 | A6 | 1228 | G |
| 80 | A6 | 1229 | G |
| 80 | A6 | 1230 | A |
| 80 | A6 | 1231 | U |
| 80 | A6 | 1234 | A |
| 80 | A6 | 1239 | U |
| 80 | A6 | 1240 | U |
| 80 | A6 | 1241 | G |
| 80 | A6 | 1242 | A |
| 80 | A6 | 1243 | G |
| 80 | A6 | 1244 | A |
| 80 | A6 | 1245 | G |
| 80 | A6 | 1246 | C |
| 80 | A6 | 1255 | G |
| 80 | A6 | 1256 | A |
| 80 | A6 | 1257 | U |
| 80 | A6 | 1258 | U |
| 80 | A6 | 1261 | G |
| 80 | A6 | 1262 | U |
| 80 | A6 | 1285 | U |
| 80 | A6 | 1286 | U |
| 80 | A6 | 1288 | G |
| 80 | A6 | 1314 | U |
| 80 | A6 | 1315 | U |
| 80 | A6 | 1316 | G |
| 80 | A6 | 1321 | A |
| 80 | A6 | 1329 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 80 | A6 | 1331 | A |
| 80 | A6 | 1343 | U |
| 80 | A6 | 1344 | A |
| 80 | A6 | 1345 | A |
| 80 | A6 | 1346 | A |
| 80 | A6 | 1354 | G |
| 80 | A6 | 1361 | U |
| 80 | A6 | 1363 | U |
| 80 | A6 | 1364 | G |
| 80 | A6 | 1371 | A |
| 80 | A6 | 1372 | U |
| 80 | A6 | 1373 | C |
| 80 | A6 | 1379 | C |
| 80 | A6 | 1390 | U |
| 80 | A6 | 1398 | U |
| 80 | A6 | 1399 | C |
| 80 | A6 | 1400 | A |
| 80 | A6 | 1402 | G |
| 80 | A6 | 1413 | U |
| 80 | A6 | 1414 | U |
| 80 | A6 | 1415 | U |
| 80 | A6 | 1425 | A |
| 80 | A6 | 1427 | A |
| 80 | A6 | 1428 | G |
| 80 | A6 | 1429 | G |
| 80 | A6 | 1433 | G |
| 80 | A6 | 1445 | G |
| 80 | A6 | 1446 | A |
| 80 | A6 | 1448 | G |
| 80 | A6 | 1449 | U |
| 80 | A6 | 1457 | C |
| 80 | A6 | 1458 | G |
| 80 | A6 | 1459 | C |
| 80 | A6 | 1461 | C |
| 80 | A6 | 1471 | A |
| 80 | A6 | 1481 | C |
| 80 | A6 | 1482 | C |
| 80 | A6 | 1486 | G |
| 80 | A6 | 1489 | U |
| 80 | A6 | 1490 | C |
| 80 | A6 | 1491 | U |
| 80 | A6 | 1492 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 80 | A6 | 1493 | A |
| 80 | A6 | 1494 | C |
| 80 | A6 | 1496 | U |
| 80 | A6 | 1497 | U |
| 80 | A6 | 1506 | G |
| 80 | A6 | 1514 | U |
| 80 | A6 | 1515 | A |
| 80 | A6 | 1516 | A |
| 80 | A6 | 1517 | U |
| 80 | A6 | 1521 | G |
| 80 | A6 | 1523 | G |
| 80 | A6 | 1524 | A |
| 80 | A6 | 1531 | G |
| 80 | A6 | 1535 | U |
| 80 | A6 | 1536 | G |
| 80 | A6 | 1537 | C |
| 80 | A6 | 1538 | U |
| 80 | A6 | 1539 | G |
| 80 | A6 | 1540 | G |
| 80 | A6 | 1554 | U |
| 80 | A6 | 1555 | A |
| 80 | A6 | 1557 | U |
| 80 | A6 | 1559 | A |
| 80 | A6 | 1569 | A |
| 80 | A6 | 1573 | A |
| 80 | A6 | 1574 | G |
| 80 | A6 | 1575 | G |
| 80 | A6 | 1582 | U |
| 80 | A6 | 1584 | G |
| 80 | A6 | 1596 | C |
| 80 | A6 | 1601 | G |
| 80 | A6 | 1616 | G |
| 80 | A6 | 1621 | U |
| 80 | A6 | 1634 | C |
| 80 | A6 | 1635 | A |
| 80 | A6 | 1637 | C |
| 80 | A6 | 1638 | G |
| 80 | A6 | 1657 | U |
| 80 | A6 | 1658 | G |
| 80 | A6 | 1665 | U |
| 80 | A6 | 1710 | U |
| 80 | A6 | 1712 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 80 | A6 | 1715 | G |
| 80 | A6 | 1716 | C |
| 80 | A6 | 1717 | G |
| 80 | A6 | 1723 | U |
| 80 | A6 | 1727 | G |
| 80 | A6 | 1731 | A |
| 80 | A6 | 1736 | G |
| 80 | A6 | 1755 | A |
| 80 | A6 | 1759 | C |
| 80 | A6 | 1760 | G |
| 80 | A6 | 1766 | A |
| 80 | A6 | 1767 | G |
| 80 | A6 | 1769 | U |
| 80 | A6 | 1770 | U |
| 80 | A6 | 1779 | U |
| 80 | A6 | 1780 | G |
| 80 | A6 | 1782 | A |
| 80 | A6 | 1783 | C |
| 80 | A6 | 1784 | C |
| 80 | A6 | 1789 | G |
| 80 | A6 | 1792 | G |
| 80 | A6 | 1793 | G |
| 80 | A6 | 1794 | A |
| 80 | A6 | 1795 | U |
| 80 | A6 | 1796 | C |
| 80 | A6 | 1799 | U |
| 80 | A6 | 1800 | A |
| 36 | A5 | 14 | U |
| 36 | A5 | 15 | C |
| 36 | A5 | 16 | A |
| 36 | A5 | 26 | A |
| 36 | A5 | 38 | U |
| 36 | A5 | 40 | A |
| 36 | A5 | 43 | A |
| 36 | A5 | 49 | A |
| 36 | A5 | 60 | A |
| 36 | A5 | 65 | A |
| 36 | A5 | 66 | A |
| 36 | A5 | 74 | G |
| 36 | A5 | 76 | G |
| 36 | A5 | 77 | A |
| 36 | A5 | 92 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A5 | 93 | C |
| 36 | A5 | 96 | G |
| 36 | A5 | 99 | A |
| 36 | A5 | 109 | A |
| 36 | A5 | 110 | G |
| 36 | A5 | 111 | C |
| 36 | A5 | 116 | A |
| 36 | A5 | 121 | A |
| 36 | A5 | 122 | A |
| 36 | A5 | 133 | U |
| 36 | A5 | 134 | U |
| 36 | A5 | 135 | C |
| 36 | A5 | 136 | G |
| 36 | A5 | 146 | U |
| 36 | A5 | 150 | A |
| 36 | A5 | 152 | U |
| 36 | A5 | 156 | G |
| 36 | A5 | 157 | A |
| 36 | A5 | 160 | G |
| 36 | A5 | 166 | C |
| 36 | A5 | 170 | G |
| 36 | A5 | 171 | G |
| 36 | A5 | 174 | C |
| 36 | A5 | 178 | U |
| 36 | A5 | 180 | C |
| 36 | A5 | 182 | U |
| 36 | A5 | 183 | G |
| 36 | A5 | 184 | U |
| 36 | A5 | 187 | A |
| 36 | A5 | 190 | U |
| 36 | A5 | 191 | U |
| 36 | A5 | 200 | C |
| 36 | A5 | 201 | A |
| 36 | A5 | 210 | U |
| 36 | A5 | 218 | G |
| 36 | A5 | 219 | A |
| 36 | A5 | 221 | A |
| 36 | A5 | 235 | A |
| 36 | A5 | 236 | G |
| 36 | A5 | 238 | A |
| 36 | A5 | 239 | G |
| 36 | A5 | 240 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A5 | 242 | C |
| 36 | A5 | 244 | G |
| 36 | A5 | 248 | U |
| 36 | A5 | 249 | U |
| 36 | A5 | 250 | U |
| 36 | A5 | 251 | G |
| 36 | A5 | 252 | U |
| 36 | A5 | 253 | A |
| 36 | A5 | 254 | A |
| 36 | A5 | 258 | G |
| 36 | A5 | 259 | C |
| 36 | A5 | 269 | G |
| 36 | A5 | 283 | G |
| 36 | A5 | 284 | A |
| 36 | A5 | 286 | U |
| 36 | A5 | 294 | U |
| 36 | A5 | 295 | A |
| 36 | A5 | 305 | U |
| 36 | A5 | 322 | U |
| 36 | A5 | 323 | A |
| 36 | A5 | 329 | U |
| 36 | A5 | 334 | A |
| 36 | A5 | 339 | C |
| 36 | A5 | 349 | A |
| 36 | A5 | 350 | C |
| 36 | A5 | 351 | A |
| 36 | A5 | 352 | A |
| 36 | A5 | 370 | U |
| 36 | A5 | 376 | G |
| 36 | A5 | 390 | G |
| 36 | A5 | 395 | A |
| 36 | A5 | 398 | A |
| 36 | A5 | 399 | A |
| 36 | A5 | 401 | U |
| 36 | A5 | 402 | A |
| 36 | A5 | 403 | C |
| 36 | A5 | 421 | G |
| 36 | A5 | 422 | A |
| 36 | A5 | 436 | A |
| 36 | A5 | 437 | G |
| 36 | A5 | 438 | A |
| 36 | A5 | 439 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A5 | 440 | A |
| 36 | A5 | 441 | U |
| 36 | A5 | 442 | G |
| 36 | A5 | 443 | G |
| 36 | A5 | 492 | U |
| 36 | A5 | 493 | G |
| 36 | A5 | 495 | G |
| 36 | A5 | 520 | U |
| 36 | A5 | 521 | A |
| 36 | A5 | 531 | G |
| 36 | A5 | 535 | G |
| 36 | A5 | 538 | G |
| 36 | A5 | 546 | C |
| 36 | A5 | 547 | G |
| 36 | A5 | 548 | G |
| 36 | A5 | 551 | A |
| 36 | A5 | 553 | U |
| 36 | A5 | 555 | U |
| 36 | A5 | 557 | A |
| 36 | A5 | 559 | A |
| 36 | A5 | 578 | A |
| 36 | A5 | 579 | G |
| 36 | A5 | 592 | A |
| 36 | A5 | 594 | U |
| 36 | A5 | 595 | G |
| 36 | A5 | 600 | G |
| 36 | A5 | 604 | G |
| 36 | A5 | 609 | G |
| 36 | A5 | 610 | G |
| 36 | A5 | 611 | A |
| 36 | A5 | 612 | U |
| 36 | A5 | 619 | A |
| 36 | A5 | 620 | U |
| 36 | A5 | 621 | A |
| 36 | A5 | 630 | A |
| 36 | A5 | 636 | C |
| 36 | A5 | 649 | A |
| 36 | A5 | 653 | A |
| 36 | A5 | 656 | A |
| 36 | A5 | 660 | A |
| 36 | A5 | 675 | C |
| 36 | A5 | 677 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A5 | 681 | U |
| 36 | A5 | 705 | A |
| 36 | A5 | 708 | G |
| 36 | A5 | 712 | G |
| 36 | A5 | 715 | A |
| 36 | A5 | 716 | A |
| 36 | A5 | 719 | U |
| 36 | A5 | 720 | A |
| 36 | A5 | 725 | G |
| 36 | A5 | 726 | G |
| 36 | A5 | 735 | A |
| 36 | A5 | 736 | A |
| 36 | A5 | 750 | G |
| 36 | A5 | 758 | C |
| 36 | A5 | 766 | U |
| 36 | A5 | 767 | U |
| 36 | A5 | 768 | C |
| 36 | A5 | 776 | U |
| 36 | A5 | 777 | U |
| 36 | A5 | 780 | A |
| 36 | A5 | 781 | G |
| 36 | A5 | 785 | G |
| 36 | A5 | 786 | A |
| 36 | A5 | 806 | A |
| 36 | A5 | 809 | G |
| 36 | A5 | 817 | A |
| 36 | A5 | 830 | A |
| 36 | A5 | 846 | A |
| 36 | A5 | 851 | C |
| 36 | A5 | 861 | C |
| 36 | A5 | 862 | U |
| 36 | A5 | 871 | U |
| 36 | A5 | 874 | U |
| 36 | A5 | 879 | U |
| 36 | A5 | 891 | G |
| 36 | A5 | 893 | C |
| 36 | A5 | 896 | A |
| 36 | A5 | 897 | U |
| 36 | A5 | 907 | G |
| 36 | A5 | 908 | G |
| 36 | A5 | 914 | A |
| 36 | A5 | 916 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A5 | 917 | A |
| 36 | A5 | 921 | A |
| 36 | A5 | 923 | C |
| 36 | A5 | 924 | G |
| 36 | A5 | 937 | G |
| 36 | A5 | 944 | C |
| 36 | A5 | 946 | U |
| 36 | A5 | 947 | G |
| 36 | A5 | 958 | C |
| 36 | A5 | 959 | C |
| 36 | A5 | 960 | U |
| 36 | A5 | 974 | G |
| 36 | A5 | 979 | U |
| 36 | A5 | 980 | A |
| 36 | A5 | 981 | U |
| 36 | A5 | 983 | A |
| 36 | A5 | 994 | G |
| 36 | A5 | 1000 | C |
| 36 | A5 | 1001 | G |
| 36 | A5 | 1002 | A |
| 36 | A5 | 1003 | A |
| 36 | A5 | 1010 | G |
| 36 | A5 | 1014 | U |
| 36 | A5 | 1015 | U |
| 36 | A5 | 1016 | C |
| 36 | A5 | 1017 | C |
| 36 | A5 | 1018 | G |
| 36 | A5 | 1020 | G |
| 36 | A5 | 1021 | G |
| 36 | A5 | 1023 | C |
| 36 | A5 | 1024 | G |
| 36 | A5 | 1025 | A |
| 36 | A5 | 1026 | A |
| 36 | A5 | 1027 | A |
| 36 | A5 | 1028 | U |
| 36 | A5 | 1029 | G |
| 36 | A5 | 1032 | C |
| 36 | A5 | 1034 | U |
| 36 | A5 | 1035 | G |
| 36 | A5 | 1047 | A |
| 36 | A5 | 1049 | C |
| 36 | A5 | 1057 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A5 | 1064 | A |
| 36 | A5 | 1065 | A |
| 36 | A5 | 1071 | U |
| 36 | A5 | 1072 | G |
| 36 | A5 | 1081 | U |
| 36 | A5 | 1082 | U |
| 36 | A5 | 1085 | A |
| 36 | A5 | 1093 | A |
| 36 | A5 | 1094 | U |
| 36 | A5 | 1095 | U |
| 36 | A5 | 1096 | U |
| 36 | A5 | 1097 | G |
| 36 | A5 | 1098 | A |
| 36 | A5 | 1103 | A |
| 36 | A5 | 1104 | G |
| 36 | A5 | 1117 | G |
| 36 | A5 | 1131 | G |
| 36 | A5 | 1153 | A |
| 36 | A5 | 1159 | A |
| 36 | A5 | 1160 | C |
| 36 | A5 | 1174 | G |
| 36 | A5 | 1178 | G |
| 36 | A5 | 1179 | A |
| 36 | A5 | 1180 | A |
| 36 | A5 | 1181 | U |
| 36 | A5 | 1182 | A |
| 36 | A5 | 1191 | U |
| 36 | A5 | 1192 | C |
| 36 | A5 | 1193 | A |
| 36 | A5 | 1201 | C |
| 36 | A5 | 1209 | G |
| 36 | A5 | 1213 | G |
| 36 | A5 | 1222 | G |
| 36 | A5 | 1223 | A |
| 36 | A5 | 1232 | C |
| 36 | A5 | 1233 | G |
| 36 | A5 | 1236 | G |
| 36 | A5 | 1237 | G |
| 36 | A5 | 1239 | C |
| 36 | A5 | 1241 | U |
| 36 | A5 | 1242 | G |
| 36 | A5 | 1243 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A5 | 1245 | A |
| 36 | A5 | 1246 | G |
| 36 | A5 | 1248 | C |
| 36 | A5 | 1258 | U |
| 36 | A5 | 1259 | A |
| 36 | A5 | 1262 | G |
| 36 | A5 | 1263 | A |
| 36 | A5 | 1264 | G |
| 36 | A5 | 1265 | U |
| 36 | A5 | 1266 | G |
| 36 | A5 | 1270 | A |
| 36 | A5 | 1281 | G |
| 36 | A5 | 1285 | G |
| 36 | A5 | 1294 | A |
| 36 | A5 | 1307 | G |
| 36 | A5 | 1308 | A |
| 36 | A5 | 1309 | U |
| 36 | A5 | 1312 | C |
| 36 | A5 | 1330 | A |
| 36 | A5 | 1332 | A |
| 36 | A5 | 1348 | U |
| 36 | A5 | 1349 | G |
| 36 | A5 | 1350 | A |
| 36 | A5 | 1351 | U |
| 36 | A5 | 1352 | A |
| 36 | A5 | 1353 | U |
| 36 | A5 | 1354 | G |
| 36 | A5 | 1355 | A |
| 36 | A5 | 1356 | U |
| 36 | A5 | 1357 | G |
| 36 | A5 | 1366 | A |
| 36 | A5 | 1385 | C |
| 36 | A5 | 1386 | A |
| 36 | A5 | 1387 | G |
| 36 | A5 | 1399 | A |
| 36 | A5 | 1400 | G |
| 36 | A5 | 1403 | C |
| 36 | A5 | 1419 | A |
| 36 | A5 | 1422 | G |
| 36 | A5 | 1428 | A |
| 36 | A5 | 1434 | G |
| 36 | A5 | 1437 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A5 | 1440 | G |
| 36 | A5 | 1446 | A |
| 36 | A5 | 1450 | G |
| 36 | A5 | 1460 | A |
| 36 | A5 | 1481 | A |
| 36 | A5 | 1482 | A |
| 36 | A5 | 1490 | A |
| 36 | A5 | 1495 | U |
| 36 | A5 | 1502 | C |
| 36 | A5 | 1503 | A |
| 36 | A5 | 1508 | C |
| 36 | A5 | 1527 | C |
| 36 | A5 | 1541 | G |
| 36 | A5 | 1542 | G |
| 36 | A5 | 1549 | U |
| 36 | A5 | 1554 | U |
| 36 | A5 | 1555 | U |
| 36 | A5 | 1556 | C |
| 36 | A5 | 1557 | A |
| 36 | A5 | 1560 | G |
| 36 | A5 | 1561 | G |
| 36 | A5 | 1562 | C |
| 36 | A5 | 1563 | C |
| 36 | A5 | 1565 | G |
| 36 | A5 | 1566 | A |
| 36 | A5 | 1567 | U |
| 36 | A5 | 1568 | U |
| 36 | A5 | 1569 | U |
| 36 | A5 | 1570 | U |
| 36 | A5 | 1571 | A |
| 36 | A5 | 1572 | U |
| 36 | A5 | 1574 | C |
| 36 | A5 | 1575 | A |
| 36 | A5 | 1576 | G |
| 36 | A5 | 1577 | G |
| 36 | A5 | 1578 | C |
| 36 | A5 | 1580 | A |
| 36 | A5 | 1581 | C |
| 36 | A5 | 1582 | C |
| 36 | A5 | 1583 | A |
| 36 | A5 | 1587 | A |
| 36 | A5 | 1589 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A5 | 1593 | A |
| 36 | A5 | 1605 | A |
| 36 | A5 | 1607 | U |
| 36 | A5 | 1608 | C |
| 36 | A5 | 1620 | U |
| 36 | A5 | 1629 | U |
| 36 | A5 | 1633 | C |
| 36 | A5 | 1635 | G |
| 36 | A5 | 1639 | C |
| 36 | A5 | 1641 | U |
| 36 | A5 | 1643 | A |
| 36 | A5 | 1644 | C |
| 36 | A5 | 1645 | U |
| 36 | A5 | 1655 | G |
| 36 | A5 | 1657 | C |
| 36 | A5 | 1680 | G |
| 36 | A5 | 1683 | A |
| 36 | A5 | 1716 | U |
| 36 | A5 | 1717 | U |
| 36 | A5 | 1718 | G |
| 36 | A5 | 1724 | U |
| 36 | A5 | 1725 | C |
| 36 | A5 | 1736 | G |
| 36 | A5 | 1750 | A |
| 36 | A5 | 1751 | G |
| 36 | A5 | 1754 | G |
| 36 | A5 | 1758 | G |
| 36 | A5 | 1760 | A |
| 36 | A5 | 1762 | C |
| 36 | A5 | 1764 | U |
| 36 | A5 | 1765 | U |
| 36 | A5 | 1766 | G |
| 36 | A5 | 1767 | C |
| 36 | A5 | 1770 | G |
| 36 | A5 | 1778 | G |
| 36 | A5 | 1780 | G |
| 36 | A5 | 1783 | U |
| 36 | A5 | 1797 | A |
| 36 | A5 | 1810 | A |
| 36 | A5 | 1812 | G |
| 36 | A5 | 1814 | A |
| 36 | A5 | 1815 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A5 | 1816 | A |
| 36 | A5 | 1817 | G |
| 36 | A5 | 1818 | U |
| 36 | A5 | 1820 | U |
| 36 | A5 | 1821 | U |
| 36 | A5 | 1835 | A |
| 36 | A5 | 1841 | A |
| 36 | A5 | 1842 | A |
| 36 | A5 | 1846 | C |
| 36 | A5 | 1849 | C |
| 36 | A5 | 1850 | A |
| 36 | A5 | 1855 | U |
| 36 | A5 | 1871 | U |
| 36 | A5 | 1876 | U |
| 36 | A5 | 1878 | G |
| 36 | A5 | 1879 | A |
| 36 | A5 | 1880 | U |
| 36 | A5 | 1905 | G |
| 36 | A5 | 1906 | G |
| 36 | A5 | 1909 | A |
| 36 | A5 | 1918 | C |
| 36 | A5 | 1927 | G |
| 36 | A5 | 1940 | G |
| 36 | A5 | 1953 | G |
| 36 | A5 | 2100 | A |
| 36 | A5 | 2101 | C |
| 36 | A5 | 2102 | U |
| 36 | A5 | 2112 | U |
| 36 | A5 | 2113 | A |
| 36 | A5 | 2114 | C |
| 36 | A5 | 2121 | G |
| 36 | A5 | 2122 | G |
| 36 | A5 | 2128 | C |
| 36 | A5 | 2131 | A |
| 36 | A5 | 2134 | G |
| 36 | A5 | 2139 | A |
| 36 | A5 | 2144 | A |
| 36 | A5 | 2158 | A |
| 36 | A5 | 2169 | G |
| 36 | A5 | 2170 | U |
| 36 | A5 | 2171 | G |
| 36 | A5 | 2192 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A5 | 2201 | G |
| 36 | A5 | 2205 | U |
| 36 | A5 | 2210 | G |
| 36 | A5 | 2213 | A |
| 36 | A5 | 2222 | A |
| 36 | A5 | 2223 | A |
| 36 | A5 | 2228 | A |
| 36 | A5 | 2229 | A |
| 36 | A5 | 2244 | A |
| 36 | A5 | 2250 | G |
| 36 | A5 | 2253 | G |
| 36 | A5 | 2255 | A |
| 36 | A5 | 2256 | A |
| 36 | A5 | 2257 | C |
| 36 | A5 | 2258 | U |
| 36 | A5 | 2264 | U |
| 36 | A5 | 2270 | A |
| 36 | A5 | 2273 | G |
| 36 | A5 | 2276 | G |
| 36 | A5 | 2278 | C |
| 36 | A5 | 2279 | A |
| 36 | A5 | 2288 | G |
| 36 | A5 | 2290 | C |
| 36 | A5 | 2294 | U |
| 36 | A5 | 2298 | U |
| 36 | A5 | 2307 | G |
| 36 | A5 | 2310 | U |
| 36 | A5 | 2313 | A |
| 36 | A5 | 2315 | G |
| 36 | A5 | 2324 | A |
| 36 | A5 | 2329 | C |
| 36 | A5 | 2334 | U |
| 36 | A5 | 2335 | G |
| 36 | A5 | 2336 | U |
| 36 | A5 | 2373 | A |
| 36 | A5 | 2374 | C |
| 36 | A5 | 2375 | G |
| 36 | A5 | 2377 | G |
| 36 | A5 | 2385 | G |
| 36 | A5 | 2388 | U |
| 36 | A5 | 2393 | G |
| 36 | A5 | 2394 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A5 | 2396 | G |
| 36 | A5 | 2397 | A |
| 36 | A5 | 2398 | A |
| 36 | A5 | 2400 | G |
| 36 | A5 | 2401 | A |
| 36 | A5 | 2402 | A |
| 36 | A5 | 2403 | G |
| 36 | A5 | 2404 | A |
| 36 | A5 | 2405 | C |
| 36 | A5 | 2406 | C |
| 36 | A5 | 2411 | U |
| 36 | A5 | 2418 | G |
| 36 | A5 | 2435 | G |
| 36 | A5 | 2436 | U |
| 36 | A5 | 2437 | G |
| 36 | A5 | 2438 | A |
| 36 | A5 | 2439 | A |
| 36 | A5 | 2440 | G |
| 36 | A5 | 2441 | A |
| 36 | A5 | 2443 | A |
| 36 | A5 | 2504 | U |
| 36 | A5 | 2505 | U |
| 36 | A5 | 2506 | U |
| 36 | A5 | 2507 | C |
| 36 | A5 | 2508 | U |
| 36 | A5 | 2510 | U |
| 36 | A5 | 2511 | A |
| 36 | A5 | 2512 | C |
| 36 | A5 | 2513 | U |
| 36 | A5 | 2514 | U |
| 36 | A5 | 2515 | A |
| 36 | A5 | 2518 | C |
| 36 | A5 | 2523 | A |
| 36 | A5 | 2524 | A |
| 36 | A5 | 2526 | C |
| 36 | A5 | 2530 | G |
| 36 | A5 | 2531 | C |
| 36 | A5 | 2532 | U |
| 36 | A5 | 2534 | G |
| 36 | A5 | 2538 | U |
| 36 | A5 | 2539 | C |
| 36 | A5 | 2540 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A5 | 2543 | U |
| 36 | A5 | 2544 | U |
| 36 | A5 | 2549 | G |
| 36 | A5 | 2552 | C |
| 36 | A5 | 2555 | G |
| 36 | A5 | 2562 | A |
| 36 | A5 | 2567 | C |
| 36 | A5 | 2568 | C |
| 36 | A5 | 2569 | A |
| 36 | A5 | 2570 | U |
| 36 | A5 | 2571 | U |
| 36 | A5 | 2572 | C |
| 36 | A5 | 2573 | G |
| 36 | A5 | 2574 | G |
| 36 | A5 | 2584 | G |
| 36 | A5 | 2585 | G |
| 36 | A5 | 2589 | G |
| 36 | A5 | 2590 | A |
| 36 | A5 | 2591 | A |
| 36 | A5 | 2593 | A |
| 36 | A5 | 2594 | C |
| 36 | A5 | 2598 | G |
| 36 | A5 | 2599 | U |
| 36 | A5 | 2606 | G |
| 36 | A5 | 2607 | G |
| 36 | A5 | 2610 | G |
| 36 | A5 | 2614 | G |
| 36 | A5 | 2615 | G |
| 36 | A5 | 2622 | C |
| 36 | A5 | 2637 | A |
| 36 | A5 | 2639 | G |
| 36 | A5 | 2652 | U |
| 36 | A5 | 2656 | A |
| 36 | A5 | 2662 | G |
| 36 | A5 | 2663 | G |
| 36 | A5 | 2667 | A |
| 36 | A5 | 2674 | A |
| 36 | A5 | 2677 | G |
| 36 | A5 | 2678 | A |
| 36 | A5 | 2681 | U |
| 36 | A5 | 2683 | U |
| 36 | A5 | 2689 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A5 | 2691 | A |
| 36 | A5 | 2694 | A |
| 36 | A5 | 2696 | A |
| 36 | A5 | 2714 | G |
| 36 | A5 | 2723 | U |
| 36 | A5 | 2728 | G |
| 36 | A5 | 2729 | U |
| 36 | A5 | 2752 | U |
| 36 | A5 | 2753 | G |
| 36 | A5 | 2762 | A |
| 36 | A5 | 2771 | U |
| 36 | A5 | 2772 | C |
| 36 | A5 | 2773 | C |
| 36 | A5 | 2776 | C |
| 36 | A5 | 2777 | G |
| 36 | A5 | 2778 | G |
| 36 | A5 | 2779 | A |
| 36 | A5 | 2796 | G |
| 36 | A5 | 2799 | A |
| 36 | A5 | 2800 | G |
| 36 | A5 | 2801 | A |
| 36 | A5 | 2810 | C |
| 36 | A5 | 2817 | A |
| 36 | A5 | 2818 | U |
| 36 | A5 | 2819 | A |
| 36 | A5 | 2822 | U |
| 36 | A5 | 2829 | U |
| 36 | A5 | 2839 | G |
| 36 | A5 | 2844 | C |
| 36 | A5 | 2845 | A |
| 36 | A5 | 2853 | A |
| 36 | A5 | 2871 | G |
| 36 | A5 | 2872 | A |
| 36 | A5 | 2873 | U |
| 36 | A5 | 2875 | U |
| 36 | A5 | 2887 | A |
| 36 | A5 | 2889 | C |
| 36 | A5 | 2896 | A |
| 36 | A5 | 2897 | A |
| 36 | A5 | 2898 | G |
| 36 | A5 | 2899 | C |
| 36 | A5 | 2904 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A5 | 2910 | A |
| 36 | A5 | 2923 | U |
| 36 | A5 | 2928 | C |
| 36 | A5 | 2935 | U |
| 36 | A5 | 2936 | A |
| 36 | A5 | 2941 | A |
| 36 | A5 | 2942 | C |
| 36 | A5 | 2945 | G |
| 36 | A5 | 2947 | G |
| 36 | A5 | 2954 | U |
| 36 | A5 | 2957 | G |
| 36 | A5 | 2970 | C |
| 36 | A5 | 2971 | A |
| 36 | A5 | 2972 | G |
| 36 | A5 | 2979 | U |
| 36 | A5 | 2983 | C |
| 36 | A5 | 2987 | A |
| 36 | A5 | 2990 | G |
| 36 | A5 | 2996 | U |
| 36 | A5 | 2997 | G |
| 36 | A5 | 3012 | A |
| 36 | A5 | 3028 | G |
| 36 | A5 | 3050 | U |
| 36 | A5 | 3056 | U |
| 36 | A5 | 3057 | U |
| 36 | A5 | 3059 | G |
| 36 | A5 | 3078 | U |
| 36 | A5 | 3079 | U |
| 36 | A5 | 3080 | G |
| 36 | A5 | 3086 | A |
| 36 | A5 | 3087 | A |
| 36 | A5 | 3092 | C |
| 36 | A5 | 3130 | A |
| 36 | A5 | 3131 | U |
| 36 | A5 | 3139 | A |
| 36 | A5 | 3142 | A |
| 36 | A5 | 3143 | C |
| 36 | A5 | 3148 | U |
| 36 | A5 | 3153 | U |
| 36 | A5 | 3154 | C |
| 36 | A5 | 3155 | U |
| 36 | A5 | 3156 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A5 | 3157 | U |
| 36 | A5 | 3158 | G |
| 36 | A5 | 3159 | C |
| 36 | A5 | 3164 | C |
| 36 | A5 | 3165 | A |
| 36 | A5 | 3166 | C |
| 36 | A5 | 3168 | A |
| 36 | A5 | 3171 | U |
| 36 | A5 | 3172 | A |
| 36 | A5 | 3173 | G |
| 36 | A5 | 3174 | A |
| 36 | A5 | 3175 | U |
| 36 | A5 | 3176 | G |
| 36 | A5 | 3177 | G |
| 36 | A5 | 3179 | U |
| 36 | A5 | 3180 | A |
| 36 | A5 | 3181 | C |
| 36 | A5 | 3187 | A |
| 36 | A5 | 3195 | U |
| 36 | A5 | 3196 | U |
| 36 | A5 | 3207 | U |
| 36 | A5 | 3217 | C |
| 36 | A5 | 3218 | A |
| 36 | A5 | 3219 | G |
| 36 | A5 | 3222 | U |
| 36 | A5 | 3223 | A |
| 36 | A5 | 3224 | G |
| 36 | A5 | 3227 | A |
| 36 | A5 | 3229 | G |
| 36 | A5 | 3238 | G |
| 36 | A5 | 3245 | A |
| 36 | A5 | 3246 | G |
| 36 | A5 | 3247 | G |
| 36 | A5 | 3251 | U |
| 36 | A5 | 3253 | G |
| 36 | A5 | 3259 | U |
| 36 | A5 | 3260 | G |
| 36 | A5 | 3269 | U |
| 36 | A5 | 3270 | U |
| 36 | A5 | 3273 | A |
| 36 | A5 | 3275 | U |
| 36 | A5 | 3276 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A5 | 3277 | U |
| 36 | A5 | 3279 | A |
| 36 | A5 | 3280 | U |
| 36 | A5 | 3282 | U |
| 36 | A5 | 3284 | G |
| 36 | A5 | 3285 | C |
| 36 | A5 | 3286 | G |
| 36 | A5 | 3288 | G |
| 36 | A5 | 3289 | G |
| 36 | A5 | 3290 | G |
| 36 | A5 | 3292 | A |
| 36 | A5 | 3294 | A |
| 36 | A5 | 3304 | U |
| 36 | A5 | 3307 | A |
| 36 | A5 | 3313 | U |
| 36 | A5 | 3316 | A |
| 36 | A5 | 3317 | U |
| 36 | A5 | 3318 | G |
| 36 | A5 | 3319 | U |
| 36 | A5 | 3320 | A |
| 36 | A5 | 3330 | A |
| 36 | A5 | 3333 | G |
| 36 | A5 | 3335 | A |
| 36 | A5 | 3336 | A |
| 36 | A5 | 3341 | U |
| 36 | A5 | 3342 | A |
| 36 | A5 | 3343 | G |
| 36 | A5 | 3345 | G |
| 36 | A5 | 3349 | C |
| 36 | A5 | 3351 | U |
| 36 | A5 | 3352 | U |
| 36 | A5 | 3354 | U |
| 36 | A5 | 3355 | U |
| 36 | A5 | 3356 | G |
| 36 | A5 | 3357 | U |
| 36 | A5 | 3358 | U |
| 36 | A5 | 3369 | G |
| 36 | A5 | 3378 | C |
| 36 | A5 | 3382 | U |
| 36 | A5 | 3383 | G |
| 36 | A5 | 3389 | U |
| 36 | A5 | 3390 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A5 | 3393 | U |
| 36 | A5 | 3396 | U |
| 37 | A7 | 7 | G |
| 37 | A7 | 22 | A |
| 37 | A7 | 27 | A |
| 37 | A7 | 33 | U |
| 37 | A7 | 38 | U |
| 37 | A7 | 42 | A |
| 37 | A7 | 54 | U |
| 37 | A7 | 61 | G |
| 37 | A7 | 65 | G |
| 37 | A7 | 66 | A |
| 37 | A7 | 73 | C |
| 37 | A7 | 74 | C |
| 37 | A7 | 93 | C |
| 37 | A7 | 101 | G |
| 37 | A7 | 102 | A |
| 37 | A7 | 103 | A |
| 37 | A7 | 104 | A |
| 37 | A7 | 112 | G |
| 38 | A8 | 21 | C |
| 38 | A8 | 34 | U |
| 38 | A8 | 35 | C |
| 38 | A8 | 48 | A |
| 38 | A8 | 52 | A |
| 38 | A8 | 53 | A |
| 38 | A8 | 59 | A |
| 38 | A8 | 62 | C |
| 38 | A8 | 63 | G |
| 38 | A8 | 79 | A |
| 38 | A8 | 80 | A |
| 38 | A8 | 81 | U |
| 38 | A8 | 83 | C |
| 38 | A8 | 84 | C |
| 38 | A8 | 86 | U |
| 38 | A8 | 87 | G |
| 38 | A8 | 90 | U |
| 38 | A8 | 95 | G |
| 38 | A8 | 104 | A |
| 38 | A8 | 105 | A |
| 38 | A8 | 106 | C |
| 38 | A8 | 111 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 38 | A8 | 113 | U |
| 38 | A8 | 122 | U |
| 38 | A8 | 125 | U |
| 38 | A8 | 126 | A |
| 38 | A8 | 127 | U |
| 38 | A8 | 138 | A |
| 38 | A8 | 152 | G |
| 38 | A8 | 156 | U |
| 38 | A8 | 157 | U |
| 38 | A8 | 158 | U |

All (413) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A2 | 2 | A |
| 1 | A2 | 25 | C |
| 1 | A2 | 45 | U |
| 1 | A2 | 68 | A |
| 1 | A2 | 73 | U |
| 1 | A2 | 74 | U |
| 1 | A2 | 76 | A |
| 1 | A2 | 103 | A |
| 1 | A2 | 114 | C |
| 1 | A2 | 126 | A |
| 1 | A2 | 130 | C |
| 1 | A2 | 131 | C |
| 1 | A2 | 132 | U |
| 1 | A2 | 133 | U |
| 1 | A2 | 136 | C |
| 1 | A2 | 139 | C |
| 1 | A2 | 144 | U |
| 1 | A2 | 158 | U |
| 1 | A2 | 187 | G |
| 1 | A2 | 217 | A |
| 1 | A2 | 218 | A |
| 1 | A2 | 232 | U |
| 1 | A2 | 239 | C |
| 1 | A2 | 240 | U |
| 1 | A2 | 278 | U |
| 1 | A2 | 280 | U |
| 1 | A2 | 320 | U |
| 1 | A2 | 400 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A2 | 417 | A |
| 1 | A2 | 484 | C |
| 1 | A2 | 495 | C |
| 1 | A2 | 497 | G |
| 1 | A2 | 498 | G |
| 1 | A2 | 499 | U |
| 1 | A2 | 501 | U |
| 1 | A2 | 503 | G |
| 1 | A2 | 507 | U |
| 1 | A2 | 512 | A |
| 1 | A2 | 542 | A |
| 1 | A2 | 543 | C |
| 1 | A2 | 555 | A |
| 1 | A2 | 558 | U |
| 1 | A2 | 582 | U |
| 1 | A2 | 685 | A |
| 1 | A2 | 704 | C |
| 1 | A2 | 720 | G |
| 1 | A2 | 721 | U |
| 1 | A2 | 734 | A |
| 1 | A2 | 755 | A |
| 1 | A2 | 781 | U |
| 1 | A2 | 782 | U |
| 1 | A2 | 794 | U |
| 1 | A2 | 811 | A |
| 1 | A2 | 815 | G |
| 1 | A2 | 819 | G |
| 1 | A2 | 823 | G |
| 1 | A2 | 829 | A |
| 1 | A2 | 913 | G |
| 1 | A2 | 1051 | G |
| 1 | A2 | 1058 | U |
| 1 | A2 | 1081 | A |
| 1 | A2 | 1137 | A |
| 1 | A2 | 1157 | A |
| 1 | A2 | 1187 | U |
| 1 | A2 | 1195 | C |
| 1 | A2 | 1196 | A |
| 1 | A2 | 1207 | C |
| 1 | A2 | 1226 | A |
| 1 | A2 | 1234 | A |
| 1 | A2 | 1244 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A2 | 1250 | U |
| 1 | A2 | 1339 | C |
| 1 | A2 | 1344 | A |
| 1 | A2 | 1370 | U |
| 1 | A2 | 1428 | G |
| 1 | A2 | 1481 | C |
| 1 | A2 | 1489 | U |
| 1 | A2 | 1490 | C |
| 1 | A2 | 1521 | G |
| 1 | A2 | 1568 | C |
| 1 | A2 | 1572 | G |
| 1 | A2 | 1573 | A |
| 1 | A2 | 1615 | C |
| 1 | A2 | 1657 | U |
| 1 | A2 | 1711 | C |
| 1 | A2 | 1761 | U |
| 36 | A1 | 13 | A |
| 36 | A1 | 43 | A |
| 36 | A1 | 65 | A |
| 36 | A1 | 99 | A |
| 36 | A1 | 169 | U |
| 36 | A1 | 210 | U |
| 36 | A1 | 223 | U |
| 36 | A1 | 239 | G |
| 36 | A1 | 282 | G |
| 36 | A1 | 397 | A |
| 36 | A1 | 439 | C |
| 36 | A1 | 517 | G |
| 36 | A1 | 547 | G |
| 36 | A1 | 558 | U |
| 36 | A1 | 588 | G |
| 36 | A1 | 594 | U |
| 36 | A1 | 619 | A |
| 36 | A1 | 620 | U |
| 36 | A1 | 637 | C |
| 36 | A1 | 648 | C |
| 36 | A1 | 715 | A |
| 36 | A1 | 719 | U |
| 36 | A1 | 726 | G |
| 36 | A1 | 763 | G |
| 36 | A1 | 764 | U |
| 36 | A1 | 816 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A1 | 873 | C |
| 36 | A1 | 896 | A |
| 36 | A1 | 908 | G |
| 36 | A1 | 916 | G |
| 36 | A1 | 979 | U |
| 36 | A1 | 981 | U |
| 36 | A1 | 993 | G |
| 36 | A1 | 1015 | U |
| 36 | A1 | 1017 | C |
| 36 | A1 | 1064 | A |
| 36 | A1 | 1094 | U |
| 36 | A1 | 1097 | G |
| 36 | A1 | 1103 | A |
| 36 | A1 | 1152 | G |
| 36 | A1 | 1222 | G |
| 36 | A1 | 1241 | U |
| 36 | A1 | 1273 | A |
| 36 | A1 | 1307 | G |
| 36 | A1 | 1317 | A |
| 36 | A1 | 1329 | U |
| 36 | A1 | 1331 | U |
| 36 | A1 | 1352 | A |
| 36 | A1 | 1355 | A |
| 36 | A1 | 1481 | A |
| 36 | A1 | 1484 | U |
| 36 | A1 | 1507 | G |
| 36 | A1 | 1554 | U |
| 36 | A1 | 1556 | C |
| 36 | A1 | 1562 | C |
| 36 | A1 | 1568 | U |
| 36 | A1 | 1580 | A |
| 36 | A1 | 1582 | C |
| 36 | A1 | 1589 | A |
| 36 | A1 | 1607 | U |
| 36 | A1 | 1716 | U |
| 36 | A1 | 1751 | G |
| 36 | A1 | 1778 | G |
| 36 | A1 | 1815 | U |
| 36 | A1 | 1816 | A |
| 36 | A1 | 1820 | U |
| 36 | A1 | 1841 | A |
| 36 | A1 | 1842 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A1 | 1846 | C |
| 36 | A1 | 1849 | C |
| 36 | A1 | 2101 | C |
| 36 | A1 | 2112 | U |
| 36 | A1 | 2116 | G |
| 36 | A1 | 2209 | U |
| 36 | A1 | 2227 | C |
| 36 | A1 | 2249 | G |
| 36 | A1 | 2281 | A |
| 36 | A1 | 2372 | A |
| 36 | A1 | 2373 | A |
| 36 | A1 | 2374 | C |
| 36 | A1 | 2403 | G |
| 36 | A1 | 2418 | G |
| 36 | A1 | 2501 | U |
| 36 | A1 | 2513 | U |
| 36 | A1 | 2522 | G |
| 36 | A1 | 2525 | G |
| 36 | A1 | 2537 | U |
| 36 | A1 | 2538 | U |
| 36 | A1 | 2541 | U |
| 36 | A1 | 2552 | C |
| 36 | A1 | 2554 | A |
| 36 | A1 | 2585 | G |
| 36 | A1 | 2593 | A |
| 36 | A1 | 2689 | A |
| 36 | A1 | 2704 | A |
| 36 | A1 | 2728 | G |
| 36 | A1 | 2752 | U |
| 36 | A1 | 2772 | C |
| 36 | A1 | 2801 | A |
| 36 | A1 | 2817 | A |
| 36 | A1 | 2818 | U |
| 36 | A1 | 2867 | C |
| 36 | A1 | 2887 | A |
| 36 | A1 | 2896 | A |
| 36 | A1 | 3056 | U |
| 36 | A1 | 3078 | U |
| 36 | A1 | 3121 | U |
| 36 | A1 | 3139 | A |
| 36 | A1 | 3156 | U |
| 36 | A1 | 3169 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A1 | 3195 | U |
| 36 | A1 | 3207 | U |
| 36 | A1 | 3217 | C |
| 36 | A1 | 3218 | A |
| 36 | A1 | 3228 | C |
| 36 | A1 | 3242 | G |
| 36 | A1 | 3269 | U |
| 36 | A1 | 3275 | U |
| 36 | A1 | 3276 | G |
| 36 | A1 | 3316 | A |
| 36 | A1 | 3317 | U |
| 36 | A1 | 3319 | U |
| 36 | A1 | 3330 | A |
| 36 | A1 | 3350 | C |
| 36 | A1 | 3351 | U |
| 36 | A1 | 3353 | G |
| 36 | A1 | 3375 | A |
| 37 | A3 | 13 | A |
| 37 | A3 | 41 | G |
| 37 | A3 | 52 | G |
| 38 | A4 | 82 | U |
| 38 | A4 | 85 | G |
| 38 | A4 | 111 | A |
| 38 | A4 | 125 | U |
| 38 | A4 | 157 | U |
| 80 | A6 | 25 | C |
| 80 | A6 | 66 | U |
| 80 | A6 | 72 | A |
| 80 | A6 | 75 | U |
| 80 | A6 | 76 | A |
| 80 | A6 | 103 | A |
| 80 | A6 | 114 | C |
| 80 | A6 | 136 | C |
| 80 | A6 | 139 | C |
| 80 | A6 | 158 | U |
| 80 | A6 | 187 | G |
| 80 | A6 | 217 | A |
| 80 | A6 | 240 | U |
| 80 | A6 | 249 | U |
| 80 | A6 | 272 | U |
| 80 | A6 | 277 | U |
| 80 | A6 | 352 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 80 | A6 | 400 | A |
| 80 | A6 | 417 | A |
| 80 | A6 | 468 | A |
| 80 | A6 | 512 | A |
| 80 | A6 | 542 | A |
| 80 | A6 | 543 | C |
| 80 | A6 | 555 | A |
| 80 | A6 | 557 | G |
| 80 | A6 | 558 | U |
| 80 | A6 | 647 | G |
| 80 | A6 | 651 | G |
| 80 | A6 | 678 | A |
| 80 | A6 | 681 | U |
| 80 | A6 | 695 | U |
| 80 | A6 | 697 | C |
| 80 | A6 | 717 | C |
| 80 | A6 | 755 | A |
| 80 | A6 | 811 | A |
| 80 | A6 | 815 | G |
| 80 | A6 | 829 | A |
| 80 | A6 | 834 | G |
| 80 | A6 | 1051 | G |
| 80 | A6 | 1058 | U |
| 80 | A6 | 1081 | A |
| 80 | A6 | 1097 | U |
| 80 | A6 | 1098 | U |
| 80 | A6 | 1196 | A |
| 80 | A6 | 1227 | A |
| 80 | A6 | 1238 | A |
| 80 | A6 | 1244 | A |
| 80 | A6 | 1255 | G |
| 80 | A6 | 1344 | A |
| 80 | A6 | 1481 | C |
| 80 | A6 | 1490 | C |
| 80 | A6 | 1491 | U |
| 80 | A6 | 1535 | U |
| 80 | A6 | 1568 | C |
| 80 | A6 | 1572 | G |
| 80 | A6 | 1573 | A |
| 80 | A6 | 1615 | C |
| 80 | A6 | 1620 | C |
| 80 | A6 | 1637 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 80 | A6 | 1657 | U |
| 36 | A5 | 43 | A |
| 36 | A5 | 65 | A |
| 36 | A5 | 93 | C |
| 36 | A5 | 151 | A |
| 36 | A5 | 169 | U |
| 36 | A5 | 183 | G |
| 36 | A5 | 217 | U |
| 36 | A5 | 238 | A |
| 36 | A5 | 282 | G |
| 36 | A5 | 397 | A |
| 36 | A5 | 436 | A |
| 36 | A5 | 438 | A |
| 36 | A5 | 439 | C |
| 36 | A5 | 545 | U |
| 36 | A5 | 546 | C |
| 36 | A5 | 588 | G |
| 36 | A5 | 611 | A |
| 36 | A5 | 619 | A |
| 36 | A5 | 647 | A |
| 36 | A5 | 705 | A |
| 36 | A5 | 715 | A |
| 36 | A5 | 719 | U |
| 36 | A5 | 726 | G |
| 36 | A5 | 735 | A |
| 36 | A5 | 765 | C |
| 36 | A5 | 786 | A |
| 36 | A5 | 816 | A |
| 36 | A5 | 873 | C |
| 36 | A5 | 896 | A |
| 36 | A5 | 908 | G |
| 36 | A5 | 916 | G |
| 36 | A5 | 937 | G |
| 36 | A5 | 979 | U |
| 36 | A5 | 993 | G |
| 36 | A5 | 1027 | A |
| 36 | A5 | 1033 | U |
| 36 | A5 | 1064 | A |
| 36 | A5 | 1081 | U |
| 36 | A5 | 1085 | A |
| 36 | A5 | 1094 | U |
| 36 | A5 | 1152 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A5 | 1181 | U |
| 36 | A5 | 1192 | C |
| 36 | A5 | 1222 | G |
| 36 | A5 | 1236 | G |
| 36 | A5 | 1238 | C |
| 36 | A5 | 1239 | C |
| 36 | A5 | 1241 | U |
| 36 | A5 | 1284 | C |
| 36 | A5 | 1307 | G |
| 36 | A5 | 1317 | A |
| 36 | A5 | 1329 | U |
| 36 | A5 | 1331 | U |
| 36 | A5 | 1352 | A |
| 36 | A5 | 1355 | A |
| 36 | A5 | 1434 | G |
| 36 | A5 | 1481 | A |
| 36 | A5 | 1507 | G |
| 36 | A5 | 1514 | G |
| 36 | A5 | 1554 | U |
| 36 | A5 | 1560 | G |
| 36 | A5 | 1568 | U |
| 36 | A5 | 1574 | C |
| 36 | A5 | 1580 | A |
| 36 | A5 | 1589 | A |
| 36 | A5 | 1607 | U |
| 36 | A5 | 1716 | U |
| 36 | A5 | 1724 | U |
| 36 | A5 | 1815 | U |
| 36 | A5 | 1816 | A |
| 36 | A5 | 1817 | G |
| 36 | A5 | 1819 | U |
| 36 | A5 | 1841 | A |
| 36 | A5 | 1842 | A |
| 36 | A5 | 1849 | C |
| 36 | A5 | 1878 | G |
| 36 | A5 | 1879 | A |
| 36 | A5 | 2101 | C |
| 36 | A5 | 2112 | U |
| 36 | A5 | 2116 | G |
| 36 | A5 | 2204 | C |
| 36 | A5 | 2209 | U |
| 36 | A5 | 2249 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | A5 | 2255 | A |
| 36 | A5 | 2257 | C |
| 36 | A5 | 2372 | A |
| 36 | A5 | 2374 | C |
| 36 | A5 | 2440 | G |
| 36 | A5 | 2507 | C |
| 36 | A5 | 2513 | U |
| 36 | A5 | 2531 | C |
| 36 | A5 | 2537 | U |
| 36 | A5 | 2539 | C |
| 36 | A5 | 2583 | C |
| 36 | A5 | 2585 | G |
| 36 | A5 | 2593 | A |
| 36 | A5 | 2662 | G |
| 36 | A5 | 2682 | C |
| 36 | A5 | 2689 | A |
| 36 | A5 | 2714 | G |
| 36 | A5 | 2728 | G |
| 36 | A5 | 2752 | U |
| 36 | A5 | 2772 | C |
| 36 | A5 | 2777 | G |
| 36 | A5 | 2801 | A |
| 36 | A5 | 2817 | A |
| 36 | A5 | 2818 | U |
| 36 | A5 | 2887 | A |
| 36 | A5 | 2896 | A |
| 36 | A5 | 2970 | C |
| 36 | A5 | 2971 | A |
| 36 | A5 | 2996 | U |
| 36 | A5 | 3056 | U |
| 36 | A5 | 3078 | U |
| 36 | A5 | 3154 | C |
| 36 | A5 | 3155 | U |
| 36 | A5 | 3167 | A |
| 36 | A5 | 3195 | U |
| 36 | A5 | 3218 | A |
| 36 | A5 | 3228 | C |
| 36 | A5 | 3259 | U |
| 36 | A5 | 3269 | U |
| 36 | A5 | 3275 | U |
| 36 | A5 | 3289 | G |
| 36 | A5 | 3317 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 36 | A5 | 3330 | A |
| 36 | A5 | 3340 | G |
| 36 | A5 | 3341 | U |
| 36 | A5 | 3357 | U |
| 38 | A8 | 111 | A |
| 38 | A8 | 126 | A |
| 38 | A8 | 156 | U |

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3566 ligands modelled in this entry, 2221 are monoatomic - leaving 1345 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 86 | OHX | A5 | 3806 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | A3 | 206 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | A1 | 3431 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | A1 | 3507 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | A6 | 1997 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | A5 | 3813 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | A1 | 3612 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | A1 | 3511 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | A5 | 3726 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | A5 | 3662 | - | 0,6,6 | - | - | - | | |
| 86 | OHX | A5 | 3471 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | A5 | 3690 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1967 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3554 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3633 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3674 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1913 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3765 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3609 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3786 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3589 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3568 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3805 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3632 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1912 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | CY | 202 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | De | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3567 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3438 | 86 | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1984 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2050 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3417 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2025 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1998 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3758 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2016 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3450 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3488 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1944 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1989 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3489 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3760 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1962 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3452 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3611 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1911 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3448 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3786 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2013 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A8 | 205 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3574 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3480 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3654 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | Bj | 103 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | A5 | 3815 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3703 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | AP | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2075 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3580 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3559 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3596 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3425 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2059 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | AC | 301 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | Bo | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3457 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2044 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3418 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3762 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2023 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3705 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1957 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | Bj | 102 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3801 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3732 | 36 | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A4 | 209 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | AN | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3761 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3606 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1903 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | DM | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3728 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3670 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3644 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3745 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3682 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3822 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3432 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1952 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2027 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3488 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3439 | 86 | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3534 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3759 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3636 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2062 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3717 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | A8 | 213 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1959 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2085 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2090 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3496 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3532 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3564 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1993 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1921 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2065 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3446 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3773 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3699 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3434 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1915 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1916 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3631 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3629 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3682 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A8 | 203 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1928 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2017 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2058 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1908 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2068 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1950 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1948 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3762 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3404 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3517 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3719 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3473 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3449 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3543 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3565 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1940 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1974 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1956 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2083 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3520 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2038 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3694 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3697 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | A5 | 3774 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2086 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3482 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A3 | 209 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3559 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3451 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2039 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3808 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2014 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3585 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3621 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3750 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3545 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3763 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3671 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3422 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3617 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3769 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2055 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3809 | 86 | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3706 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1972 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A4 | 208 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A4 | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3689 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3808 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1958 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3791 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1919 | 86 | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2021 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3685 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3525 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2052 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3718 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3450 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3748 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3823 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1992 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3462 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3540 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3655 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3791 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2045 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | A1 | 3678 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3563 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3744 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1912 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3618 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1922 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1990 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2002 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3517 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3625 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1910 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1992 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2078 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A4 | 213 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2098 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3455 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3579 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3770 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3499 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | BB | 401 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3709 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3710 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3789 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3659 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | Db | 101 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3540 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2035 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3689 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3792 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3734 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3526 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2012 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3740 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | Dj | 104 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | DJ | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3608 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3673 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3725 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3612 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3625 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3753 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1939 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3768 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | A6 | 2016 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3603 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3426 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3796 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1920 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1947 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1907 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | CL | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3627 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3666 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1973 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3526 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3560 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2028 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1903 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3496 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1943 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | AI | 301 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3628 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1978 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | Do | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3690 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2026 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3456 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2085 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3792 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3734 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | Dg | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3667 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2001 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1918 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3583 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3566 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A7 | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2071 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A8 | 202 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2018 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2049 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3607 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3683 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1997 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3755 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3452 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | A2 | 1926 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3705 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3512 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | AL | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3464 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3777 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3746 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3647 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1914 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3726 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3622 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3665 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3527 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3714 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3624 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3628 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2077 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3467 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3585 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3813 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3755 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3801 | 86 | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3487 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3539 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3575 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3805 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3557 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3597 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3441 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1953 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2082 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3409 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3424 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3499 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2041 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3688 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3720 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3423 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3490 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3472 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3639 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2004 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1954 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | A2 | 2047 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3800 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3614 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3549 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3749 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3776 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2032 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3580 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3530 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3620 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3512 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3616 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3696 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3501 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3665 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3636 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2069 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3788 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2073 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3521 | 86 | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2031 | - | 0,5,6 | - | - | - | - | - |
| 86 | OHX | DO | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3472 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3444 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1981 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3757 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A7 | 211 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3613 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3422 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A7 | 207 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A8 | 219 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1946 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3623 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3441 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3704 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1924 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3530 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2023 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3604 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3642 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2005 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3715 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3694 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | A6 | 2080 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3503 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1991 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3536 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3415 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3401 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2011 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3778 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3787 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1987 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1986 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3520 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3534 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3747 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3779 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1955 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1964 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1902 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3454 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3643 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3637 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2093 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3750 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1947 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3458 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3481 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3691 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3508 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3546 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3653 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3649 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3697 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3504 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3537 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3597 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3565 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3677 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3685 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1935 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3602 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3599 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3769 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3721 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | CB | 301 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3710 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3586 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3481 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3506 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2015 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3550 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1909 | 86 | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3739 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A4 | 203 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3429 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3802 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A4 | 207 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1917 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3556 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1906 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | BB | 402 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3555 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2015 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3474 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1941 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3640 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3735 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3662 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3408 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1967 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2033 | 86 | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3480 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3420 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3748 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1925 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | CG | 301 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2050 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1977 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3680 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3752 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3515 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2096 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1990 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1968 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3707 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3497 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1994 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | BD | 301 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3795 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3455 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1962 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1951 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3608 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3698 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A7 | 206 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3447 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3802 | 86,36 | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3476 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3516 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | DR | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3601 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3709 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3491 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3810 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3812 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A3 | 208 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3730 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3626 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3587 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3418 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3648 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1957 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3641 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | DC | 401 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3814 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1970 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3756 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3736 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3577 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3475 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2062 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3650 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3414 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3493 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2051 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3575 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3646 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3518 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3586 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3495 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | A1 | 3562 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A7 | 205 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1927 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2099 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3470 | 86 | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3494 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3778 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2068 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | BO | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3639 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1950 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A8 | 217 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3661 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3500 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3464 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3811 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3584 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2022 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2060 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3654 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3556 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3407 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1901 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2074 | 1 | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3566 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3535 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | BP | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3477 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3818 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3402 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3600 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3656 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2054 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3723 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2039 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | Cd | 101 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2041 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3757 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3466 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3486 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2049 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3649 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2046 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | A5 | 3469 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1949 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3467 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A7 | 203 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2055 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3756 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2073 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3784 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3430 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3698 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2029 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3779 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3651 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3794 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3793 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2061 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3620 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3811 | 36 | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3461 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3538 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3722 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3605 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3632 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3501 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3522 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3790 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1961 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3423 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3535 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3505 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | DB | 401 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3411 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2076 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1942 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3443 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3687 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2078 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2048 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3660 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3693 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A7 | 213 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3513 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3814 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | A1 | 3492 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2024 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3722 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3588 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1936 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3433 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1922 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2002 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3785 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3669 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3796 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | DI | 302 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | DD | 301 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1902 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1982 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | Bj | 101 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3788 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1964 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | CI | 301 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A8 | 211 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3623 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3544 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3542 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3752 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3681 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1999 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A7 | 208 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3675 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1988 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3468 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3541 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2094 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3519 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3679 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3711 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3522 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | CJ | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3695 | 36 | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3615 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3551 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3531 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3416 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1983 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | A1 | 3766 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3605 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3417 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3463 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3809 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3453 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3509 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3561 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1973 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3582 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3407 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2028 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2081 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2067 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2020 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1940 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1943 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3434 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1963 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1978 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1955 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3797 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3581 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3548 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3506 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3671 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3463 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2013 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3576 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3653 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A8 | 207 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2034 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3440 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3712 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2040 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | DG | 301 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1932 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3459 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3765 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3546 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | BR | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3640 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3821 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | A1 | 3515 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3615 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2042 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2044 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3578 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3804 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | BI | 304 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3510 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2040 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2006 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3569 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3738 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3435 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3549 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1926 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3439 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3478 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3561 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3686 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3602 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3782 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3521 | 86 | 0,6,6 | - | - | - | - | - |
| 86 | OHX | CN | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A8 | 204 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3516 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3553 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3431 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3634 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3611 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1944 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1917 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3781 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3446 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3804 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2066 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3576 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2079 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3476 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1996 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3462 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3772 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3780 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3634 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | A6 | 1953 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1931 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3498 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3729 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3655 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3413 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3570 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3618 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2065 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3706 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1975 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1934 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3664 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2047 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3747 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3558 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1905 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3572 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2086 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1929 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3643 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2087 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3693 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3730 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2036 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3603 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3533 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3754 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3412 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3767 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2060 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1938 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3626 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1981 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3803 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3562 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3807 | 86 | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3426 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | DC | 402 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1921 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2088 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3785 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2037 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | A5 | 3502 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2072 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3684 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1916 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3780 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A8 | 218 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3475 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1933 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3725 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3607 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1958 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1923 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1937 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3533 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3466 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2011 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3629 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | Ad | 101 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3645 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A8 | 212 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3477 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2051 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3495 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3527 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A8 | 214 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3419 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3510 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3594 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3720 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3483 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3723 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1979 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1985 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2008 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3652 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2084 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | CP | 202 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3486 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2007 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3436 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3635 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3420 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3657 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | A1 | 3727 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3471 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | Dh | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3807 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3672 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3687 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3508 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3670 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1995 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1980 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1904 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3749 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3427 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3742 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2064 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3425 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | Ag | 401 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | BI | 301 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1959 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3790 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3594 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1935 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3746 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3445 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3647 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1966 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3609 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3519 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3701 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3768 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3657 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3714 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3727 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3708 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A8 | 210 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3469 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3438 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2058 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3737 | 86 | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2053 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3494 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3692 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3487 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | A5 | 3696 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3572 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3483 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | Bb | 101 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3428 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3590 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3523 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2000 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3435 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3436 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2038 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2056 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3708 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1930 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3672 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A3 | 207 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2029 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3816 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | DB | 402 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A4 | 214 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1977 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3645 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3574 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2014 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3799 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2033 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3415 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3663 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3583 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1968 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3445 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2063 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1945 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1994 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3763 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2089 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3541 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3761 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3669 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3658 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3737 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3578 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2095 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | A5 | 3798 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1976 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2021 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3692 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3741 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2019 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1942 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1960 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3613 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3630 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3713 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3460 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3797 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A4 | 204 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3433 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3563 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1965 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3638 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1969 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2009 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3681 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1939 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3564 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A3 | 202 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3582 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3550 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3717 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3456 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3401 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3695 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A3 | 205 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2022 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A4 | 215 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3673 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1907 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3524 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1931 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3468 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3525 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3787 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1915 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1914 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2045 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | A1 | 3770 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3437 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1976 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3789 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3427 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1952 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3449 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3637 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2046 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3816 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2010 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2091 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3595 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3610 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3543 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3798 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3509 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2012 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3806 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3776 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3739 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3622 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3630 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3621 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3403 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A3 | 213 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3591 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3659 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3764 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3599 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1913 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3529 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1971 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3729 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3781 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3547 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3641 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1984 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2025 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3478 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A8 | 220 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A7 | 209 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3555 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | A1 | 3474 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3803 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3666 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1989 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3514 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3783 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3764 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3610 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3799 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A4 | 210 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1949 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3573 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3820 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3718 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3453 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3528 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3547 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A4 | 212 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3619 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1987 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2075 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3680 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3545 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1966 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | CP | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2059 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3644 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1938 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3678 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3490 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3751 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | Cg | 401 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2030 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3498 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3721 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3667 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1961 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3552 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3724 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2076 | 86 | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3528 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3638 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1986 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | A2 | 2030 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3579 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1980 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3676 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3593 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3514 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3740 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3557 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | CG | 302 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2024 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A8 | 216 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1936 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1975 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2057 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3753 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3410 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2003 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1982 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3688 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2043 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A4 | 206 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3815 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3442 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A3 | 210 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1928 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3604 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3484 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1985 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | DP | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2008 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2070 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1905 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3592 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A3 | 212 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1948 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2036 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1988 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A7 | 202 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A7 | 204 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3539 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3704 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2081 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3424 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | A1 | 3482 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2092 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2083 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3421 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3652 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3518 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3552 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3724 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1954 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3744 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3470 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1974 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1956 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3502 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3465 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2035 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3538 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2084 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2037 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2069 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | CS | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3760 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3553 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3751 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A8 | 208 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1933 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3454 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3648 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3700 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2005 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3663 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3558 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1951 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3458 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3571 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3507 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3635 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2097 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1924 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3735 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3461 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2034 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3473 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | A2 | 1972 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3812 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3658 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3777 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1906 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2007 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1932 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3537 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1941 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3741 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3674 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3523 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1911 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3598 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3443 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A8 | 206 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3485 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3701 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3489 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3775 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2006 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | DH | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3691 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | BI | 303 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3683 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3590 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3713 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3451 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3413 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1999 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A4 | 202 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1971 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3554 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3428 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2018 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3460 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3491 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A3 | 211 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1930 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3598 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3405 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3568 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1960 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | A1 | 3429 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3617 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1925 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3588 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | DI | 301 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3716 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3485 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3775 | 86 | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2066 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | Df | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3573 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3793 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3616 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3493 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2056 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3745 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3771 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1998 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3677 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2043 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3767 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1909 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3731 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1918 | 86 | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3668 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3567 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1993 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3571 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3758 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1934 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | BI | 302 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3551 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1920 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1901 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3430 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3524 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3743 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3497 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3421 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3703 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2054 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | DA | 302 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3700 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | A5 | 3702 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2063 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3732 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3716 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A3 | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3595 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2026 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3531 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3733 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3783 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A7 | 210 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | DV | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1965 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3686 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | Bf | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3513 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3536 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2100 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3759 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2072 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A7 | 212 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2057 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3402 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3601 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2003 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3642 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3668 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3810 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2071 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2061 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3403 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1923 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3581 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1937 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3414 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | BT | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3444 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3447 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3795 | 86 | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3548 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3743 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3619 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1904 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | A5 | 3773 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2048 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2001 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A3 | 204 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3479 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1919 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2010 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A3 | 203 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3702 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | BA | 301 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3664 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1979 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2000 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3699 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2017 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1927 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3593 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3631 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2052 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1970 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3587 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A8 | 215 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2077 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | BN | 301 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3774 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3733 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3738 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3596 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3542 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1995 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2064 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | BP | 202 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3600 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3736 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3782 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2082 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3719 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3711 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3577 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A4 | 211 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3661 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2087 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3614 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | A5 | 3416 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3766 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3650 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3660 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | CY | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2258 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2004 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2053 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3675 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2032 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3624 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3479 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3707 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3511 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3784 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1945 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3606 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2027 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3505 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2074 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2031 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1908 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2067 | 86 | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3432 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2070 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3712 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1946 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3651 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3459 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1929 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3500 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3503 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3754 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2080 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1991 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A4 | 205 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3819 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3676 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3656 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3569 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2042 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3544 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2019 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | A1 | 3731 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3772 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3465 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A8 | 209 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1910 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3684 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1969 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2009 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3529 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3570 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3457 | 86 | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3794 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3592 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3646 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3484 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3591 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 1983 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | DQ | 201 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3442 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3679 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3728 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1963 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3440 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3504 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3627 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3419 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 2079 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3560 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3406 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3800 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A2 | 1996 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | BC | 401 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3532 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3742 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3584 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3633 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3437 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3817 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A6 | 2020 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3492 | 86 | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A1 | 3589 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3715 | - | 0,6,6 | - | - | - | - | - |
| 86 | OHX | A5 | 3448 | - | 0,6,6 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 86 | OHX | A5 | 3771 | - | 0,6,6 | - | - | - | - | - |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

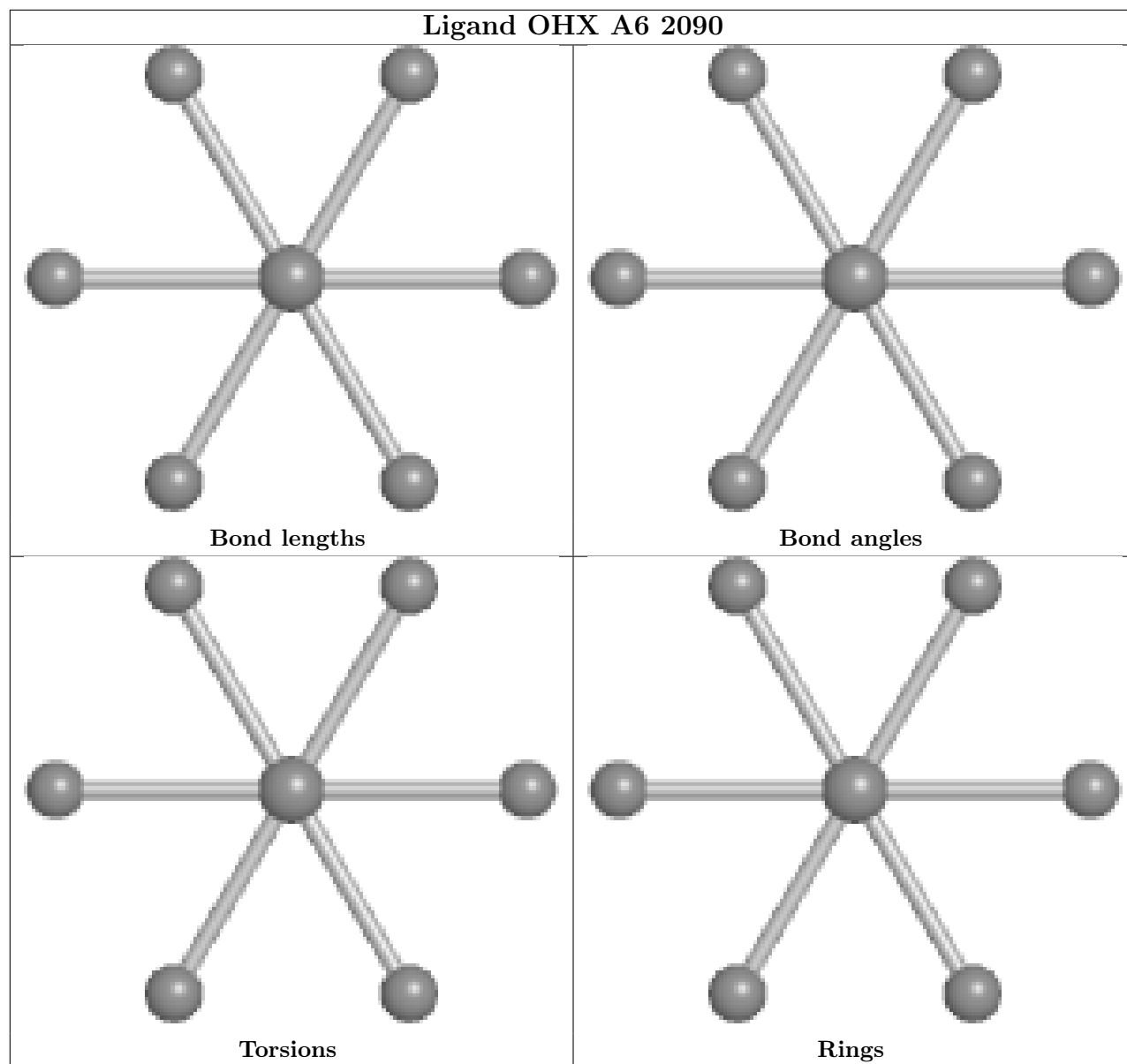
There are no torsion outliers.

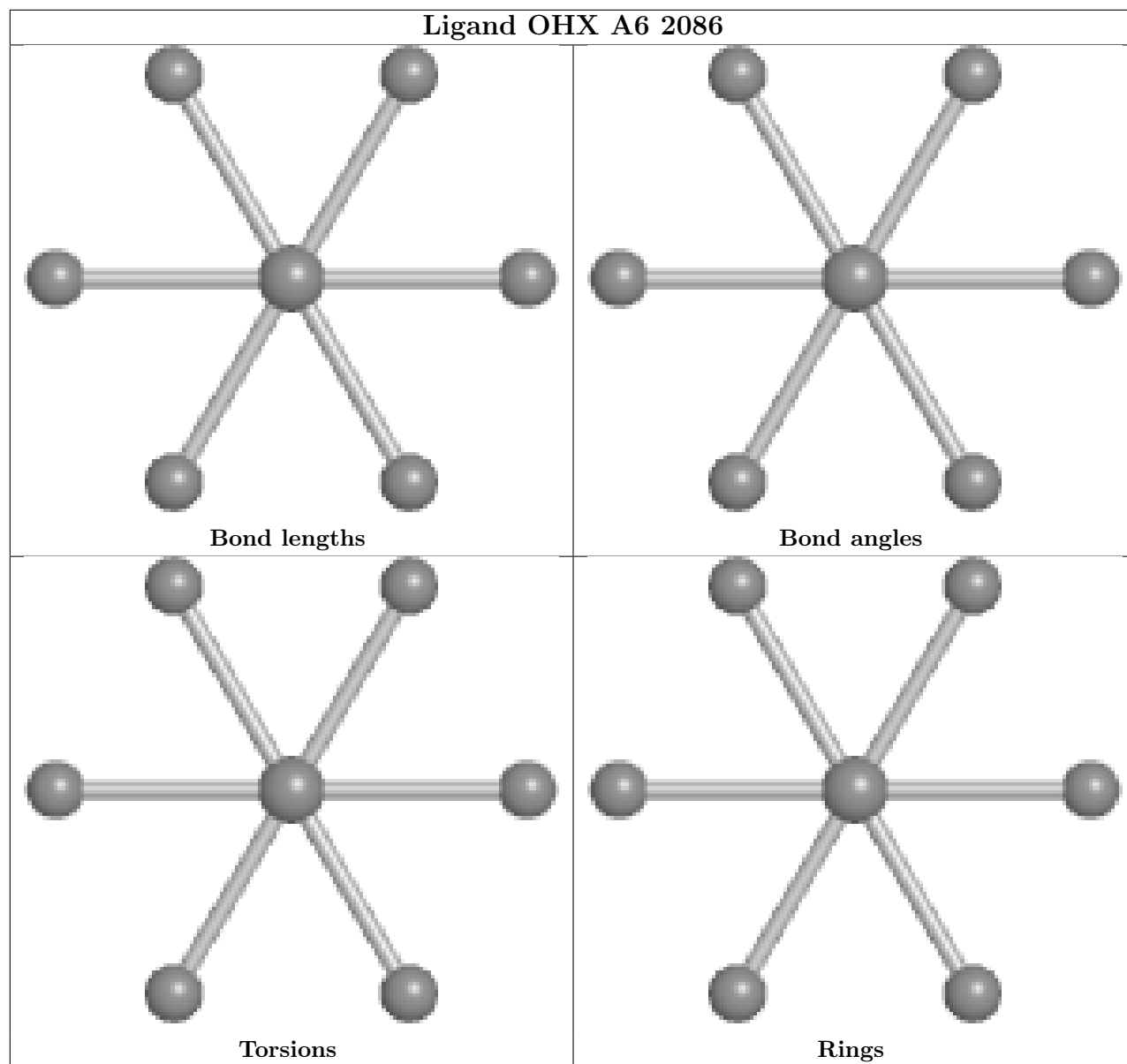
There are no ring outliers.

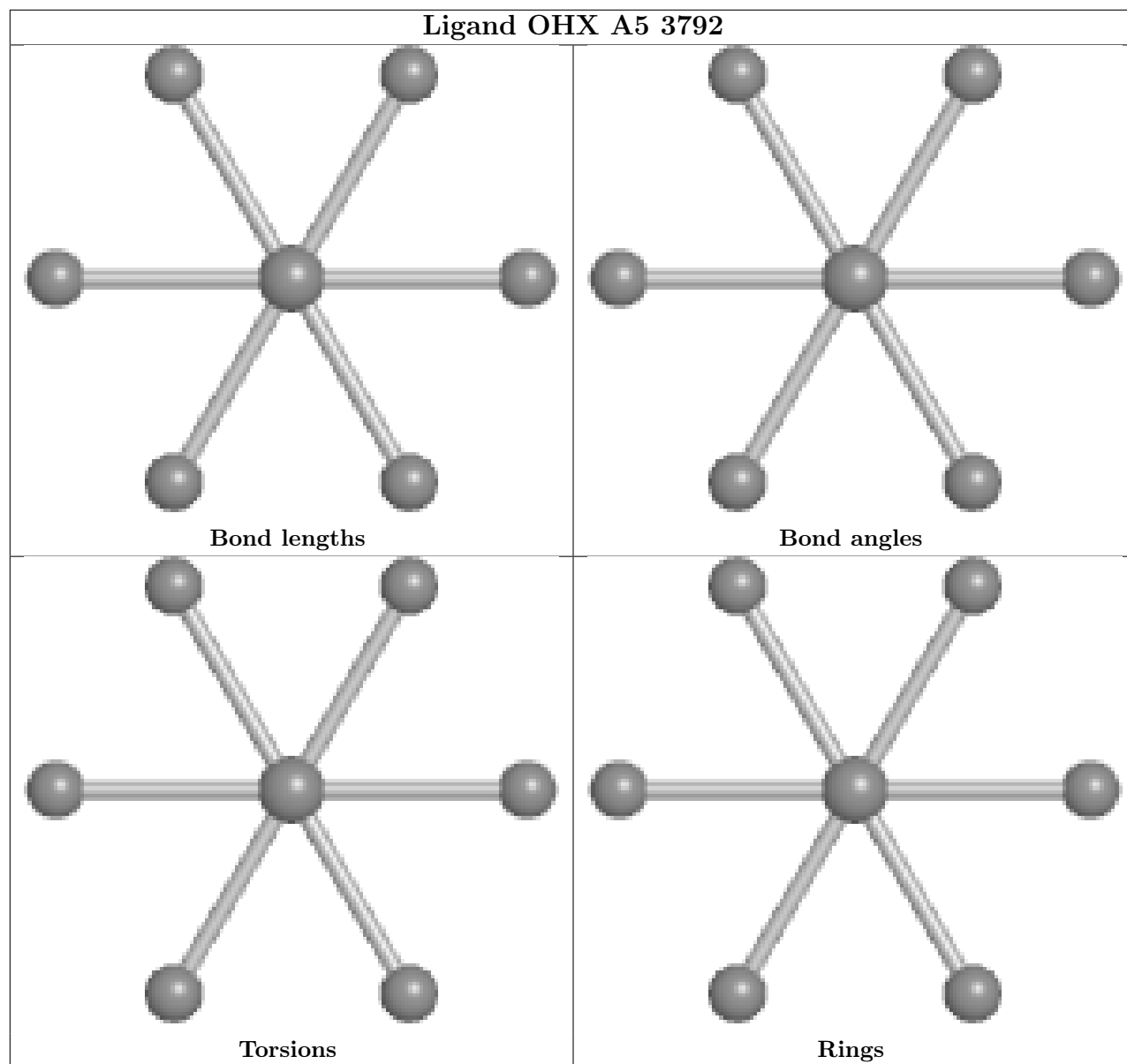
2 monomers are involved in 2 short contacts:

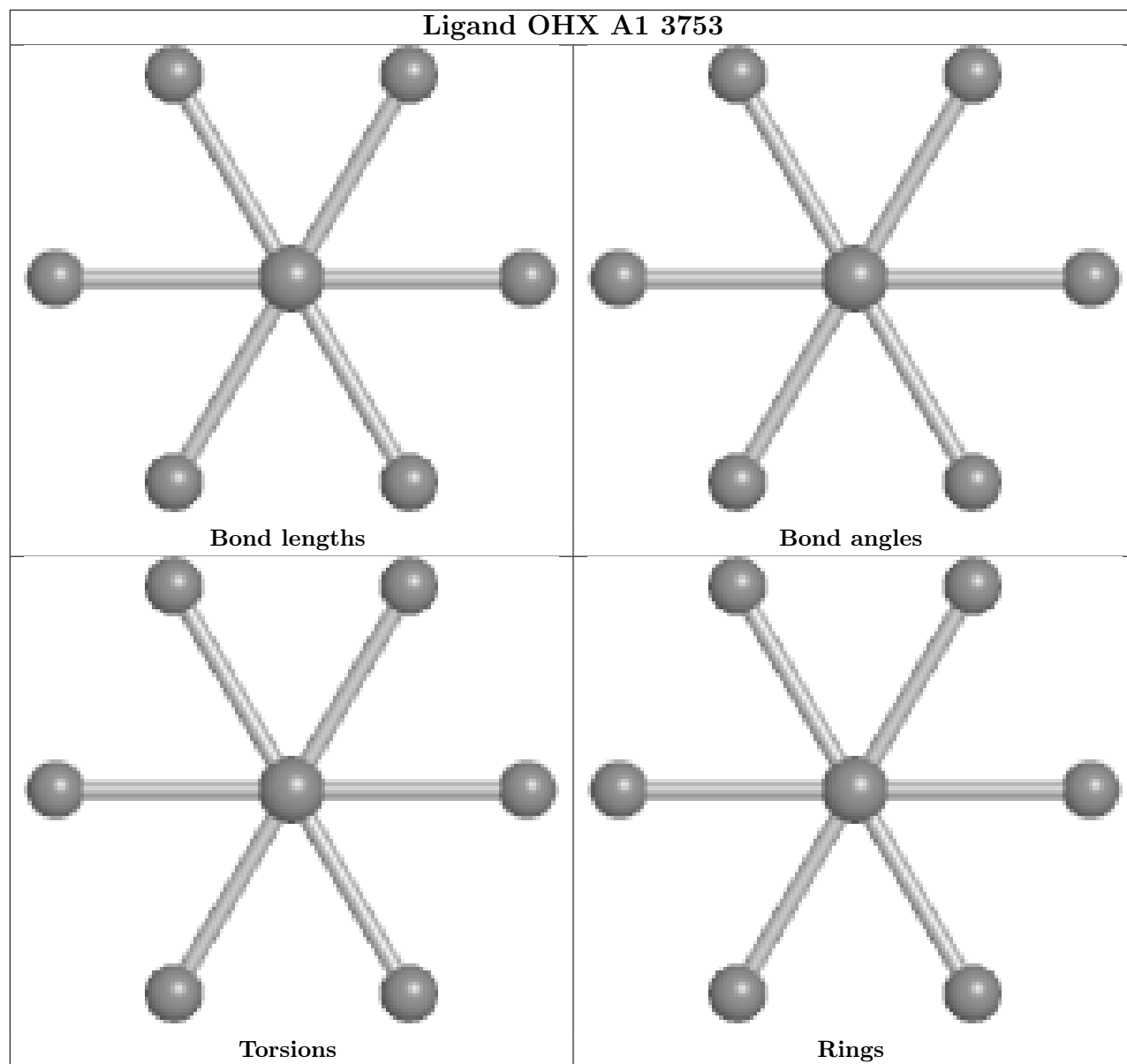
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 86 | CG | 301 | OHX | 0 | 1 |
| 86 | A1 | 3788 | OHX | 0 | 1 |

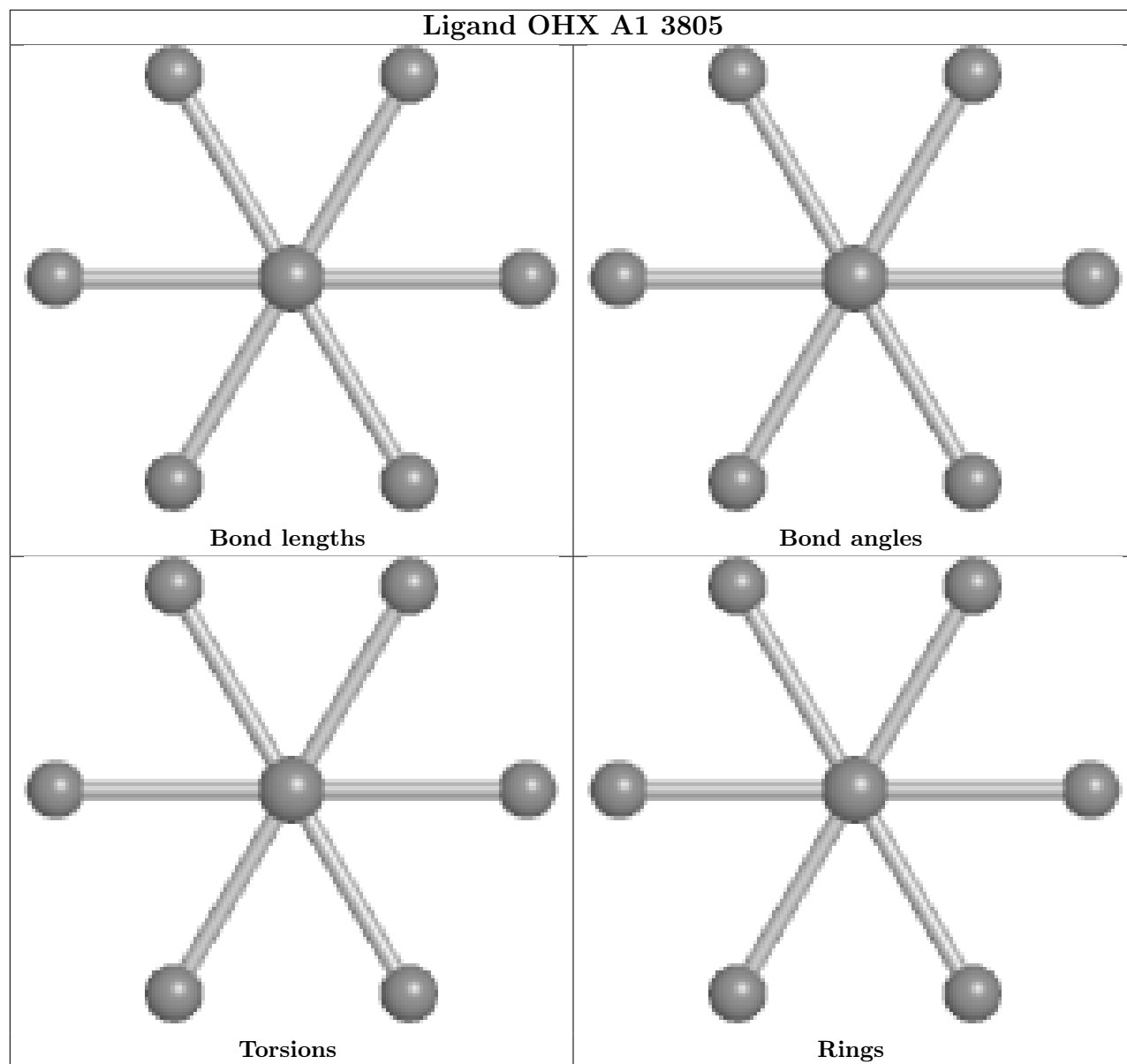
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

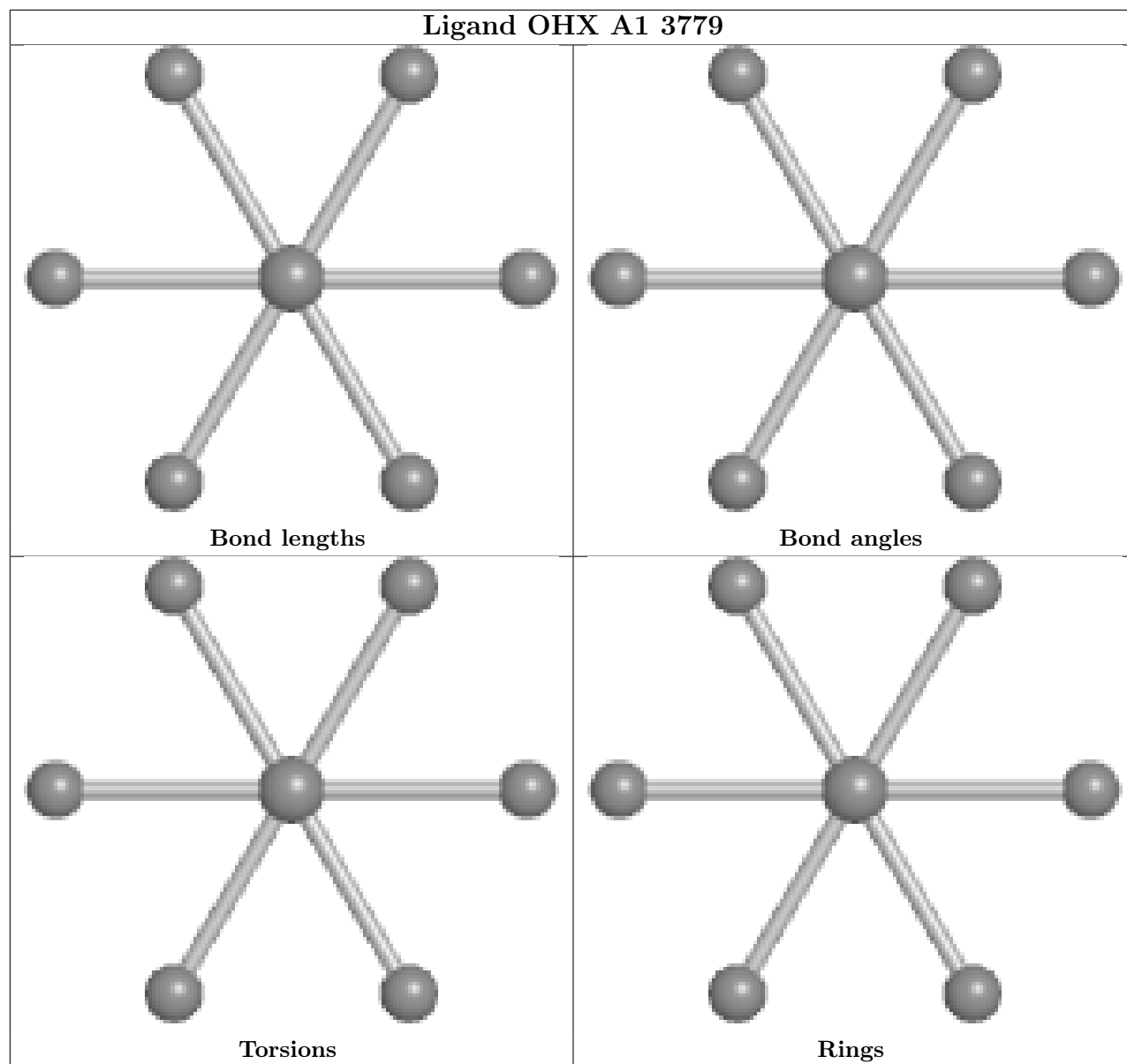


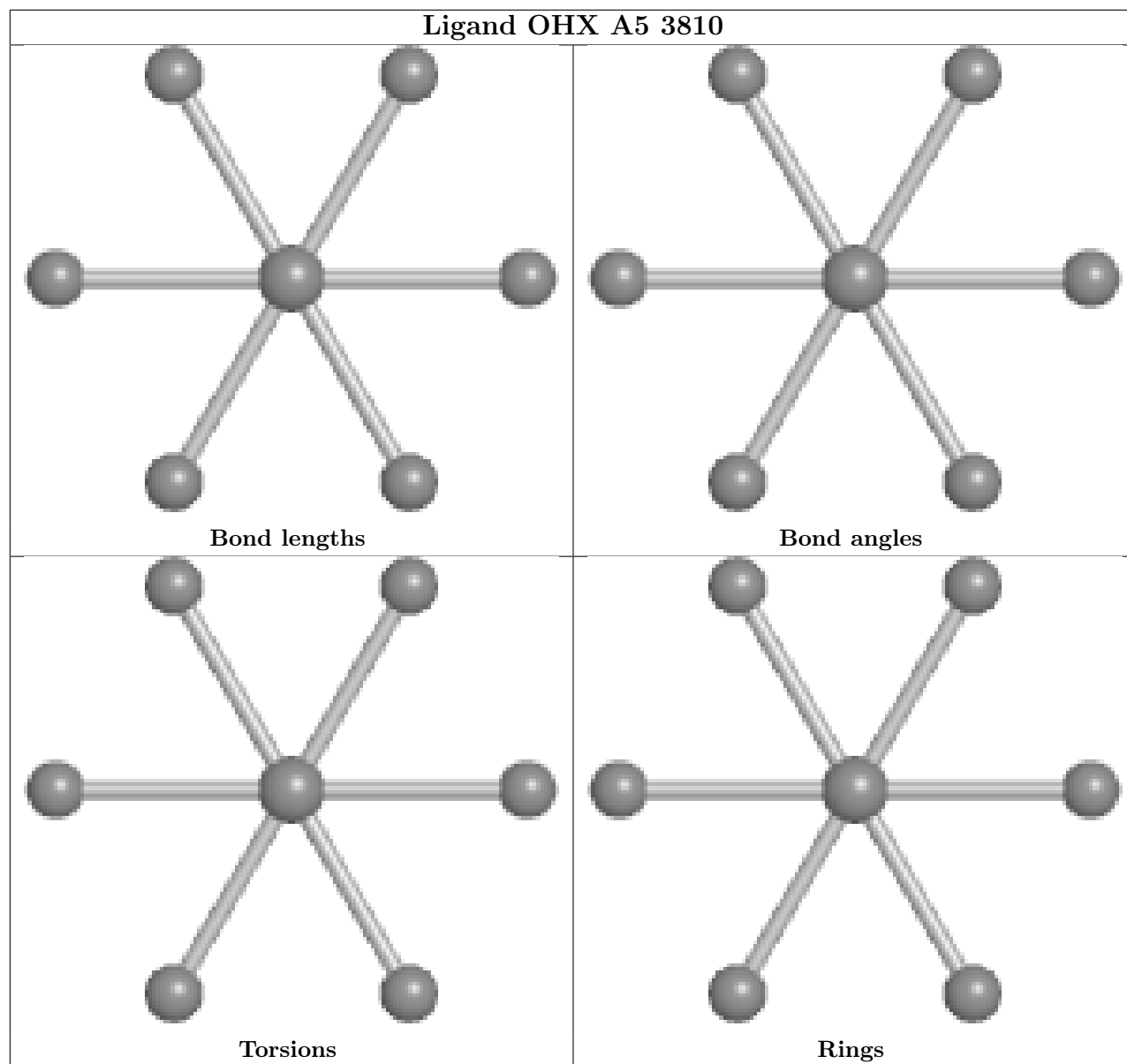


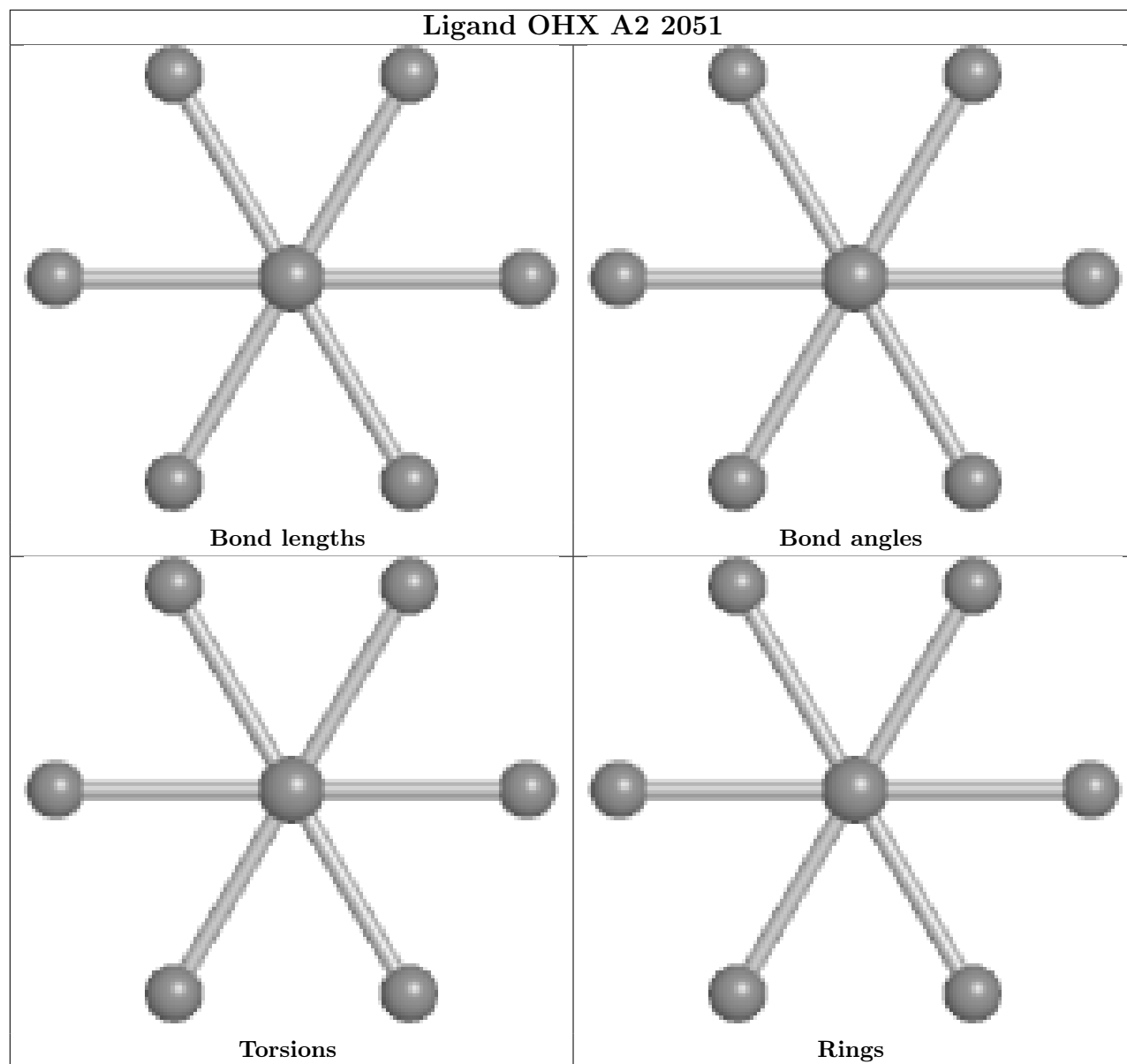


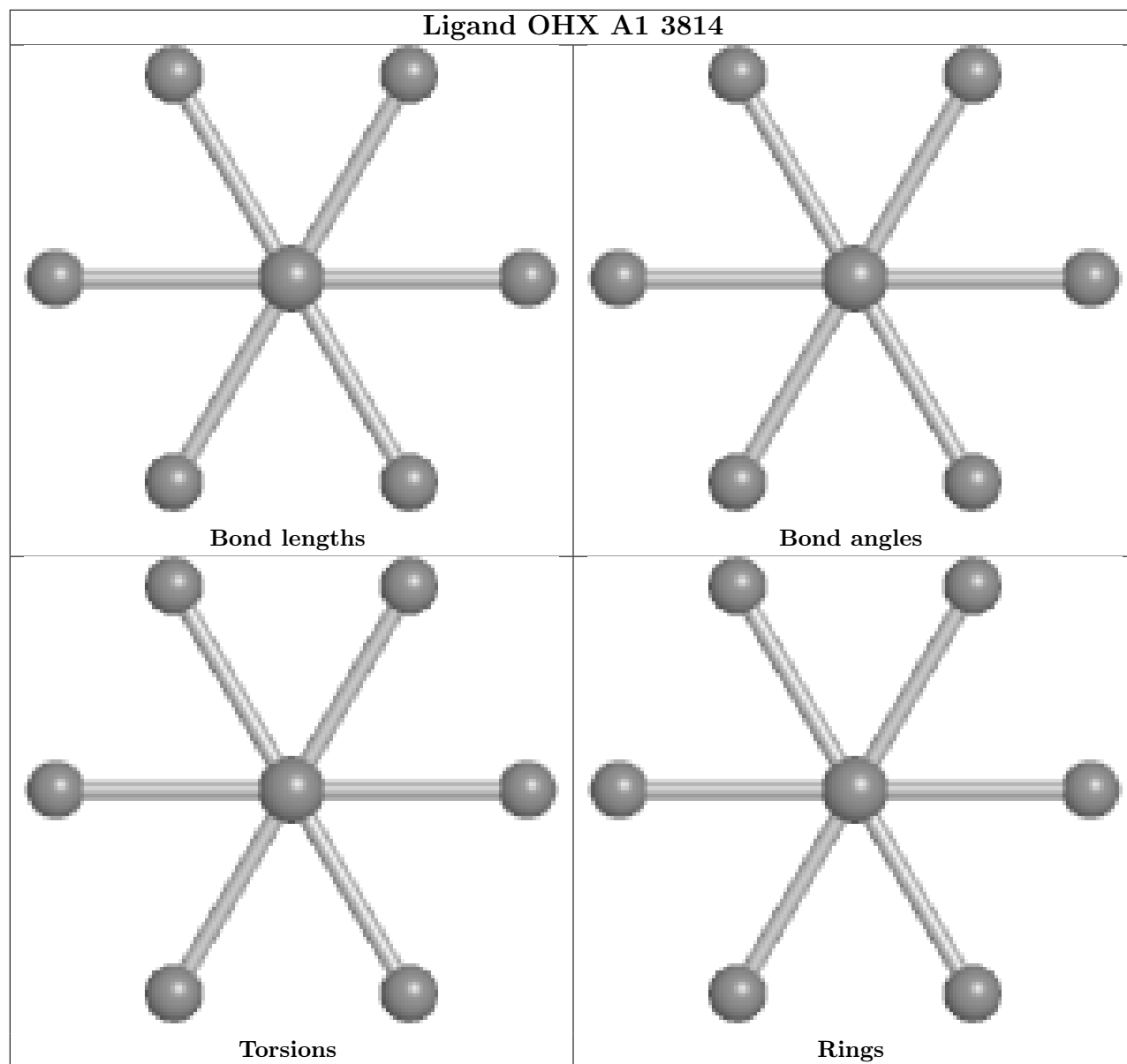


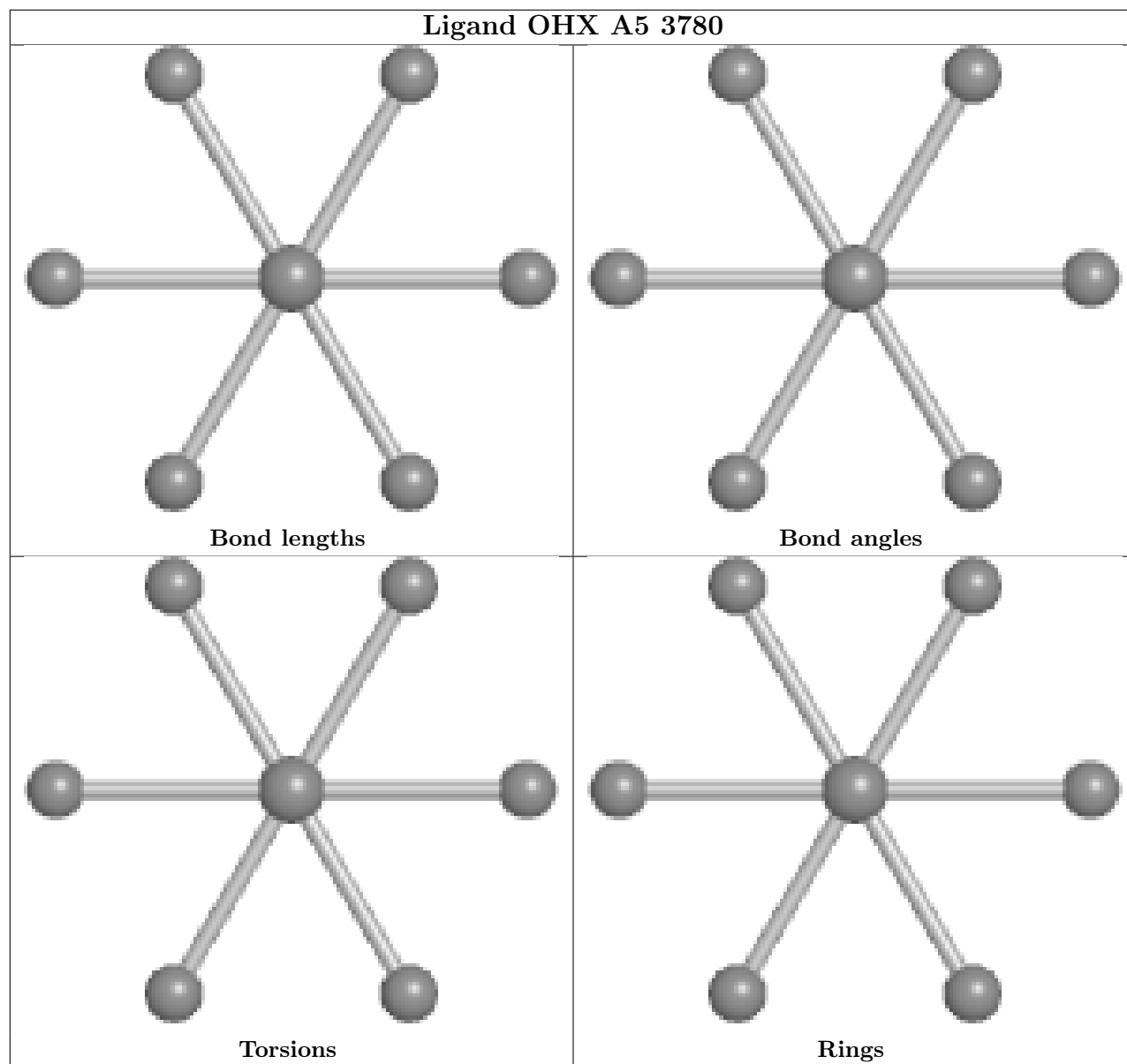


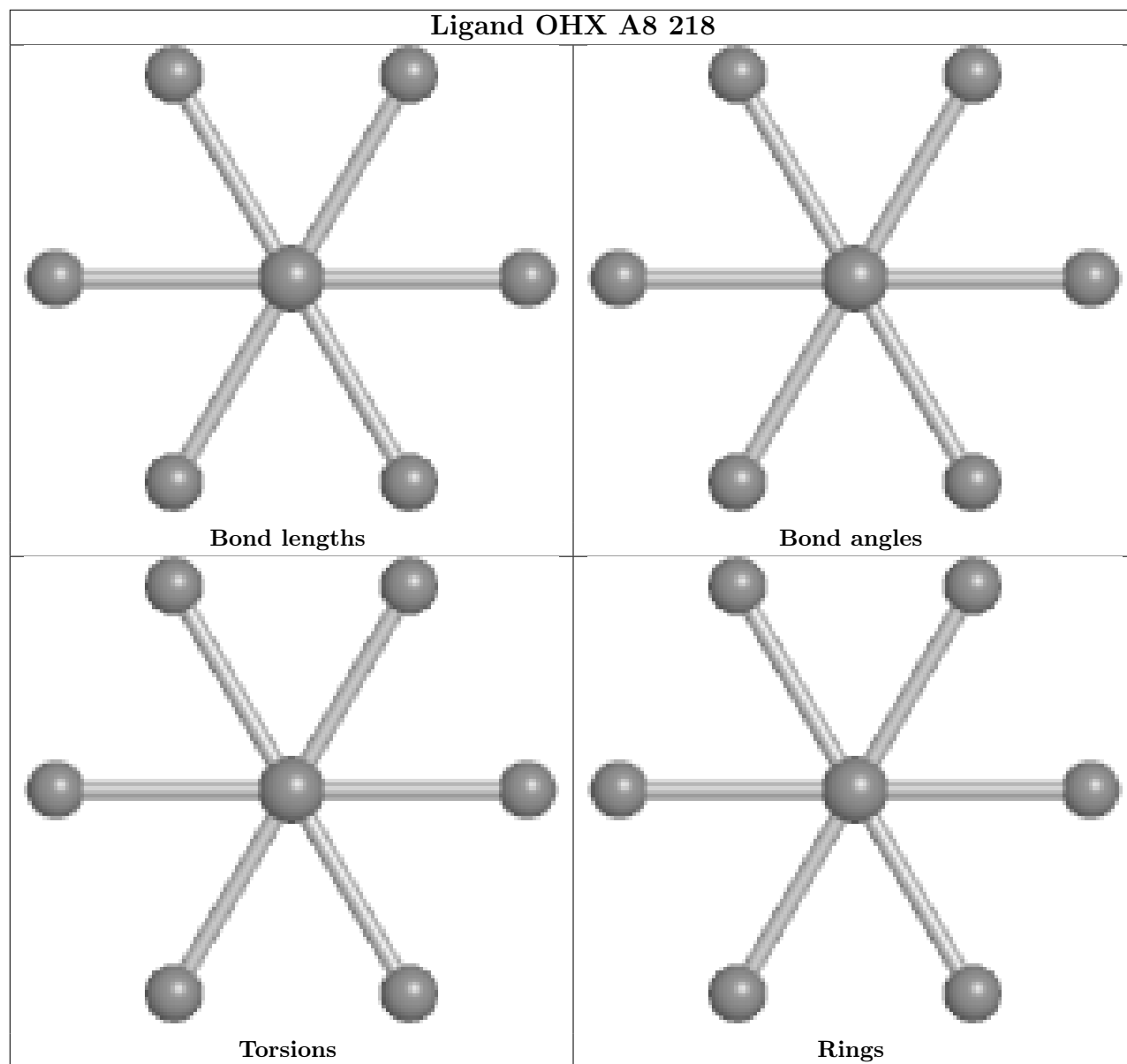


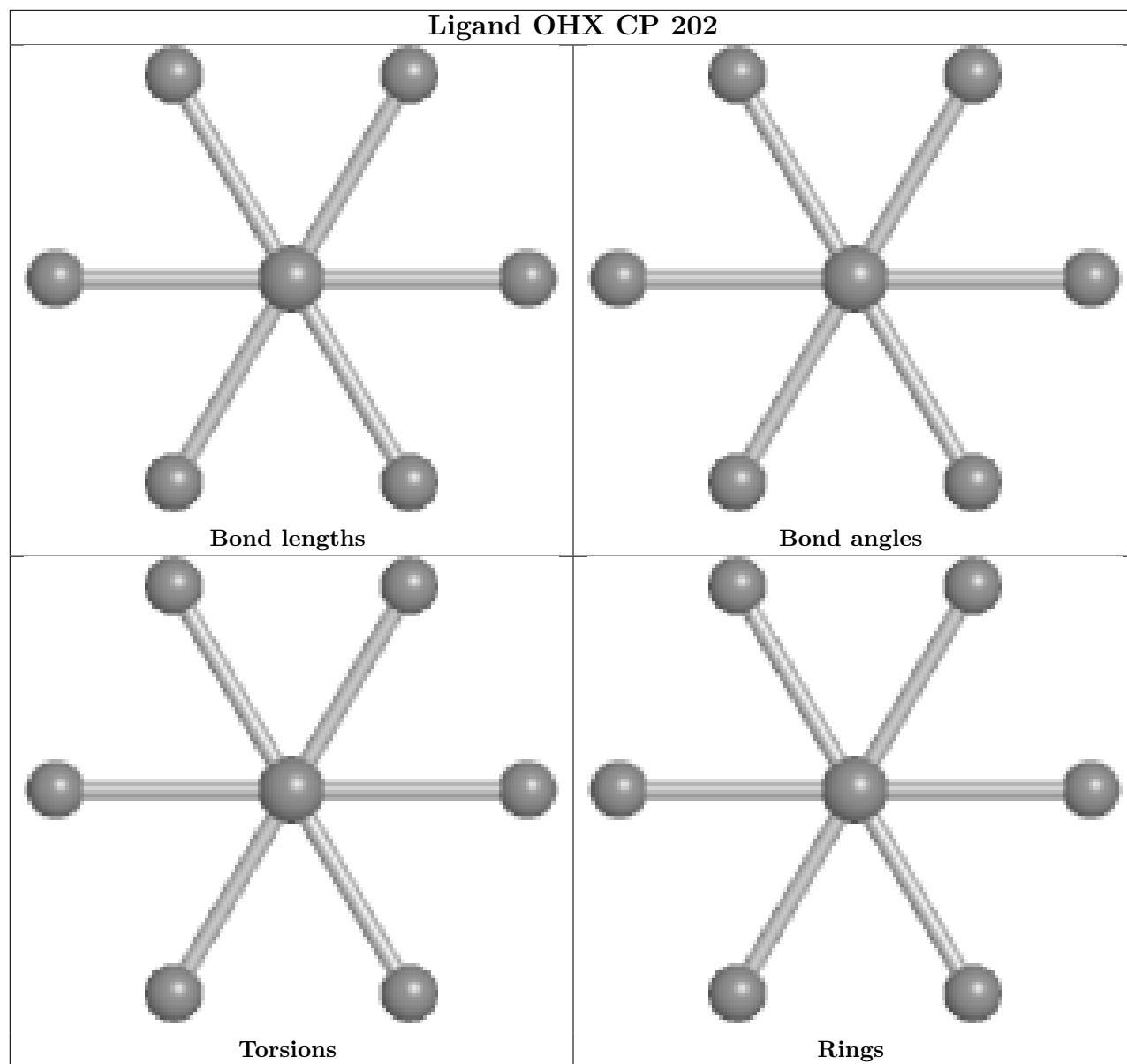


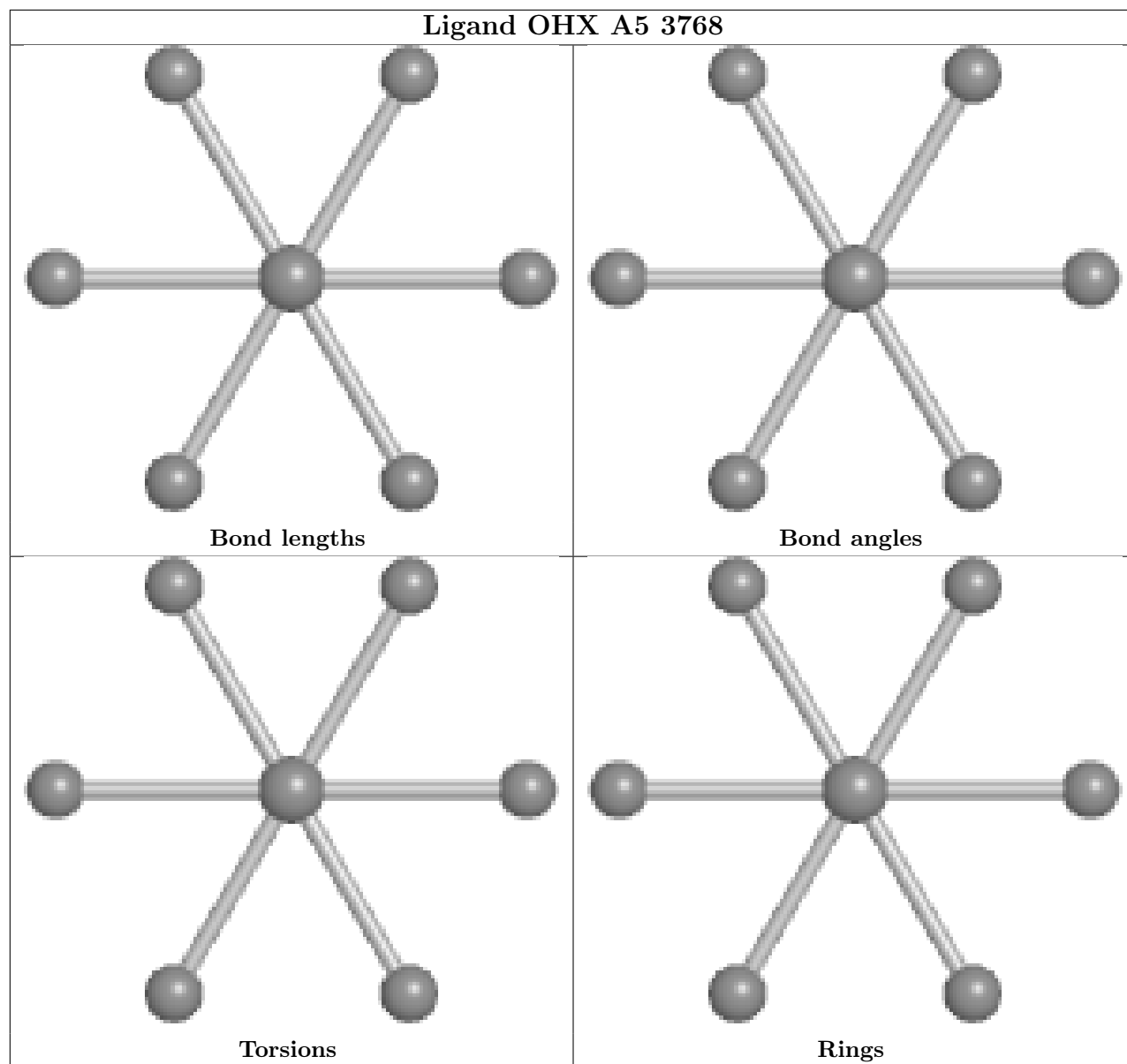


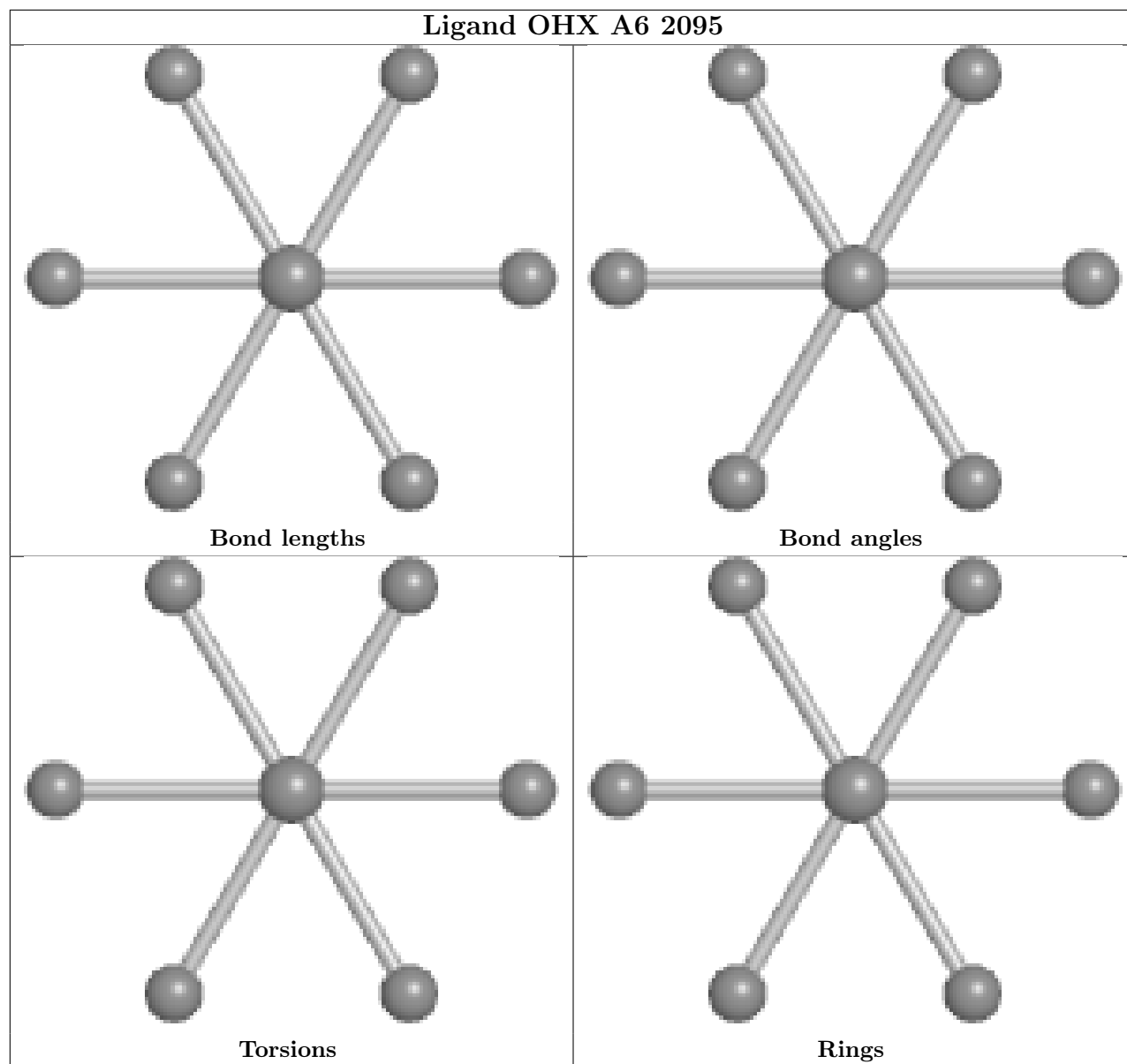


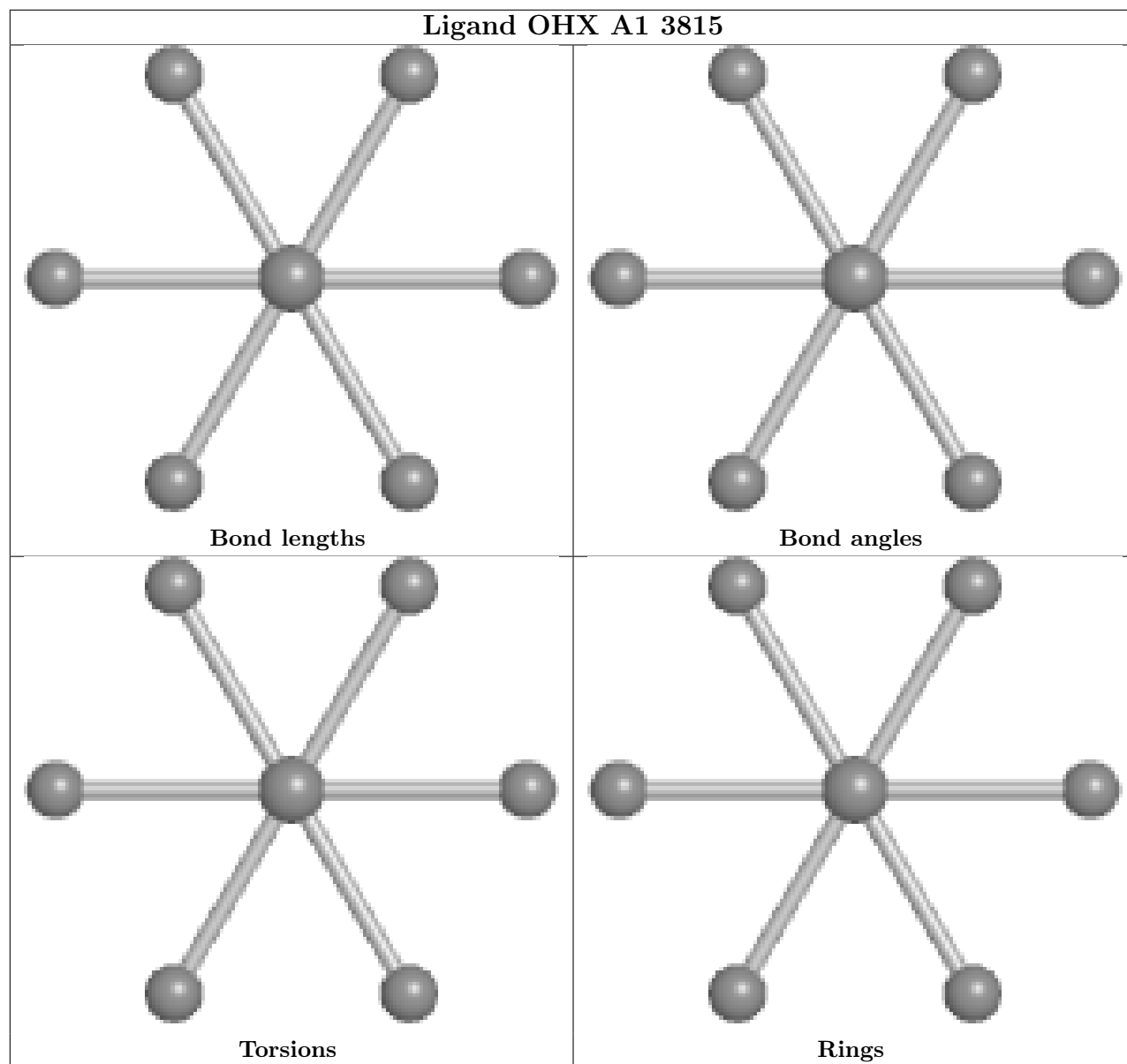


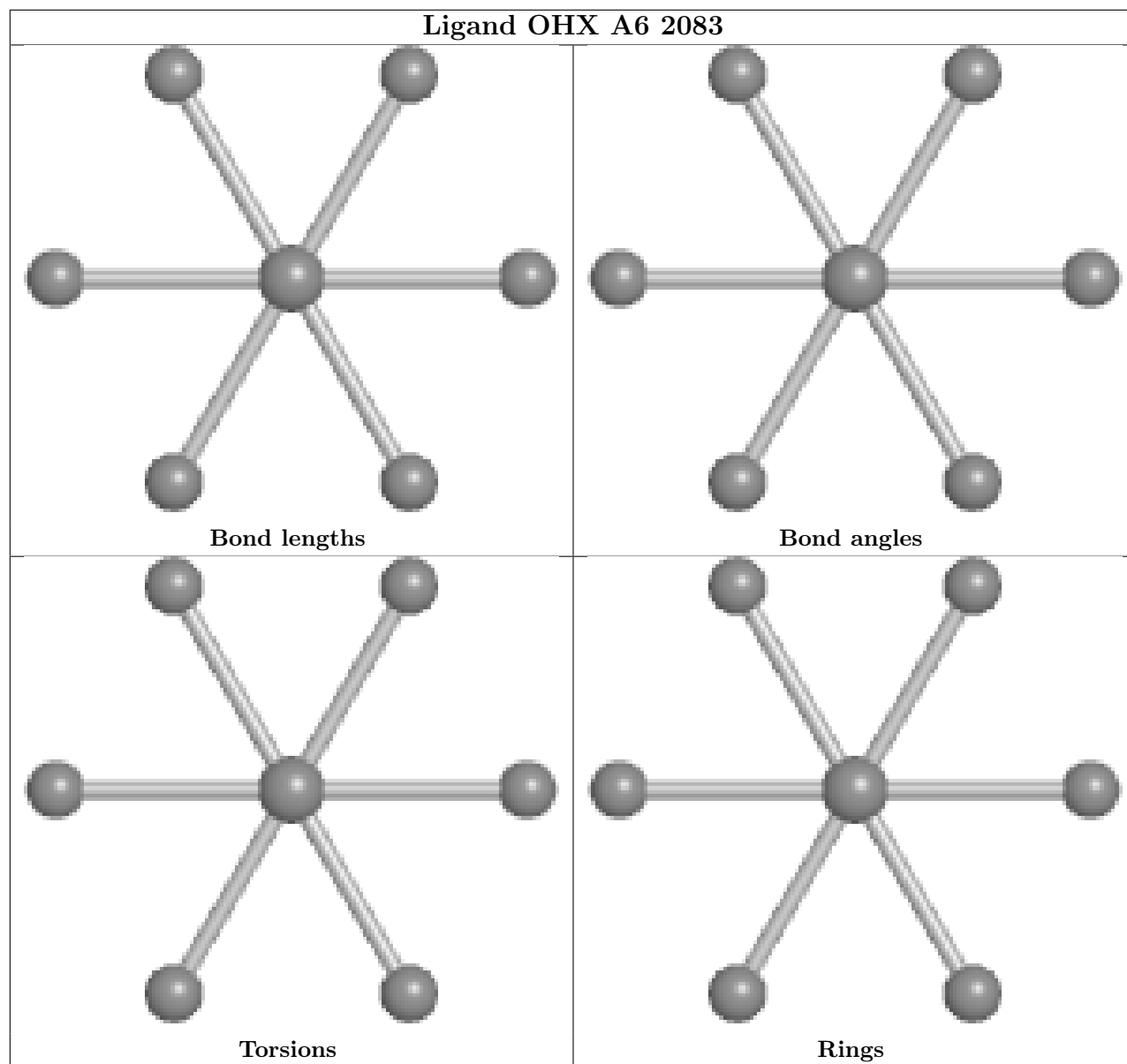


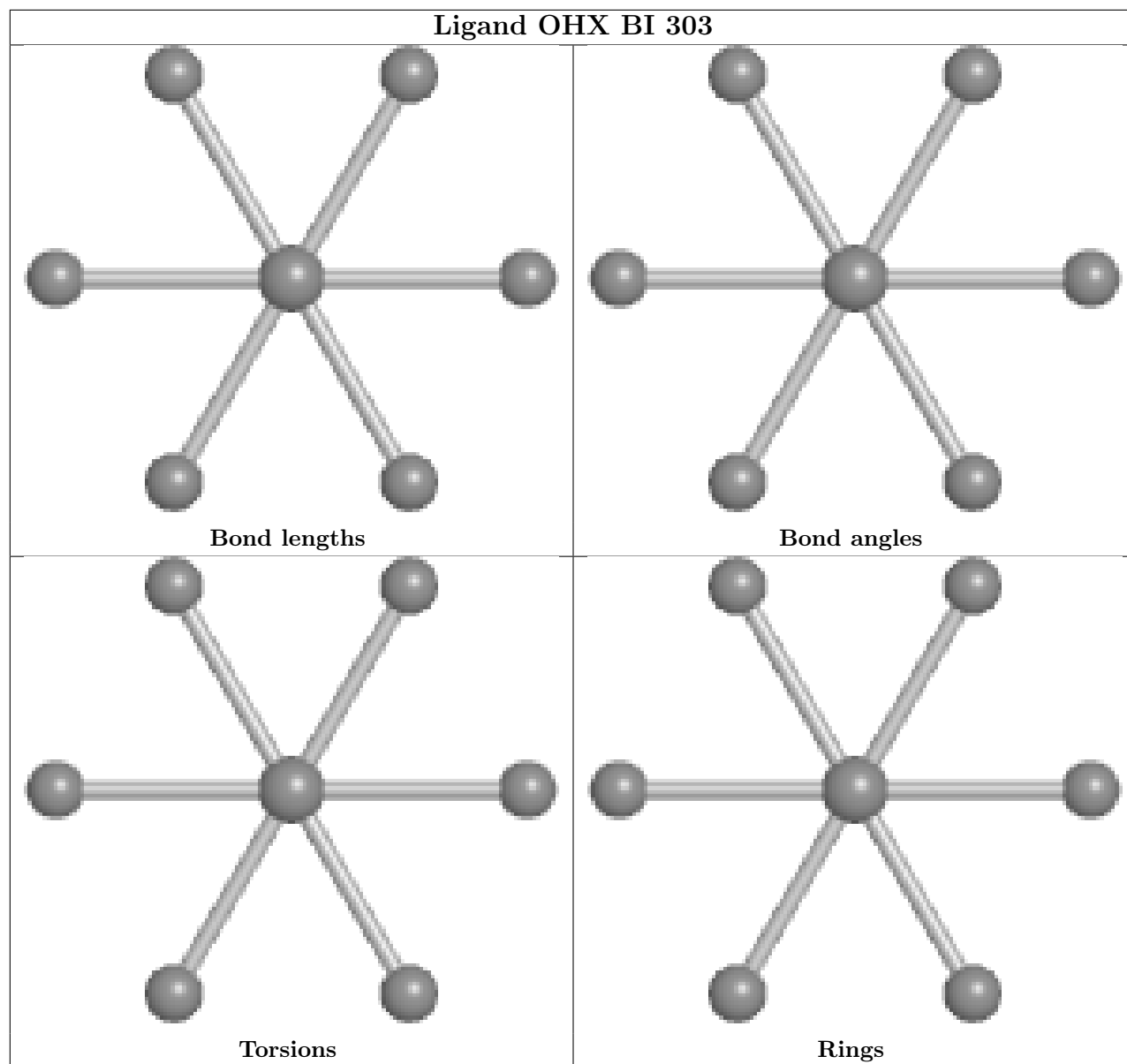


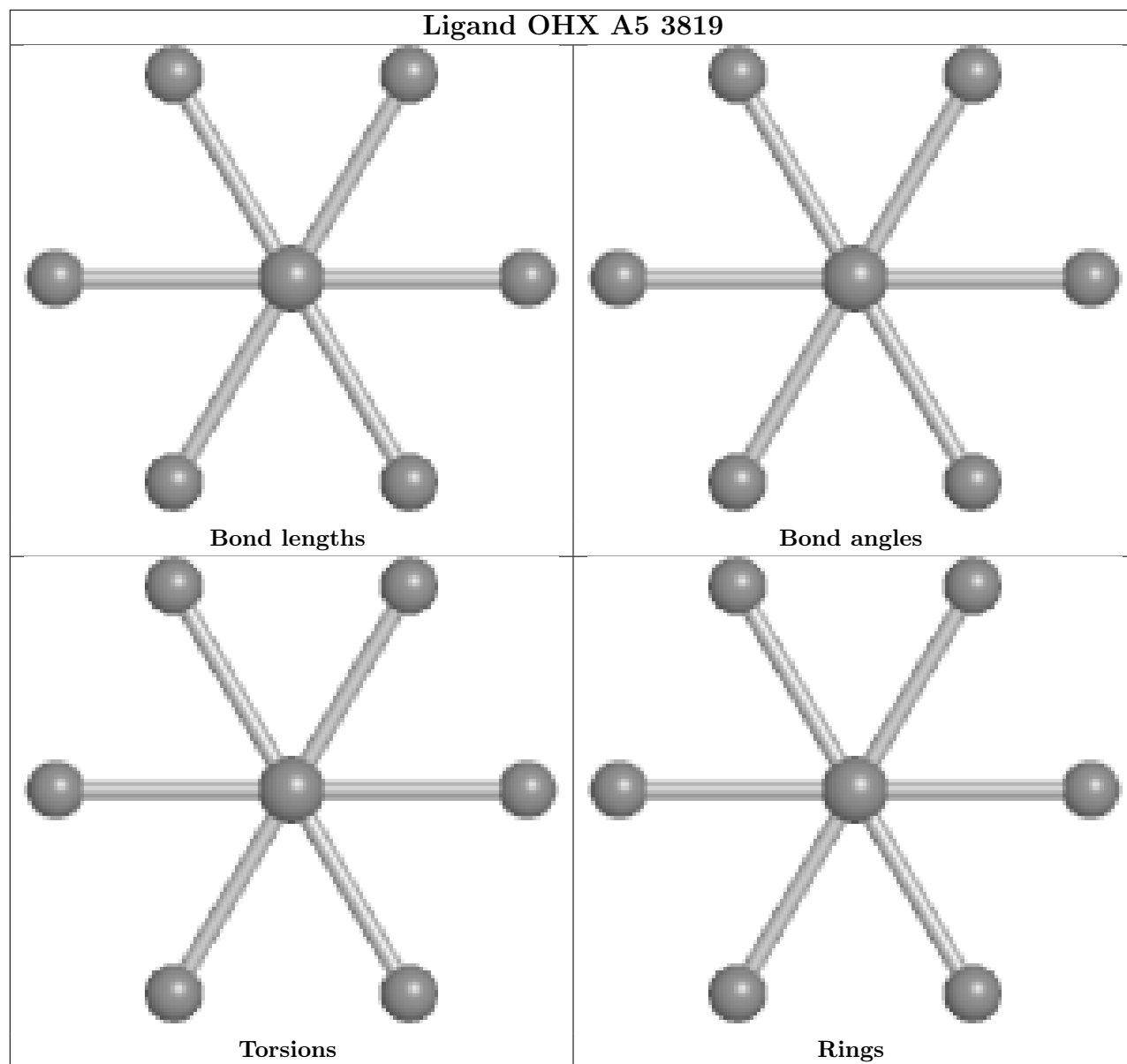












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data 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 | A2 | 1767/1800 (98%) | 0.00 | 39 (2%) 62 33 | 49, 88, 220, 373 | 0 |
| 2 | AA | 206/252 (81%) | 0.20 | 5 (2%) 59 30 | 71, 111, 170, 202 | 0 |
| 2 | CA | 206/252 (81%) | 0.14 | 2 (0%) 82 59 | 60, 90, 133, 228 | 0 |
| 3 | AB | 214/255 (83%) | 0.64 | 28 (13%) 3 1 | 79, 144, 219, 256 | 0 |
| 3 | CB | 216/255 (84%) | 0.04 | 0 100 100 | 59, 85, 127, 171 | 0 |
| 4 | AC | 217/254 (85%) | 0.09 | 2 (0%) 84 63 | 60, 91, 130, 170 | 0 |
| 4 | CC | 217/254 (85%) | 0.09 | 6 (2%) 53 25 | 50, 75, 127, 193 | 0 |
| 5 | AD | 223/240 (92%) | 0.34 | 8 (3%) 42 17 | 69, 97, 154, 222 | 0 |
| 5 | CD | 223/240 (92%) | 0.23 | 4 (1%) 68 40 | 56, 91, 144, 182 | 0 |
| 6 | AE | 260/261 (99%) | 0.24 | 8 (3%) 49 21 | 60, 89, 131, 187 | 0 |
| 6 | CE | 260/261 (99%) | 0.02 | 1 (0%) 92 79 | 48, 74, 112, 237 | 0 |
| 7 | AF | 206/225 (91%) | 0.22 | 9 (4%) 34 13 | 72, 116, 160, 231 | 0 |
| 7 | CF | 206/225 (91%) | 0.12 | 6 (2%) 51 23 | 53, 87, 143, 207 | 0 |
| 8 | AG | 226/236 (95%) | 0.38 | 7 (3%) 49 21 | 58, 102, 153, 209 | 0 |
| 8 | CG | 218/236 (92%) | 0.22 | 6 (2%) 53 25 | 49, 83, 140, 239 | 0 |
| 9 | AH | 184/190 (96%) | 0.23 | 2 (1%) 80 56 | 75, 121, 178, 259 | 0 |
| 9 | CH | 186/190 (97%) | 0.06 | 2 (1%) 80 56 | 64, 102, 162, 222 | 0 |
| 10 | AI | 188/200 (94%) | 0.11 | 4 (2%) 63 34 | 48, 76, 132, 165 | 0 |
| 10 | CI | 188/200 (94%) | -0.01 | 0 100 100 | 41, 68, 116, 154 | 0 |
| 11 | AJ | 185/197 (93%) | 0.69 | 13 (7%) 16 5 | 70, 101, 163, 231 | 0 |
| 11 | CJ | 185/197 (93%) | 0.13 | 3 (1%) 72 44 | 55, 78, 138, 196 | 0 |
| 12 | AK | 96/105 (91%) | 0.21 | 1 (1%) 82 59 | 71, 101, 164, 198 | 0 |
| 12 | CK | 96/105 (91%) | 0.71 | 10 (10%) 6 2 | 77, 116, 163, 222 | 0 |
| 13 | AL | 155/156 (99%) | 0.48 | 13 (8%) 11 3 | 48, 71, 176, 236 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|---------------|--------|--------------|-----------------------|-------|
| 13 | CL | 146/156 (93%) | 0.37 | 9 (6%) 20 7 | 41, 63, 134, 219 | 0 |
| 14 | AM | 124/143 (86%) | 0.80 | 24 (19%) 1 0 | 97, 148, 209, 234 | 0 |
| 14 | CM | 124/143 (86%) | 1.84 | 40 (32%) 0 0 | 121, 191, 250, 311 | 0 |
| 15 | AN | 150/151 (99%) | 0.08 | 1 (0%) 87 69 | 57, 89, 127, 183 | 0 |
| 15 | CN | 150/151 (99%) | -0.22 | 0 100 100 | 49, 73, 109, 130 | 0 |
| 16 | AO | 127/137 (92%) | 0.85 | 18 (14%) 2 1 | 61, 134, 179, 240 | 0 |
| 16 | CO | 128/137 (93%) | 0.08 | 1 (0%) 86 65 | 50, 84, 118, 140 | 0 |
| 17 | AP | 124/142 (87%) | 0.35 | 2 (1%) 72 44 | 68, 93, 167, 197 | 0 |
| 17 | CP | 135/142 (95%) | 0.16 | 10 (7%) 14 4 | 61, 93, 166, 196 | 0 |
| 18 | AQ | 141/143 (98%) | 0.67 | 12 (8%) 10 3 | 72, 100, 138, 155 | 0 |
| 18 | CQ | 142/143 (99%) | 0.33 | 4 (2%) 53 25 | 53, 79, 121, 171 | 0 |
| 19 | AR | 120/136 (88%) | 0.06 | 2 (1%) 70 41 | 66, 112, 180, 214 | 0 |
| 19 | CR | 117/136 (86%) | 0.01 | 2 (1%) 70 41 | 58, 88, 142, 199 | 0 |
| 20 | AS | 145/146 (99%) | 0.66 | 15 (10%) 6 2 | 57, 104, 156, 182 | 0 |
| 20 | CS | 145/146 (99%) | 0.03 | 2 (1%) 75 49 | 56, 79, 138, 165 | 0 |
| 21 | AT | 143/144 (99%) | 0.37 | 4 (2%) 53 25 | 73, 102, 147, 180 | 0 |
| 21 | CT | 143/144 (99%) | 0.03 | 0 100 100 | 48, 74, 114, 181 | 0 |
| 22 | AU | 107/121 (88%) | 0.69 | 10 (9%) 8 3 | 64, 102, 189, 226 | 0 |
| 22 | CU | 110/121 (90%) | 0.83 | 12 (10%) 5 2 | 56, 93, 183, 243 | 0 |
| 23 | AV | 87/87 (100%) | 0.13 | 0 100 100 | 75, 102, 151, 169 | 0 |
| 23 | CV | 87/87 (100%) | -0.03 | 1 (1%) 80 56 | 54, 79, 118, 185 | 0 |
| 24 | AW | 129/130 (99%) | 0.03 | 0 100 100 | 58, 82, 103, 121 | 0 |
| 24 | CW | 129/130 (99%) | 0.00 | 0 100 100 | 40, 62, 77, 98 | 0 |
| 25 | AX | 144/145 (99%) | 0.24 | 1 (0%) 87 69 | 48, 68, 98, 150 | 0 |
| 25 | CX | 144/145 (99%) | -0.04 | 0 100 100 | 37, 53, 80, 139 | 0 |
| 26 | AY | 134/135 (99%) | 0.29 | 3 (2%) 62 33 | 70, 106, 166, 216 | 0 |
| 26 | CY | 134/135 (99%) | 0.06 | 3 (2%) 62 33 | 57, 84, 143, 191 | 0 |
| 27 | AZ | 70/108 (64%) | 0.49 | 5 (7%) 16 5 | 88, 132, 172, 235 | 0 |
| 27 | CZ | 69/108 (63%) | 0.30 | 5 (7%) 15 4 | 68, 103, 151, 196 | 0 |
| 28 | Aa | 97/119 (81%) | 1.31 | 24 (24%) 0 0 | 69, 113, 206, 223 | 0 |
| 28 | Ca | 97/119 (81%) | 0.27 | 1 (1%) 82 59 | 54, 79, 129, 165 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 29 | Ab | 81/82 (98%) | 0.22 | 3 (3%) 41 17 | 68, 102, 188, 225 | 0 |
| 29 | Cb | 81/82 (98%) | 0.06 | 0 100 100 | 51, 85, 170, 203 | 0 |
| 30 | Ac | 63/67 (94%) | 0.36 | 3 (4%) 30 11 | 86, 130, 182, 204 | 0 |
| 30 | Cc | 63/67 (94%) | 0.54 | 6 (9%) 8 3 | 74, 107, 155, 180 | 0 |
| 31 | Ad | 53/56 (94%) | 0.23 | 2 (3%) 40 16 | 64, 76, 106, 155 | 0 |
| 31 | Cd | 53/56 (94%) | 0.35 | 3 (5%) 23 8 | 51, 69, 108, 168 | 0 |
| 32 | Ae | 60/63 (95%) | 0.87 | 10 (16%) 1 0 | 56, 103, 179, 270 | 0 |
| 32 | Ce | 62/63 (98%) | 0.09 | 4 (6%) 18 5 | 47, 84, 184, 218 | 0 |
| 33 | Af | 51/152 (33%) | 0.56 | 5 (9%) 7 2 | 92, 138, 186, 202 | 0 |
| 33 | Cf | 51/152 (33%) | 1.39 | 11 (21%) 0 0 | 113, 172, 222, 254 | 0 |
| 34 | Ag | 318/319 (99%) | 0.21 | 10 (3%) 49 21 | 74, 113, 171, 237 | 0 |
| 34 | Cg | 318/319 (99%) | 0.51 | 17 (5%) 26 10 | 73, 105, 158, 232 | 0 |
| 35 | Ah | 121/273 (44%) | 0.39 | 6 (4%) 28 10 | 54, 99, 162, 212 | 0 |
| 36 | A1 | 3149/3396 (92%) | 0.03 | 23 (0%) 87 69 | 29, 54, 168, 351 | 0 |
| 36 | A5 | 3150/3396 (92%) | 0.06 | 36 (1%) 80 56 | 28, 52, 157, 346 | 0 |
| 37 | A3 | 121/121 (100%) | -0.10 | 0 100 100 | 34, 72, 92, 118 | 0 |
| 37 | A7 | 121/121 (100%) | 0.03 | 0 100 100 | 31, 57, 74, 144 | 0 |
| 38 | A4 | 158/158 (100%) | 0.05 | 1 (0%) 89 72 | 37, 58, 112, 223 | 0 |
| 38 | A8 | 158/158 (100%) | 0.02 | 1 (0%) 89 72 | 39, 65, 128, 263 | 0 |
| 39 | BA | 252/254 (99%) | 0.03 | 1 (0%) 92 79 | 27, 53, 78, 150 | 0 |
| 39 | DA | 252/254 (99%) | 0.11 | 7 (2%) 53 25 | 29, 55, 83, 177 | 0 |
| 40 | BB | 386/387 (99%) | -0.05 | 1 (0%) 94 84 | 26, 58, 86, 187 | 0 |
| 40 | DB | 386/387 (99%) | -0.21 | 0 100 100 | 20, 44, 69, 188 | 0 |
| 41 | BC | 361/362 (99%) | -0.23 | 0 100 100 | 26, 50, 86, 132 | 0 |
| 41 | DC | 361/362 (99%) | -0.16 | 0 100 100 | 30, 56, 90, 136 | 0 |
| 42 | BD | 296/297 (99%) | -0.05 | 2 (0%) 87 69 | 47, 81, 132, 223 | 0 |
| 42 | DD | 294/297 (98%) | -0.07 | 2 (0%) 87 69 | 38, 58, 110, 205 | 0 |
| 43 | BE | 156/176 (88%) | -0.23 | 0 100 100 | 34, 52, 89, 152 | 0 |
| 43 | DE | 157/176 (89%) | -0.11 | 2 (1%) 77 51 | 37, 54, 97, 160 | 0 |
| 44 | BF | 222/244 (90%) | -0.23 | 1 (0%) 91 75 | 31, 46, 87, 247 | 0 |
| 44 | DF | 223/244 (91%) | -0.22 | 0 100 100 | 26, 44, 99, 196 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|----------|
| 45 | BG | 233/256 (91%) | -0.05 | 1 (0%) 92 79 | 52, 79, 148, 255 | 0 |
| 45 | DG | 231/256 (90%) | 0.05 | 3 (1%) 77 51 | 63, 88, 132, 196 | 0 |
| 46 | BH | 191/191 (100%) | 0.03 | 1 (0%) 91 75 | 44, 65, 99, 197 | 0 |
| 46 | DH | 191/191 (100%) | -0.26 | 1 (0%) 91 75 | 30, 47, 83, 206 | 0 |
| 47 | BI | 211/221 (95%) | -0.09 | 1 (0%) 91 75 | 37, 60, 121, 229 | 0 |
| 47 | DI | 213/221 (96%) | 0.12 | 4 (1%) 66 37 | 34, 60, 106, 207 | 0 |
| 48 | BJ | 169/174 (97%) | 0.18 | 2 (1%) 79 54 | 50, 84, 123, 151 | 0 |
| 48 | DJ | 169/174 (97%) | -0.11 | 0 100 100 | 40, 64, 98, 123 | 0 |
| 49 | BL | 193/199 (96%) | -0.22 | 0 100 100 | 30, 57, 126, 216 | 0 |
| 49 | DL | 194/199 (97%) | 0.06 | 0 100 100 | 38, 69, 134, 174 | 0 |
| 50 | BM | 136/138 (98%) | -0.14 | 0 100 100 | 37, 55, 92, 132 | 0 |
| 50 | DM | 137/138 (99%) | -0.30 | 0 100 100 | 30, 47, 83, 153 | 0 |
| 51 | BN | 203/204 (99%) | -0.06 | 0 100 100 | 32, 52, 68, 92 | 0 |
| 51 | DN | 203/204 (99%) | 0.09 | 0 100 100 | 37, 60, 82, 104 | 0 |
| 52 | BO | 217/219 (99%) | 0.02 | 0 100 100 | 26, 51, 97, 114 | 40 (18%) |
| 52 | DO | 217/219 (99%) | -0.00 | 0 100 100 | 22, 41, 91, 118 | 40 (18%) |
| 53 | BP | 183/184 (99%) | 0.23 | 7 (3%) 40 16 | 30, 49, 149, 224 | 0 |
| 53 | DP | 155/184 (84%) | -0.20 | 0 100 100 | 30, 44, 72, 161 | 0 |
| 54 | BQ | 185/186 (99%) | -0.17 | 0 100 100 | 33, 48, 68, 107 | 0 |
| 54 | DQ | 185/186 (99%) | -0.08 | 0 100 100 | 35, 54, 73, 125 | 0 |
| 55 | BR | 188/189 (99%) | 0.00 | 3 (1%) 72 44 | 45, 71, 170, 201 | 0 |
| 55 | DR | 188/189 (99%) | -0.04 | 4 (2%) 63 34 | 36, 64, 142, 199 | 0 |
| 56 | BS | 172/172 (100%) | -0.06 | 2 (1%) 79 54 | 36, 51, 85, 123 | 0 |
| 56 | DS | 172/172 (100%) | -0.20 | 2 (1%) 79 54 | 26, 44, 72, 141 | 0 |
| 57 | BT | 159/160 (99%) | -0.18 | 0 100 100 | 33, 52, 111, 149 | 0 |
| 57 | DT | 159/160 (99%) | -0.13 | 0 100 100 | 30, 46, 97, 120 | 0 |
| 58 | BU | 100/121 (82%) | -0.02 | 3 (3%) 50 22 | 79, 108, 150, 180 | 0 |
| 58 | DU | 98/121 (80%) | 0.36 | 7 (7%) 16 5 | 67, 97, 128, 168 | 0 |
| 59 | BV | 136/137 (99%) | -0.02 | 0 100 100 | 35, 57, 95, 182 | 0 |
| 59 | DV | 136/137 (99%) | -0.03 | 3 (2%) 62 33 | 26, 42, 78, 210 | 0 |
| 60 | BW | 98/155 (63%) | 1.53 | 22 (22%) 0 0 | 47, 77, 244, 306 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|---------------|--------|--------------|-----------------------|-------|
| 60 | DW | 135/155 (87%) | 0.36 | 10 (7%) 14 4 | 36, 94, 192, 249 | 0 |
| 61 | BX | 121/142 (85%) | -0.03 | 1 (0%) 86 65 | 41, 68, 99, 152 | 0 |
| 61 | DX | 120/142 (84%) | 0.07 | 1 (0%) 86 65 | 46, 71, 108, 135 | 0 |
| 62 | BY | 126/127 (99%) | -0.10 | 1 (0%) 86 65 | 38, 59, 91, 150 | 0 |
| 62 | DY | 126/127 (99%) | 0.08 | 0 100 100 | 39, 66, 102, 168 | 0 |
| 63 | BZ | 135/136 (99%) | 0.23 | 3 (2%) 62 33 | 68, 94, 138, 162 | 0 |
| 63 | DZ | 135/136 (99%) | 0.23 | 3 (2%) 62 33 | 68, 103, 142, 170 | 0 |
| 64 | Ba | 148/149 (99%) | -0.07 | 0 100 100 | 26, 50, 89, 116 | 0 |
| 64 | Da | 148/149 (99%) | 0.00 | 0 100 100 | 28, 55, 93, 142 | 0 |
| 65 | Bb | 58/59 (98%) | 0.10 | 1 (1%) 70 41 | 33, 58, 119, 142 | 0 |
| 65 | Db | 58/59 (98%) | 0.10 | 2 (3%) 45 19 | 35, 59, 123, 160 | 0 |
| 66 | Bc | 97/105 (92%) | -0.05 | 0 100 100 | 63, 88, 129, 171 | 0 |
| 66 | Dc | 100/105 (95%) | 0.19 | 4 (4%) 38 15 | 59, 86, 154, 173 | 0 |
| 67 | Bd | 109/113 (96%) | 0.12 | 3 (2%) 53 25 | 40, 66, 132, 202 | 0 |
| 67 | Dd | 109/113 (96%) | -0.08 | 0 100 100 | 34, 57, 126, 199 | 0 |
| 68 | Be | 127/130 (97%) | 0.00 | 3 (2%) 59 30 | 22, 42, 65, 149 | 0 |
| 68 | De | 127/130 (97%) | -0.07 | 2 (1%) 72 44 | 25, 47, 77, 136 | 0 |
| 69 | Bf | 106/107 (99%) | -0.13 | 1 (0%) 84 63 | 30, 41, 73, 139 | 0 |
| 69 | Df | 106/107 (99%) | -0.15 | 0 100 100 | 27, 40, 75, 119 | 0 |
| 70 | Bg | 112/121 (92%) | 0.29 | 3 (2%) 54 26 | 44, 71, 134, 197 | 0 |
| 70 | Dg | 112/121 (92%) | 0.09 | 2 (1%) 68 40 | 41, 72, 139, 191 | 0 |
| 71 | Bh | 119/120 (99%) | -0.08 | 1 (0%) 86 65 | 42, 68, 104, 119 | 0 |
| 71 | Dh | 119/120 (99%) | 0.07 | 1 (0%) 86 65 | 51, 75, 109, 149 | 0 |
| 72 | Bi | 99/100 (99%) | -0.03 | 0 100 100 | 45, 69, 111, 172 | 0 |
| 72 | Di | 99/100 (99%) | 0.06 | 1 (1%) 82 59 | 57, 75, 116, 171 | 0 |
| 73 | Bj | 87/88 (98%) | 0.06 | 1 (1%) 80 56 | 35, 45, 74, 216 | 0 |
| 73 | Dj | 87/88 (98%) | 0.28 | 2 (2%) 60 31 | 30, 50, 91, 241 | 0 |
| 74 | Bk | 77/78 (98%) | -0.21 | 0 100 100 | 65, 95, 146, 168 | 0 |
| 74 | Dk | 77/78 (98%) | 0.16 | 1 (1%) 77 51 | 64, 98, 138, 153 | 0 |
| 75 | Bl | 50/51 (98%) | 0.23 | 0 100 100 | 37, 59, 80, 95 | 0 |
| 75 | Dl | 50/51 (98%) | 0.19 | 1 (2%) 65 36 | 44, 59, 82, 102 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|---------|
| 76 | Bm | 52/128 (40%) | 0.01 | 2 (3%) 40 16 | 42, 55, 82, 139 | 0 |
| 76 | Dm | 52/128 (40%) | 0.01 | 1 (1%) 66 37 | 30, 39, 68, 106 | 0 |
| 77 | Bn | 25/25 (100%) | 0.49 | 1 (4%) 38 15 | 49, 62, 79, 94 | 0 |
| 77 | Dn | 25/25 (100%) | 0.28 | 0 100 100 | 37, 55, 72, 99 | 0 |
| 78 | Bo | 105/106 (99%) | 0.07 | 1 (0%) 82 59 | 35, 60, 97, 219 | 0 |
| 78 | Do | 105/106 (99%) | 0.05 | 2 (1%) 66 37 | 37, 59, 101, 157 | 0 |
| 79 | Bp | 91/92 (98%) | -0.11 | 0 100 100 | 40, 61, 104, 126 | 0 |
| 79 | Dp | 91/92 (98%) | -0.07 | 1 (1%) 80 56 | 29, 60, 96, 111 | 0 |
| 80 | A6 | 1769/1800 (98%) | 0.02 | 32 (1%) 68 40 | 38, 72, 189, 360 | 0 |
| 81 | Ch | 63/273 (23%) | 0.52 | 5 (7%) 12 4 | 50, 99, 156, 183 | 0 |
| 82 | DK | 0/155 | - | - | - | - |
| 83 | Dq | 120/312 (38%) | 0.53 | 7 (5%) 23 7 | 70, 109, 166, 232 | 0 |
| 84 | Dr | 0/47 | - | - | - | - |
| 85 | Ds | 0/46 | - | - | - | - |
| All | All | 32947/35856 (91%) | 0.09 | 713 (2%) 62 33 | 20, 71, 157, 373 | 80 (0%) |

All (713) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 60 | BW | 76 | VAL | 21.3 |
| 16 | AO | 15 | GLY | 17.6 |
| 60 | BW | 75 | THR | 16.9 |
| 60 | BW | 86 | SER | 14.2 |
| 33 | Cf | 145 | HIS | 13.6 |
| 14 | CM | 20 | ALA | 13.6 |
| 13 | CL | 3 | THR | 13.2 |
| 53 | BP | 161 | ALA | 12.6 |
| 60 | BW | 85 | ALA | 11.9 |
| 1 | A2 | 1693 | A | 11.4 |
| 36 | A1 | 1955 | U | 11.1 |
| 14 | CM | 21 | GLU | 10.9 |
| 60 | BW | 84 | GLY | 10.5 |
| 40 | BB | 387 | LEU | 10.0 |
| 53 | BP | 184 | ALA | 9.8 |
| 3 | AB | 20 | VAL | 9.7 |
| 73 | Dj | 88 | ALA | 9.0 |
| 1 | A2 | 1708 | U | 9.0 |
| 11 | AJ | 181 | ALA | 8.8 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 47 | DI | 221 | ALA | 8.5 |
| 14 | CM | 22 | VAL | 8.2 |
| 1 | A2 | 656 | G | 8.2 |
| 22 | CU | 98 | GLN | 8.2 |
| 36 | A1 | 1350 | A | 7.9 |
| 1 | A2 | 1692 | G | 7.9 |
| 78 | Bo | 106 | PHE | 7.9 |
| 14 | CM | 23 | THR | 7.9 |
| 71 | Dh | 120 | ALA | 7.8 |
| 28 | Aa | 62 | TYR | 7.7 |
| 14 | CM | 126 | TRP | 7.6 |
| 1 | A2 | 1709 | C | 7.6 |
| 33 | Af | 145 | HIS | 7.4 |
| 33 | Cf | 110 | ALA | 7.3 |
| 12 | CK | 93 | GLN | 7.1 |
| 14 | AM | 85 | LYS | 7.1 |
| 12 | CK | 98 | THR | 7.1 |
| 14 | CM | 105 | LYS | 7.0 |
| 14 | CM | 85 | LYS | 6.9 |
| 14 | CM | 84 | ASN | 6.9 |
| 36 | A5 | 2873 | U | 6.9 |
| 60 | BW | 69 | LYS | 6.8 |
| 83 | Dq | 192 | ASP | 6.8 |
| 13 | AL | 145 | ALA | 6.8 |
| 4 | CC | 90 | THR | 6.7 |
| 36 | A1 | 1349 | G | 6.6 |
| 36 | A5 | 2503 | G | 6.5 |
| 17 | CP | 4 | ALA | 6.5 |
| 36 | A1 | 1351 | U | 6.4 |
| 66 | Dc | 6 | SER | 6.4 |
| 1 | A2 | 134 | U | 6.3 |
| 36 | A5 | 2506 | U | 6.3 |
| 1 | A2 | 658 | C | 6.2 |
| 17 | CP | 135 | THR | 6.2 |
| 60 | BW | 88 | ASP | 6.2 |
| 32 | Ae | 46 | ASN | 6.2 |
| 34 | Cg | 2 | ALA | 6.1 |
| 73 | Dj | 87 | SER | 6.1 |
| 1 | A2 | 1059 | U | 6.1 |
| 60 | BW | 89 | LEU | 6.0 |
| 22 | AU | 121 | ASN | 6.0 |
| 36 | A5 | 1349 | G | 6.0 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 47 | DI | 111 | LEU | 5.9 |
| 60 | BW | 83 | THR | 5.9 |
| 60 | BW | 90 | ILE | 5.8 |
| 39 | DA | 253 | GLN | 5.8 |
| 31 | Cd | 4 | GLU | 5.8 |
| 36 | A5 | 1350 | A | 5.8 |
| 34 | Cg | 214 | ALA | 5.6 |
| 14 | CM | 56 | GLU | 5.6 |
| 1 | A2 | 1711 | C | 5.5 |
| 73 | Bj | 87 | SER | 5.5 |
| 11 | AJ | 95 | TYR | 5.5 |
| 56 | BS | 1 | MET | 5.5 |
| 11 | AJ | 182 | GLU | 5.4 |
| 33 | Cf | 134 | ASN | 5.4 |
| 63 | DZ | 2 | ALA | 5.4 |
| 3 | AB | 26 | ARG | 5.4 |
| 42 | DD | 296 | GLN | 5.3 |
| 59 | DV | 2 | SER | 5.3 |
| 80 | A6 | 493 | U | 5.3 |
| 1 | A2 | 719 | U | 5.3 |
| 36 | A5 | 1566 | A | 5.2 |
| 60 | BW | 87 | LEU | 5.2 |
| 3 | AB | 138 | PHE | 5.2 |
| 31 | Ad | 4 | GLU | 5.1 |
| 7 | AF | 152 | GLY | 5.1 |
| 80 | A6 | 718 | U | 5.1 |
| 36 | A5 | 2505 | U | 5.1 |
| 11 | CJ | 2 | PRO | 5.1 |
| 13 | CL | 2 | SER | 5.0 |
| 22 | CU | 121 | ASN | 5.0 |
| 36 | A5 | 1025 | A | 5.0 |
| 22 | CU | 107 | THR | 5.0 |
| 10 | AI | 21 | PHE | 5.0 |
| 7 | AF | 37 | GLN | 5.0 |
| 34 | Cg | 3 | SER | 4.9 |
| 14 | CM | 128 | ALA | 4.9 |
| 11 | AJ | 2 | PRO | 4.9 |
| 27 | AZ | 88 | ILE | 4.9 |
| 29 | Ab | 38 | PRO | 4.9 |
| 35 | Ah | 88 | ARG | 4.8 |
| 1 | A2 | 1690 | G | 4.7 |
| 60 | BW | 77 | LYS | 4.7 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 36 | A1 | 1352 | A | 4.7 |
| 13 | CL | 5 | LEU | 4.7 |
| 60 | BW | 78 | ALA | 4.7 |
| 7 | CF | 37 | GLN | 4.6 |
| 8 | CG | 169 | TYR | 4.6 |
| 1 | A2 | 135 | A | 4.6 |
| 38 | A4 | 82 | U | 4.6 |
| 7 | AF | 36 | ALA | 4.5 |
| 29 | Ab | 41 | LEU | 4.5 |
| 14 | CM | 124 | LYS | 4.5 |
| 68 | Be | 128 | LEU | 4.5 |
| 32 | Ae | 61 | SER | 4.5 |
| 31 | Cd | 5 | ASN | 4.5 |
| 13 | CL | 145 | ALA | 4.5 |
| 80 | A6 | 678 | A | 4.5 |
| 36 | A5 | 1567 | U | 4.5 |
| 12 | CK | 94 | GLU | 4.4 |
| 18 | AQ | 143 | ARG | 4.4 |
| 2 | CA | 186 | GLY | 4.4 |
| 22 | CU | 18 | GLN | 4.4 |
| 27 | AZ | 71 | ILE | 4.4 |
| 20 | AS | 32 | LEU | 4.4 |
| 11 | AJ | 186 | GLU | 4.3 |
| 61 | BX | 24 | LEU | 4.3 |
| 1 | A2 | 715 | U | 4.3 |
| 1 | A2 | 913 | G | 4.3 |
| 61 | DX | 23 | ALA | 4.3 |
| 1 | A2 | 657 | U | 4.3 |
| 80 | A6 | 506 | A | 4.3 |
| 55 | DR | 184 | LEU | 4.3 |
| 53 | BP | 162 | GLU | 4.2 |
| 13 | AL | 148 | LYS | 4.2 |
| 36 | A1 | 1569 | U | 4.2 |
| 81 | Ch | 83 | LYS | 4.2 |
| 53 | BP | 160 | ALA | 4.2 |
| 79 | Dp | 2 | ALA | 4.2 |
| 60 | BW | 95 | SER | 4.2 |
| 14 | CM | 123 | VAL | 4.2 |
| 2 | AA | 28 | ASN | 4.2 |
| 14 | CM | 125 | ASN | 4.2 |
| 47 | DI | 112 | GLN | 4.1 |
| 80 | A6 | 494 | U | 4.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 13 | AL | 146 | ALA | 4.1 |
| 62 | BY | 127 | GLU | 4.1 |
| 7 | AF | 41 | LYS | 4.1 |
| 36 | A5 | 2504 | U | 4.1 |
| 16 | AO | 16 | VAL | 4.1 |
| 13 | AL | 2 | SER | 4.1 |
| 3 | AB | 46 | THR | 4.1 |
| 45 | DG | 120 | LYS | 4.1 |
| 32 | Ae | 54 | ARG | 4.1 |
| 17 | AP | 89 | MET | 4.1 |
| 9 | CH | 187 | SER | 4.1 |
| 34 | Ag | 102 | ARG | 4.0 |
| 60 | DW | 66 | GLU | 4.0 |
| 80 | A6 | 1710 | U | 4.0 |
| 22 | CU | 105 | GLN | 4.0 |
| 17 | CP | 5 | VAL | 4.0 |
| 33 | Af | 143 | LYS | 4.0 |
| 13 | CL | 4 | GLU | 4.0 |
| 17 | CP | 136 | SER | 4.0 |
| 17 | CP | 134 | THR | 3.9 |
| 36 | A1 | 1568 | U | 3.9 |
| 8 | CG | 216 | LEU | 3.9 |
| 39 | DA | 249 | SER | 3.9 |
| 18 | AQ | 20 | ALA | 3.9 |
| 28 | Aa | 63 | ALA | 3.9 |
| 60 | DW | 67 | VAL | 3.9 |
| 1 | A2 | 1710 | U | 3.9 |
| 11 | AJ | 180 | LYS | 3.9 |
| 3 | AB | 25 | THR | 3.9 |
| 28 | Aa | 65 | PRO | 3.9 |
| 2 | AA | 44 | GLY | 3.8 |
| 1 | A2 | 261 | U | 3.8 |
| 80 | A6 | 679 | U | 3.8 |
| 59 | DV | 3 | GLY | 3.8 |
| 20 | AS | 145 | ARG | 3.8 |
| 11 | AJ | 3 | ARG | 3.8 |
| 1 | A2 | 506 | A | 3.8 |
| 80 | A6 | 495 | C | 3.8 |
| 18 | AQ | 141 | SER | 3.8 |
| 3 | AB | 94 | LYS | 3.7 |
| 60 | DW | 133 | THR | 3.7 |
| 16 | AO | 41 | ARG | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 60 | BW | 68 | ALA | 3.7 |
| 1 | A2 | 1691 | A | 3.7 |
| 14 | CM | 127 | GLY | 3.7 |
| 14 | AM | 137 | MET | 3.7 |
| 35 | Ah | 85 | SER | 3.7 |
| 36 | A5 | 1352 | A | 3.7 |
| 3 | AB | 102 | GLY | 3.6 |
| 1 | A2 | 495 | C | 3.6 |
| 13 | AL | 156 | PHE | 3.6 |
| 28 | Aa | 2 | PRO | 3.6 |
| 67 | Bd | 82 | GLU | 3.6 |
| 55 | DR | 187 | GLU | 3.6 |
| 13 | AL | 151 | LYS | 3.6 |
| 20 | AS | 2 | SER | 3.6 |
| 60 | DW | 68 | ALA | 3.6 |
| 34 | Ag | 319 | ASN | 3.6 |
| 14 | CM | 121 | VAL | 3.5 |
| 36 | A1 | 2539 | C | 3.5 |
| 21 | AT | 71 | VAL | 3.5 |
| 60 | DW | 130 | SER | 3.5 |
| 1 | A2 | 1370 | U | 3.5 |
| 36 | A5 | 1351 | U | 3.5 |
| 20 | AS | 39 | GLY | 3.5 |
| 36 | A5 | 1568 | U | 3.5 |
| 38 | A8 | 81 | U | 3.5 |
| 13 | AL | 152 | GLN | 3.5 |
| 59 | DV | 4 | ASN | 3.5 |
| 1 | A2 | 194 | U | 3.5 |
| 14 | CM | 41 | LEU | 3.5 |
| 36 | A1 | 1952 | G | 3.5 |
| 14 | CM | 133 | LEU | 3.5 |
| 12 | CK | 25 | LYS | 3.5 |
| 28 | Aa | 8 | ASN | 3.4 |
| 32 | Ce | 63 | GLN | 3.4 |
| 16 | AO | 79 | VAL | 3.4 |
| 39 | BA | 253 | GLN | 3.4 |
| 36 | A1 | 1566 | A | 3.4 |
| 18 | AQ | 29 | ILE | 3.4 |
| 36 | A5 | 1580 | A | 3.4 |
| 1 | A2 | 238 | U | 3.4 |
| 33 | Cf | 111 | GLU | 3.4 |
| 70 | Bg | 110 | GLU | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 80 | A6 | 658 | C | 3.4 |
| 35 | Ah | 89 | ARG | 3.3 |
| 14 | CM | 92 | ALA | 3.3 |
| 16 | AO | 27 | PHE | 3.3 |
| 18 | AQ | 132 | LYS | 3.3 |
| 53 | BP | 183 | ALA | 3.3 |
| 18 | AQ | 11 | GLY | 3.3 |
| 60 | BW | 94 | ARG | 3.3 |
| 80 | A6 | 490 | C | 3.3 |
| 18 | AQ | 36 | ILE | 3.3 |
| 60 | BW | 67 | VAL | 3.3 |
| 27 | CZ | 86 | GLU | 3.3 |
| 32 | Ae | 53 | LYS | 3.3 |
| 30 | Cc | 65 | ARG | 3.3 |
| 26 | CY | 2 | SER | 3.3 |
| 36 | A1 | 2873 | U | 3.3 |
| 16 | AO | 17 | ALA | 3.3 |
| 14 | CM | 33 | ARG | 3.2 |
| 22 | AU | 94 | GLU | 3.2 |
| 14 | CM | 59 | LEU | 3.2 |
| 20 | AS | 146 | ALA | 3.2 |
| 33 | Cf | 112 | GLY | 3.2 |
| 3 | AB | 21 | VAL | 3.2 |
| 76 | Dm | 128 | LYS | 3.2 |
| 20 | AS | 21 | ASN | 3.2 |
| 76 | Bm | 77 | ILE | 3.2 |
| 13 | CL | 30 | ARG | 3.2 |
| 20 | CS | 146 | ALA | 3.2 |
| 28 | Aa | 45 | VAL | 3.2 |
| 18 | CQ | 143 | ARG | 3.2 |
| 13 | AL | 30 | ARG | 3.2 |
| 28 | Aa | 20 | PRO | 3.2 |
| 56 | DS | 1 | MET | 3.2 |
| 4 | CC | 84 | LYS | 3.2 |
| 35 | Ah | 84 | LYS | 3.2 |
| 32 | Ae | 2 | ALA | 3.2 |
| 66 | Dc | 7 | GLN | 3.2 |
| 36 | A5 | 1764 | U | 3.2 |
| 47 | DI | 103 | LEU | 3.2 |
| 14 | AM | 108 | ARG | 3.2 |
| 43 | DE | 129 | GLU | 3.1 |
| 67 | Bd | 79 | ARG | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 4 | AC | 250 | GLN | 3.1 |
| 3 | AB | 131 | ASP | 3.1 |
| 28 | Aa | 98 | PRO | 3.1 |
| 80 | A6 | 1708 | U | 3.1 |
| 12 | CK | 64 | TYR | 3.1 |
| 42 | DD | 270 | LYS | 3.1 |
| 14 | CM | 43 | ARG | 3.1 |
| 18 | AQ | 142 | TYR | 3.1 |
| 30 | Cc | 67 | ARG | 3.1 |
| 36 | A1 | 1570 | U | 3.1 |
| 18 | CQ | 114 | ARG | 3.1 |
| 17 | CP | 7 | ALA | 3.1 |
| 44 | BF | 27 | ALA | 3.1 |
| 58 | DU | 52 | ASN | 3.1 |
| 36 | A5 | 1581 | C | 3.1 |
| 80 | A6 | 1371 | A | 3.1 |
| 66 | Dc | 105 | ALA | 3.1 |
| 19 | CR | 87 | GLU | 3.1 |
| 22 | AU | 105 | GLN | 3.1 |
| 80 | A6 | 656 | G | 3.1 |
| 60 | BW | 66 | GLU | 3.1 |
| 3 | AB | 140 | ILE | 3.1 |
| 27 | CZ | 88 | ILE | 3.1 |
| 36 | A5 | 1569 | U | 3.1 |
| 36 | A5 | 2874 | G | 3.1 |
| 14 | CM | 62 | LEU | 3.0 |
| 14 | CM | 112 | ALA | 3.0 |
| 22 | AU | 19 | ILE | 3.0 |
| 14 | CM | 116 | VAL | 3.0 |
| 36 | A1 | 2205 | U | 3.0 |
| 22 | CU | 99 | ILE | 3.0 |
| 8 | AG | 154 | ARG | 3.0 |
| 80 | A6 | 676 | G | 3.0 |
| 3 | AB | 84 | ILE | 3.0 |
| 13 | AL | 3 | THR | 3.0 |
| 3 | AB | 101 | HIS | 3.0 |
| 5 | CD | 151 | LYS | 3.0 |
| 65 | Bb | 25 | LYS | 3.0 |
| 36 | A5 | 2403 | G | 3.0 |
| 36 | A5 | 2871 | G | 3.0 |
| 9 | AH | 98 | ILE | 3.0 |
| 20 | AS | 15 | LEU | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 58 | BU | 9 | GLN | 3.0 |
| 21 | AT | 5 | SER | 2.9 |
| 22 | AU | 120 | SER | 2.9 |
| 16 | AO | 89 | THR | 2.9 |
| 3 | AB | 130 | SER | 2.9 |
| 26 | AY | 70 | VAL | 2.9 |
| 7 | AF | 43 | PHE | 2.9 |
| 81 | Ch | 52 | PRO | 2.9 |
| 8 | AG | 190 | GLN | 2.9 |
| 14 | AM | 62 | LEU | 2.9 |
| 28 | Aa | 18 | VAL | 2.9 |
| 81 | Ch | 50 | ASN | 2.9 |
| 13 | CL | 146 | ALA | 2.9 |
| 1 | A2 | 493 | U | 2.9 |
| 36 | A5 | 3275 | U | 2.9 |
| 34 | Cg | 92 | TRP | 2.9 |
| 14 | AM | 36 | LEU | 2.9 |
| 14 | CM | 31 | VAL | 2.9 |
| 33 | Cf | 147 | VAL | 2.9 |
| 34 | Ag | 51 | ASP | 2.9 |
| 20 | AS | 8 | GLN | 2.9 |
| 22 | CU | 17 | GLN | 2.9 |
| 39 | DA | 248 | GLY | 2.9 |
| 5 | CD | 86 | LEU | 2.8 |
| 22 | CU | 93 | LEU | 2.8 |
| 8 | AG | 175 | ILE | 2.8 |
| 22 | CU | 97 | VAL | 2.8 |
| 11 | AJ | 5 | PRO | 2.8 |
| 14 | AM | 141 | SER | 2.8 |
| 35 | Ah | 87 | THR | 2.8 |
| 32 | Ce | 62 | VAL | 2.8 |
| 60 | BW | 98 | PRO | 2.8 |
| 3 | AB | 29 | TRP | 2.8 |
| 36 | A1 | 3155 | U | 2.8 |
| 1 | A2 | 1686 | C | 2.8 |
| 1 | A2 | 280 | U | 2.8 |
| 80 | A6 | 487 | G | 2.8 |
| 80 | A6 | 677 | G | 2.8 |
| 3 | AB | 47 | LEU | 2.8 |
| 14 | CM | 114 | LYS | 2.8 |
| 28 | Aa | 85 | ARG | 2.8 |
| 27 | AZ | 89 | ILE | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 34 | Cg | 244 | ALA | 2.8 |
| 4 | CC | 89 | GLN | 2.8 |
| 12 | CK | 43 | ILE | 2.8 |
| 83 | Dq | 44 | GLU | 2.8 |
| 5 | AD | 218 | LEU | 2.8 |
| 20 | AS | 17 | LEU | 2.8 |
| 36 | A5 | 2539 | C | 2.8 |
| 1 | A2 | 718 | U | 2.7 |
| 36 | A5 | 2971 | A | 2.7 |
| 1 | A2 | 1688 | U | 2.7 |
| 18 | AQ | 66 | ARG | 2.7 |
| 27 | AZ | 69 | LEU | 2.7 |
| 67 | Bd | 4 | LEU | 2.7 |
| 14 | CM | 64 | SER | 2.7 |
| 33 | Cf | 104 | SER | 2.7 |
| 63 | BZ | 2 | ALA | 2.7 |
| 8 | CG | 133 | LEU | 2.7 |
| 14 | AM | 84 | ASN | 2.7 |
| 32 | Ce | 49 | LEU | 2.7 |
| 78 | Do | 106 | PHE | 2.7 |
| 5 | AD | 142 | LEU | 2.7 |
| 36 | A1 | 1581 | C | 2.7 |
| 36 | A5 | 1016 | C | 2.7 |
| 80 | A6 | 1709 | C | 2.7 |
| 33 | Af | 148 | TYR | 2.7 |
| 56 | DS | 2 | ALA | 2.7 |
| 70 | Bg | 78 | GLY | 2.7 |
| 42 | BD | 293 | LEU | 2.7 |
| 32 | Ae | 42 | ARG | 2.7 |
| 81 | Ch | 53 | ARG | 2.7 |
| 18 | CQ | 142 | TYR | 2.7 |
| 14 | CM | 28 | LEU | 2.7 |
| 27 | AZ | 73 | GLY | 2.7 |
| 58 | BU | 108 | TYR | 2.7 |
| 3 | AB | 50 | LYS | 2.7 |
| 20 | AS | 19 | ASN | 2.7 |
| 3 | AB | 103 | MET | 2.7 |
| 8 | CG | 162 | VAL | 2.7 |
| 7 | CF | 154 | ALA | 2.7 |
| 17 | CP | 9 | LYS | 2.6 |
| 20 | AS | 18 | LEU | 2.6 |
| 13 | AL | 155 | LYS | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 55 | DR | 181 | ARG | 2.6 |
| 33 | Af | 149 | LYS | 2.6 |
| 42 | BD | 296 | GLN | 2.6 |
| 6 | AE | 261 | LEU | 2.6 |
| 3 | AB | 106 | THR | 2.6 |
| 36 | A5 | 1565 | G | 2.6 |
| 16 | AO | 82 | LYS | 2.6 |
| 12 | CK | 95 | ARG | 2.6 |
| 34 | Cg | 167 | VAL | 2.6 |
| 34 | Cg | 314 | GLN | 2.6 |
| 34 | Cg | 279 | ALA | 2.6 |
| 60 | BW | 74 | LYS | 2.6 |
| 71 | Bh | 120 | ALA | 2.6 |
| 1 | A2 | 1362 | U | 2.6 |
| 36 | A1 | 3154 | C | 2.6 |
| 8 | AG | 149 | LYS | 2.6 |
| 68 | De | 128 | LEU | 2.6 |
| 7 | CF | 155 | ALA | 2.6 |
| 16 | AO | 11 | SER | 2.6 |
| 14 | AM | 110 | GLY | 2.6 |
| 58 | DU | 14 | THR | 2.6 |
| 60 | DW | 69 | LYS | 2.6 |
| 16 | AO | 76 | ILE | 2.6 |
| 36 | A1 | 1353 | U | 2.6 |
| 39 | DA | 250 | GLN | 2.6 |
| 32 | Ae | 51 | ASN | 2.6 |
| 18 | AQ | 54 | LEU | 2.6 |
| 34 | Cg | 165 | ASP | 2.6 |
| 48 | BJ | 11 | ASP | 2.6 |
| 5 | AD | 50 | ILE | 2.6 |
| 4 | CC | 92 | ALA | 2.5 |
| 28 | Aa | 49 | ALA | 2.5 |
| 45 | BG | 116 | VAL | 2.5 |
| 28 | Aa | 31 | PRO | 2.5 |
| 80 | A6 | 721 | U | 2.5 |
| 20 | AS | 76 | PRO | 2.5 |
| 22 | AU | 20 | ILE | 2.5 |
| 28 | Aa | 61 | GLU | 2.5 |
| 12 | CK | 97 | PRO | 2.5 |
| 80 | A6 | 239 | C | 2.5 |
| 7 | AF | 70 | VAL | 2.5 |
| 22 | AU | 53 | LYS | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 60 | DW | 135 | SER | 2.5 |
| 6 | AE | 25 | GLY | 2.5 |
| 16 | AO | 75 | GLY | 2.5 |
| 58 | DU | 13 | LYS | 2.5 |
| 34 | Cg | 252 | LEU | 2.5 |
| 14 | CM | 82 | PRO | 2.5 |
| 2 | CA | 185 | ARG | 2.5 |
| 3 | AB | 132 | ASP | 2.5 |
| 34 | Cg | 319 | ASN | 2.5 |
| 33 | Cf | 125 | THR | 2.5 |
| 81 | Ch | 51 | ARG | 2.5 |
| 7 | AF | 71 | ALA | 2.5 |
| 27 | CZ | 50 | ILE | 2.5 |
| 55 | BR | 186 | LYS | 2.5 |
| 83 | Dq | 88 | PHE | 2.5 |
| 1 | A2 | 716 | C | 2.5 |
| 14 | AM | 129 | GLU | 2.5 |
| 26 | CY | 133 | ASN | 2.5 |
| 7 | CF | 151 | GLY | 2.5 |
| 28 | Aa | 35 | ALA | 2.5 |
| 58 | DU | 33 | TYR | 2.5 |
| 3 | AB | 85 | LYS | 2.4 |
| 11 | CJ | 148 | VAL | 2.4 |
| 30 | Ac | 44 | VAL | 2.4 |
| 8 | CG | 22 | HIS | 2.4 |
| 14 | AM | 26 | ASP | 2.4 |
| 10 | AI | 200 | LYS | 2.4 |
| 22 | AU | 84 | MET | 2.4 |
| 3 | AB | 93 | GLY | 2.4 |
| 39 | DA | 247 | ARG | 2.4 |
| 14 | AM | 136 | ILE | 2.4 |
| 72 | Di | 100 | HIS | 2.4 |
| 29 | Ab | 32 | PHE | 2.4 |
| 14 | AM | 111 | ASN | 2.4 |
| 13 | AL | 4 | GLU | 2.4 |
| 1 | A2 | 132 | U | 2.4 |
| 36 | A5 | 1570 | U | 2.4 |
| 80 | A6 | 657 | U | 2.4 |
| 9 | CH | 93 | LEU | 2.4 |
| 75 | Dl | 2 | ALA | 2.4 |
| 28 | Aa | 69 | ASN | 2.4 |
| 2 | AA | 40 | ALA | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 27 | CZ | 37 | GLN | 2.4 |
| 45 | DG | 109 | LEU | 2.4 |
| 36 | A5 | 2507 | C | 2.4 |
| 63 | DZ | 56 | LYS | 2.4 |
| 14 | CM | 25 | GLU | 2.4 |
| 28 | Aa | 46 | GLU | 2.4 |
| 14 | CM | 87 | PRO | 2.4 |
| 5 | AD | 143 | ARG | 2.4 |
| 46 | DH | 191 | LEU | 2.4 |
| 36 | A1 | 2522 | G | 2.4 |
| 13 | CL | 116 | ARG | 2.4 |
| 47 | BI | 221 | ALA | 2.4 |
| 20 | AS | 69 | ILE | 2.4 |
| 4 | CC | 87 | GLN | 2.4 |
| 80 | A6 | 1711 | C | 2.4 |
| 46 | BH | 134 | ILE | 2.4 |
| 83 | Dq | 100 | ILE | 2.4 |
| 3 | AB | 209 | ASN | 2.4 |
| 28 | Aa | 60 | PRO | 2.4 |
| 22 | CU | 104 | THR | 2.4 |
| 34 | Ag | 79 | TYR | 2.4 |
| 34 | Cg | 79 | TYR | 2.4 |
| 26 | AY | 125 | LEU | 2.4 |
| 6 | AE | 134 | LYS | 2.3 |
| 80 | A6 | 719 | U | 2.3 |
| 17 | AP | 101 | ALA | 2.3 |
| 3 | AB | 184 | LEU | 2.3 |
| 14 | AM | 59 | LEU | 2.3 |
| 12 | CK | 92 | ILE | 2.3 |
| 43 | DE | 130 | ILE | 2.3 |
| 55 | BR | 170 | ARG | 2.3 |
| 17 | CP | 6 | ASN | 2.3 |
| 2 | AA | 185 | ARG | 2.3 |
| 13 | AL | 149 | ALA | 2.3 |
| 30 | Cc | 66 | LEU | 2.3 |
| 13 | AL | 147 | GLY | 2.3 |
| 6 | AE | 123 | LEU | 2.3 |
| 18 | CQ | 141 | SER | 2.3 |
| 80 | A6 | 675 | U | 2.3 |
| 80 | A6 | 653 | C | 2.3 |
| 1 | A2 | 714 | G | 2.3 |
| 26 | AY | 132 | ARG | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 4 | CC | 88 | LYS | 2.3 |
| 22 | CU | 14 | GLN | 2.3 |
| 33 | Cf | 151 | ASN | 2.3 |
| 36 | A5 | 440 | A | 2.3 |
| 14 | AM | 32 | LEU | 2.3 |
| 34 | Ag | 115 | ILE | 2.3 |
| 6 | AE | 260 | GLY | 2.3 |
| 13 | CL | 147 | GLY | 2.3 |
| 1 | A2 | 494 | U | 2.3 |
| 18 | AQ | 92 | TYR | 2.3 |
| 6 | AE | 22 | LYS | 2.3 |
| 14 | AM | 88 | LEU | 2.3 |
| 5 | AD | 217 | ILE | 2.3 |
| 14 | CM | 60 | VAL | 2.3 |
| 36 | A5 | 1572 | U | 2.3 |
| 53 | BP | 157 | VAL | 2.3 |
| 7 | AF | 151 | GLY | 2.3 |
| 33 | Cf | 143 | LYS | 2.3 |
| 16 | AO | 114 | ARG | 2.3 |
| 3 | AB | 55 | LYS | 2.3 |
| 31 | Ad | 5 | ASN | 2.3 |
| 6 | CE | 261 | LEU | 2.3 |
| 36 | A1 | 1103 | A | 2.3 |
| 60 | DW | 132 | GLY | 2.3 |
| 34 | Cg | 51 | ASP | 2.3 |
| 16 | AO | 103 | ARG | 2.3 |
| 27 | CZ | 71 | ILE | 2.3 |
| 12 | CK | 79 | TYR | 2.3 |
| 16 | AO | 13 | VAL | 2.3 |
| 34 | Ag | 253 | ALA | 2.3 |
| 1 | A2 | 729 | G | 2.2 |
| 63 | BZ | 99 | GLU | 2.2 |
| 20 | CS | 18 | LEU | 2.2 |
| 39 | DA | 252 | THR | 2.2 |
| 80 | A6 | 1491 | U | 2.2 |
| 80 | A6 | 1399 | C | 2.2 |
| 14 | CM | 63 | VAL | 2.2 |
| 21 | AT | 50 | ALA | 2.2 |
| 22 | AU | 54 | GLY | 2.2 |
| 36 | A1 | 2445 | A | 2.2 |
| 32 | Ae | 48 | THR | 2.2 |
| 80 | A6 | 794 | U | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 3 | AB | 28 | GLU | 2.2 |
| 36 | A5 | 2444 | C | 2.2 |
| 80 | A6 | 491 | C | 2.2 |
| 7 | CF | 156 | ARG | 2.2 |
| 4 | AC | 34 | GLY | 2.2 |
| 32 | Ce | 2 | ALA | 2.2 |
| 28 | Aa | 17 | HIS | 2.2 |
| 28 | Aa | 66 | LYS | 2.2 |
| 14 | CM | 86 | VAL | 2.2 |
| 66 | Dc | 100 | ILE | 2.2 |
| 17 | CP | 103 | ASN | 2.2 |
| 20 | AS | 44 | ASN | 2.2 |
| 34 | Cg | 227 | ALA | 2.2 |
| 16 | AO | 80 | HIS | 2.2 |
| 30 | Ac | 67 | ARG | 2.2 |
| 8 | AG | 182 | GLN | 2.2 |
| 33 | Af | 151 | ASN | 2.2 |
| 3 | AB | 83 | LYS | 2.2 |
| 3 | AB | 216 | LYS | 2.2 |
| 16 | AO | 116 | GLU | 2.2 |
| 3 | AB | 104 | ASP | 2.2 |
| 28 | Aa | 83 | ILE | 2.2 |
| 7 | CF | 152 | GLY | 2.2 |
| 36 | A1 | 1762 | C | 2.2 |
| 14 | CM | 137 | MET | 2.2 |
| 39 | DA | 143 | GLU | 2.2 |
| 11 | AJ | 87 | SER | 2.2 |
| 80 | A6 | 1398 | U | 2.2 |
| 26 | CY | 134 | ALA | 2.2 |
| 58 | BU | 89 | LEU | 2.2 |
| 35 | Ah | 101 | ASP | 2.2 |
| 83 | Dq | 104 | ARG | 2.2 |
| 14 | AM | 28 | LEU | 2.2 |
| 14 | AM | 50 | LYS | 2.2 |
| 55 | BR | 173 | ARG | 2.2 |
| 34 | Cg | 121 | MET | 2.2 |
| 2 | AA | 32 | HIS | 2.2 |
| 10 | AI | 199 | LYS | 2.2 |
| 14 | AM | 128 | ALA | 2.2 |
| 32 | Ae | 45 | VAL | 2.2 |
| 33 | Cf | 108 | VAL | 2.2 |
| 17 | CP | 128 | HIS | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 34 | Ag | 181 | TRP | 2.1 |
| 65 | Db | 22 | LYS | 2.2 |
| 65 | Db | 25 | LYS | 2.2 |
| 1 | A2 | 711 | U | 2.1 |
| 1 | A2 | 1687 | U | 2.1 |
| 70 | Dg | 33 | GLN | 2.1 |
| 7 | AF | 68 | ILE | 2.1 |
| 18 | AQ | 39 | VAL | 2.1 |
| 30 | Cc | 43 | ASN | 2.1 |
| 21 | AT | 80 | TYR | 2.1 |
| 10 | AI | 8 | ARG | 2.1 |
| 32 | Ae | 39 | LEU | 2.1 |
| 15 | AN | 61 | THR | 2.1 |
| 34 | Cg | 253 | ALA | 2.1 |
| 48 | BJ | 96 | PHE | 2.1 |
| 22 | CU | 102 | ARG | 2.1 |
| 30 | Cc | 9 | LEU | 2.1 |
| 5 | AD | 54 | ARG | 2.1 |
| 14 | CM | 113 | ARG | 2.1 |
| 63 | DZ | 4 | PHE | 2.1 |
| 60 | DW | 65 | GLU | 2.1 |
| 74 | Dk | 69 | LEU | 2.1 |
| 80 | A6 | 651 | G | 2.1 |
| 1 | A2 | 696 | C | 2.1 |
| 6 | AE | 54 | TYR | 2.1 |
| 28 | Aa | 68 | TYR | 2.1 |
| 36 | A1 | 1567 | U | 2.1 |
| 8 | CG | 147 | LEU | 2.1 |
| 11 | AJ | 177 | ALA | 2.1 |
| 14 | CM | 26 | ASP | 2.1 |
| 55 | DR | 183 | ALA | 2.1 |
| 14 | AM | 83 | GLU | 2.1 |
| 36 | A5 | 1564 | U | 2.1 |
| 31 | Cd | 6 | VAL | 2.1 |
| 34 | Ag | 43 | ILE | 2.1 |
| 83 | Dq | 80 | VAL | 2.1 |
| 28 | Aa | 64 | LEU | 2.1 |
| 76 | Bm | 128 | LYS | 2.1 |
| 56 | BS | 2 | ALA | 2.1 |
| 1 | A2 | 492 | A | 2.1 |
| 34 | Ag | 313 | TRP | 2.1 |
| 28 | Ca | 11 | ASN | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 34 | Cg | 53 | LYS | 2.1 |
| 36 | A5 | 2538 | U | 2.1 |
| 11 | AJ | 179 | ARG | 2.1 |
| 58 | DU | 15 | PHE | 2.1 |
| 53 | BP | 156 | ALA | 2.1 |
| 14 | CM | 122 | VAL | 2.1 |
| 11 | CJ | 3 | ARG | 2.1 |
| 12 | AK | 66 | TYR | 2.1 |
| 60 | BW | 65 | GLU | 2.1 |
| 11 | AJ | 6 | ARG | 2.1 |
| 23 | CV | 44 | ARG | 2.1 |
| 34 | Ag | 3 | SER | 2.1 |
| 14 | CM | 74 | LEU | 2.1 |
| 36 | A5 | 249 | U | 2.1 |
| 1 | A2 | 717 | C | 2.1 |
| 5 | AD | 122 | VAL | 2.1 |
| 28 | Aa | 89 | ARG | 2.1 |
| 69 | Bf | 60 | ARG | 2.1 |
| 45 | DG | 121 | SER | 2.1 |
| 58 | DU | 11 | ILE | 2.1 |
| 19 | AR | 2 | GLY | 2.1 |
| 30 | Ac | 66 | LEU | 2.1 |
| 8 | AG | 156 | PHE | 2.1 |
| 68 | De | 16 | LYS | 2.1 |
| 36 | A1 | 1764 | U | 2.1 |
| 36 | A5 | 1763 | U | 2.1 |
| 60 | BW | 81 | PRO | 2.1 |
| 80 | A6 | 501 | U | 2.1 |
| 6 | AE | 133 | LYS | 2.0 |
| 16 | AO | 78 | ALA | 2.0 |
| 58 | DU | 98 | THR | 2.0 |
| 68 | Be | 127 | ALA | 2.0 |
| 78 | Do | 54 | THR | 2.0 |
| 14 | AM | 89 | ILE | 2.0 |
| 20 | AS | 35 | ILE | 2.0 |
| 14 | CM | 40 | GLY | 2.0 |
| 5 | CD | 178 | ARG | 2.0 |
| 19 | CR | 62 | GLN | 2.0 |
| 14 | AM | 41 | LEU | 2.0 |
| 60 | DW | 129 | LYS | 2.0 |
| 25 | AX | 144 | ARG | 2.0 |
| 22 | AU | 87 | HIS | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 14 | AM | 20 | ALA | 2.0 |
| 16 | CO | 112 | ILE | 2.0 |
| 28 | Aa | 67 | THR | 2.0 |
| 63 | BZ | 70 | PRO | 2.0 |
| 80 | A6 | 194 | U | 2.0 |
| 11 | AJ | 97 | LEU | 2.0 |
| 77 | Bn | 25 | LYS | 2.0 |
| 14 | AM | 104 | GLY | 2.0 |
| 16 | AO | 44 | GLY | 2.0 |
| 19 | AR | 123 | ASN | 2.0 |
| 36 | A5 | 1017 | C | 2.0 |
| 5 | AD | 179 | GLN | 2.0 |
| 8 | AG | 199 | GLN | 2.0 |
| 14 | AM | 107 | ASP | 2.0 |
| 68 | Be | 26 | HIS | 2.0 |
| 70 | Bg | 113 | LYS | 2.0 |
| 83 | Dq | 25 | LEU | 2.0 |
| 36 | A5 | 1571 | A | 2.0 |
| 30 | Cc | 45 | LYS | 2.0 |
| 70 | Dg | 102 | LYS | 2.0 |
| 5 | CD | 142 | LEU | 2.0 |
| 9 | AH | 58 | LEU | 2.0 |

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

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

6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

6.4 Ligands [\(i\)](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|----------------------------|-------|
| 87 | MG | A2 | 2209 | 1/1 | -0.15 | 0.41 | 96,96,96,96 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|----------------------------|-------|
| 87 | MG | A2 | 2227 | 1/1 | -0.10 | 0.19 | 106,106,106,106 | 0 |
| 87 | MG | A1 | 4299 | 1/1 | -0.05 | 0.41 | 84,84,84,84 | 0 |
| 87 | MG | A5 | 4515 | 1/1 | 0.02 | 0.41 | 109,109,109,109 | 0 |
| 87 | MG | A1 | 4230 | 1/1 | 0.08 | 0.38 | 91,91,91,91 | 0 |
| 87 | MG | A6 | 2250 | 1/1 | 0.10 | 0.46 | 96,96,96,96 | 0 |
| 87 | MG | A5 | 4203 | 1/1 | 0.12 | 0.29 | 82,82,82,82 | 0 |
| 87 | MG | A5 | 4353 | 1/1 | 0.13 | 0.61 | 71,71,71,71 | 0 |
| 88 | ZN | Ab | 101 | 1/1 | 0.13 | 0.12 | 327,327,327,327 | 0 |
| 87 | MG | A5 | 4099 | 1/1 | 0.14 | 0.30 | 93,93,93,93 | 0 |
| 87 | MG | A1 | 4150 | 1/1 | 0.16 | 0.60 | 95,95,95,95 | 0 |
| 87 | MG | A1 | 4481 | 1/1 | 0.18 | 0.32 | 97,97,97,97 | 0 |
| 87 | MG | A6 | 2259 | 1/1 | 0.19 | 0.66 | 119,119,119,119 | 0 |
| 87 | MG | A5 | 4177 | 1/1 | 0.19 | 0.42 | 65,65,65,65 | 0 |
| 87 | MG | A5 | 4254 | 1/1 | 0.20 | 0.66 | 103,103,103,103 | 0 |
| 87 | MG | A6 | 2316 | 1/1 | 0.21 | 0.58 | 112,112,112,112 | 0 |
| 87 | MG | AB | 301 | 1/1 | 0.23 | 0.33 | 98,98,98,98 | 0 |
| 87 | MG | A1 | 4109 | 1/1 | 0.23 | 0.37 | 80,80,80,80 | 0 |
| 87 | MG | A1 | 4147 | 1/1 | 0.24 | 0.34 | 73,73,73,73 | 0 |
| 87 | MG | A1 | 4477 | 1/1 | 0.25 | 0.29 | 108,108,108,108 | 0 |
| 87 | MG | A5 | 4478 | 1/1 | 0.25 | 0.37 | 81,81,81,81 | 0 |
| 87 | MG | A5 | 4581 | 1/1 | 0.26 | 0.36 | 97,97,97,97 | 0 |
| 87 | MG | A1 | 3921 | 1/1 | 0.26 | 0.26 | 87,87,87,87 | 0 |
| 87 | MG | A1 | 3919 | 1/1 | 0.27 | 0.98 | 138,138,138,138 | 0 |
| 87 | MG | A5 | 4552 | 1/1 | 0.27 | 0.30 | 84,84,84,84 | 0 |
| 87 | MG | A1 | 3851 | 1/1 | 0.27 | 0.26 | 53,53,53,53 | 0 |
| 87 | MG | DJ | 202 | 1/1 | 0.27 | 0.28 | 81,81,81,81 | 0 |
| 87 | MG | A5 | 4497 | 1/1 | 0.27 | 0.29 | 76,76,76,76 | 0 |
| 87 | MG | A1 | 4448 | 1/1 | 0.29 | 0.33 | 66,66,66,66 | 0 |
| 87 | MG | A2 | 2219 | 1/1 | 0.29 | 0.24 | 93,93,93,93 | 0 |
| 87 | MG | A5 | 4485 | 1/1 | 0.30 | 0.61 | 77,77,77,77 | 0 |
| 87 | MG | DM | 203 | 1/1 | 0.31 | 0.28 | 94,94,94,94 | 0 |
| 87 | MG | A1 | 4454 | 1/1 | 0.33 | 0.35 | 81,81,81,81 | 0 |
| 87 | MG | A2 | 2221 | 1/1 | 0.34 | 0.34 | 83,83,83,83 | 0 |
| 87 | MG | A1 | 4359 | 1/1 | 0.34 | 0.27 | 70,70,70,70 | 0 |
| 87 | MG | A6 | 2308 | 1/1 | 0.34 | 0.40 | 81,81,81,81 | 0 |
| 87 | MG | A1 | 4104 | 1/1 | 0.34 | 0.21 | 65,65,65,65 | 0 |
| 87 | MG | A5 | 4320 | 1/1 | 0.34 | 0.24 | 117,117,117,117 | 0 |
| 87 | MG | A1 | 4387 | 1/1 | 0.35 | 0.54 | 89,89,89,89 | 0 |
| 87 | MG | A1 | 4495 | 1/1 | 0.35 | 0.45 | 109,109,109,109 | 0 |
| 87 | MG | A1 | 4232 | 1/1 | 0.35 | 0.57 | 75,75,75,75 | 0 |
| 87 | MG | A5 | 4207 | 1/1 | 0.35 | 0.38 | 102,102,102,102 | 0 |
| 87 | MG | A2 | 2211 | 1/1 | 0.36 | 0.76 | 94,94,94,94 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87 | MG | A2 | 2156 | 1/1 | 0.36 | 0.33 | 70,70,70,70 | 0 |
| 87 | MG | A8 | 237 | 1/1 | 0.37 | 0.27 | 85,85,85,85 | 0 |
| 87 | MG | A5 | 4084 | 1/1 | 0.37 | 0.79 | 112,112,112,112 | 0 |
| 87 | MG | A6 | 2337 | 1/1 | 0.38 | 0.29 | 127,127,127,127 | 0 |
| 87 | MG | A2 | 2208 | 1/1 | 0.38 | 0.24 | 109,109,109,109 | 0 |
| 87 | MG | A5 | 4576 | 1/1 | 0.38 | 0.31 | 77,77,77,77 | 0 |
| 87 | MG | A1 | 4228 | 1/1 | 0.38 | 0.33 | 82,82,82,82 | 0 |
| 87 | MG | AJ | 201 | 1/1 | 0.39 | 0.29 | 82,82,82,82 | 0 |
| 87 | MG | A5 | 4230 | 1/1 | 0.39 | 0.30 | 78,78,78,78 | 0 |
| 87 | MG | A1 | 4369 | 1/1 | 0.39 | 0.27 | 85,85,85,85 | 0 |
| 87 | MG | A6 | 2133 | 1/1 | 0.39 | 0.29 | 65,65,65,65 | 0 |
| 87 | MG | A1 | 4501 | 1/1 | 0.40 | 1.01 | 103,103,103,103 | 0 |
| 87 | MG | A5 | 4283 | 1/1 | 0.40 | 0.69 | 79,79,79,79 | 0 |
| 87 | MG | A6 | 2255 | 1/1 | 0.40 | 0.30 | 81,81,81,81 | 0 |
| 87 | MG | A6 | 2244 | 1/1 | 0.41 | 0.65 | 97,97,97,97 | 0 |
| 87 | MG | A6 | 2278 | 1/1 | 0.41 | 0.72 | 64,64,64,64 | 0 |
| 87 | MG | A5 | 4341 | 1/1 | 0.41 | 0.27 | 96,96,96,96 | 0 |
| 87 | MG | A1 | 4325 | 1/1 | 0.41 | 0.31 | 67,67,67,67 | 0 |
| 87 | MG | A1 | 4370 | 1/1 | 0.41 | 0.25 | 104,104,104,104 | 0 |
| 87 | MG | A5 | 4318 | 1/1 | 0.43 | 0.15 | 83,83,83,83 | 0 |
| 87 | MG | A5 | 4569 | 1/1 | 0.43 | 1.00 | 103,103,103,103 | 0 |
| 87 | MG | A6 | 2249 | 1/1 | 0.44 | 0.22 | 71,71,71,71 | 0 |
| 87 | MG | A5 | 4575 | 1/1 | 0.44 | 0.50 | 68,68,68,68 | 0 |
| 87 | MG | A1 | 4478 | 1/1 | 0.44 | 0.25 | 100,100,100,100 | 0 |
| 87 | MG | A1 | 4502 | 1/1 | 0.44 | 0.25 | 93,93,93,93 | 0 |
| 87 | MG | CY | 203 | 1/1 | 0.44 | 0.24 | 109,109,109,109 | 0 |
| 87 | MG | A1 | 4256 | 1/1 | 0.44 | 0.18 | 86,86,86,86 | 0 |
| 87 | MG | A6 | 2262 | 1/1 | 0.44 | 0.49 | 101,101,101,101 | 0 |
| 87 | MG | A1 | 4364 | 1/1 | 0.44 | 0.23 | 92,92,92,92 | 0 |
| 87 | MG | A1 | 4313 | 1/1 | 0.45 | 0.22 | 105,105,105,105 | 0 |
| 87 | MG | A3 | 229 | 1/1 | 0.45 | 0.31 | 99,99,99,99 | 0 |
| 87 | MG | A5 | 4543 | 1/1 | 0.45 | 0.18 | 78,78,78,78 | 0 |
| 87 | MG | A5 | 4464 | 1/1 | 0.45 | 0.51 | 85,85,85,85 | 0 |
| 87 | MG | A2 | 2166 | 1/1 | 0.45 | 0.34 | 90,90,90,90 | 0 |
| 87 | MG | A5 | 4324 | 1/1 | 0.45 | 0.23 | 80,80,80,80 | 0 |
| 87 | MG | A1 | 4155 | 1/1 | 0.46 | 0.73 | 88,88,88,88 | 0 |
| 87 | MG | A5 | 3929 | 1/1 | 0.46 | 0.33 | 80,80,80,80 | 0 |
| 87 | MG | A2 | 2254 | 1/1 | 0.46 | 0.22 | 61,61,61,61 | 0 |
| 87 | MG | A1 | 4337 | 1/1 | 0.46 | 0.54 | 108,108,108,108 | 0 |
| 87 | MG | A2 | 2222 | 1/1 | 0.46 | 0.64 | 103,103,103,103 | 0 |
| 87 | MG | A3 | 230 | 1/1 | 0.47 | 0.48 | 85,85,85,85 | 0 |
| 87 | MG | A6 | 2129 | 1/1 | 0.47 | 0.28 | 66,66,66,66 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | A5 | 4392 | 1/1 | 0.47 | 0.25 | 64,64,64,64 | 0 |
| 87 | MG | A2 | 2092 | 1/1 | 0.47 | 0.24 | 69,69,69,69 | 0 |
| 87 | MG | A6 | 2182 | 1/1 | 0.47 | 0.15 | 63,63,63,63 | 0 |
| 87 | MG | A6 | 2312 | 1/1 | 0.47 | 0.38 | 85,85,85,85 | 0 |
| 87 | MG | A1 | 4088 | 1/1 | 0.48 | 0.29 | 90,90,90,90 | 0 |
| 87 | MG | A5 | 4479 | 1/1 | 0.48 | 0.38 | 64,64,64,64 | 0 |
| 87 | MG | A2 | 2187 | 1/1 | 0.48 | 0.21 | 90,90,90,90 | 0 |
| 87 | MG | A5 | 4414 | 1/1 | 0.48 | 1.28 | 101,101,101,101 | 0 |
| 87 | MG | A1 | 3994 | 1/1 | 0.48 | 0.38 | 64,64,64,64 | 0 |
| 87 | MG | A5 | 4493 | 1/1 | 0.49 | 0.24 | 76,76,76,76 | 0 |
| 87 | MG | A1 | 4048 | 1/1 | 0.50 | 0.21 | 67,67,67,67 | 0 |
| 87 | MG | Cd | 102 | 1/1 | 0.50 | 0.24 | 75,75,75,75 | 0 |
| 87 | MG | DB | 413 | 1/1 | 0.50 | 0.34 | 101,101,101,101 | 0 |
| 87 | MG | A2 | 2167 | 1/1 | 0.50 | 0.33 | 72,72,72,72 | 0 |
| 87 | MG | A1 | 4274 | 1/1 | 0.50 | 0.37 | 87,87,87,87 | 0 |
| 87 | MG | A2 | 2256 | 1/1 | 0.50 | 0.71 | 80,80,80,80 | 0 |
| 87 | MG | A5 | 4263 | 1/1 | 0.51 | 0.27 | 72,72,72,72 | 0 |
| 87 | MG | A1 | 4319 | 1/1 | 0.51 | 0.31 | 76,76,76,76 | 0 |
| 87 | MG | A5 | 4503 | 1/1 | 0.51 | 0.33 | 72,72,72,72 | 0 |
| 87 | MG | A1 | 4135 | 1/1 | 0.51 | 0.41 | 96,96,96,96 | 0 |
| 87 | MG | A1 | 4239 | 1/1 | 0.51 | 0.28 | 60,60,60,60 | 0 |
| 87 | MG | A5 | 4545 | 1/1 | 0.51 | 0.39 | 94,94,94,94 | 0 |
| 87 | MG | A1 | 4241 | 1/1 | 0.51 | 0.38 | 74,74,74,74 | 0 |
| 87 | MG | A5 | 4075 | 1/1 | 0.51 | 0.38 | 60,60,60,60 | 0 |
| 87 | MG | A1 | 4249 | 1/1 | 0.51 | 0.34 | 73,73,73,73 | 0 |
| 87 | MG | A5 | 4377 | 1/1 | 0.51 | 0.32 | 85,85,85,85 | 0 |
| 87 | MG | A1 | 4184 | 1/1 | 0.51 | 0.36 | 81,81,81,81 | 0 |
| 87 | MG | A1 | 4221 | 1/1 | 0.51 | 0.16 | 92,92,92,92 | 0 |
| 87 | MG | A1 | 4288 | 1/1 | 0.51 | 0.38 | 81,81,81,81 | 0 |
| 87 | MG | BV | 201 | 1/1 | 0.51 | 0.22 | 95,95,95,95 | 0 |
| 87 | MG | A1 | 3922 | 1/1 | 0.51 | 0.45 | 107,107,107,107 | 0 |
| 86 | OHX | A6 | 2095 | 7/7 | 0.51 | 0.46 | 213,213,213,213 | 7 |
| 87 | MG | A1 | 4047 | 1/1 | 0.52 | 0.24 | 98,98,98,98 | 0 |
| 87 | MG | A5 | 4486 | 1/1 | 0.52 | 0.56 | 94,94,94,94 | 0 |
| 87 | MG | AI | 302 | 1/1 | 0.52 | 0.27 | 66,66,66,66 | 0 |
| 87 | MG | A1 | 4273 | 1/1 | 0.52 | 0.42 | 85,85,85,85 | 0 |
| 87 | MG | A5 | 4359 | 1/1 | 0.52 | 0.21 | 86,86,86,86 | 0 |
| 87 | MG | A6 | 2317 | 1/1 | 0.52 | 0.94 | 82,82,82,82 | 0 |
| 87 | MG | CQ | 202 | 1/1 | 0.53 | 0.29 | 85,85,85,85 | 0 |
| 87 | MG | A6 | 2293 | 1/1 | 0.53 | 0.21 | 78,78,78,78 | 0 |
| 87 | MG | A1 | 4137 | 1/1 | 0.53 | 0.33 | 84,84,84,84 | 0 |
| 87 | MG | DT | 203 | 1/1 | 0.53 | 0.34 | 80,80,80,80 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | A1 | 4489 | 1/1 | 0.53 | 0.31 | 94,94,94,94 | 0 |
| 87 | MG | A5 | 4518 | 1/1 | 0.54 | 1.25 | 144,144,144,144 | 0 |
| 87 | MG | A5 | 3897 | 1/1 | 0.54 | 0.38 | 100,100,100,100 | 0 |
| 87 | MG | A2 | 2181 | 1/1 | 0.54 | 0.17 | 79,79,79,79 | 0 |
| 87 | MG | CF | 302 | 1/1 | 0.54 | 0.25 | 73,73,73,73 | 0 |
| 86 | OHX | A6 | 2083 | 7/7 | 0.54 | 0.64 | 214,214,214,214 | 7 |
| 87 | MG | A1 | 4201 | 1/1 | 0.54 | 0.65 | 65,65,65,65 | 0 |
| 87 | MG | A6 | 2209 | 1/1 | 0.54 | 0.23 | 79,79,79,79 | 0 |
| 87 | MG | A1 | 4153 | 1/1 | 0.55 | 0.24 | 96,96,96,96 | 0 |
| 87 | MG | A6 | 2296 | 1/1 | 0.55 | 2.16 | 119,119,119,119 | 0 |
| 86 | OHX | A5 | 3817 | 7/7 | 0.55 | 0.19 | 205,205,205,205 | 7 |
| 87 | MG | A6 | 2282 | 1/1 | 0.55 | 0.39 | 83,83,83,83 | 0 |
| 87 | MG | A5 | 4251 | 1/1 | 0.55 | 0.38 | 85,85,85,85 | 0 |
| 87 | MG | BS | 202 | 1/1 | 0.56 | 0.35 | 84,84,84,84 | 0 |
| 87 | MG | A1 | 3918 | 1/1 | 0.56 | 0.29 | 83,83,83,83 | 0 |
| 87 | MG | A5 | 4214 | 1/1 | 0.56 | 0.32 | 66,66,66,66 | 0 |
| 87 | MG | A6 | 2103 | 1/1 | 0.56 | 0.36 | 64,64,64,64 | 0 |
| 87 | MG | A5 | 4495 | 1/1 | 0.56 | 0.31 | 88,88,88,88 | 0 |
| 87 | MG | A5 | 4241 | 1/1 | 0.56 | 0.34 | 106,106,106,106 | 0 |
| 87 | MG | A1 | 4213 | 1/1 | 0.56 | 0.19 | 79,79,79,79 | 0 |
| 87 | MG | A2 | 2123 | 1/1 | 0.56 | 0.39 | 81,81,81,81 | 0 |
| 87 | MG | A1 | 4103 | 1/1 | 0.56 | 0.24 | 74,74,74,74 | 0 |
| 87 | MG | A1 | 4252 | 1/1 | 0.56 | 0.28 | 121,121,121,121 | 0 |
| 87 | MG | A2 | 2236 | 1/1 | 0.56 | 0.10 | 100,100,100,100 | 0 |
| 87 | MG | A1 | 3987 | 1/1 | 0.57 | 0.22 | 57,57,57,57 | 0 |
| 87 | MG | A2 | 2231 | 1/1 | 0.57 | 0.32 | 75,75,75,75 | 0 |
| 87 | MG | BQ | 202 | 1/1 | 0.57 | 0.83 | 80,80,80,80 | 0 |
| 87 | MG | A1 | 4395 | 1/1 | 0.57 | 0.16 | 97,97,97,97 | 0 |
| 87 | MG | A6 | 2335 | 1/1 | 0.57 | 0.69 | 84,84,84,84 | 0 |
| 87 | MG | A5 | 4349 | 1/1 | 0.57 | 1.82 | 79,79,79,79 | 0 |
| 87 | MG | A1 | 4282 | 1/1 | 0.57 | 0.41 | 92,92,92,92 | 0 |
| 87 | MG | A5 | 3826 | 1/1 | 0.58 | 0.45 | 63,63,63,63 | 0 |
| 87 | MG | A2 | 2194 | 1/1 | 0.58 | 0.48 | 113,113,113,113 | 0 |
| 87 | MG | A1 | 4301 | 1/1 | 0.58 | 0.13 | 118,118,118,118 | 0 |
| 87 | MG | Ba | 205 | 1/1 | 0.58 | 0.27 | 69,69,69,69 | 0 |
| 87 | MG | A2 | 2147 | 1/1 | 0.58 | 0.20 | 93,93,93,93 | 0 |
| 87 | MG | BA | 302 | 1/1 | 0.59 | 0.40 | 63,63,63,63 | 0 |
| 87 | MG | A6 | 2132 | 1/1 | 0.59 | 0.23 | 81,81,81,81 | 0 |
| 87 | MG | A5 | 3920 | 1/1 | 0.59 | 0.31 | 83,83,83,83 | 0 |
| 87 | MG | A1 | 4069 | 1/1 | 0.59 | 0.24 | 69,69,69,69 | 0 |
| 87 | MG | A2 | 2135 | 1/1 | 0.59 | 0.12 | 54,54,54,54 | 0 |
| 87 | MG | A7 | 228 | 1/1 | 0.59 | 0.44 | 85,85,85,85 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87 | MG | A1 | 4233 | 1/1 | 0.59 | 0.24 | 79,79,79,79 | 0 |
| 87 | MG | A6 | 2222 | 1/1 | 0.59 | 0.22 | 86,86,86,86 | 0 |
| 87 | MG | A6 | 2240 | 1/1 | 0.59 | 0.21 | 95,95,95,95 | 0 |
| 87 | MG | A2 | 2243 | 1/1 | 0.59 | 0.30 | 86,86,86,86 | 0 |
| 87 | MG | A1 | 4059 | 1/1 | 0.59 | 0.43 | 84,84,84,84 | 0 |
| 87 | MG | A5 | 4549 | 1/1 | 0.59 | 0.46 | 70,70,70,70 | 0 |
| 87 | MG | A1 | 4420 | 1/1 | 0.60 | 0.61 | 73,73,73,73 | 0 |
| 87 | MG | A6 | 2324 | 1/1 | 0.60 | 0.26 | 74,74,74,74 | 0 |
| 87 | MG | A6 | 2334 | 1/1 | 0.60 | 0.36 | 72,72,72,72 | 0 |
| 87 | MG | A5 | 4476 | 1/1 | 0.60 | 0.50 | 86,86,86,86 | 0 |
| 87 | MG | A1 | 4141 | 1/1 | 0.60 | 0.40 | 53,53,53,53 | 0 |
| 87 | MG | A5 | 4571 | 1/1 | 0.60 | 0.36 | 84,84,84,84 | 0 |
| 87 | MG | A5 | 4312 | 1/1 | 0.60 | 0.39 | 87,87,87,87 | 0 |
| 87 | MG | Ad | 102 | 1/1 | 0.60 | 0.13 | 89,89,89,89 | 0 |
| 87 | MG | A5 | 4146 | 1/1 | 0.60 | 0.25 | 80,80,80,80 | 0 |
| 87 | MG | A1 | 3920 | 1/1 | 0.60 | 0.24 | 53,53,53,53 | 0 |
| 87 | MG | A1 | 4291 | 1/1 | 0.60 | 0.18 | 112,112,112,112 | 0 |
| 87 | MG | A6 | 2245 | 1/1 | 0.60 | 0.18 | 82,82,82,82 | 0 |
| 87 | MG | A1 | 4244 | 1/1 | 0.60 | 0.32 | 52,52,52,52 | 0 |
| 87 | MG | A1 | 4357 | 1/1 | 0.60 | 0.32 | 89,89,89,89 | 0 |
| 87 | MG | A6 | 2169 | 1/1 | 0.60 | 0.33 | 77,77,77,77 | 0 |
| 87 | MG | A5 | 4529 | 1/1 | 0.60 | 0.53 | 91,91,91,91 | 0 |
| 87 | MG | A1 | 4465 | 1/1 | 0.61 | 0.37 | 92,92,92,92 | 0 |
| 87 | MG | A5 | 3872 | 1/1 | 0.61 | 0.31 | 81,81,81,81 | 0 |
| 87 | MG | A1 | 4222 | 1/1 | 0.61 | 0.25 | 73,73,73,73 | 0 |
| 87 | MG | A1 | 4277 | 1/1 | 0.61 | 0.73 | 89,89,89,89 | 0 |
| 87 | MG | A6 | 2134 | 1/1 | 0.61 | 0.35 | 67,67,67,67 | 0 |
| 87 | MG | A6 | 2328 | 1/1 | 0.61 | 0.21 | 87,87,87,87 | 0 |
| 87 | MG | BI | 305 | 1/1 | 0.61 | 0.24 | 84,84,84,84 | 0 |
| 87 | MG | A1 | 3928 | 1/1 | 0.61 | 0.43 | 88,88,88,88 | 0 |
| 87 | MG | A5 | 4319 | 1/1 | 0.61 | 0.19 | 86,86,86,86 | 0 |
| 87 | MG | A5 | 4492 | 1/1 | 0.61 | 0.42 | 73,73,73,73 | 0 |
| 87 | MG | A6 | 2184 | 1/1 | 0.61 | 0.20 | 67,67,67,67 | 0 |
| 87 | MG | A1 | 4190 | 1/1 | 0.61 | 0.27 | 98,98,98,98 | 0 |
| 87 | MG | A5 | 4191 | 1/1 | 0.61 | 0.29 | 99,99,99,99 | 0 |
| 87 | MG | DC | 406 | 1/1 | 0.61 | 0.30 | 111,111,111,111 | 0 |
| 87 | MG | A5 | 4502 | 1/1 | 0.61 | 0.28 | 84,84,84,84 | 0 |
| 86 | OHX | BI | 303 | 7/7 | 0.61 | 0.46 | 215,215,215,215 | 7 |
| 87 | MG | DO | 207 | 1/1 | 0.61 | 0.53 | 109,109,109,109 | 0 |
| 87 | MG | A1 | 4058 | 1/1 | 0.61 | 0.27 | 97,97,97,97 | 0 |
| 87 | MG | A2 | 2182 | 1/1 | 0.61 | 0.21 | 78,78,78,78 | 0 |
| 87 | MG | BO | 202 | 1/1 | 0.62 | 0.20 | 77,77,77,77 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | A1 | 3991 | 1/1 | 0.62 | 0.40 | 52,52,52,52 | 0 |
| 87 | MG | A2 | 2193 | 1/1 | 0.62 | 0.25 | 79,79,79,79 | 0 |
| 87 | MG | A1 | 3898 | 1/1 | 0.62 | 0.23 | 64,64,64,64 | 0 |
| 87 | MG | A5 | 4135 | 1/1 | 0.62 | 0.43 | 73,73,73,73 | 0 |
| 87 | MG | A1 | 4087 | 1/1 | 0.62 | 0.25 | 67,67,67,67 | 0 |
| 87 | MG | A2 | 2201 | 1/1 | 0.62 | 0.15 | 96,96,96,96 | 0 |
| 87 | MG | A5 | 4179 | 1/1 | 0.62 | 0.23 | 71,71,71,71 | 0 |
| 87 | MG | A5 | 4390 | 1/1 | 0.62 | 0.21 | 70,70,70,70 | 0 |
| 87 | MG | DQ | 202 | 1/1 | 0.62 | 0.28 | 88,88,88,88 | 0 |
| 87 | MG | A6 | 2299 | 1/1 | 0.62 | 0.75 | 84,84,84,84 | 0 |
| 87 | MG | A1 | 4089 | 1/1 | 0.62 | 0.18 | 89,89,89,89 | 0 |
| 88 | ZN | Cb | 101 | 1/1 | 0.62 | 0.33 | 305,305,305,305 | 0 |
| 87 | MG | A1 | 4493 | 1/1 | 0.63 | 0.36 | 66,66,66,66 | 0 |
| 87 | MG | A5 | 4067 | 1/1 | 0.63 | 0.33 | 61,61,61,61 | 0 |
| 86 | OHX | A1 | 3779 | 7/7 | 0.63 | 0.46 | 164,164,164,164 | 7 |
| 87 | MG | A5 | 4081 | 1/1 | 0.63 | 0.41 | 79,79,79,79 | 0 |
| 87 | MG | A5 | 4244 | 1/1 | 0.63 | 0.17 | 82,82,82,82 | 0 |
| 86 | OHX | A2 | 2082 | 7/7 | 0.63 | 0.23 | 225,225,225,225 | 7 |
| 87 | MG | CS | 203 | 1/1 | 0.63 | 0.12 | 71,71,71,71 | 0 |
| 87 | MG | A1 | 4344 | 1/1 | 0.63 | 0.20 | 88,88,88,88 | 0 |
| 87 | MG | A5 | 4267 | 1/1 | 0.63 | 0.28 | 88,88,88,88 | 0 |
| 87 | MG | A1 | 4217 | 1/1 | 0.63 | 0.17 | 57,57,57,57 | 0 |
| 86 | OHX | A5 | 3792 | 7/7 | 0.63 | 0.40 | 217,217,217,217 | 7 |
| 87 | MG | A6 | 2332 | 1/1 | 0.63 | 0.41 | 80,80,80,80 | 0 |
| 87 | MG | A1 | 4068 | 1/1 | 0.63 | 0.35 | 78,78,78,78 | 0 |
| 87 | MG | A5 | 4482 | 1/1 | 0.63 | 0.73 | 79,79,79,79 | 0 |
| 87 | MG | A6 | 2254 | 1/1 | 0.63 | 0.17 | 69,69,69,69 | 0 |
| 87 | MG | A5 | 4253 | 1/1 | 0.64 | 0.28 | 75,75,75,75 | 0 |
| 87 | MG | A1 | 4436 | 1/1 | 0.64 | 0.13 | 115,115,115,115 | 0 |
| 87 | MG | A1 | 4447 | 1/1 | 0.64 | 0.58 | 104,104,104,104 | 0 |
| 87 | MG | A5 | 4211 | 1/1 | 0.64 | 0.35 | 77,77,77,77 | 0 |
| 87 | MG | A5 | 4162 | 1/1 | 0.64 | 0.20 | 70,70,70,70 | 0 |
| 87 | MG | A5 | 4164 | 1/1 | 0.64 | 0.13 | 87,87,87,87 | 0 |
| 87 | MG | A5 | 3839 | 1/1 | 0.64 | 0.19 | 48,48,48,48 | 0 |
| 87 | MG | Dq | 401 | 1/1 | 0.64 | 0.12 | 81,81,81,81 | 0 |
| 87 | MG | A6 | 2187 | 1/1 | 0.64 | 0.23 | 64,64,64,64 | 0 |
| 87 | MG | A5 | 4121 | 1/1 | 0.64 | 0.23 | 55,55,55,55 | 0 |
| 87 | MG | A2 | 2168 | 1/1 | 0.65 | 0.28 | 78,78,78,78 | 0 |
| 87 | MG | A5 | 4224 | 1/1 | 0.65 | 0.27 | 58,58,58,58 | 0 |
| 87 | MG | DF | 303 | 1/1 | 0.65 | 0.28 | 73,73,73,73 | 0 |
| 87 | MG | A5 | 4561 | 1/1 | 0.65 | 0.58 | 111,111,111,111 | 0 |
| 87 | MG | A5 | 4351 | 1/1 | 0.65 | 0.38 | 85,85,85,85 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87 | MG | A5 | 4087 | 1/1 | 0.65 | 0.28 | 86,86,86,86 | 0 |
| 87 | MG | A6 | 2128 | 1/1 | 0.65 | 0.36 | 81,81,81,81 | 0 |
| 87 | MG | A2 | 2245 | 1/1 | 0.65 | 0.16 | 71,71,71,71 | 0 |
| 87 | MG | A6 | 2333 | 1/1 | 0.65 | 1.27 | 99,99,99,99 | 0 |
| 87 | MG | A5 | 3860 | 1/1 | 0.65 | 0.29 | 66,66,66,66 | 0 |
| 87 | MG | A6 | 2158 | 1/1 | 0.65 | 0.46 | 66,66,66,66 | 0 |
| 87 | MG | A5 | 4445 | 1/1 | 0.66 | 0.29 | 65,65,65,65 | 0 |
| 87 | MG | A5 | 4556 | 1/1 | 0.66 | 0.31 | 73,73,73,73 | 0 |
| 87 | MG | A1 | 3836 | 1/1 | 0.66 | 0.31 | 48,48,48,48 | 0 |
| 87 | MG | A5 | 3965 | 1/1 | 0.66 | 0.38 | 64,64,64,64 | 0 |
| 87 | MG | Bo | 202 | 1/1 | 0.66 | 0.37 | 82,82,82,82 | 0 |
| 87 | MG | Bo | 203 | 1/1 | 0.66 | 0.38 | 79,79,79,79 | 0 |
| 87 | MG | A2 | 2145 | 1/1 | 0.66 | 0.33 | 71,71,71,71 | 0 |
| 87 | MG | A1 | 4281 | 1/1 | 0.66 | 0.23 | 74,74,74,74 | 0 |
| 87 | MG | A7 | 226 | 1/1 | 0.66 | 0.19 | 74,74,74,74 | 0 |
| 87 | MG | A2 | 2242 | 1/1 | 0.66 | 0.15 | 105,105,105,105 | 0 |
| 87 | MG | A5 | 4347 | 1/1 | 0.66 | 0.26 | 78,78,78,78 | 0 |
| 87 | MG | A1 | 4242 | 1/1 | 0.66 | 0.17 | 84,84,84,84 | 0 |
| 87 | MG | A1 | 3932 | 1/1 | 0.66 | 0.29 | 30,30,30,30 | 0 |
| 87 | MG | A5 | 4131 | 1/1 | 0.66 | 0.23 | 85,85,85,85 | 0 |
| 87 | MG | DH | 202 | 1/1 | 0.66 | 0.62 | 73,73,73,73 | 0 |
| 86 | OHX | A2 | 2077 | 7/7 | 0.66 | 0.31 | 206,206,206,206 | 7 |
| 87 | MG | A5 | 4375 | 1/1 | 0.66 | 0.82 | 65,65,65,65 | 0 |
| 87 | MG | A2 | 2141 | 1/1 | 0.66 | 0.28 | 68,68,68,68 | 0 |
| 87 | MG | A2 | 2207 | 1/1 | 0.66 | 0.34 | 76,76,76,76 | 0 |
| 87 | MG | A1 | 4198 | 1/1 | 0.66 | 0.24 | 79,79,79,79 | 0 |
| 87 | MG | De | 203 | 1/1 | 0.66 | 1.56 | 109,109,109,109 | 0 |
| 87 | MG | A5 | 4397 | 1/1 | 0.66 | 0.17 | 101,101,101,101 | 0 |
| 87 | MG | A1 | 4404 | 1/1 | 0.66 | 0.28 | 80,80,80,80 | 0 |
| 88 | ZN | Bo | 205 | 1/1 | 0.66 | 0.14 | 209,209,209,209 | 0 |
| 87 | MG | A5 | 4420 | 1/1 | 0.66 | 0.26 | 93,93,93,93 | 0 |
| 87 | MG | A5 | 4334 | 1/1 | 0.67 | 0.11 | 109,109,109,109 | 0 |
| 87 | MG | A5 | 4078 | 1/1 | 0.67 | 0.30 | 49,49,49,49 | 0 |
| 87 | MG | A1 | 4492 | 1/1 | 0.67 | 0.21 | 100,100,100,100 | 0 |
| 86 | OHX | BI | 304 | 7/7 | 0.67 | 0.36 | 193,193,193,193 | 7 |
| 87 | MG | A5 | 4086 | 1/1 | 0.67 | 0.28 | 59,59,59,59 | 0 |
| 87 | MG | A1 | 3847 | 1/1 | 0.67 | 0.15 | 74,74,74,74 | 0 |
| 87 | MG | A1 | 4156 | 1/1 | 0.67 | 0.24 | 75,75,75,75 | 0 |
| 87 | MG | A1 | 4206 | 1/1 | 0.67 | 0.21 | 55,55,55,55 | 0 |
| 87 | MG | A1 | 4057 | 1/1 | 0.67 | 0.25 | 63,63,63,63 | 0 |
| 87 | MG | A5 | 4379 | 1/1 | 0.67 | 0.40 | 45,45,45,45 | 0 |
| 87 | MG | A1 | 4368 | 1/1 | 0.67 | 0.71 | 80,80,80,80 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | A5 | 4138 | 1/1 | 0.67 | 0.39 | 77,77,77,77 | 0 |
| 87 | MG | A5 | 3888 | 1/1 | 0.67 | 0.24 | 64,64,64,64 | 0 |
| 87 | MG | A5 | 4157 | 1/1 | 0.67 | 0.19 | 56,56,56,56 | 0 |
| 87 | MG | A6 | 2275 | 1/1 | 0.67 | 0.18 | 63,63,63,63 | 0 |
| 87 | MG | A6 | 2195 | 1/1 | 0.67 | 0.32 | 93,93,93,93 | 0 |
| 87 | MG | A1 | 4483 | 1/1 | 0.67 | 0.20 | 72,72,72,72 | 0 |
| 87 | MG | A1 | 4290 | 1/1 | 0.67 | 0.25 | 69,69,69,69 | 0 |
| 87 | MG | BI | 307 | 1/1 | 0.67 | 2.09 | 81,81,81,81 | 0 |
| 87 | MG | BN | 304 | 1/1 | 0.67 | 0.33 | 80,80,80,80 | 0 |
| 87 | MG | A1 | 4487 | 1/1 | 0.68 | 0.23 | 80,80,80,80 | 0 |
| 87 | MG | A3 | 231 | 1/1 | 0.68 | 0.34 | 92,92,92,92 | 0 |
| 87 | MG | Bj | 107 | 1/1 | 0.68 | 0.44 | 101,101,101,101 | 0 |
| 87 | MG | A6 | 2326 | 1/1 | 0.68 | 0.19 | 117,117,117,117 | 0 |
| 87 | MG | A5 | 4217 | 1/1 | 0.68 | 0.40 | 83,83,83,83 | 0 |
| 87 | MG | A1 | 3940 | 1/1 | 0.68 | 0.37 | 51,51,51,51 | 0 |
| 87 | MG | BG | 301 | 1/1 | 0.68 | 0.28 | 91,91,91,91 | 0 |
| 87 | MG | A2 | 2111 | 1/1 | 0.68 | 0.18 | 69,69,69,69 | 0 |
| 87 | MG | A5 | 4137 | 1/1 | 0.68 | 0.20 | 104,104,104,104 | 0 |
| 87 | MG | AP | 202 | 1/1 | 0.68 | 0.30 | 88,88,88,88 | 0 |
| 87 | MG | A5 | 4364 | 1/1 | 0.68 | 0.23 | 76,76,76,76 | 0 |
| 87 | MG | A6 | 2284 | 1/1 | 0.68 | 0.55 | 107,107,107,107 | 0 |
| 87 | MG | A1 | 4207 | 1/1 | 0.68 | 0.17 | 85,85,85,85 | 0 |
| 87 | MG | A5 | 4056 | 1/1 | 0.68 | 0.23 | 78,78,78,78 | 0 |
| 87 | MG | A5 | 4382 | 1/1 | 0.68 | 0.62 | 99,99,99,99 | 0 |
| 87 | MG | A1 | 4479 | 1/1 | 0.68 | 0.26 | 74,74,74,74 | 0 |
| 87 | MG | BP | 207 | 1/1 | 0.68 | 0.26 | 65,65,65,65 | 0 |
| 87 | MG | A5 | 4540 | 1/1 | 0.68 | 0.21 | 94,94,94,94 | 0 |
| 87 | MG | A1 | 4333 | 1/1 | 0.68 | 0.85 | 68,68,68,68 | 0 |
| 87 | MG | A5 | 4315 | 1/1 | 0.68 | 0.24 | 106,106,106,106 | 0 |
| 87 | MG | A5 | 4419 | 1/1 | 0.68 | 0.28 | 65,65,65,65 | 0 |
| 87 | MG | A1 | 4450 | 1/1 | 0.68 | 0.24 | 68,68,68,68 | 0 |
| 87 | MG | A5 | 4441 | 1/1 | 0.68 | 0.22 | 61,61,61,61 | 0 |
| 87 | MG | A5 | 4399 | 1/1 | 0.69 | 0.27 | 64,64,64,64 | 0 |
| 87 | MG | A5 | 4402 | 1/1 | 0.69 | 0.68 | 91,91,91,91 | 0 |
| 87 | MG | A1 | 3894 | 1/1 | 0.69 | 0.33 | 43,43,43,43 | 0 |
| 87 | MG | A5 | 4554 | 1/1 | 0.69 | 0.55 | 86,86,86,86 | 0 |
| 87 | MG | A1 | 4284 | 1/1 | 0.69 | 0.29 | 87,87,87,87 | 0 |
| 87 | MG | A5 | 4557 | 1/1 | 0.69 | 0.27 | 69,69,69,69 | 0 |
| 87 | MG | A2 | 2224 | 1/1 | 0.69 | 0.20 | 77,77,77,77 | 0 |
| 87 | MG | A5 | 3862 | 1/1 | 0.69 | 0.48 | 82,82,82,82 | 0 |
| 87 | MG | A5 | 4330 | 1/1 | 0.69 | 0.19 | 86,86,86,86 | 0 |
| 87 | MG | A5 | 4333 | 1/1 | 0.69 | 0.39 | 75,75,75,75 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | A5 | 4115 | 1/1 | 0.69 | 0.37 | 69,69,69,69 | 0 |
| 87 | MG | A5 | 4338 | 1/1 | 0.69 | 0.31 | 93,93,93,93 | 0 |
| 87 | MG | A2 | 2188 | 1/1 | 0.69 | 0.20 | 82,82,82,82 | 0 |
| 87 | MG | A2 | 2191 | 1/1 | 0.69 | 0.23 | 91,91,91,91 | 0 |
| 87 | MG | A8 | 235 | 1/1 | 0.69 | 0.79 | 79,79,79,79 | 0 |
| 87 | MG | A6 | 2281 | 1/1 | 0.69 | 0.44 | 75,75,75,75 | 0 |
| 87 | MG | A1 | 4507 | 1/1 | 0.69 | 0.30 | 90,90,90,90 | 0 |
| 87 | MG | A5 | 4488 | 1/1 | 0.69 | 0.93 | 81,81,81,81 | 0 |
| 87 | MG | A6 | 2243 | 1/1 | 0.69 | 0.27 | 74,74,74,74 | 0 |
| 87 | MG | A5 | 3933 | 1/1 | 0.69 | 0.36 | 74,74,74,74 | 0 |
| 87 | MG | DH | 203 | 1/1 | 0.69 | 0.55 | 72,72,72,72 | 0 |
| 87 | MG | A2 | 2152 | 1/1 | 0.69 | 0.28 | 88,88,88,88 | 0 |
| 87 | MG | A5 | 4372 | 1/1 | 0.69 | 0.84 | 74,74,74,74 | 0 |
| 87 | MG | A5 | 4256 | 1/1 | 0.69 | 0.69 | 81,81,81,81 | 0 |
| 87 | MG | AN | 202 | 1/1 | 0.69 | 0.13 | 63,63,63,63 | 0 |
| 87 | MG | A5 | 4511 | 1/1 | 0.69 | 0.66 | 68,68,68,68 | 0 |
| 87 | MG | A6 | 2246 | 1/1 | 0.69 | 0.41 | 78,78,78,78 | 0 |
| 87 | MG | A1 | 4182 | 1/1 | 0.69 | 0.20 | 81,81,81,81 | 0 |
| 87 | MG | A5 | 4285 | 1/1 | 0.69 | 0.57 | 68,68,68,68 | 0 |
| 87 | MG | A4 | 242 | 1/1 | 0.69 | 0.21 | 81,81,81,81 | 0 |
| 87 | MG | A1 | 3870 | 1/1 | 0.69 | 0.40 | 57,57,57,57 | 0 |
| 87 | MG | A2 | 2226 | 1/1 | 0.70 | 0.40 | 87,87,87,87 | 0 |
| 87 | MG | A2 | 2158 | 1/1 | 0.70 | 0.22 | 71,71,71,71 | 0 |
| 86 | OHX | A1 | 3814 | 7/7 | 0.70 | 0.53 | 221,221,221,221 | 7 |
| 87 | MG | A1 | 4258 | 1/1 | 0.70 | 0.18 | 67,67,67,67 | 0 |
| 87 | MG | A6 | 2287 | 1/1 | 0.70 | 1.05 | 96,96,96,96 | 0 |
| 87 | MG | A1 | 4422 | 1/1 | 0.70 | 0.24 | 68,68,68,68 | 0 |
| 87 | MG | A5 | 4562 | 1/1 | 0.70 | 0.28 | 69,69,69,69 | 0 |
| 87 | MG | A1 | 4431 | 1/1 | 0.70 | 0.36 | 59,59,59,59 | 0 |
| 87 | MG | A6 | 2215 | 1/1 | 0.70 | 0.18 | 56,56,56,56 | 0 |
| 87 | MG | A5 | 4323 | 1/1 | 0.70 | 0.34 | 64,64,64,64 | 0 |
| 87 | MG | A2 | 2196 | 1/1 | 0.70 | 0.54 | 131,131,131,131 | 0 |
| 87 | MG | Ba | 207 | 1/1 | 0.70 | 0.81 | 89,89,89,89 | 0 |
| 87 | MG | A7 | 221 | 1/1 | 0.70 | 0.30 | 82,82,82,82 | 0 |
| 87 | MG | A5 | 4188 | 1/1 | 0.70 | 0.37 | 78,78,78,78 | 0 |
| 87 | MG | A1 | 4175 | 1/1 | 0.70 | 0.09 | 69,69,69,69 | 0 |
| 87 | MG | A5 | 4337 | 1/1 | 0.70 | 0.47 | 70,70,70,70 | 0 |
| 87 | MG | B1 | 4500 | 1/1 | 0.70 | 0.53 | 77,77,77,77 | 0 |
| 87 | MG | A1 | 3914 | 1/1 | 0.70 | 0.19 | 73,73,73,73 | 0 |
| 87 | MG | A5 | 4491 | 1/1 | 0.70 | 0.57 | 82,82,82,82 | 0 |
| 87 | MG | A5 | 3992 | 1/1 | 0.70 | 0.32 | 57,57,57,57 | 0 |
| 87 | MG | A2 | 2237 | 1/1 | 0.70 | 0.16 | 90,90,90,90 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | A1 | 4451 | 1/1 | 0.70 | 0.44 | 75,75,75,75 | 0 |
| 87 | MG | A2 | 2238 | 1/1 | 0.70 | 0.40 | 92,92,92,92 | 0 |
| 87 | MG | DJ | 203 | 1/1 | 0.70 | 0.26 | 80,80,80,80 | 0 |
| 86 | OHX | A5 | 3819 | 7/7 | 0.70 | 0.56 | 238,238,238,238 | 7 |
| 87 | MG | A2 | 2091 | 1/1 | 0.70 | 0.38 | 81,81,81,81 | 0 |
| 87 | MG | A2 | 2170 | 1/1 | 0.70 | 0.41 | 88,88,88,88 | 0 |
| 87 | MG | A2 | 2253 | 1/1 | 0.70 | 0.16 | 89,89,89,89 | 0 |
| 87 | MG | A6 | 2267 | 1/1 | 0.70 | 0.24 | 72,72,72,72 | 0 |
| 87 | MG | CP | 203 | 1/1 | 0.70 | 0.63 | 63,63,63,63 | 0 |
| 87 | MG | A1 | 4298 | 1/1 | 0.70 | 0.65 | 95,95,95,95 | 0 |
| 87 | MG | A6 | 2276 | 1/1 | 0.70 | 0.36 | 105,105,105,105 | 0 |
| 87 | MG | A5 | 4264 | 1/1 | 0.70 | 0.41 | 103,103,103,103 | 0 |
| 87 | MG | A2 | 2139 | 1/1 | 0.71 | 0.19 | 81,81,81,81 | 0 |
| 87 | MG | A5 | 4317 | 1/1 | 0.71 | 0.41 | 63,63,63,63 | 0 |
| 87 | MG | A5 | 3871 | 1/1 | 0.71 | 0.24 | 56,56,56,56 | 0 |
| 87 | MG | A6 | 2315 | 1/1 | 0.71 | 0.26 | 84,84,84,84 | 0 |
| 87 | MG | A5 | 3880 | 1/1 | 0.71 | 0.26 | 45,45,45,45 | 0 |
| 87 | MG | A5 | 4447 | 1/1 | 0.71 | 0.23 | 61,61,61,61 | 0 |
| 87 | MG | A4 | 245 | 1/1 | 0.71 | 0.42 | 90,90,90,90 | 0 |
| 87 | MG | A1 | 4176 | 1/1 | 0.71 | 0.07 | 84,84,84,84 | 0 |
| 87 | MG | A5 | 3906 | 1/1 | 0.71 | 0.30 | 56,56,56,56 | 0 |
| 87 | MG | A1 | 4035 | 1/1 | 0.71 | 0.12 | 59,59,59,59 | 0 |
| 87 | MG | A1 | 4238 | 1/1 | 0.71 | 0.19 | 69,69,69,69 | 0 |
| 86 | OHX | A1 | 3805 | 7/7 | 0.71 | 0.41 | 209,209,209,209 | 7 |
| 87 | MG | A1 | 4187 | 1/1 | 0.71 | 0.73 | 90,90,90,90 | 0 |
| 87 | MG | A1 | 3863 | 1/1 | 0.71 | 0.24 | 125,125,125,125 | 0 |
| 87 | MG | A6 | 2273 | 1/1 | 0.71 | 0.22 | 90,90,90,90 | 0 |
| 87 | MG | A2 | 2233 | 1/1 | 0.71 | 0.13 | 80,80,80,80 | 0 |
| 87 | MG | A5 | 4229 | 1/1 | 0.71 | 0.38 | 81,81,81,81 | 0 |
| 87 | MG | BP | 211 | 1/1 | 0.71 | 0.73 | 123,123,123,123 | 0 |
| 87 | MG | A2 | 2177 | 1/1 | 0.71 | 0.30 | 83,83,83,83 | 0 |
| 87 | MG | CL | 202 | 1/1 | 0.71 | 0.31 | 82,82,82,82 | 0 |
| 87 | MG | CL | 204 | 1/1 | 0.71 | 0.49 | 83,83,83,83 | 0 |
| 87 | MG | A1 | 4425 | 1/1 | 0.71 | 0.21 | 106,106,106,106 | 0 |
| 87 | MG | A2 | 2210 | 1/1 | 0.71 | 0.42 | 81,81,81,81 | 0 |
| 87 | MG | A1 | 4143 | 1/1 | 0.71 | 0.24 | 70,70,70,70 | 0 |
| 87 | MG | A1 | 3907 | 1/1 | 0.71 | 0.30 | 50,50,50,50 | 0 |
| 87 | MG | A5 | 4538 | 1/1 | 0.71 | 0.37 | 67,67,67,67 | 0 |
| 87 | MG | A1 | 3943 | 1/1 | 0.71 | 0.33 | 59,59,59,59 | 0 |
| 87 | MG | A1 | 4071 | 1/1 | 0.71 | 0.20 | 71,71,71,71 | 0 |
| 87 | MG | A2 | 2255 | 1/1 | 0.71 | 0.08 | 107,107,107,107 | 0 |
| 87 | MG | A5 | 3854 | 1/1 | 0.71 | 0.31 | 74,74,74,74 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86 | OHX | A1 | 3753 | 7/7 | 0.71 | 0.97 | 243,243,243,243 | 7 |
| 87 | MG | A1 | 4105 | 1/1 | 0.72 | 0.27 | 84,84,84,84 | 0 |
| 87 | MG | A6 | 2140 | 1/1 | 0.72 | 0.23 | 61,61,61,61 | 0 |
| 86 | OHX | A2 | 2047 | 7/7 | 0.72 | 0.32 | 188,188,188,188 | 7 |
| 87 | MG | A1 | 3817 | 1/1 | 0.72 | 0.39 | 63,63,63,63 | 0 |
| 87 | MG | A6 | 2173 | 1/1 | 0.72 | 0.22 | 71,71,71,71 | 0 |
| 87 | MG | A5 | 4565 | 1/1 | 0.72 | 0.16 | 87,87,87,87 | 0 |
| 87 | MG | A5 | 4192 | 1/1 | 0.72 | 0.37 | 95,95,95,95 | 0 |
| 87 | MG | A5 | 4194 | 1/1 | 0.72 | 0.40 | 88,88,88,88 | 0 |
| 86 | OHX | A1 | 3786 | 7/7 | 0.72 | 0.31 | 184,184,184,184 | 7 |
| 87 | MG | A5 | 4040 | 1/1 | 0.72 | 0.24 | 46,46,46,46 | 0 |
| 87 | MG | A5 | 4335 | 1/1 | 0.72 | 0.36 | 94,94,94,94 | 0 |
| 87 | MG | A2 | 2155 | 1/1 | 0.72 | 0.29 | 86,86,86,86 | 0 |
| 87 | MG | A1 | 4269 | 1/1 | 0.72 | 0.74 | 87,87,87,87 | 0 |
| 87 | MG | A6 | 2194 | 1/1 | 0.72 | 0.17 | 67,67,67,67 | 0 |
| 87 | MG | A5 | 4076 | 1/1 | 0.72 | 0.30 | 64,64,64,64 | 0 |
| 87 | MG | BV | 205 | 1/1 | 0.72 | 0.81 | 68,68,68,68 | 0 |
| 87 | MG | A6 | 2200 | 1/1 | 0.72 | 0.23 | 82,82,82,82 | 0 |
| 87 | MG | DC | 405 | 1/1 | 0.72 | 0.67 | 72,72,72,72 | 0 |
| 87 | MG | A1 | 4385 | 1/1 | 0.72 | 0.86 | 65,65,65,65 | 0 |
| 87 | MG | A1 | 4474 | 1/1 | 0.72 | 0.29 | 72,72,72,72 | 0 |
| 87 | MG | A2 | 2172 | 1/1 | 0.72 | 0.22 | 69,69,69,69 | 0 |
| 87 | MG | A6 | 2233 | 1/1 | 0.72 | 0.39 | 63,63,63,63 | 0 |
| 87 | MG | A5 | 3852 | 1/1 | 0.72 | 0.23 | 49,49,49,49 | 0 |
| 87 | MG | A5 | 4514 | 1/1 | 0.72 | 1.55 | 98,98,98,98 | 0 |
| 87 | MG | A4 | 234 | 1/1 | 0.72 | 0.31 | 74,74,74,74 | 0 |
| 87 | MG | A1 | 4317 | 1/1 | 0.72 | 0.28 | 92,92,92,92 | 0 |
| 86 | OHX | A2 | 2028 | 7/7 | 0.72 | 0.38 | 180,180,180,180 | 7 |
| 87 | MG | A1 | 4480 | 1/1 | 0.72 | 0.55 | 91,91,91,91 | 0 |
| 87 | MG | Db | 102 | 1/1 | 0.72 | 1.28 | 70,70,70,70 | 0 |
| 86 | OHX | A1 | 3778 | 7/7 | 0.72 | 0.37 | 150,150,150,150 | 7 |
| 87 | MG | A1 | 3891 | 1/1 | 0.72 | 0.22 | 58,58,58,58 | 0 |
| 87 | MG | A5 | 4297 | 1/1 | 0.72 | 0.34 | 56,56,56,56 | 0 |
| 87 | MG | A1 | 3925 | 1/1 | 0.72 | 0.21 | 40,40,40,40 | 0 |
| 86 | OHX | A1 | 3815 | 7/7 | 0.72 | 0.53 | 183,183,183,183 | 7 |
| 88 | ZN | Do | 203 | 1/1 | 0.72 | 0.15 | 181,181,181,181 | 0 |
| 87 | MG | A1 | 4161 | 1/1 | 0.73 | 0.29 | 73,73,73,73 | 0 |
| 87 | MG | A5 | 4440 | 1/1 | 0.73 | 0.64 | 76,76,76,76 | 0 |
| 87 | MG | A5 | 3923 | 1/1 | 0.73 | 0.28 | 68,68,68,68 | 0 |
| 86 | OHX | A8 | 218 | 7/7 | 0.73 | 0.45 | 221,221,221,221 | 7 |
| 87 | MG | A1 | 3405 | 1/1 | 0.73 | 0.18 | 71,71,71,71 | 0 |
| 87 | MG | A1 | 4374 | 1/1 | 0.73 | 1.18 | 60,60,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | A5 | 4189 | 1/1 | 0.73 | 0.37 | 96,96,96,96 | 0 |
| 87 | MG | A4 | 229 | 1/1 | 0.73 | 0.16 | 54,54,54,54 | 0 |
| 87 | MG | A5 | 4024 | 1/1 | 0.73 | 0.37 | 42,42,42,42 | 0 |
| 87 | MG | A1 | 3857 | 1/1 | 0.73 | 0.26 | 53,53,53,53 | 0 |
| 87 | MG | A4 | 240 | 1/1 | 0.73 | 0.29 | 72,72,72,72 | 0 |
| 87 | MG | A1 | 4226 | 1/1 | 0.73 | 0.83 | 63,63,63,63 | 0 |
| 87 | MG | A6 | 2231 | 1/1 | 0.73 | 0.32 | 69,69,69,69 | 0 |
| 87 | MG | A6 | 2288 | 1/1 | 0.73 | 0.50 | 106,106,106,106 | 0 |
| 87 | MG | Ca | 201 | 1/1 | 0.73 | 0.28 | 67,67,67,67 | 0 |
| 87 | MG | DB | 415 | 1/1 | 0.73 | 0.29 | 91,91,91,91 | 0 |
| 87 | MG | A1 | 4264 | 1/1 | 0.73 | 0.23 | 65,65,65,65 | 0 |
| 87 | MG | A6 | 2116 | 1/1 | 0.73 | 0.25 | 80,80,80,80 | 0 |
| 87 | MG | A2 | 2203 | 1/1 | 0.73 | 0.33 | 68,68,68,68 | 0 |
| 87 | MG | A1 | 4271 | 1/1 | 0.73 | 0.24 | 58,58,58,58 | 0 |
| 87 | MG | A5 | 4089 | 1/1 | 0.73 | 0.20 | 81,81,81,81 | 0 |
| 87 | MG | A5 | 4250 | 1/1 | 0.73 | 0.61 | 110,110,110,110 | 0 |
| 87 | MG | A1 | 4037 | 1/1 | 0.73 | 0.17 | 83,83,83,83 | 0 |
| 87 | MG | A5 | 4100 | 1/1 | 0.73 | 0.33 | 86,86,86,86 | 0 |
| 87 | MG | A1 | 4042 | 1/1 | 0.73 | 0.33 | 68,68,68,68 | 0 |
| 87 | MG | A1 | 4194 | 1/1 | 0.73 | 0.32 | 96,96,96,96 | 0 |
| 87 | MG | A5 | 4126 | 1/1 | 0.73 | 0.27 | 100,100,100,100 | 0 |
| 87 | MG | A1 | 3912 | 1/1 | 0.73 | 0.66 | 84,84,84,84 | 0 |
| 87 | MG | A1 | 4444 | 1/1 | 0.73 | 1.27 | 81,81,81,81 | 0 |
| 87 | MG | A1 | 3868 | 1/1 | 0.73 | 0.26 | 55,55,55,55 | 0 |
| 87 | MG | A6 | 2258 | 1/1 | 0.73 | 0.22 | 71,71,71,71 | 0 |
| 86 | OHX | A3 | 213 | 7/7 | 0.73 | 0.22 | 195,195,195,195 | 7 |
| 87 | MG | A1 | 3876 | 1/1 | 0.73 | 0.38 | 68,68,68,68 | 0 |
| 87 | MG | A5 | 4314 | 1/1 | 0.73 | 0.21 | 56,56,56,56 | 0 |
| 87 | MG | Bj | 106 | 1/1 | 0.74 | 0.34 | 75,75,75,75 | 0 |
| 87 | MG | A5 | 4043 | 1/1 | 0.74 | 0.28 | 35,35,35,35 | 0 |
| 87 | MG | A6 | 2196 | 1/1 | 0.74 | 0.57 | 83,83,83,83 | 0 |
| 87 | MG | A2 | 2098 | 1/1 | 0.74 | 0.30 | 62,62,62,62 | 0 |
| 87 | MG | A1 | 4440 | 1/1 | 0.74 | 0.61 | 55,55,55,55 | 0 |
| 87 | MG | A6 | 2210 | 1/1 | 0.74 | 0.25 | 72,72,72,72 | 0 |
| 87 | MG | A2 | 2101 | 1/1 | 0.74 | 0.12 | 59,59,59,59 | 0 |
| 87 | MG | BA | 306 | 1/1 | 0.74 | 0.43 | 74,74,74,74 | 0 |
| 87 | MG | A7 | 222 | 1/1 | 0.74 | 0.38 | 94,94,94,94 | 0 |
| 87 | MG | A5 | 3408 | 1/1 | 0.74 | 0.62 | 63,63,63,63 | 0 |
| 86 | OHX | A6 | 2087 | 7/7 | 0.74 | 0.23 | 205,205,205,205 | 7 |
| 87 | MG | A8 | 228 | 1/1 | 0.74 | 0.33 | 86,86,86,86 | 0 |
| 87 | MG | A6 | 2106 | 1/1 | 0.74 | 0.34 | 64,64,64,64 | 0 |
| 87 | MG | A5 | 3848 | 1/1 | 0.74 | 0.32 | 77,77,77,77 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | DA | 301 | 1/1 | 0.74 | 0.23 | 86,86,86,86 | 0 |
| 87 | MG | A2 | 2149 | 1/1 | 0.74 | 0.28 | 83,83,83,83 | 0 |
| 86 | OHX | A5 | 3798 | 7/7 | 0.74 | 0.27 | 202,202,202,202 | 7 |
| 87 | MG | A5 | 3859 | 1/1 | 0.74 | 0.23 | 50,50,50,50 | 0 |
| 86 | OHX | A5 | 3811 | 7/7 | 0.74 | 0.30 | 214,214,214,214 | 7 |
| 87 | MG | A1 | 4149 | 1/1 | 0.74 | 0.17 | 74,74,74,74 | 0 |
| 87 | MG | A1 | 4189 | 1/1 | 0.74 | 0.21 | 59,59,59,59 | 0 |
| 87 | MG | A1 | 4285 | 1/1 | 0.74 | 0.31 | 64,64,64,64 | 0 |
| 87 | MG | A5 | 4381 | 1/1 | 0.74 | 0.24 | 96,96,96,96 | 0 |
| 87 | MG | A6 | 2321 | 1/1 | 0.74 | 0.48 | 93,93,93,93 | 0 |
| 87 | MG | A5 | 4385 | 1/1 | 0.74 | 0.30 | 74,74,74,74 | 0 |
| 87 | MG | A1 | 4060 | 1/1 | 0.74 | 0.20 | 67,67,67,67 | 0 |
| 86 | OHX | A6 | 2074 | 7/7 | 0.74 | 0.32 | 176,176,176,176 | 7 |
| 87 | MG | A4 | 217 | 1/1 | 0.74 | 0.38 | 69,69,69,69 | 0 |
| 87 | MG | BV | 202 | 1/1 | 0.74 | 0.22 | 73,73,73,73 | 0 |
| 87 | MG | A6 | 2179 | 1/1 | 0.74 | 0.20 | 47,47,47,47 | 0 |
| 87 | MG | A1 | 4108 | 1/1 | 0.74 | 0.23 | 60,60,60,60 | 0 |
| 87 | MG | A1 | 4427 | 1/1 | 0.74 | 0.26 | 77,77,77,77 | 0 |
| 87 | MG | A6 | 2272 | 1/1 | 0.74 | 0.31 | 115,115,115,115 | 0 |
| 87 | MG | A1 | 4362 | 1/1 | 0.74 | 0.19 | 85,85,85,85 | 0 |
| 87 | MG | Bj | 104 | 1/1 | 0.74 | 0.29 | 86,86,86,86 | 0 |
| 87 | MG | A1 | 4459 | 1/1 | 0.75 | 0.39 | 88,88,88,88 | 0 |
| 87 | MG | A1 | 4463 | 1/1 | 0.75 | 0.20 | 76,76,76,76 | 0 |
| 86 | OHX | A1 | 3774 | 7/7 | 0.75 | 0.18 | 206,206,206,206 | 7 |
| 87 | MG | BJ | 201 | 1/1 | 0.75 | 0.18 | 81,81,81,81 | 0 |
| 87 | MG | A1 | 4467 | 1/1 | 0.75 | 0.30 | 68,68,68,68 | 0 |
| 86 | OHX | A6 | 2060 | 7/7 | 0.75 | 0.27 | 165,165,165,165 | 7 |
| 87 | MG | BO | 205 | 1/1 | 0.75 | 0.82 | 58,58,58,58 | 0 |
| 87 | MG | A5 | 3988 | 1/1 | 0.75 | 0.35 | 51,51,51,51 | 0 |
| 87 | MG | A1 | 4132 | 1/1 | 0.75 | 0.17 | 64,64,64,64 | 0 |
| 86 | OHX | A5 | 3777 | 7/7 | 0.75 | 0.34 | 187,187,187,187 | 7 |
| 87 | MG | A5 | 4231 | 1/1 | 0.75 | 0.17 | 105,105,105,105 | 0 |
| 87 | MG | A5 | 4035 | 1/1 | 0.75 | 0.14 | 39,39,39,39 | 0 |
| 86 | OHX | A2 | 2075 | 7/7 | 0.75 | 0.28 | 204,204,204,204 | 7 |
| 86 | OHX | A2 | 2037 | 7/7 | 0.75 | 0.38 | 197,197,197,197 | 7 |
| 87 | MG | A1 | 4276 | 1/1 | 0.75 | 0.26 | 95,95,95,95 | 0 |
| 87 | MG | A2 | 2212 | 1/1 | 0.75 | 0.34 | 100,100,100,100 | 0 |
| 87 | MG | A7 | 219 | 1/1 | 0.75 | 0.23 | 71,71,71,71 | 0 |
| 87 | MG | A1 | 4219 | 1/1 | 0.75 | 0.16 | 85,85,85,85 | 0 |
| 87 | MG | Ba | 203 | 1/1 | 0.75 | 0.22 | 70,70,70,70 | 0 |
| 87 | MG | A5 | 4423 | 1/1 | 0.75 | 0.33 | 82,82,82,82 | 0 |
| 87 | MG | A2 | 2215 | 1/1 | 0.75 | 0.34 | 86,86,86,86 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | A1 | 4390 | 1/1 | 0.75 | 0.22 | 82,82,82,82 | 0 |
| 87 | MG | A8 | 233 | 1/1 | 0.75 | 0.30 | 78,78,78,78 | 0 |
| 86 | OHX | A5 | 3799 | 7/7 | 0.75 | 0.29 | 168,168,168,168 | 7 |
| 87 | MG | A2 | 2197 | 1/1 | 0.75 | 0.25 | 80,80,80,80 | 0 |
| 87 | MG | A2 | 2097 | 1/1 | 0.75 | 0.22 | 78,78,78,78 | 0 |
| 87 | MG | A1 | 4082 | 1/1 | 0.75 | 0.20 | 73,73,73,73 | 0 |
| 87 | MG | A5 | 4094 | 1/1 | 0.75 | 0.31 | 69,69,69,69 | 0 |
| 87 | MG | A1 | 4085 | 1/1 | 0.75 | 0.18 | 35,35,35,35 | 0 |
| 87 | MG | A3 | 220 | 1/1 | 0.75 | 0.46 | 83,83,83,83 | 0 |
| 87 | MG | A1 | 4086 | 1/1 | 0.75 | 0.55 | 58,58,58,58 | 0 |
| 87 | MG | A1 | 4236 | 1/1 | 0.75 | 0.34 | 73,73,73,73 | 0 |
| 87 | MG | A1 | 4432 | 1/1 | 0.75 | 0.76 | 79,79,79,79 | 0 |
| 87 | MG | A6 | 2119 | 1/1 | 0.75 | 0.26 | 70,70,70,70 | 0 |
| 87 | MG | A5 | 3831 | 1/1 | 0.75 | 0.19 | 37,37,37,37 | 0 |
| 87 | MG | A2 | 2247 | 1/1 | 0.75 | 0.23 | 86,86,86,86 | 0 |
| 87 | MG | A4 | 226 | 1/1 | 0.75 | 0.34 | 70,70,70,70 | 0 |
| 87 | MG | A1 | 4011 | 1/1 | 0.75 | 0.23 | 50,50,50,50 | 0 |
| 87 | MG | A2 | 2159 | 1/1 | 0.75 | 0.26 | 88,88,88,88 | 0 |
| 87 | MG | A1 | 4095 | 1/1 | 0.75 | 0.27 | 56,56,56,56 | 0 |
| 87 | MG | Dd | 201 | 1/1 | 0.75 | 0.31 | 77,77,77,77 | 0 |
| 87 | MG | A2 | 2225 | 1/1 | 0.75 | 0.44 | 79,79,79,79 | 0 |
| 87 | MG | A6 | 2156 | 1/1 | 0.75 | 0.36 | 62,62,62,62 | 0 |
| 87 | MG | A1 | 4038 | 1/1 | 0.75 | 0.22 | 89,89,89,89 | 0 |
| 87 | MG | A6 | 2166 | 1/1 | 0.75 | 0.26 | 64,64,64,64 | 0 |
| 87 | MG | A1 | 4041 | 1/1 | 0.75 | 0.21 | 70,70,70,70 | 0 |
| 87 | MG | A1 | 4193 | 1/1 | 0.75 | 0.35 | 72,72,72,72 | 0 |
| 87 | MG | A3 | 222 | 1/1 | 0.76 | 0.17 | 66,66,66,66 | 0 |
| 87 | MG | A5 | 4095 | 1/1 | 0.76 | 0.27 | 79,79,79,79 | 0 |
| 87 | MG | A1 | 4148 | 1/1 | 0.76 | 0.21 | 94,94,94,94 | 0 |
| 87 | MG | A5 | 3870 | 1/1 | 0.76 | 0.33 | 56,56,56,56 | 0 |
| 87 | MG | A5 | 4108 | 1/1 | 0.76 | 0.30 | 74,74,74,74 | 0 |
| 87 | MG | A5 | 4394 | 1/1 | 0.76 | 0.22 | 73,73,73,73 | 0 |
| 87 | MG | A5 | 4111 | 1/1 | 0.76 | 0.25 | 65,65,65,65 | 0 |
| 87 | MG | A1 | 4376 | 1/1 | 0.76 | 0.68 | 71,71,71,71 | 0 |
| 87 | MG | A1 | 4310 | 1/1 | 0.76 | 1.21 | 67,67,67,67 | 0 |
| 87 | MG | A5 | 4272 | 1/1 | 0.76 | 0.18 | 69,69,69,69 | 0 |
| 87 | MG | A5 | 4273 | 1/1 | 0.76 | 1.30 | 75,75,75,75 | 0 |
| 87 | MG | A5 | 4580 | 1/1 | 0.76 | 0.19 | 82,82,82,82 | 0 |
| 87 | MG | A5 | 4279 | 1/1 | 0.76 | 1.08 | 63,63,63,63 | 0 |
| 87 | MG | A2 | 2095 | 1/1 | 0.76 | 0.24 | 63,63,63,63 | 0 |
| 87 | MG | A1 | 4316 | 1/1 | 0.76 | 0.70 | 65,65,65,65 | 0 |
| 87 | MG | A1 | 4470 | 1/1 | 0.76 | 0.13 | 97,97,97,97 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87 | MG | A1 | 3990 | 1/1 | 0.76 | 0.43 | 54,54,54,54 | 0 |
| 87 | MG | A1 | 4396 | 1/1 | 0.76 | 0.16 | 74,74,74,74 | 0 |
| 87 | MG | A5 | 4451 | 1/1 | 0.76 | 0.31 | 80,80,80,80 | 0 |
| 87 | MG | A8 | 229 | 1/1 | 0.76 | 0.21 | 95,95,95,95 | 0 |
| 87 | MG | A2 | 2179 | 1/1 | 0.76 | 0.25 | 81,81,81,81 | 0 |
| 87 | MG | A5 | 4153 | 1/1 | 0.76 | 0.24 | 83,83,83,83 | 0 |
| 86 | OHX | A6 | 2090 | 7/7 | 0.76 | 0.47 | 212,212,212,212 | 7 |
| 87 | MG | A2 | 2160 | 1/1 | 0.76 | 0.37 | 66,66,66,66 | 0 |
| 87 | MG | A5 | 3951 | 1/1 | 0.76 | 0.27 | 40,40,40,40 | 0 |
| 87 | MG | A1 | 4074 | 1/1 | 0.76 | 0.12 | 57,57,57,57 | 0 |
| 87 | MG | A6 | 2280 | 1/1 | 0.76 | 0.39 | 79,79,79,79 | 0 |
| 87 | MG | A1 | 4341 | 1/1 | 0.76 | 0.25 | 118,118,118,118 | 0 |
| 87 | MG | A6 | 2105 | 1/1 | 0.76 | 0.22 | 78,78,78,78 | 0 |
| 87 | MG | A6 | 2211 | 1/1 | 0.76 | 0.14 | 86,86,86,86 | 0 |
| 87 | MG | A6 | 2285 | 1/1 | 0.76 | 0.26 | 74,74,74,74 | 0 |
| 87 | MG | A1 | 4342 | 1/1 | 0.76 | 0.21 | 79,79,79,79 | 0 |
| 87 | MG | A5 | 4196 | 1/1 | 0.76 | 0.10 | 66,66,66,66 | 0 |
| 87 | MG | A1 | 4255 | 1/1 | 0.76 | 0.32 | 87,87,87,87 | 0 |
| 87 | MG | A5 | 4059 | 1/1 | 0.76 | 0.32 | 71,71,71,71 | 0 |
| 87 | MG | A1 | 3906 | 1/1 | 0.76 | 0.34 | 91,91,91,91 | 0 |
| 87 | MG | A1 | 4144 | 1/1 | 0.76 | 0.82 | 82,82,82,82 | 0 |
| 87 | MG | A1 | 4289 | 1/1 | 0.76 | 0.28 | 74,74,74,74 | 0 |
| 87 | MG | A5 | 4355 | 1/1 | 0.76 | 0.19 | 66,66,66,66 | 0 |
| 87 | MG | A5 | 3840 | 1/1 | 0.76 | 0.15 | 26,26,26,26 | 0 |
| 87 | MG | A1 | 4260 | 1/1 | 0.76 | 0.23 | 75,75,75,75 | 0 |
| 87 | MG | A5 | 3851 | 1/1 | 0.76 | 0.30 | 45,45,45,45 | 0 |
| 87 | MG | A1 | 4261 | 1/1 | 0.76 | 0.31 | 79,79,79,79 | 0 |
| 86 | OHX | A5 | 3665 | 7/7 | 0.76 | 0.23 | 184,184,184,184 | 7 |
| 87 | MG | A1 | 4212 | 1/1 | 0.76 | 0.26 | 67,67,67,67 | 0 |
| 86 | OHX | A5 | 3768 | 7/7 | 0.77 | 0.75 | 198,198,198,198 | 7 |
| 87 | MG | A1 | 4257 | 1/1 | 0.77 | 0.15 | 88,88,88,88 | 0 |
| 87 | MG | A1 | 4443 | 1/1 | 0.77 | 0.39 | 65,65,65,65 | 0 |
| 86 | OHX | A5 | 3770 | 7/7 | 0.77 | 0.29 | 198,198,198,198 | 7 |
| 87 | MG | A1 | 4324 | 1/1 | 0.77 | 0.20 | 79,79,79,79 | 0 |
| 87 | MG | A6 | 2271 | 1/1 | 0.77 | 0.28 | 95,95,95,95 | 0 |
| 87 | MG | A1 | 4014 | 1/1 | 0.77 | 0.40 | 56,56,56,56 | 0 |
| 87 | MG | A5 | 4410 | 1/1 | 0.77 | 0.69 | 66,66,66,66 | 0 |
| 87 | MG | A5 | 3907 | 1/1 | 0.77 | 0.35 | 75,75,75,75 | 0 |
| 87 | MG | A5 | 3915 | 1/1 | 0.77 | 0.26 | 78,78,78,78 | 0 |
| 87 | MG | A5 | 4579 | 1/1 | 0.77 | 0.71 | 57,57,57,57 | 0 |
| 87 | MG | A5 | 3916 | 1/1 | 0.77 | 0.27 | 49,49,49,49 | 0 |
| 87 | MG | A6 | 2336 | 1/1 | 0.77 | 0.43 | 93,93,93,93 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | A1 | 4326 | 1/1 | 0.77 | 1.26 | 80,80,80,80 | 0 |
| 87 | MG | A1 | 4110 | 1/1 | 0.77 | 0.19 | 71,71,71,71 | 0 |
| 87 | MG | AC | 302 | 1/1 | 0.77 | 0.27 | 74,74,74,74 | 0 |
| 87 | MG | A6 | 2118 | 1/1 | 0.77 | 0.32 | 57,57,57,57 | 0 |
| 87 | MG | A5 | 4155 | 1/1 | 0.77 | 0.45 | 95,95,95,95 | 0 |
| 87 | MG | A5 | 3955 | 1/1 | 0.77 | 0.32 | 62,62,62,62 | 0 |
| 87 | MG | A1 | 3822 | 1/1 | 0.77 | 0.21 | 50,50,50,50 | 0 |
| 86 | OHX | CP | 202 | 7/7 | 0.77 | 0.63 | 221,221,221,221 | 7 |
| 87 | MG | A5 | 4322 | 1/1 | 0.77 | 0.39 | 61,61,61,61 | 0 |
| 87 | MG | A6 | 2218 | 1/1 | 0.77 | 0.23 | 53,53,53,53 | 0 |
| 87 | MG | A1 | 4343 | 1/1 | 0.77 | 0.39 | 78,78,78,78 | 0 |
| 87 | MG | A1 | 4408 | 1/1 | 0.77 | 0.79 | 81,81,81,81 | 0 |
| 87 | MG | DB | 414 | 1/1 | 0.77 | 1.34 | 76,76,76,76 | 0 |
| 87 | MG | A5 | 4039 | 1/1 | 0.77 | 0.34 | 63,63,63,63 | 0 |
| 87 | MG | A6 | 2232 | 1/1 | 0.77 | 0.29 | 77,77,77,77 | 0 |
| 87 | MG | A1 | 4411 | 1/1 | 0.77 | 0.23 | 94,94,94,94 | 0 |
| 87 | MG | A5 | 4045 | 1/1 | 0.77 | 0.29 | 63,63,63,63 | 0 |
| 87 | MG | A1 | 4224 | 1/1 | 0.77 | 0.22 | 72,72,72,72 | 0 |
| 87 | MG | A6 | 2138 | 1/1 | 0.77 | 0.36 | 94,94,94,94 | 0 |
| 86 | OHX | A2 | 2087 | 7/7 | 0.77 | 0.19 | 196,196,196,196 | 7 |
| 87 | MG | A5 | 4072 | 1/1 | 0.77 | 0.27 | 56,56,56,56 | 0 |
| 87 | MG | A6 | 2306 | 1/1 | 0.77 | 0.16 | 103,103,103,103 | 0 |
| 87 | MG | A2 | 2241 | 1/1 | 0.77 | 0.47 | 108,108,108,108 | 0 |
| 87 | MG | A5 | 4220 | 1/1 | 0.77 | 0.37 | 82,82,82,82 | 0 |
| 87 | MG | A2 | 2206 | 1/1 | 0.77 | 0.15 | 78,78,78,78 | 0 |
| 87 | MG | A5 | 4079 | 1/1 | 0.77 | 0.24 | 67,67,67,67 | 0 |
| 87 | MG | A4 | 235 | 1/1 | 0.77 | 0.14 | 119,119,119,119 | 0 |
| 87 | MG | A1 | 4363 | 1/1 | 0.77 | 0.34 | 46,46,46,46 | 0 |
| 87 | MG | A5 | 4541 | 1/1 | 0.77 | 0.52 | 107,107,107,107 | 0 |
| 87 | MG | A6 | 2253 | 1/1 | 0.77 | 0.29 | 85,85,85,85 | 0 |
| 87 | MG | A1 | 4278 | 1/1 | 0.77 | 0.24 | 67,67,67,67 | 0 |
| 87 | MG | A5 | 4088 | 1/1 | 0.77 | 0.18 | 41,41,41,41 | 0 |
| 87 | MG | A6 | 2323 | 1/1 | 0.77 | 0.26 | 77,77,77,77 | 0 |
| 87 | MG | A5 | 4572 | 1/1 | 0.78 | 0.24 | 77,77,77,77 | 0 |
| 87 | MG | A2 | 2115 | 1/1 | 0.78 | 0.32 | 78,78,78,78 | 0 |
| 87 | MG | Be | 201 | 1/1 | 0.78 | 0.60 | 88,88,88,88 | 0 |
| 87 | MG | BE | 201 | 1/1 | 0.78 | 0.27 | 55,55,55,55 | 0 |
| 87 | MG | A1 | 4327 | 1/1 | 0.78 | 0.14 | 108,108,108,108 | 0 |
| 87 | MG | A5 | 4477 | 1/1 | 0.78 | 0.48 | 66,66,66,66 | 0 |
| 87 | MG | A5 | 3925 | 1/1 | 0.78 | 0.23 | 57,57,57,57 | 0 |
| 87 | MG | A1 | 4329 | 1/1 | 0.78 | 0.65 | 85,85,85,85 | 0 |
| 87 | MG | A5 | 4345 | 1/1 | 0.78 | 0.74 | 77,77,77,77 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87 | MG | A1 | 3995 | 1/1 | 0.78 | 0.28 | 63,63,63,63 | 0 |
| 87 | MG | A2 | 2094 | 1/1 | 0.78 | 0.36 | 68,68,68,68 | 0 |
| 87 | MG | A7 | 229 | 1/1 | 0.78 | 1.04 | 98,98,98,98 | 0 |
| 87 | MG | BL | 201 | 1/1 | 0.78 | 0.23 | 51,51,51,51 | 0 |
| 87 | MG | A6 | 2101 | 1/1 | 0.78 | 0.31 | 51,51,51,51 | 0 |
| 87 | MG | A1 | 3896 | 1/1 | 0.78 | 0.25 | 40,40,40,40 | 0 |
| 87 | MG | A4 | 220 | 1/1 | 0.78 | 0.45 | 70,70,70,70 | 0 |
| 87 | MG | A5 | 4021 | 1/1 | 0.78 | 0.31 | 35,35,35,35 | 0 |
| 87 | MG | A2 | 2169 | 1/1 | 0.78 | 0.19 | 105,105,105,105 | 0 |
| 87 | MG | A6 | 2261 | 1/1 | 0.78 | 0.24 | 76,76,76,76 | 0 |
| 87 | MG | A6 | 2322 | 1/1 | 0.78 | 0.52 | 77,77,77,77 | 0 |
| 87 | MG | A2 | 2133 | 1/1 | 0.78 | 0.17 | 72,72,72,72 | 0 |
| 87 | MG | A4 | 231 | 1/1 | 0.78 | 0.30 | 45,45,45,45 | 0 |
| 87 | MG | A1 | 4464 | 1/1 | 0.78 | 0.26 | 63,63,63,63 | 0 |
| 87 | MG | A6 | 2121 | 1/1 | 0.78 | 0.37 | 64,64,64,64 | 0 |
| 87 | MG | A5 | 4387 | 1/1 | 0.78 | 0.38 | 93,93,93,93 | 0 |
| 87 | MG | A6 | 2126 | 1/1 | 0.78 | 0.22 | 78,78,78,78 | 0 |
| 87 | MG | A1 | 4164 | 1/1 | 0.78 | 0.27 | 78,78,78,78 | 0 |
| 87 | MG | A1 | 4321 | 1/1 | 0.78 | 0.16 | 88,88,88,88 | 0 |
| 87 | MG | A2 | 2232 | 1/1 | 0.78 | 0.26 | 125,125,125,125 | 0 |
| 87 | MG | A6 | 2227 | 1/1 | 0.78 | 0.28 | 67,67,67,67 | 0 |
| 87 | MG | A1 | 4473 | 1/1 | 0.78 | 0.27 | 111,111,111,111 | 0 |
| 87 | MG | A5 | 4409 | 1/1 | 0.78 | 0.45 | 59,59,59,59 | 0 |
| 87 | MG | A5 | 3896 | 1/1 | 0.78 | 0.34 | 67,67,67,67 | 0 |
| 87 | MG | A6 | 2338 | 1/1 | 0.78 | 0.50 | 80,80,80,80 | 0 |
| 87 | MG | A5 | 4083 | 1/1 | 0.78 | 0.23 | 70,70,70,70 | 0 |
| 87 | MG | Df | 203 | 1/1 | 0.78 | 0.26 | 93,93,93,93 | 0 |
| 87 | MG | A5 | 4202 | 1/1 | 0.78 | 0.41 | 45,45,45,45 | 0 |
| 87 | MG | A5 | 3898 | 1/1 | 0.78 | 0.25 | 44,44,44,44 | 0 |
| 87 | MG | A5 | 4206 | 1/1 | 0.78 | 0.19 | 110,110,110,110 | 0 |
| 87 | MG | A4 | 249 | 1/1 | 0.78 | 0.29 | 75,75,75,75 | 0 |
| 86 | OHX | A5 | 3765 | 7/7 | 0.78 | 0.21 | 201,201,201,201 | 7 |
| 87 | MG | A5 | 3989 | 1/1 | 0.79 | 0.41 | 76,76,76,76 | 0 |
| 87 | MG | A1 | 4129 | 1/1 | 0.79 | 0.24 | 75,75,75,75 | 0 |
| 87 | MG | A5 | 4002 | 1/1 | 0.79 | 0.33 | 40,40,40,40 | 0 |
| 87 | MG | A1 | 4072 | 1/1 | 0.79 | 0.26 | 73,73,73,73 | 0 |
| 87 | MG | A6 | 2157 | 1/1 | 0.79 | 0.41 | 70,70,70,70 | 0 |
| 87 | MG | A1 | 4419 | 1/1 | 0.79 | 0.49 | 79,79,79,79 | 0 |
| 87 | MG | A1 | 3848 | 1/1 | 0.79 | 0.42 | 75,75,75,75 | 0 |
| 86 | OHX | A5 | 3693 | 7/7 | 0.79 | 0.27 | 181,181,181,181 | 7 |
| 87 | MG | BR | 203 | 1/1 | 0.79 | 0.26 | 65,65,65,65 | 0 |
| 87 | MG | A5 | 4544 | 1/1 | 0.79 | 0.38 | 79,79,79,79 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | A1 | 4334 | 1/1 | 0.79 | 0.38 | 104,104,104,104 | 0 |
| 86 | OHX | A6 | 2086 | 7/7 | 0.79 | 0.78 | 215,215,215,215 | 7 |
| 87 | MG | A5 | 4360 | 1/1 | 0.79 | 0.23 | 85,85,85,85 | 0 |
| 87 | MG | A1 | 4339 | 1/1 | 0.79 | 0.65 | 97,97,97,97 | 0 |
| 86 | OHX | A5 | 3816 | 7/7 | 0.79 | 0.27 | 195,195,195,195 | 7 |
| 87 | MG | A5 | 4374 | 1/1 | 0.79 | 0.42 | 95,95,95,95 | 0 |
| 87 | MG | Ba | 201 | 1/1 | 0.79 | 0.36 | 66,66,66,66 | 0 |
| 87 | MG | A5 | 4218 | 1/1 | 0.79 | 0.22 | 57,57,57,57 | 0 |
| 87 | MG | A1 | 3974 | 1/1 | 0.79 | 0.25 | 35,35,35,35 | 0 |
| 87 | MG | A1 | 3978 | 1/1 | 0.79 | 0.40 | 73,73,73,73 | 0 |
| 87 | MG | A1 | 4248 | 1/1 | 0.79 | 0.71 | 78,78,78,78 | 0 |
| 87 | MG | A5 | 4384 | 1/1 | 0.79 | 0.25 | 77,77,77,77 | 0 |
| 87 | MG | A1 | 4356 | 1/1 | 0.79 | 0.26 | 65,65,65,65 | 0 |
| 87 | MG | A3 | 232 | 1/1 | 0.79 | 0.24 | 95,95,95,95 | 0 |
| 86 | OHX | A1 | 3765 | 7/7 | 0.79 | 0.35 | 173,173,173,173 | 7 |
| 86 | OHX | A1 | 3745 | 7/7 | 0.79 | 0.29 | 178,178,178,178 | 7 |
| 87 | MG | A5 | 4247 | 1/1 | 0.79 | 0.18 | 64,64,64,64 | 0 |
| 87 | MG | A1 | 4360 | 1/1 | 0.79 | 0.53 | 88,88,88,88 | 0 |
| 87 | MG | A1 | 4101 | 1/1 | 0.79 | 0.33 | 86,86,86,86 | 0 |
| 87 | MG | A1 | 4453 | 1/1 | 0.79 | 1.13 | 114,114,114,114 | 0 |
| 87 | MG | A5 | 3875 | 1/1 | 0.79 | 0.35 | 78,78,78,78 | 0 |
| 86 | OHX | A6 | 2061 | 7/7 | 0.79 | 0.29 | 172,172,172,172 | 7 |
| 87 | MG | A5 | 4258 | 1/1 | 0.79 | 0.32 | 70,70,70,70 | 0 |
| 87 | MG | A8 | 201 | 1/1 | 0.79 | 0.17 | 92,92,92,92 | 0 |
| 87 | MG | A5 | 3887 | 1/1 | 0.79 | 0.41 | 84,84,84,84 | 0 |
| 87 | MG | A1 | 3888 | 1/1 | 0.79 | 0.30 | 67,67,67,67 | 0 |
| 87 | MG | A5 | 4265 | 1/1 | 0.79 | 1.24 | 80,80,80,80 | 0 |
| 87 | MG | A5 | 4424 | 1/1 | 0.79 | 0.47 | 86,86,86,86 | 0 |
| 87 | MG | A5 | 4425 | 1/1 | 0.79 | 0.28 | 65,65,65,65 | 0 |
| 87 | MG | A5 | 4432 | 1/1 | 0.79 | 0.41 | 95,95,95,95 | 0 |
| 87 | MG | A6 | 2104 | 1/1 | 0.79 | 0.30 | 68,68,68,68 | 0 |
| 87 | MG | A6 | 2238 | 1/1 | 0.79 | 0.19 | 73,73,73,73 | 0 |
| 86 | OHX | A5 | 3785 | 7/7 | 0.79 | 0.35 | 126,126,126,126 | 7 |
| 87 | MG | DC | 404 | 1/1 | 0.79 | 0.34 | 70,70,70,70 | 0 |
| 87 | MG | A1 | 4302 | 1/1 | 0.79 | 0.57 | 114,114,114,114 | 0 |
| 87 | MG | A1 | 4259 | 1/1 | 0.79 | 0.24 | 102,102,102,102 | 0 |
| 86 | OHX | A1 | 3796 | 7/7 | 0.79 | 0.29 | 174,174,174,174 | 7 |
| 87 | MG | A5 | 4471 | 1/1 | 0.79 | 0.18 | 61,61,61,61 | 0 |
| 87 | MG | A5 | 4130 | 1/1 | 0.79 | 0.28 | 49,49,49,49 | 0 |
| 87 | MG | A5 | 4309 | 1/1 | 0.79 | 0.80 | 64,64,64,64 | 0 |
| 87 | MG | A6 | 2329 | 1/1 | 0.79 | 1.14 | 138,138,138,138 | 0 |
| 86 | OHX | A2 | 2051 | 7/7 | 0.79 | 0.52 | 209,209,209,209 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | A1 | 4263 | 1/1 | 0.79 | 1.37 | 71,71,71,71 | 0 |
| 87 | MG | A1 | 4016 | 1/1 | 0.79 | 0.34 | 40,40,40,40 | 0 |
| 87 | MG | A1 | 4118 | 1/1 | 0.79 | 0.18 | 74,74,74,74 | 0 |
| 87 | MG | A1 | 4323 | 1/1 | 0.79 | 0.14 | 92,92,92,92 | 0 |
| 87 | MG | A1 | 4178 | 1/1 | 0.79 | 0.17 | 70,70,70,70 | 0 |
| 87 | MG | A1 | 4398 | 1/1 | 0.79 | 0.28 | 49,49,49,49 | 0 |
| 87 | MG | A5 | 3960 | 1/1 | 0.79 | 0.24 | 49,49,49,49 | 0 |
| 87 | MG | A1 | 4122 | 1/1 | 0.79 | 0.28 | 57,57,57,57 | 0 |
| 87 | MG | A5 | 4169 | 1/1 | 0.79 | 0.20 | 90,90,90,90 | 0 |
| 87 | MG | A5 | 4172 | 1/1 | 0.79 | 0.32 | 67,67,67,67 | 0 |
| 87 | MG | A1 | 4407 | 1/1 | 0.79 | 0.66 | 113,113,113,113 | 0 |
| 87 | MG | A5 | 4510 | 1/1 | 0.79 | 1.84 | 86,86,86,86 | 0 |
| 87 | MG | A5 | 4181 | 1/1 | 0.80 | 0.29 | 80,80,80,80 | 0 |
| 87 | MG | A5 | 4186 | 1/1 | 0.80 | 0.23 | 84,84,84,84 | 0 |
| 87 | MG | A6 | 2189 | 1/1 | 0.80 | 0.32 | 42,42,42,42 | 0 |
| 87 | MG | A1 | 3875 | 1/1 | 0.80 | 0.15 | 60,60,60,60 | 0 |
| 87 | MG | A1 | 4508 | 1/1 | 0.80 | 0.39 | 58,58,58,58 | 0 |
| 86 | OHX | A1 | 3726 | 7/7 | 0.80 | 0.22 | 178,178,178,178 | 7 |
| 87 | MG | A6 | 2197 | 1/1 | 0.80 | 0.20 | 74,74,74,74 | 0 |
| 87 | MG | A5 | 4435 | 1/1 | 0.80 | 0.18 | 87,87,87,87 | 0 |
| 86 | OHX | A1 | 3793 | 7/7 | 0.80 | 0.29 | 232,232,232,232 | 7 |
| 87 | MG | A1 | 4215 | 1/1 | 0.80 | 0.18 | 65,65,65,65 | 0 |
| 87 | MG | A1 | 4133 | 1/1 | 0.80 | 0.25 | 91,91,91,91 | 0 |
| 86 | OHX | A5 | 3810 | 7/7 | 0.80 | 0.55 | 199,199,199,199 | 7 |
| 86 | OHX | A5 | 3780 | 7/7 | 0.80 | 0.43 | 211,211,211,211 | 7 |
| 87 | MG | CG | 304 | 1/1 | 0.80 | 0.30 | 72,72,72,72 | 0 |
| 87 | MG | A6 | 2216 | 1/1 | 0.80 | 0.13 | 64,64,64,64 | 0 |
| 87 | MG | A7 | 227 | 1/1 | 0.80 | 0.55 | 100,100,100,100 | 0 |
| 87 | MG | A4 | 216 | 1/1 | 0.80 | 0.42 | 64,64,64,64 | 0 |
| 87 | MG | A5 | 4091 | 1/1 | 0.80 | 0.12 | 54,54,54,54 | 0 |
| 87 | MG | A5 | 4344 | 1/1 | 0.80 | 0.48 | 66,66,66,66 | 0 |
| 86 | OHX | A6 | 2099 | 7/7 | 0.80 | 0.35 | 184,184,184,184 | 7 |
| 86 | OHX | A1 | 3734 | 7/7 | 0.80 | 0.28 | 190,190,190,190 | 7 |
| 87 | MG | A8 | 231 | 1/1 | 0.80 | 0.23 | 71,71,71,71 | 0 |
| 87 | MG | Af | 201 | 1/1 | 0.80 | 0.13 | 88,88,88,88 | 0 |
| 87 | MG | CX | 201 | 1/1 | 0.80 | 0.31 | 68,68,68,68 | 0 |
| 87 | MG | A1 | 4145 | 1/1 | 0.80 | 0.22 | 54,54,54,54 | 0 |
| 87 | MG | A5 | 4490 | 1/1 | 0.80 | 0.25 | 90,90,90,90 | 0 |
| 87 | MG | A5 | 4235 | 1/1 | 0.80 | 0.23 | 75,75,75,75 | 0 |
| 86 | OHX | A5 | 3818 | 7/7 | 0.80 | 0.62 | 226,226,226,226 | 7 |
| 87 | MG | A1 | 4192 | 1/1 | 0.80 | 0.28 | 86,86,86,86 | 0 |
| 87 | MG | A1 | 3908 | 1/1 | 0.80 | 0.18 | 64,64,64,64 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | A5 | 4370 | 1/1 | 0.80 | 0.21 | 59,59,59,59 | 0 |
| 87 | MG | A5 | 4124 | 1/1 | 0.80 | 0.17 | 78,78,78,78 | 0 |
| 87 | MG | DD | 302 | 1/1 | 0.80 | 0.18 | 66,66,66,66 | 0 |
| 87 | MG | A4 | 237 | 1/1 | 0.80 | 0.29 | 94,94,94,94 | 0 |
| 87 | MG | A1 | 3909 | 1/1 | 0.80 | 0.44 | 67,67,67,67 | 0 |
| 87 | MG | A1 | 4303 | 1/1 | 0.80 | 0.36 | 105,105,105,105 | 0 |
| 87 | MG | A5 | 4134 | 1/1 | 0.80 | 0.22 | 84,84,84,84 | 0 |
| 87 | MG | A5 | 3993 | 1/1 | 0.80 | 0.26 | 25,25,25,25 | 0 |
| 87 | MG | A5 | 4000 | 1/1 | 0.80 | 0.44 | 53,53,53,53 | 0 |
| 87 | MG | Ba | 208 | 1/1 | 0.80 | 0.53 | 68,68,68,68 | 0 |
| 87 | MG | A1 | 4073 | 1/1 | 0.80 | 0.13 | 57,57,57,57 | 0 |
| 87 | MG | A5 | 4022 | 1/1 | 0.80 | 0.46 | 52,52,52,52 | 0 |
| 87 | MG | DY | 201 | 1/1 | 0.80 | 0.27 | 59,59,59,59 | 0 |
| 87 | MG | A2 | 2185 | 1/1 | 0.80 | 0.14 | 72,72,72,72 | 0 |
| 87 | MG | A6 | 2319 | 1/1 | 0.80 | 0.22 | 64,64,64,64 | 0 |
| 87 | MG | A6 | 2320 | 1/1 | 0.80 | 1.56 | 117,117,117,117 | 0 |
| 87 | MG | A1 | 3977 | 1/1 | 0.80 | 0.31 | 76,76,76,76 | 0 |
| 87 | MG | A1 | 4462 | 1/1 | 0.80 | 0.42 | 71,71,71,71 | 0 |
| 87 | MG | BD | 302 | 1/1 | 0.80 | 0.22 | 79,79,79,79 | 0 |
| 87 | MG | A5 | 4405 | 1/1 | 0.80 | 0.89 | 69,69,69,69 | 0 |
| 87 | MG | A1 | 4503 | 1/1 | 0.80 | 1.26 | 77,77,77,77 | 0 |
| 87 | MG | A1 | 4504 | 1/1 | 0.80 | 1.16 | 98,98,98,98 | 0 |
| 87 | MG | BO | 209 | 1/1 | 0.81 | 1.55 | 95,95,95,95 | 0 |
| 87 | MG | A5 | 4378 | 1/1 | 0.81 | 1.17 | 75,75,75,75 | 0 |
| 87 | MG | A5 | 4110 | 1/1 | 0.81 | 0.17 | 63,63,63,63 | 0 |
| 87 | MG | CS | 202 | 1/1 | 0.81 | 0.41 | 63,63,63,63 | 0 |
| 86 | OHX | A2 | 2054 | 7/7 | 0.81 | 0.18 | 227,227,227,227 | 7 |
| 87 | MG | A1 | 4423 | 1/1 | 0.81 | 0.57 | 85,85,85,85 | 0 |
| 86 | OHX | A5 | 3734 | 7/7 | 0.81 | 0.31 | 208,208,208,208 | 7 |
| 86 | OHX | A5 | 3748 | 7/7 | 0.81 | 0.27 | 183,183,183,183 | 7 |
| 87 | MG | A5 | 3986 | 1/1 | 0.81 | 0.27 | 53,53,53,53 | 0 |
| 87 | MG | BR | 204 | 1/1 | 0.81 | 0.35 | 67,67,67,67 | 0 |
| 87 | MG | A5 | 4558 | 1/1 | 0.81 | 0.44 | 63,63,63,63 | 0 |
| 87 | MG | A5 | 4393 | 1/1 | 0.81 | 0.79 | 97,97,97,97 | 0 |
| 87 | MG | A5 | 4262 | 1/1 | 0.81 | 0.23 | 60,60,60,60 | 0 |
| 86 | OHX | A1 | 3732 | 7/7 | 0.81 | 0.26 | 166,166,166,166 | 7 |
| 87 | MG | A1 | 3404 | 1/1 | 0.81 | 0.28 | 74,74,74,74 | 0 |
| 87 | MG | A5 | 4136 | 1/1 | 0.81 | 0.28 | 46,46,46,46 | 0 |
| 87 | MG | A6 | 2242 | 1/1 | 0.81 | 0.37 | 87,87,87,87 | 0 |
| 87 | MG | A5 | 3995 | 1/1 | 0.81 | 0.39 | 53,53,53,53 | 0 |
| 87 | MG | A5 | 4139 | 1/1 | 0.81 | 0.20 | 99,99,99,99 | 0 |
| 87 | MG | A1 | 3882 | 1/1 | 0.81 | 0.31 | 47,47,47,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87 | MG | A5 | 4151 | 1/1 | 0.81 | 0.14 | 64,64,64,64 | 0 |
| 87 | MG | A6 | 2147 | 1/1 | 0.81 | 0.28 | 44,44,44,44 | 0 |
| 87 | MG | A7 | 215 | 1/1 | 0.81 | 0.26 | 46,46,46,46 | 0 |
| 87 | MG | A5 | 4294 | 1/1 | 0.81 | 0.21 | 62,62,62,62 | 0 |
| 87 | MG | A5 | 4004 | 1/1 | 0.81 | 0.43 | 55,55,55,55 | 0 |
| 87 | MG | A5 | 4156 | 1/1 | 0.81 | 0.28 | 65,65,65,65 | 0 |
| 87 | MG | A5 | 4428 | 1/1 | 0.81 | 0.10 | 75,75,75,75 | 0 |
| 87 | MG | A5 | 4431 | 1/1 | 0.81 | 0.38 | 118,118,118,118 | 0 |
| 87 | MG | A5 | 3845 | 1/1 | 0.81 | 0.31 | 51,51,51,51 | 0 |
| 87 | MG | A4 | 232 | 1/1 | 0.81 | 0.22 | 74,74,74,74 | 0 |
| 87 | MG | A5 | 4023 | 1/1 | 0.81 | 0.39 | 44,44,44,44 | 0 |
| 87 | MG | A6 | 2318 | 1/1 | 0.81 | 0.22 | 68,68,68,68 | 0 |
| 86 | OHX | A6 | 2068 | 7/7 | 0.81 | 0.55 | 217,217,217,217 | 7 |
| 87 | MG | A1 | 4247 | 1/1 | 0.81 | 0.24 | 74,74,74,74 | 0 |
| 87 | MG | A5 | 3856 | 1/1 | 0.81 | 0.33 | 54,54,54,54 | 0 |
| 87 | MG | A1 | 4112 | 1/1 | 0.81 | 0.21 | 58,58,58,58 | 0 |
| 87 | MG | A6 | 2168 | 1/1 | 0.81 | 0.33 | 77,77,77,77 | 0 |
| 87 | MG | A1 | 4490 | 1/1 | 0.81 | 0.28 | 77,77,77,77 | 0 |
| 87 | MG | DB | 412 | 1/1 | 0.81 | 0.48 | 70,70,70,70 | 0 |
| 87 | MG | A1 | 4115 | 1/1 | 0.81 | 0.36 | 62,62,62,62 | 0 |
| 86 | OHX | A6 | 2071 | 7/7 | 0.81 | 0.44 | 160,160,160,160 | 7 |
| 86 | OHX | A6 | 2073 | 7/7 | 0.81 | 0.22 | 186,186,186,186 | 7 |
| 87 | MG | A1 | 4167 | 1/1 | 0.81 | 1.06 | 66,66,66,66 | 0 |
| 87 | MG | A5 | 4483 | 1/1 | 0.81 | 0.49 | 112,112,112,112 | 0 |
| 87 | MG | A5 | 4336 | 1/1 | 0.81 | 0.46 | 77,77,77,77 | 0 |
| 87 | MG | A5 | 3879 | 1/1 | 0.81 | 0.25 | 61,61,61,61 | 0 |
| 87 | MG | A1 | 3826 | 1/1 | 0.81 | 0.19 | 51,51,51,51 | 0 |
| 87 | MG | A2 | 2259 | 1/1 | 0.81 | 0.51 | 63,63,63,63 | 0 |
| 87 | MG | A1 | 4399 | 1/1 | 0.81 | 0.54 | 85,85,85,85 | 0 |
| 87 | MG | A5 | 3895 | 1/1 | 0.81 | 0.26 | 32,32,32,32 | 0 |
| 87 | MG | A1 | 4177 | 1/1 | 0.81 | 0.90 | 76,76,76,76 | 0 |
| 87 | MG | A5 | 4212 | 1/1 | 0.81 | 0.19 | 73,73,73,73 | 0 |
| 87 | MG | A5 | 4496 | 1/1 | 0.81 | 0.23 | 77,77,77,77 | 0 |
| 86 | OHX | A5 | 3778 | 7/7 | 0.81 | 0.20 | 153,153,153,153 | 7 |
| 87 | MG | A5 | 4499 | 1/1 | 0.81 | 0.39 | 76,76,76,76 | 0 |
| 86 | OHX | A6 | 2051 | 7/7 | 0.81 | 0.21 | 167,167,167,167 | 7 |
| 87 | MG | Da | 203 | 1/1 | 0.81 | 0.21 | 54,54,54,54 | 0 |
| 86 | OHX | A5 | 3822 | 7/7 | 0.81 | 0.60 | 205,205,205,205 | 7 |
| 87 | MG | A5 | 4219 | 1/1 | 0.81 | 0.33 | 74,74,74,74 | 0 |
| 87 | MG | De | 202 | 1/1 | 0.81 | 0.73 | 52,52,52,52 | 0 |
| 87 | MG | CE | 301 | 1/1 | 0.81 | 0.16 | 57,57,57,57 | 0 |
| 87 | MG | A3 | 228 | 1/1 | 0.81 | 0.35 | 81,81,81,81 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | BL | 203 | 1/1 | 0.81 | 0.21 | 61,61,61,61 | 0 |
| 86 | OHX | A6 | 2052 | 7/7 | 0.81 | 0.14 | 211,211,211,211 | 7 |
| 87 | MG | A1 | 3981 | 1/1 | 0.81 | 0.35 | 41,41,41,41 | 0 |
| 87 | MG | A5 | 4533 | 1/1 | 0.81 | 0.19 | 83,83,83,83 | 0 |
| 87 | MG | A1 | 4472 | 1/1 | 0.81 | 0.27 | 86,86,86,86 | 0 |
| 87 | MG | Bj | 108 | 1/1 | 0.82 | 1.98 | 66,66,66,66 | 0 |
| 86 | OHX | A1 | 3772 | 7/7 | 0.82 | 0.27 | 171,171,171,171 | 7 |
| 87 | MG | A5 | 4517 | 1/1 | 0.82 | 0.54 | 73,73,73,73 | 0 |
| 87 | MG | A6 | 2302 | 1/1 | 0.82 | 0.17 | 108,108,108,108 | 0 |
| 87 | MG | A5 | 4522 | 1/1 | 0.82 | 0.26 | 73,73,73,73 | 0 |
| 87 | MG | A1 | 4012 | 1/1 | 0.82 | 0.38 | 41,41,41,41 | 0 |
| 87 | MG | A2 | 2148 | 1/1 | 0.82 | 0.24 | 89,89,89,89 | 0 |
| 87 | MG | A5 | 4363 | 1/1 | 0.82 | 0.29 | 83,83,83,83 | 0 |
| 87 | MG | A6 | 2309 | 1/1 | 0.82 | 0.39 | 105,105,105,105 | 0 |
| 87 | MG | A5 | 4365 | 1/1 | 0.82 | 0.28 | 80,80,80,80 | 0 |
| 87 | MG | A1 | 4268 | 1/1 | 0.82 | 0.19 | 65,65,65,65 | 0 |
| 87 | MG | A1 | 3850 | 1/1 | 0.82 | 0.36 | 64,64,64,64 | 0 |
| 86 | OHX | A5 | 3800 | 7/7 | 0.82 | 0.27 | 203,203,203,203 | 7 |
| 87 | MG | A6 | 2224 | 1/1 | 0.82 | 0.12 | 47,47,47,47 | 0 |
| 87 | MG | A1 | 4154 | 1/1 | 0.82 | 0.20 | 91,91,91,91 | 0 |
| 87 | MG | A1 | 4484 | 1/1 | 0.82 | 1.48 | 106,106,106,106 | 0 |
| 87 | MG | A5 | 4228 | 1/1 | 0.82 | 0.35 | 82,82,82,82 | 0 |
| 87 | MG | A1 | 3852 | 1/1 | 0.82 | 0.26 | 70,70,70,70 | 0 |
| 86 | OHX | A2 | 2079 | 7/7 | 0.82 | 0.22 | 157,157,157,157 | 7 |
| 87 | MG | A5 | 4383 | 1/1 | 0.82 | 0.29 | 69,69,69,69 | 0 |
| 87 | MG | A5 | 3884 | 1/1 | 0.82 | 0.29 | 54,54,54,54 | 0 |
| 87 | MG | A5 | 3885 | 1/1 | 0.82 | 0.18 | 58,58,58,58 | 0 |
| 86 | OHX | A5 | 3769 | 7/7 | 0.82 | 0.28 | 169,169,169,169 | 7 |
| 86 | OHX | A2 | 2069 | 7/7 | 0.82 | 0.46 | 191,191,191,191 | 7 |
| 87 | MG | A5 | 4246 | 1/1 | 0.82 | 0.35 | 38,38,38,38 | 0 |
| 87 | MG | A1 | 4430 | 1/1 | 0.82 | 0.35 | 67,67,67,67 | 0 |
| 86 | OHX | A2 | 2072 | 7/7 | 0.82 | 0.38 | 207,207,207,207 | 7 |
| 87 | MG | A5 | 4395 | 1/1 | 0.82 | 0.92 | 58,58,58,58 | 0 |
| 87 | MG | A1 | 4498 | 1/1 | 0.82 | 0.23 | 60,60,60,60 | 0 |
| 86 | OHX | A1 | 3599 | 7/7 | 0.82 | 0.27 | 196,196,196,196 | 7 |
| 87 | MG | A5 | 3902 | 1/1 | 0.82 | 0.15 | 31,31,31,31 | 0 |
| 87 | MG | A6 | 2330 | 1/1 | 0.82 | 0.35 | 80,80,80,80 | 0 |
| 87 | MG | A1 | 4053 | 1/1 | 0.82 | 0.19 | 76,76,76,76 | 0 |
| 87 | MG | A5 | 3914 | 1/1 | 0.82 | 0.42 | 69,69,69,69 | 0 |
| 87 | MG | A7 | 224 | 1/1 | 0.82 | 0.15 | 69,69,69,69 | 0 |
| 87 | MG | A1 | 3937 | 1/1 | 0.82 | 0.39 | 40,40,40,40 | 0 |
| 87 | MG | A2 | 2239 | 1/1 | 0.82 | 0.18 | 92,92,92,92 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87 | MG | AS | 202 | 1/1 | 0.82 | 0.51 | 63,63,63,63 | 0 |
| 87 | MG | A6 | 2146 | 1/1 | 0.82 | 0.25 | 49,49,49,49 | 0 |
| 87 | MG | BP | 208 | 1/1 | 0.82 | 0.16 | 52,52,52,52 | 0 |
| 87 | MG | A5 | 3926 | 1/1 | 0.82 | 0.31 | 53,53,53,53 | 0 |
| 87 | MG | A5 | 4427 | 1/1 | 0.82 | 0.47 | 102,102,102,102 | 0 |
| 87 | MG | A5 | 4277 | 1/1 | 0.82 | 0.56 | 85,85,85,85 | 0 |
| 87 | MG | A6 | 2154 | 1/1 | 0.82 | 0.36 | 56,56,56,56 | 0 |
| 87 | MG | A1 | 4119 | 1/1 | 0.82 | 0.24 | 78,78,78,78 | 0 |
| 87 | MG | A5 | 3941 | 1/1 | 0.82 | 0.27 | 51,51,51,51 | 0 |
| 87 | MG | A5 | 4292 | 1/1 | 0.82 | 0.26 | 113,113,113,113 | 0 |
| 87 | MG | DA | 303 | 1/1 | 0.82 | 0.25 | 53,53,53,53 | 0 |
| 87 | MG | DB | 408 | 1/1 | 0.82 | 0.29 | 67,67,67,67 | 0 |
| 87 | MG | A5 | 3944 | 1/1 | 0.82 | 0.20 | 36,36,36,36 | 0 |
| 87 | MG | AX | 201 | 1/1 | 0.82 | 0.14 | 70,70,70,70 | 0 |
| 87 | MG | A1 | 4293 | 1/1 | 0.82 | 1.13 | 110,110,110,110 | 0 |
| 87 | MG | A5 | 4149 | 1/1 | 0.82 | 0.25 | 63,63,63,63 | 0 |
| 87 | MG | A1 | 4188 | 1/1 | 0.82 | 0.35 | 82,82,82,82 | 0 |
| 87 | MG | A1 | 4452 | 1/1 | 0.82 | 2.08 | 112,112,112,112 | 0 |
| 87 | MG | A1 | 4063 | 1/1 | 0.82 | 0.23 | 73,73,73,73 | 0 |
| 87 | MG | A2 | 2240 | 1/1 | 0.82 | 0.53 | 97,97,97,97 | 0 |
| 87 | MG | A1 | 4455 | 1/1 | 0.82 | 0.24 | 79,79,79,79 | 0 |
| 87 | MG | DG | 302 | 1/1 | 0.82 | 0.43 | 65,65,65,65 | 0 |
| 87 | MG | A6 | 2181 | 1/1 | 0.82 | 0.31 | 77,77,77,77 | 0 |
| 87 | MG | A5 | 4480 | 1/1 | 0.82 | 0.19 | 76,76,76,76 | 0 |
| 87 | MG | A6 | 2277 | 1/1 | 0.82 | 0.26 | 79,79,79,79 | 0 |
| 87 | MG | A2 | 2214 | 1/1 | 0.82 | 0.23 | 75,75,75,75 | 0 |
| 87 | MG | CZ | 201 | 1/1 | 0.82 | 0.21 | 74,74,74,74 | 0 |
| 87 | MG | A5 | 4329 | 1/1 | 0.82 | 0.42 | 86,86,86,86 | 0 |
| 87 | MG | DO | 208 | 1/1 | 0.82 | 0.45 | 77,77,77,77 | 0 |
| 87 | MG | A5 | 4174 | 1/1 | 0.82 | 0.18 | 75,75,75,75 | 0 |
| 86 | OHX | A1 | 3664 | 7/7 | 0.82 | 0.15 | 207,207,207,207 | 7 |
| 87 | MG | A1 | 4307 | 1/1 | 0.82 | 0.24 | 71,71,71,71 | 0 |
| 86 | OHX | BP | 201 | 7/7 | 0.82 | 0.41 | 115,115,115,115 | 7 |
| 87 | MG | A5 | 3412 | 1/1 | 0.82 | 0.71 | 68,68,68,68 | 0 |
| 86 | OHX | A5 | 3786 | 7/7 | 0.82 | 0.41 | 238,238,238,238 | 7 |
| 87 | MG | A1 | 4200 | 1/1 | 0.82 | 0.26 | 71,71,71,71 | 0 |
| 86 | OHX | DM | 201 | 7/7 | 0.82 | 0.23 | 208,208,208,208 | 7 |
| 87 | MG | A5 | 4498 | 1/1 | 0.82 | 0.27 | 90,90,90,90 | 0 |
| 87 | MG | Dp | 102 | 1/1 | 0.82 | 0.28 | 63,63,63,63 | 0 |
| 87 | MG | A5 | 4038 | 1/1 | 0.82 | 0.20 | 42,42,42,42 | 0 |
| 86 | OHX | BR | 201 | 7/7 | 0.82 | 0.18 | 181,181,181,181 | 7 |
| 86 | OHX | A1 | 3709 | 7/7 | 0.82 | 0.19 | 176,176,176,176 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | A5 | 4348 | 1/1 | 0.82 | 0.43 | 58,58,58,58 | 0 |
| 87 | MG | A5 | 4198 | 1/1 | 0.82 | 0.22 | 58,58,58,58 | 0 |
| 87 | MG | A6 | 2310 | 1/1 | 0.83 | 0.28 | 89,89,89,89 | 0 |
| 87 | MG | A6 | 2205 | 1/1 | 0.83 | 0.26 | 72,72,72,72 | 0 |
| 87 | MG | A6 | 2207 | 1/1 | 0.83 | 0.12 | 57,57,57,57 | 0 |
| 87 | MG | A1 | 4134 | 1/1 | 0.83 | 0.27 | 69,69,69,69 | 0 |
| 87 | MG | A1 | 4352 | 1/1 | 0.83 | 0.20 | 93,93,93,93 | 0 |
| 87 | MG | A1 | 4354 | 1/1 | 0.83 | 0.21 | 61,61,61,61 | 0 |
| 87 | MG | A6 | 2212 | 1/1 | 0.83 | 0.16 | 91,91,91,91 | 0 |
| 87 | MG | A1 | 3839 | 1/1 | 0.83 | 0.29 | 64,64,64,64 | 0 |
| 87 | MG | A5 | 3890 | 1/1 | 0.83 | 0.35 | 82,82,82,82 | 0 |
| 86 | OHX | AC | 301 | 7/7 | 0.83 | 0.86 | 213,213,213,213 | 7 |
| 87 | MG | A2 | 2108 | 1/1 | 0.83 | 0.17 | 56,56,56,56 | 0 |
| 86 | OHX | A1 | 3792 | 7/7 | 0.83 | 0.58 | 213,213,213,213 | 7 |
| 87 | MG | A1 | 4458 | 1/1 | 0.83 | 0.77 | 92,92,92,92 | 0 |
| 87 | MG | A5 | 4568 | 1/1 | 0.83 | 0.38 | 64,64,64,64 | 0 |
| 87 | MG | Bm | 201 | 1/1 | 0.83 | 0.62 | 68,68,68,68 | 0 |
| 87 | MG | A4 | 230 | 1/1 | 0.83 | 0.30 | 71,71,71,71 | 0 |
| 87 | MG | A2 | 2113 | 1/1 | 0.83 | 0.41 | 80,80,80,80 | 0 |
| 87 | MG | A2 | 2249 | 1/1 | 0.83 | 0.19 | 85,85,85,85 | 0 |
| 87 | MG | A4 | 233 | 1/1 | 0.83 | 0.20 | 57,57,57,57 | 0 |
| 86 | OHX | A5 | 3688 | 7/7 | 0.83 | 0.17 | 212,212,212,212 | 7 |
| 87 | MG | A1 | 3946 | 1/1 | 0.83 | 0.34 | 41,41,41,41 | 0 |
| 87 | MG | A5 | 3922 | 1/1 | 0.83 | 0.20 | 54,54,54,54 | 0 |
| 86 | OHX | A1 | 3759 | 7/7 | 0.83 | 0.50 | 149,149,149,149 | 7 |
| 87 | MG | A1 | 4227 | 1/1 | 0.83 | 0.19 | 52,52,52,52 | 0 |
| 87 | MG | A1 | 4468 | 1/1 | 0.83 | 1.20 | 79,79,79,79 | 0 |
| 87 | MG | A5 | 3927 | 1/1 | 0.83 | 0.32 | 49,49,49,49 | 0 |
| 87 | MG | A2 | 2132 | 1/1 | 0.83 | 0.10 | 77,77,77,77 | 0 |
| 87 | MG | A1 | 4084 | 1/1 | 0.83 | 0.34 | 67,67,67,67 | 0 |
| 86 | OHX | A5 | 3823 | 7/7 | 0.83 | 0.12 | 225,225,225,225 | 7 |
| 87 | MG | A5 | 4434 | 1/1 | 0.83 | 0.37 | 72,72,72,72 | 0 |
| 86 | OHX | A7 | 213 | 7/7 | 0.83 | 0.28 | 181,181,181,181 | 7 |
| 87 | MG | A7 | 230 | 1/1 | 0.83 | 0.22 | 61,61,61,61 | 0 |
| 87 | MG | A7 | 233 | 1/1 | 0.83 | 0.27 | 60,60,60,60 | 0 |
| 87 | MG | A7 | 235 | 1/1 | 0.83 | 0.38 | 74,74,74,74 | 0 |
| 87 | MG | BC | 406 | 1/1 | 0.83 | 0.29 | 61,61,61,61 | 0 |
| 87 | MG | A2 | 2137 | 1/1 | 0.83 | 0.21 | 97,97,97,97 | 0 |
| 87 | MG | A5 | 3958 | 1/1 | 0.83 | 0.26 | 64,64,64,64 | 0 |
| 87 | MG | A1 | 4159 | 1/1 | 0.83 | 0.26 | 84,84,84,84 | 0 |
| 86 | OHX | A8 | 215 | 7/7 | 0.83 | 0.33 | 151,151,151,151 | 7 |
| 87 | MG | A5 | 4452 | 1/1 | 0.83 | 0.84 | 57,57,57,57 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86 | OHX | A8 | 217 | 7/7 | 0.83 | 0.33 | 169,169,169,169 | 7 |
| 87 | MG | A2 | 2186 | 1/1 | 0.83 | 0.28 | 76,76,76,76 | 0 |
| 87 | MG | A1 | 4403 | 1/1 | 0.83 | 0.17 | 71,71,71,71 | 0 |
| 87 | MG | DB | 404 | 1/1 | 0.83 | 0.29 | 68,68,68,68 | 0 |
| 86 | OHX | A1 | 3728 | 7/7 | 0.83 | 0.16 | 203,203,203,203 | 7 |
| 86 | OHX | A2 | 2074 | 7/7 | 0.83 | 0.26 | 191,191,191,191 | 7 |
| 87 | MG | A1 | 3897 | 1/1 | 0.83 | 0.30 | 75,75,75,75 | 0 |
| 87 | MG | A2 | 2230 | 1/1 | 0.83 | 0.15 | 94,94,94,94 | 0 |
| 87 | MG | A1 | 3903 | 1/1 | 0.83 | 0.29 | 85,85,85,85 | 0 |
| 87 | MG | A5 | 3410 | 1/1 | 0.83 | 0.27 | 61,61,61,61 | 0 |
| 87 | MG | A1 | 4183 | 1/1 | 0.83 | 0.27 | 51,51,51,51 | 0 |
| 87 | MG | BP | 203 | 1/1 | 0.83 | 0.36 | 71,71,71,71 | 0 |
| 86 | OHX | A5 | 3763 | 7/7 | 0.83 | 0.48 | 197,197,197,197 | 7 |
| 86 | OHX | A1 | 3810 | 7/7 | 0.83 | 0.66 | 199,199,199,199 | 7 |
| 87 | MG | A5 | 4028 | 1/1 | 0.83 | 0.41 | 47,47,47,47 | 0 |
| 86 | OHX | A2 | 2084 | 7/7 | 0.83 | 0.18 | 183,183,183,183 | 7 |
| 87 | MG | A5 | 4036 | 1/1 | 0.83 | 0.17 | 60,60,60,60 | 0 |
| 87 | MG | A5 | 3841 | 1/1 | 0.83 | 0.33 | 44,44,44,44 | 0 |
| 87 | MG | A2 | 2154 | 1/1 | 0.83 | 0.34 | 74,74,74,74 | 0 |
| 87 | MG | DM | 202 | 1/1 | 0.83 | 0.24 | 70,70,70,70 | 0 |
| 87 | MG | A5 | 4205 | 1/1 | 0.83 | 0.28 | 79,79,79,79 | 0 |
| 87 | MG | A5 | 4352 | 1/1 | 0.83 | 0.29 | 67,67,67,67 | 0 |
| 87 | MG | A1 | 4116 | 1/1 | 0.83 | 0.39 | 65,65,65,65 | 0 |
| 87 | MG | DP | 204 | 1/1 | 0.83 | 0.29 | 78,78,78,78 | 0 |
| 87 | MG | A5 | 3850 | 1/1 | 0.83 | 0.33 | 55,55,55,55 | 0 |
| 87 | MG | A5 | 4210 | 1/1 | 0.83 | 0.26 | 79,79,79,79 | 0 |
| 87 | MG | DV | 204 | 1/1 | 0.83 | 1.04 | 83,83,83,83 | 0 |
| 87 | MG | A5 | 4506 | 1/1 | 0.83 | 0.27 | 80,80,80,80 | 0 |
| 86 | OHX | A1 | 3738 | 7/7 | 0.83 | 0.33 | 138,138,138,138 | 7 |
| 87 | MG | A5 | 4053 | 1/1 | 0.83 | 0.35 | 65,65,65,65 | 0 |
| 87 | MG | A6 | 2185 | 1/1 | 0.83 | 0.19 | 71,71,71,71 | 0 |
| 87 | MG | A2 | 2200 | 1/1 | 0.83 | 0.16 | 88,88,88,88 | 0 |
| 87 | MG | A1 | 3819 | 1/1 | 0.83 | 0.11 | 63,63,63,63 | 0 |
| 87 | MG | A5 | 4371 | 1/1 | 0.83 | 0.23 | 90,90,90,90 | 0 |
| 87 | MG | A1 | 4125 | 1/1 | 0.83 | 0.25 | 56,56,56,56 | 0 |
| 87 | MG | A3 | 221 | 1/1 | 0.83 | 0.13 | 69,69,69,69 | 0 |
| 87 | MG | A5 | 4531 | 1/1 | 0.83 | 0.26 | 65,65,65,65 | 0 |
| 86 | OHX | A2 | 2065 | 7/7 | 0.83 | 0.34 | 166,166,166,166 | 7 |
| 86 | OHX | A5 | 3772 | 7/7 | 0.83 | 0.58 | 137,137,137,137 | 7 |
| 88 | ZN | Cf | 501 | 1/1 | 0.83 | 0.16 | 152,152,152,152 | 0 |
| 87 | MG | A2 | 2099 | 1/1 | 0.83 | 0.20 | 53,53,53,53 | 0 |
| 87 | MG | A5 | 4508 | 1/1 | 0.84 | 0.17 | 67,67,67,67 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|----------------|------|-------|------|------|----------------------------|-------|
| 87 | MG | A5 | 4159 | 1/1 | 0.84 | 0.26 | 64,64,64,64 | 0 |
| 86 | OHX | A2 | 2060 | 7/7 | 0.84 | 0.35 | 168,168,168,168 | 7 |
| 87 | MG | A5 | 4513 | 1/1 | 0.84 | 0.43 | 53,53,53,53 | 0 |
| 86 | OHX | A2 | 2080 | 7/7 | 0.84 | 0.12 | 191,191,191,191 | 7 |
| 87 | MG | A5 | 4340 | 1/1 | 0.84 | 0.80 | 61,61,61,61 | 0 |
| 87 | MG | A5 | 4166 | 1/1 | 0.84 | 0.27 | 57,57,57,57 | 0 |
| 86 | OHX | A2 | 2032 | 7/7 | 0.84 | 0.15 | 200,200,200,200 | 7 |
| 86 | OHX | BB | 402 | 7/7 | 0.84 | 0.23 | 173,173,173,173 | 7 |
| 86 | OHX | A1 | 3788 | 7/7 | 0.84 | 0.59 | 232,232,232,232 | 7 |
| 87 | MG | A5 | 4530 | 1/1 | 0.84 | 0.55 | 113,113,113,113 | 0 |
| 87 | MG | A2 | 2250 | 1/1 | 0.84 | 0.06 | 97,97,97,97 | 0 |
| 87 | MG | A2 | 2122 | 1/1 | 0.84 | 0.20 | 74,74,74,74 | 0 |
| 87 | MG | A1 | 3854 | 1/1 | 0.84 | 0.21 | 57,57,57,57 | 0 |
| 87 | MG | A5 | 4182 | 1/1 | 0.84 | 0.30 | 66,66,66,66 | 0 |
| 87 | MG | CI | 303 | 1/1 | 0.84 | 0.20 | 62,62,62,62 | 0 |
| 87 | MG | A5 | 4354 | 1/1 | 0.84 | 0.72 | 60,60,60,60 | 0 |
| 87 | MG | A1 | 4077 | 1/1 | 0.84 | 0.34 | 77,77,77,77 | 0 |
| 87 | MG | B ₀ | 204 | 1/1 | 0.84 | 0.15 | 76,76,76,76 | 0 |
| 87 | MG | A5 | 4546 | 1/1 | 0.84 | 0.47 | 66,66,66,66 | 0 |
| 87 | MG | A1 | 4080 | 1/1 | 0.84 | 0.17 | 60,60,60,60 | 0 |
| 87 | MG | A4 | 228 | 1/1 | 0.84 | 0.26 | 70,70,70,70 | 0 |
| 87 | MG | A1 | 4162 | 1/1 | 0.84 | 0.35 | 79,79,79,79 | 0 |
| 87 | MG | A1 | 4331 | 1/1 | 0.84 | 0.30 | 62,62,62,62 | 0 |
| 87 | MG | A1 | 3945 | 1/1 | 0.84 | 0.34 | 50,50,50,50 | 0 |
| 87 | MG | A5 | 4199 | 1/1 | 0.84 | 0.43 | 70,70,70,70 | 0 |
| 86 | OHX | A1 | 3697 | 7/7 | 0.84 | 0.27 | 182,182,182,182 | 7 |
| 87 | MG | A1 | 4335 | 1/1 | 0.84 | 0.42 | 86,86,86,86 | 0 |
| 87 | MG | A1 | 3953 | 1/1 | 0.84 | 0.36 | 43,43,43,43 | 0 |
| 87 | MG | A1 | 3969 | 1/1 | 0.84 | 0.35 | 49,49,49,49 | 0 |
| 87 | MG | A2 | 2130 | 1/1 | 0.84 | 0.14 | 56,56,56,56 | 0 |
| 87 | MG | A5 | 4208 | 1/1 | 0.84 | 0.21 | 75,75,75,75 | 0 |
| 87 | MG | A5 | 4380 | 1/1 | 0.84 | 0.71 | 89,89,89,89 | 0 |
| 87 | MG | A6 | 2127 | 1/1 | 0.84 | 0.40 | 41,41,41,41 | 0 |
| 87 | MG | A2 | 2217 | 1/1 | 0.84 | 0.50 | 117,117,117,117 | 0 |
| 87 | MG | A2 | 2257 | 1/1 | 0.84 | 0.56 | 75,75,75,75 | 0 |
| 87 | MG | A6 | 2264 | 1/1 | 0.84 | 0.16 | 62,62,62,62 | 0 |
| 87 | MG | A5 | 3838 | 1/1 | 0.84 | 0.39 | 39,39,39,39 | 0 |
| 87 | MG | A6 | 2265 | 1/1 | 0.84 | 0.17 | 73,73,73,73 | 0 |
| 87 | MG | A7 | 217 | 1/1 | 0.84 | 0.36 | 55,55,55,55 | 0 |
| 87 | MG | A1 | 3874 | 1/1 | 0.84 | 0.29 | 60,60,60,60 | 0 |
| 87 | MG | A6 | 2270 | 1/1 | 0.84 | 0.43 | 90,90,90,90 | 0 |
| 87 | MG | A5 | 4222 | 1/1 | 0.84 | 0.30 | 75,75,75,75 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | A5 | 4054 | 1/1 | 0.84 | 0.24 | 71,71,71,71 | 0 |
| 87 | MG | A5 | 4225 | 1/1 | 0.84 | 0.32 | 66,66,66,66 | 0 |
| 86 | OHX | A2 | 2083 | 7/7 | 0.84 | 0.57 | 185,185,185,185 | 7 |
| 87 | MG | A1 | 3989 | 1/1 | 0.84 | 0.26 | 42,42,42,42 | 0 |
| 87 | MG | A5 | 4401 | 1/1 | 0.84 | 0.18 | 64,64,64,64 | 0 |
| 87 | MG | A5 | 4066 | 1/1 | 0.84 | 0.20 | 73,73,73,73 | 0 |
| 87 | MG | A6 | 2135 | 1/1 | 0.84 | 0.23 | 58,58,58,58 | 0 |
| 87 | MG | A6 | 2137 | 1/1 | 0.84 | 0.33 | 71,71,71,71 | 0 |
| 86 | OHX | A6 | 2089 | 7/7 | 0.84 | 0.21 | 212,212,212,212 | 7 |
| 87 | MG | A5 | 3853 | 1/1 | 0.84 | 0.27 | 67,67,67,67 | 0 |
| 87 | MG | A5 | 4245 | 1/1 | 0.84 | 0.23 | 66,66,66,66 | 0 |
| 87 | MG | A5 | 4077 | 1/1 | 0.84 | 0.37 | 55,55,55,55 | 0 |
| 86 | OHX | A5 | 3776 | 7/7 | 0.84 | 0.24 | 184,184,184,184 | 7 |
| 87 | MG | A1 | 3884 | 1/1 | 0.84 | 0.30 | 64,64,64,64 | 0 |
| 86 | OHX | A2 | 2058 | 7/7 | 0.84 | 0.29 | 201,201,201,201 | 7 |
| 87 | MG | A1 | 4001 | 1/1 | 0.84 | 0.31 | 50,50,50,50 | 0 |
| 87 | MG | A1 | 4275 | 1/1 | 0.84 | 0.34 | 74,74,74,74 | 0 |
| 87 | MG | A5 | 3867 | 1/1 | 0.84 | 0.21 | 27,27,27,27 | 0 |
| 87 | MG | AI | 303 | 1/1 | 0.84 | 0.56 | 73,73,73,73 | 0 |
| 86 | OHX | A6 | 2050 | 7/7 | 0.84 | 0.16 | 206,206,206,206 | 7 |
| 87 | MG | A2 | 2140 | 1/1 | 0.84 | 0.39 | 69,69,69,69 | 0 |
| 87 | MG | A1 | 4015 | 1/1 | 0.84 | 0.36 | 63,63,63,63 | 0 |
| 86 | OHX | A6 | 2097 | 7/7 | 0.84 | 0.25 | 181,181,181,181 | 7 |
| 87 | MG | BN | 305 | 1/1 | 0.84 | 1.37 | 56,56,56,56 | 0 |
| 87 | MG | A6 | 2175 | 1/1 | 0.84 | 0.28 | 62,62,62,62 | 0 |
| 87 | MG | A5 | 4449 | 1/1 | 0.84 | 1.43 | 122,122,122,122 | 0 |
| 87 | MG | A6 | 2178 | 1/1 | 0.84 | 0.25 | 71,71,71,71 | 0 |
| 87 | MG | BN | 306 | 1/1 | 0.84 | 0.55 | 55,55,55,55 | 0 |
| 87 | MG | A5 | 4453 | 1/1 | 0.84 | 0.57 | 66,66,66,66 | 0 |
| 87 | MG | A5 | 4463 | 1/1 | 0.84 | 0.10 | 89,89,89,89 | 0 |
| 87 | MG | A1 | 4375 | 1/1 | 0.84 | 0.32 | 51,51,51,51 | 0 |
| 87 | MG | A1 | 4021 | 1/1 | 0.84 | 0.32 | 54,54,54,54 | 0 |
| 87 | MG | A5 | 4473 | 1/1 | 0.84 | 0.83 | 94,94,94,94 | 0 |
| 87 | MG | A2 | 2144 | 1/1 | 0.84 | 0.27 | 57,57,57,57 | 0 |
| 86 | OHX | A5 | 3782 | 7/7 | 0.84 | 0.29 | 169,169,169,169 | 7 |
| 87 | MG | A5 | 4293 | 1/1 | 0.84 | 0.33 | 76,76,76,76 | 0 |
| 87 | MG | A1 | 4214 | 1/1 | 0.84 | 0.58 | 55,55,55,55 | 0 |
| 87 | MG | A1 | 4391 | 1/1 | 0.84 | 0.85 | 89,89,89,89 | 0 |
| 86 | OHX | DR | 201 | 7/7 | 0.84 | 0.21 | 171,171,171,171 | 7 |
| 86 | OHX | A1 | 3799 | 7/7 | 0.84 | 0.16 | 165,165,165,165 | 7 |
| 86 | OHX | A1 | 3804 | 7/7 | 0.84 | 0.34 | 152,152,152,152 | 7 |
| 87 | MG | A5 | 3911 | 1/1 | 0.84 | 0.15 | 82,82,82,82 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86 | OHX | A5 | 3790 | 7/7 | 0.84 | 0.20 | 157,157,157,157 | 7 |
| 87 | MG | A1 | 4401 | 1/1 | 0.84 | 0.26 | 69,69,69,69 | 0 |
| 87 | MG | A6 | 2204 | 1/1 | 0.84 | 0.17 | 70,70,70,70 | 0 |
| 86 | OHX | A5 | 3658 | 7/7 | 0.84 | 0.32 | 141,141,141,141 | 7 |
| 86 | OHX | A6 | 2054 | 7/7 | 0.84 | 0.28 | 169,169,169,169 | 7 |
| 87 | MG | A1 | 4142 | 1/1 | 0.84 | 0.35 | 68,68,68,68 | 0 |
| 86 | OHX | A2 | 2085 | 7/7 | 0.84 | 0.44 | 200,200,200,200 | 7 |
| 87 | MG | A5 | 4152 | 1/1 | 0.84 | 0.18 | 79,79,79,79 | 0 |
| 86 | OHX | A2 | 2070 | 7/7 | 0.84 | 0.18 | 202,202,202,202 | 7 |
| 87 | MG | A5 | 4332 | 1/1 | 0.84 | 0.10 | 73,73,73,73 | 0 |
| 87 | MG | A1 | 4415 | 1/1 | 0.84 | 0.70 | 85,85,85,85 | 0 |
| 87 | MG | A1 | 4309 | 1/1 | 0.84 | 0.51 | 99,99,99,99 | 0 |
| 87 | MG | A1 | 3830 | 1/1 | 0.84 | 0.28 | 60,60,60,60 | 0 |
| 87 | MG | A1 | 4424 | 1/1 | 0.85 | 0.31 | 50,50,50,50 | 0 |
| 87 | MG | A5 | 4291 | 1/1 | 0.85 | 0.73 | 78,78,78,78 | 0 |
| 87 | MG | A1 | 3869 | 1/1 | 0.85 | 0.26 | 69,69,69,69 | 0 |
| 87 | MG | BL | 202 | 1/1 | 0.85 | 0.35 | 78,78,78,78 | 0 |
| 87 | MG | A5 | 3858 | 1/1 | 0.85 | 0.31 | 43,43,43,43 | 0 |
| 86 | OHX | A6 | 2069 | 7/7 | 0.85 | 0.17 | 206,206,206,206 | 7 |
| 87 | MG | A1 | 3871 | 1/1 | 0.85 | 0.30 | 48,48,48,48 | 0 |
| 87 | MG | A5 | 4426 | 1/1 | 0.85 | 0.27 | 70,70,70,70 | 0 |
| 87 | MG | A5 | 4311 | 1/1 | 0.85 | 0.24 | 78,78,78,78 | 0 |
| 87 | MG | A1 | 4283 | 1/1 | 0.85 | 0.91 | 91,91,91,91 | 0 |
| 87 | MG | A6 | 2235 | 1/1 | 0.85 | 0.25 | 77,77,77,77 | 0 |
| 87 | MG | A6 | 2236 | 1/1 | 0.85 | 0.20 | 76,76,76,76 | 0 |
| 87 | MG | A1 | 4347 | 1/1 | 0.85 | 0.35 | 86,86,86,86 | 0 |
| 87 | MG | A5 | 4042 | 1/1 | 0.85 | 0.24 | 75,75,75,75 | 0 |
| 87 | MG | A2 | 2199 | 1/1 | 0.85 | 0.16 | 72,72,72,72 | 0 |
| 86 | OHX | BI | 302 | 7/7 | 0.85 | 0.29 | 177,177,177,177 | 7 |
| 87 | MG | A5 | 4049 | 1/1 | 0.85 | 0.29 | 70,70,70,70 | 0 |
| 87 | MG | A1 | 4170 | 1/1 | 0.85 | 0.13 | 50,50,50,50 | 0 |
| 86 | OHX | A1 | 3812 | 7/7 | 0.85 | 0.54 | 187,187,187,187 | 7 |
| 87 | MG | A6 | 2141 | 1/1 | 0.85 | 0.41 | 78,78,78,78 | 0 |
| 87 | MG | A1 | 4445 | 1/1 | 0.85 | 0.46 | 69,69,69,69 | 0 |
| 87 | MG | A1 | 3818 | 1/1 | 0.85 | 0.19 | 63,63,63,63 | 0 |
| 86 | OHX | A5 | 3781 | 7/7 | 0.85 | 0.14 | 199,199,199,199 | 7 |
| 87 | MG | A1 | 3821 | 1/1 | 0.85 | 0.47 | 71,71,71,71 | 0 |
| 87 | MG | A5 | 3891 | 1/1 | 0.85 | 0.24 | 50,50,50,50 | 0 |
| 86 | OHX | A5 | 3750 | 7/7 | 0.85 | 0.22 | 199,199,199,199 | 7 |
| 86 | OHX | A5 | 3762 | 7/7 | 0.85 | 0.41 | 153,153,153,153 | 7 |
| 86 | OHX | A1 | 3736 | 7/7 | 0.85 | 0.23 | 174,174,174,174 | 7 |
| 87 | MG | A1 | 3976 | 1/1 | 0.85 | 0.48 | 66,66,66,66 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86 | OHX | A6 | 2077 | 7/7 | 0.85 | 0.17 | 197,197,197,197 | 7 |
| 87 | MG | AB | 302 | 1/1 | 0.85 | 0.13 | 63,63,63,63 | 0 |
| 87 | MG | A1 | 3902 | 1/1 | 0.85 | 0.26 | 47,47,47,47 | 0 |
| 87 | MG | A8 | 234 | 1/1 | 0.85 | 0.46 | 64,64,64,64 | 0 |
| 87 | MG | A1 | 4253 | 1/1 | 0.85 | 0.26 | 110,110,110,110 | 0 |
| 87 | MG | A5 | 4216 | 1/1 | 0.85 | 0.32 | 80,80,80,80 | 0 |
| 87 | MG | A1 | 4382 | 1/1 | 0.85 | 0.25 | 81,81,81,81 | 0 |
| 87 | MG | A6 | 2180 | 1/1 | 0.85 | 0.49 | 87,87,87,87 | 0 |
| 87 | MG | DA | 305 | 1/1 | 0.85 | 1.20 | 69,69,69,69 | 0 |
| 87 | MG | A1 | 3984 | 1/1 | 0.85 | 0.35 | 51,51,51,51 | 0 |
| 87 | MG | A5 | 3917 | 1/1 | 0.85 | 0.36 | 44,44,44,44 | 0 |
| 87 | MG | A5 | 3918 | 1/1 | 0.85 | 0.27 | 79,79,79,79 | 0 |
| 87 | MG | A5 | 4223 | 1/1 | 0.85 | 0.30 | 78,78,78,78 | 0 |
| 87 | MG | A1 | 3841 | 1/1 | 0.85 | 0.20 | 47,47,47,47 | 0 |
| 87 | MG | A1 | 3846 | 1/1 | 0.85 | 0.21 | 37,37,37,37 | 0 |
| 87 | MG | A5 | 4226 | 1/1 | 0.85 | 0.35 | 76,76,76,76 | 0 |
| 87 | MG | A1 | 4195 | 1/1 | 0.85 | 0.13 | 83,83,83,83 | 0 |
| 87 | MG | A5 | 4104 | 1/1 | 0.85 | 0.24 | 52,52,52,52 | 0 |
| 86 | OHX | CG | 302 | 7/7 | 0.85 | 0.29 | 197,197,197,197 | 7 |
| 86 | OHX | A6 | 2082 | 7/7 | 0.85 | 0.25 | 180,180,180,180 | 7 |
| 87 | MG | A4 | 236 | 1/1 | 0.85 | 0.16 | 100,100,100,100 | 0 |
| 86 | OHX | A1 | 3737 | 7/7 | 0.85 | 0.16 | 183,183,183,183 | 7 |
| 86 | OHX | A1 | 3723 | 7/7 | 0.85 | 0.24 | 161,161,161,161 | 7 |
| 87 | MG | A5 | 3934 | 1/1 | 0.85 | 0.23 | 61,61,61,61 | 0 |
| 86 | OHX | Dg | 201 | 7/7 | 0.85 | 0.37 | 153,153,153,153 | 7 |
| 87 | MG | A5 | 3943 | 1/1 | 0.85 | 0.39 | 38,38,38,38 | 0 |
| 87 | MG | A1 | 3915 | 1/1 | 0.85 | 0.23 | 32,32,32,32 | 0 |
| 87 | MG | A5 | 4132 | 1/1 | 0.85 | 0.26 | 66,66,66,66 | 0 |
| 87 | MG | A1 | 3917 | 1/1 | 0.85 | 0.19 | 31,31,31,31 | 0 |
| 87 | MG | A5 | 4520 | 1/1 | 0.85 | 0.25 | 81,81,81,81 | 0 |
| 87 | MG | DP | 207 | 1/1 | 0.85 | 1.09 | 64,64,64,64 | 0 |
| 86 | OHX | A5 | 3775 | 7/7 | 0.85 | 0.30 | 152,152,152,152 | 7 |
| 87 | MG | A5 | 4527 | 1/1 | 0.85 | 0.22 | 78,78,78,78 | 0 |
| 87 | MG | A1 | 4151 | 1/1 | 0.85 | 0.34 | 71,71,71,71 | 0 |
| 87 | MG | A5 | 4257 | 1/1 | 0.85 | 0.29 | 70,70,70,70 | 0 |
| 87 | MG | A6 | 2290 | 1/1 | 0.85 | 0.18 | 82,82,82,82 | 0 |
| 87 | MG | A5 | 4389 | 1/1 | 0.85 | 0.82 | 66,66,66,66 | 0 |
| 87 | MG | BB | 404 | 1/1 | 0.85 | 0.28 | 57,57,57,57 | 0 |
| 86 | OHX | A1 | 3729 | 7/7 | 0.85 | 0.37 | 167,167,167,167 | 7 |
| 87 | MG | A2 | 2161 | 1/1 | 0.85 | 0.23 | 58,58,58,58 | 0 |
| 87 | MG | A1 | 4336 | 1/1 | 0.85 | 0.20 | 80,80,80,80 | 0 |
| 87 | MG | Df | 205 | 1/1 | 0.85 | 0.43 | 76,76,76,76 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87 | MG | A5 | 3847 | 1/1 | 0.85 | 0.32 | 61,61,61,61 | 0 |
| 87 | MG | A5 | 4270 | 1/1 | 0.85 | 0.26 | 57,57,57,57 | 0 |
| 86 | OHX | A5 | 3813 | 7/7 | 0.85 | 0.22 | 191,191,191,191 | 7 |
| 87 | MG | A5 | 3849 | 1/1 | 0.85 | 0.31 | 41,41,41,41 | 0 |
| 87 | MG | A1 | 4034 | 1/1 | 0.85 | 0.18 | 46,46,46,46 | 0 |
| 87 | MG | A1 | 4340 | 1/1 | 0.85 | 0.67 | 96,96,96,96 | 0 |
| 87 | MG | A6 | 2220 | 1/1 | 0.85 | 0.13 | 91,91,91,91 | 0 |
| 87 | MG | A6 | 2228 | 1/1 | 0.86 | 0.21 | 89,89,89,89 | 0 |
| 87 | MG | BC | 403 | 1/1 | 0.86 | 0.48 | 72,72,72,72 | 0 |
| 87 | MG | A1 | 4405 | 1/1 | 0.86 | 0.40 | 61,61,61,61 | 0 |
| 87 | MG | A5 | 4542 | 1/1 | 0.86 | 1.22 | 59,59,59,59 | 0 |
| 87 | MG | A5 | 4085 | 1/1 | 0.86 | 0.28 | 79,79,79,79 | 0 |
| 86 | OHX | A1 | 3783 | 7/7 | 0.86 | 0.21 | 152,152,152,152 | 7 |
| 86 | OHX | A1 | 3768 | 7/7 | 0.86 | 0.37 | 137,137,137,137 | 7 |
| 87 | MG | BF | 4102 | 1/1 | 0.86 | 0.38 | 76,76,76,76 | 0 |
| 87 | MG | A5 | 4233 | 1/1 | 0.86 | 0.19 | 91,91,91,91 | 0 |
| 87 | MG | A1 | 4485 | 1/1 | 0.86 | 0.14 | 93,93,93,93 | 0 |
| 87 | MG | A5 | 4090 | 1/1 | 0.86 | 0.34 | 45,45,45,45 | 0 |
| 87 | MG | A1 | 4486 | 1/1 | 0.86 | 0.38 | 55,55,55,55 | 0 |
| 87 | MG | A1 | 4410 | 1/1 | 0.86 | 0.45 | 69,69,69,69 | 0 |
| 87 | MG | A1 | 4338 | 1/1 | 0.86 | 0.58 | 84,84,84,84 | 0 |
| 87 | MG | A5 | 4097 | 1/1 | 0.86 | 0.24 | 37,37,37,37 | 0 |
| 86 | OHX | CN | 201 | 7/7 | 0.86 | 0.22 | 174,174,174,174 | 7 |
| 87 | MG | A5 | 4563 | 1/1 | 0.86 | 0.35 | 89,89,89,89 | 0 |
| 86 | OHX | A1 | 3690 | 7/7 | 0.86 | 0.24 | 178,178,178,178 | 7 |
| 87 | MG | A1 | 4093 | 1/1 | 0.86 | 0.22 | 55,55,55,55 | 0 |
| 87 | MG | A1 | 3825 | 1/1 | 0.86 | 0.16 | 47,47,47,47 | 0 |
| 87 | MG | A5 | 4570 | 1/1 | 0.86 | 0.64 | 76,76,76,76 | 0 |
| 87 | MG | A5 | 4255 | 1/1 | 0.86 | 0.25 | 72,72,72,72 | 0 |
| 86 | OHX | A1 | 3809 | 7/7 | 0.86 | 0.15 | 192,192,192,192 | 7 |
| 87 | MG | A6 | 2145 | 1/1 | 0.86 | 0.28 | 46,46,46,46 | 0 |
| 87 | MG | A5 | 4114 | 1/1 | 0.86 | 0.19 | 38,38,38,38 | 0 |
| 87 | MG | A5 | 4260 | 1/1 | 0.86 | 0.64 | 80,80,80,80 | 0 |
| 87 | MG | A5 | 4261 | 1/1 | 0.86 | 0.24 | 71,71,71,71 | 0 |
| 87 | MG | A1 | 4499 | 1/1 | 0.86 | 0.22 | 65,65,65,65 | 0 |
| 87 | MG | A5 | 4118 | 1/1 | 0.86 | 0.26 | 57,57,57,57 | 0 |
| 86 | OHX | A1 | 3604 | 7/7 | 0.86 | 0.21 | 254,254,254,254 | 7 |
| 87 | MG | A7 | 218 | 1/1 | 0.86 | 0.42 | 43,43,43,43 | 0 |
| 86 | OHX | A6 | 2094 | 7/7 | 0.86 | 0.19 | 180,180,180,180 | 7 |
| 87 | MG | BO | 206 | 1/1 | 0.86 | 0.70 | 69,69,69,69 | 0 |
| 87 | MG | A1 | 4351 | 1/1 | 0.86 | 0.11 | 97,97,97,97 | 0 |
| 87 | MG | A1 | 4296 | 1/1 | 0.86 | 0.36 | 94,94,94,94 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87 | MG | CX | 202 | 1/1 | 0.86 | 0.57 | 81,81,81,81 | 0 |
| 87 | MG | A5 | 4276 | 1/1 | 0.86 | 0.23 | 60,60,60,60 | 0 |
| 87 | MG | A1 | 4297 | 1/1 | 0.86 | 0.56 | 94,94,94,94 | 0 |
| 87 | MG | A1 | 4197 | 1/1 | 0.86 | 0.16 | 74,74,74,74 | 0 |
| 87 | MG | A5 | 3945 | 1/1 | 0.86 | 0.26 | 56,56,56,56 | 0 |
| 87 | MG | A1 | 4250 | 1/1 | 0.86 | 0.30 | 56,56,56,56 | 0 |
| 87 | MG | A6 | 2171 | 1/1 | 0.86 | 0.21 | 77,77,77,77 | 0 |
| 87 | MG | A1 | 4300 | 1/1 | 0.86 | 0.27 | 76,76,76,76 | 0 |
| 87 | MG | A8 | 223 | 1/1 | 0.86 | 0.34 | 50,50,50,50 | 0 |
| 86 | OHX | A2 | 2050 | 7/7 | 0.86 | 0.19 | 181,181,181,181 | 7 |
| 87 | MG | A3 | 223 | 1/1 | 0.86 | 0.19 | 75,75,75,75 | 0 |
| 87 | MG | A5 | 3966 | 1/1 | 0.86 | 0.38 | 56,56,56,56 | 0 |
| 87 | MG | A5 | 3971 | 1/1 | 0.86 | 0.36 | 53,53,53,53 | 0 |
| 86 | OHX | A5 | 3794 | 7/7 | 0.86 | 0.20 | 179,179,179,179 | 7 |
| 87 | MG | A5 | 4458 | 1/1 | 0.86 | 0.64 | 76,76,76,76 | 0 |
| 87 | MG | A5 | 4459 | 1/1 | 0.86 | 1.14 | 84,84,84,84 | 0 |
| 87 | MG | A5 | 4154 | 1/1 | 0.86 | 0.22 | 54,54,54,54 | 0 |
| 87 | MG | A5 | 3827 | 1/1 | 0.86 | 0.39 | 67,67,67,67 | 0 |
| 87 | MG | A1 | 3889 | 1/1 | 0.86 | 0.43 | 74,74,74,74 | 0 |
| 87 | MG | A1 | 4306 | 1/1 | 0.86 | 0.13 | 68,68,68,68 | 0 |
| 86 | OHX | A1 | 3681 | 7/7 | 0.86 | 0.18 | 146,146,146,146 | 7 |
| 87 | MG | A5 | 3994 | 1/1 | 0.86 | 0.34 | 39,39,39,39 | 0 |
| 87 | MG | A2 | 2198 | 1/1 | 0.86 | 0.27 | 80,80,80,80 | 0 |
| 87 | MG | A5 | 3998 | 1/1 | 0.86 | 0.37 | 41,41,41,41 | 0 |
| 87 | MG | A1 | 4158 | 1/1 | 0.86 | 0.28 | 87,87,87,87 | 0 |
| 87 | MG | A1 | 4373 | 1/1 | 0.86 | 0.51 | 56,56,56,56 | 0 |
| 86 | OHX | A5 | 3735 | 7/7 | 0.86 | 0.26 | 149,149,149,149 | 7 |
| 87 | MG | A5 | 4011 | 1/1 | 0.86 | 0.29 | 54,54,54,54 | 0 |
| 87 | MG | A6 | 2192 | 1/1 | 0.86 | 0.34 | 81,81,81,81 | 0 |
| 87 | MG | A2 | 2110 | 1/1 | 0.86 | 0.32 | 57,57,57,57 | 0 |
| 86 | OHX | A6 | 2098 | 7/7 | 0.86 | 0.30 | 144,144,144,144 | 7 |
| 87 | MG | A2 | 2251 | 1/1 | 0.86 | 0.28 | 77,77,77,77 | 0 |
| 87 | MG | A1 | 4383 | 1/1 | 0.86 | 0.11 | 62,62,62,62 | 0 |
| 87 | MG | A6 | 2294 | 1/1 | 0.86 | 0.16 | 54,54,54,54 | 0 |
| 87 | MG | A1 | 4384 | 1/1 | 0.86 | 0.32 | 61,61,61,61 | 0 |
| 87 | MG | A6 | 2201 | 1/1 | 0.86 | 0.21 | 72,72,72,72 | 0 |
| 87 | MG | A5 | 3857 | 1/1 | 0.86 | 0.30 | 53,53,53,53 | 0 |
| 87 | MG | A6 | 2202 | 1/1 | 0.86 | 0.27 | 71,71,71,71 | 0 |
| 86 | OHX | A5 | 3802 | 7/7 | 0.86 | 0.36 | 151,151,151,151 | 7 |
| 87 | MG | A2 | 2114 | 1/1 | 0.86 | 0.41 | 84,84,84,84 | 0 |
| 87 | MG | A1 | 4174 | 1/1 | 0.86 | 0.16 | 57,57,57,57 | 0 |
| 87 | MG | A1 | 4223 | 1/1 | 0.86 | 0.31 | 79,79,79,79 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87 | MG | A5 | 4050 | 1/1 | 0.86 | 0.20 | 39,39,39,39 | 0 |
| 87 | MG | A1 | 4392 | 1/1 | 0.86 | 1.45 | 86,86,86,86 | 0 |
| 87 | MG | A6 | 2314 | 1/1 | 0.86 | 1.38 | 112,112,112,112 | 0 |
| 87 | MG | A1 | 4078 | 1/1 | 0.86 | 0.20 | 80,80,80,80 | 0 |
| 87 | MG | Da | 204 | 1/1 | 0.86 | 0.58 | 52,52,52,52 | 0 |
| 87 | MG | A1 | 4079 | 1/1 | 0.86 | 0.26 | 75,75,75,75 | 0 |
| 87 | MG | A5 | 4060 | 1/1 | 0.86 | 0.32 | 57,57,57,57 | 0 |
| 87 | MG | A6 | 2213 | 1/1 | 0.86 | 0.11 | 65,65,65,65 | 0 |
| 86 | OHX | A5 | 3808 | 7/7 | 0.86 | 0.37 | 182,182,182,182 | 7 |
| 87 | MG | A1 | 4033 | 1/1 | 0.86 | 0.26 | 48,48,48,48 | 0 |
| 87 | MG | A5 | 4073 | 1/1 | 0.86 | 0.36 | 66,66,66,66 | 0 |
| 87 | MG | Dg | 203 | 1/1 | 0.86 | 1.38 | 88,88,88,88 | 0 |
| 87 | MG | A5 | 4524 | 1/1 | 0.86 | 0.17 | 85,85,85,85 | 0 |
| 87 | MG | A5 | 4526 | 1/1 | 0.86 | 0.40 | 83,83,83,83 | 0 |
| 87 | MG | A1 | 4229 | 1/1 | 0.86 | 0.17 | 89,89,89,89 | 0 |
| 87 | MG | A1 | 4402 | 1/1 | 0.86 | 0.18 | 65,65,65,65 | 0 |
| 87 | MG | A6 | 2111 | 1/1 | 0.86 | 0.12 | 51,51,51,51 | 0 |
| 87 | MG | A1 | 3965 | 1/1 | 0.86 | 0.41 | 80,80,80,80 | 0 |
| 87 | MG | A1 | 3968 | 1/1 | 0.86 | 0.20 | 68,68,68,68 | 0 |
| 87 | MG | A1 | 4332 | 1/1 | 0.87 | 0.33 | 74,74,74,74 | 0 |
| 87 | MG | A1 | 3950 | 1/1 | 0.87 | 0.21 | 48,48,48,48 | 0 |
| 87 | MG | A1 | 4497 | 1/1 | 0.87 | 0.18 | 79,79,79,79 | 0 |
| 87 | MG | A1 | 3952 | 1/1 | 0.87 | 0.32 | 89,89,89,89 | 0 |
| 87 | MG | A1 | 4267 | 1/1 | 0.87 | 0.25 | 82,82,82,82 | 0 |
| 87 | MG | A5 | 4536 | 1/1 | 0.87 | 0.31 | 73,73,73,73 | 0 |
| 86 | OHX | A5 | 3647 | 7/7 | 0.87 | 0.11 | 204,204,204,204 | 7 |
| 87 | MG | BQ | 201 | 1/1 | 0.87 | 0.58 | 65,65,65,65 | 0 |
| 87 | MG | A1 | 4199 | 1/1 | 0.87 | 0.32 | 74,74,74,74 | 0 |
| 87 | MG | A1 | 4270 | 1/1 | 0.87 | 0.43 | 57,57,57,57 | 0 |
| 86 | OHX | A1 | 3512 | 7/7 | 0.87 | 0.49 | 197,197,197,197 | 7 |
| 87 | MG | A6 | 2186 | 1/1 | 0.87 | 0.72 | 104,104,104,104 | 0 |
| 87 | MG | A1 | 3887 | 1/1 | 0.87 | 0.21 | 54,54,54,54 | 0 |
| 86 | OHX | A1 | 3773 | 7/7 | 0.87 | 0.30 | 159,159,159,159 | 7 |
| 87 | MG | A6 | 2190 | 1/1 | 0.87 | 0.10 | 74,74,74,74 | 0 |
| 86 | OHX | A6 | 2013 | 7/7 | 0.87 | 0.24 | 180,180,180,180 | 7 |
| 87 | MG | A6 | 2305 | 1/1 | 0.87 | 0.23 | 76,76,76,76 | 0 |
| 87 | MG | A6 | 2193 | 1/1 | 0.87 | 0.16 | 75,75,75,75 | 0 |
| 86 | OHX | A6 | 2023 | 7/7 | 0.87 | 0.23 | 177,177,177,177 | 7 |
| 87 | MG | A5 | 3883 | 1/1 | 0.87 | 0.23 | 36,36,36,36 | 0 |
| 86 | OHX | A5 | 3698 | 7/7 | 0.87 | 0.20 | 173,173,173,173 | 7 |
| 87 | MG | A2 | 2129 | 1/1 | 0.87 | 0.30 | 59,59,59,59 | 0 |
| 87 | MG | A3 | 227 | 1/1 | 0.87 | 0.64 | 59,59,59,59 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87 | MG | A1 | 4433 | 1/1 | 0.87 | 0.76 | 67,67,67,67 | 0 |
| 87 | MG | A5 | 4567 | 1/1 | 0.87 | 0.27 | 59,59,59,59 | 0 |
| 86 | OHX | A5 | 3711 | 7/7 | 0.87 | 0.19 | 164,164,164,164 | 7 |
| 87 | MG | Bd | 201 | 1/1 | 0.87 | 0.48 | 106,106,106,106 | 0 |
| 87 | MG | A1 | 4437 | 1/1 | 0.87 | 0.18 | 60,60,60,60 | 0 |
| 87 | MG | Bg | 201 | 1/1 | 0.87 | 0.17 | 63,63,63,63 | 0 |
| 87 | MG | A5 | 4243 | 1/1 | 0.87 | 0.23 | 45,45,45,45 | 0 |
| 87 | MG | A6 | 2206 | 1/1 | 0.87 | 0.20 | 63,63,63,63 | 0 |
| 87 | MG | A1 | 4438 | 1/1 | 0.87 | 0.47 | 82,82,82,82 | 0 |
| 87 | MG | A5 | 4577 | 1/1 | 0.87 | 0.52 | 76,76,76,76 | 0 |
| 87 | MG | A5 | 3899 | 1/1 | 0.87 | 0.23 | 73,73,73,73 | 0 |
| 86 | OHX | A1 | 3808 | 7/7 | 0.87 | 0.21 | 194,194,194,194 | 7 |
| 87 | MG | A1 | 4353 | 1/1 | 0.87 | 0.21 | 77,77,77,77 | 0 |
| 86 | OHX | A1 | 3564 | 7/7 | 0.87 | 0.23 | 136,136,136,136 | 7 |
| 87 | MG | A1 | 4220 | 1/1 | 0.87 | 0.20 | 103,103,103,103 | 0 |
| 87 | MG | A5 | 3912 | 1/1 | 0.87 | 0.43 | 77,77,77,77 | 0 |
| 87 | MG | A5 | 4415 | 1/1 | 0.87 | 0.28 | 75,75,75,75 | 0 |
| 87 | MG | A1 | 3837 | 1/1 | 0.87 | 0.27 | 68,68,68,68 | 0 |
| 87 | MG | A2 | 2173 | 1/1 | 0.87 | 0.16 | 82,82,82,82 | 0 |
| 87 | MG | A5 | 4422 | 1/1 | 0.87 | 0.51 | 52,52,52,52 | 0 |
| 87 | MG | A5 | 4101 | 1/1 | 0.87 | 0.18 | 64,64,64,64 | 0 |
| 87 | MG | A1 | 3840 | 1/1 | 0.87 | 0.36 | 59,59,59,59 | 0 |
| 86 | OHX | DD | 301 | 7/7 | 0.87 | 0.28 | 134,134,134,134 | 7 |
| 87 | MG | A2 | 2178 | 1/1 | 0.87 | 0.24 | 73,73,73,73 | 0 |
| 86 | OHX | A5 | 3789 | 7/7 | 0.87 | 0.28 | 165,165,165,165 | 7 |
| 87 | MG | A1 | 4365 | 1/1 | 0.87 | 0.20 | 66,66,66,66 | 0 |
| 87 | MG | A6 | 2225 | 1/1 | 0.87 | 0.23 | 59,59,59,59 | 0 |
| 87 | MG | A7 | 239 | 1/1 | 0.87 | 0.27 | 71,71,71,71 | 0 |
| 86 | OHX | A1 | 3700 | 7/7 | 0.87 | 0.35 | 185,185,185,185 | 7 |
| 87 | MG | A8 | 221 | 1/1 | 0.87 | 0.16 | 33,33,33,33 | 0 |
| 86 | OHX | A2 | 2061 | 7/7 | 0.87 | 0.31 | 142,142,142,142 | 7 |
| 87 | MG | A1 | 3916 | 1/1 | 0.87 | 0.33 | 73,73,73,73 | 0 |
| 87 | MG | A1 | 4460 | 1/1 | 0.87 | 0.20 | 67,67,67,67 | 0 |
| 87 | MG | A5 | 4129 | 1/1 | 0.87 | 0.62 | 94,94,94,94 | 0 |
| 87 | MG | A1 | 4372 | 1/1 | 0.87 | 0.23 | 71,71,71,71 | 0 |
| 87 | MG | A1 | 4163 | 1/1 | 0.87 | 0.35 | 81,81,81,81 | 0 |
| 87 | MG | A5 | 3938 | 1/1 | 0.87 | 0.30 | 45,45,45,45 | 0 |
| 87 | MG | A1 | 4097 | 1/1 | 0.87 | 0.35 | 73,73,73,73 | 0 |
| 87 | MG | A6 | 2122 | 1/1 | 0.87 | 0.28 | 55,55,55,55 | 0 |
| 87 | MG | A1 | 4165 | 1/1 | 0.87 | 0.35 | 57,57,57,57 | 0 |
| 87 | MG | A5 | 4455 | 1/1 | 0.87 | 0.67 | 60,60,60,60 | 0 |
| 86 | OHX | A5 | 3752 | 7/7 | 0.87 | 0.28 | 127,127,127,127 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | A1 | 4169 | 1/1 | 0.87 | 0.33 | 80,80,80,80 | 0 |
| 87 | MG | BB | 403 | 1/1 | 0.87 | 0.21 | 53,53,53,53 | 0 |
| 87 | MG | A1 | 4304 | 1/1 | 0.87 | 0.58 | 102,102,102,102 | 0 |
| 87 | MG | A5 | 4300 | 1/1 | 0.87 | 0.60 | 51,51,51,51 | 0 |
| 87 | MG | A5 | 4472 | 1/1 | 0.87 | 0.41 | 75,75,75,75 | 0 |
| 87 | MG | A5 | 4307 | 1/1 | 0.87 | 0.09 | 78,78,78,78 | 0 |
| 87 | MG | A5 | 4308 | 1/1 | 0.87 | 0.71 | 52,52,52,52 | 0 |
| 87 | MG | A2 | 2142 | 1/1 | 0.87 | 0.38 | 65,65,65,65 | 0 |
| 87 | MG | A5 | 3964 | 1/1 | 0.87 | 0.37 | 57,57,57,57 | 0 |
| 87 | MG | DD | 307 | 1/1 | 0.87 | 0.69 | 77,77,77,77 | 0 |
| 87 | MG | A1 | 3853 | 1/1 | 0.87 | 0.11 | 43,43,43,43 | 0 |
| 86 | OHX | A2 | 2062 | 7/7 | 0.87 | 0.20 | 196,196,196,196 | 7 |
| 87 | MG | A6 | 2252 | 1/1 | 0.87 | 0.36 | 117,117,117,117 | 0 |
| 87 | MG | A5 | 3974 | 1/1 | 0.87 | 0.42 | 40,40,40,40 | 0 |
| 87 | MG | A6 | 2136 | 1/1 | 0.87 | 0.27 | 48,48,48,48 | 0 |
| 87 | MG | A1 | 3855 | 1/1 | 0.87 | 0.19 | 40,40,40,40 | 0 |
| 86 | OHX | A1 | 3616 | 7/7 | 0.87 | 0.25 | 117,117,117,117 | 7 |
| 87 | MG | A5 | 4489 | 1/1 | 0.87 | 0.25 | 82,82,82,82 | 0 |
| 87 | MG | A5 | 4161 | 1/1 | 0.87 | 0.21 | 51,51,51,51 | 0 |
| 87 | MG | A2 | 2190 | 1/1 | 0.87 | 0.14 | 82,82,82,82 | 0 |
| 86 | OHX | A1 | 3758 | 7/7 | 0.87 | 0.22 | 139,139,139,139 | 7 |
| 87 | MG | A5 | 4326 | 1/1 | 0.87 | 0.25 | 75,75,75,75 | 0 |
| 87 | MG | A5 | 4327 | 1/1 | 0.87 | 0.20 | 94,94,94,94 | 0 |
| 86 | OHX | A2 | 2076 | 7/7 | 0.87 | 0.14 | 185,185,185,185 | 7 |
| 87 | MG | A5 | 4168 | 1/1 | 0.87 | 0.26 | 74,74,74,74 | 0 |
| 87 | MG | A1 | 3934 | 1/1 | 0.87 | 0.27 | 46,46,46,46 | 0 |
| 87 | MG | DY | 202 | 1/1 | 0.87 | 0.24 | 55,55,55,55 | 0 |
| 87 | MG | A5 | 3829 | 1/1 | 0.87 | 0.18 | 35,35,35,35 | 0 |
| 86 | OHX | A1 | 3666 | 7/7 | 0.87 | 0.23 | 142,142,142,142 | 7 |
| 87 | MG | A5 | 3834 | 1/1 | 0.87 | 0.43 | 59,59,59,59 | 0 |
| 87 | MG | A5 | 3835 | 1/1 | 0.87 | 0.31 | 49,49,49,49 | 0 |
| 86 | OHX | A2 | 2019 | 7/7 | 0.87 | 0.17 | 174,174,174,174 | 7 |
| 87 | MG | A5 | 4014 | 1/1 | 0.87 | 0.33 | 54,54,54,54 | 0 |
| 87 | MG | A1 | 4050 | 1/1 | 0.87 | 0.28 | 63,63,63,63 | 0 |
| 87 | MG | A5 | 4187 | 1/1 | 0.87 | 0.38 | 78,78,78,78 | 0 |
| 86 | OHX | A5 | 3771 | 7/7 | 0.87 | 0.29 | 176,176,176,176 | 7 |
| 87 | MG | A1 | 4488 | 1/1 | 0.87 | 0.29 | 73,73,73,73 | 0 |
| 87 | MG | A6 | 2164 | 1/1 | 0.87 | 0.32 | 57,57,57,57 | 0 |
| 87 | MG | A5 | 4027 | 1/1 | 0.87 | 0.41 | 53,53,53,53 | 0 |
| 87 | MG | A1 | 4127 | 1/1 | 0.87 | 0.19 | 65,65,65,65 | 0 |
| 87 | MG | A5 | 4033 | 1/1 | 0.87 | 0.12 | 31,31,31,31 | 0 |
| 86 | OHX | A1 | 3770 | 7/7 | 0.87 | 0.21 | 179,179,179,179 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86 | OHX | A5 | 3774 | 7/7 | 0.87 | 0.28 | 148,148,148,148 | 7 |
| 86 | OHX | DP | 201 | 7/7 | 0.88 | 0.34 | 155,155,155,155 | 7 |
| 87 | MG | A5 | 3947 | 1/1 | 0.88 | 0.18 | 40,40,40,40 | 0 |
| 87 | MG | A1 | 3831 | 1/1 | 0.88 | 0.36 | 56,56,56,56 | 0 |
| 87 | MG | A1 | 4179 | 1/1 | 0.88 | 0.31 | 69,69,69,69 | 0 |
| 87 | MG | BR | 202 | 1/1 | 0.88 | 0.23 | 58,58,58,58 | 0 |
| 87 | MG | A1 | 4180 | 1/1 | 0.88 | 0.81 | 79,79,79,79 | 0 |
| 87 | MG | A5 | 3961 | 1/1 | 0.88 | 0.25 | 55,55,55,55 | 0 |
| 87 | MG | A1 | 4181 | 1/1 | 0.88 | 0.35 | 61,61,61,61 | 0 |
| 87 | MG | BR | 205 | 1/1 | 0.88 | 0.75 | 99,99,99,99 | 0 |
| 87 | MG | A1 | 3929 | 1/1 | 0.88 | 0.33 | 75,75,75,75 | 0 |
| 87 | MG | A5 | 3968 | 1/1 | 0.88 | 0.19 | 50,50,50,50 | 0 |
| 87 | MG | A5 | 4171 | 1/1 | 0.88 | 0.24 | 108,108,108,108 | 0 |
| 86 | OHX | A6 | 2037 | 7/7 | 0.88 | 0.25 | 138,138,138,138 | 7 |
| 87 | MG | A1 | 4491 | 1/1 | 0.88 | 0.85 | 80,80,80,80 | 0 |
| 87 | MG | A5 | 3982 | 1/1 | 0.88 | 0.23 | 52,52,52,52 | 0 |
| 86 | OHX | A6 | 2043 | 7/7 | 0.88 | 0.20 | 156,156,156,156 | 7 |
| 87 | MG | A5 | 4534 | 1/1 | 0.88 | 1.30 | 72,72,72,72 | 0 |
| 87 | MG | A5 | 4180 | 1/1 | 0.88 | 0.26 | 81,81,81,81 | 0 |
| 87 | MG | A5 | 4537 | 1/1 | 0.88 | 0.12 | 83,83,83,83 | 0 |
| 87 | MG | A6 | 2214 | 1/1 | 0.88 | 0.25 | 53,53,53,53 | 0 |
| 87 | MG | A1 | 3838 | 1/1 | 0.88 | 0.25 | 67,67,67,67 | 0 |
| 86 | OHX | A6 | 2047 | 7/7 | 0.88 | 0.23 | 156,156,156,156 | 7 |
| 87 | MG | A1 | 4496 | 1/1 | 0.88 | 0.96 | 82,82,82,82 | 0 |
| 87 | MG | A1 | 3942 | 1/1 | 0.88 | 0.33 | 38,38,38,38 | 0 |
| 87 | MG | A5 | 4356 | 1/1 | 0.88 | 0.46 | 74,74,74,74 | 0 |
| 87 | MG | A6 | 2221 | 1/1 | 0.88 | 0.50 | 69,69,69,69 | 0 |
| 86 | OHX | A1 | 3708 | 7/7 | 0.88 | 0.18 | 158,158,158,158 | 7 |
| 87 | MG | A5 | 4547 | 1/1 | 0.88 | 0.83 | 88,88,88,88 | 0 |
| 86 | OHX | CI | 301 | 7/7 | 0.88 | 0.17 | 172,172,172,172 | 7 |
| 87 | MG | CY | 204 | 1/1 | 0.88 | 0.14 | 56,56,56,56 | 0 |
| 87 | MG | A1 | 4092 | 1/1 | 0.88 | 0.31 | 66,66,66,66 | 0 |
| 87 | MG | A5 | 4369 | 1/1 | 0.88 | 0.81 | 69,69,69,69 | 0 |
| 87 | MG | A1 | 3844 | 1/1 | 0.88 | 0.21 | 48,48,48,48 | 0 |
| 87 | MG | A1 | 4292 | 1/1 | 0.88 | 0.23 | 67,67,67,67 | 0 |
| 86 | OHX | A1 | 3655 | 7/7 | 0.88 | 0.23 | 150,150,150,150 | 7 |
| 86 | OHX | A5 | 3779 | 7/7 | 0.88 | 0.40 | 167,167,167,167 | 7 |
| 87 | MG | A2 | 2175 | 1/1 | 0.88 | 0.36 | 68,68,68,68 | 0 |
| 87 | MG | A3 | 214 | 1/1 | 0.88 | 0.31 | 70,70,70,70 | 0 |
| 87 | MG | A5 | 4026 | 1/1 | 0.88 | 0.40 | 53,53,53,53 | 0 |
| 87 | MG | A1 | 3960 | 1/1 | 0.88 | 0.19 | 54,54,54,54 | 0 |
| 86 | OHX | A1 | 3712 | 7/7 | 0.88 | 0.46 | 180,180,180,180 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86 | OHX | A5 | 3405 | 7/7 | 0.88 | 0.31 | 118,118,118,118 | 7 |
| 87 | MG | A5 | 3833 | 1/1 | 0.88 | 0.33 | 54,54,54,54 | 0 |
| 86 | OHX | A5 | 3532 | 7/7 | 0.88 | 0.17 | 164,164,164,164 | 7 |
| 87 | MG | A3 | 224 | 1/1 | 0.88 | 0.21 | 62,62,62,62 | 0 |
| 87 | MG | A3 | 226 | 1/1 | 0.88 | 0.21 | 69,69,69,69 | 0 |
| 86 | OHX | A2 | 2025 | 7/7 | 0.88 | 0.14 | 219,219,219,219 | 7 |
| 86 | OHX | A6 | 2057 | 7/7 | 0.88 | 0.43 | 134,134,134,134 | 7 |
| 87 | MG | A6 | 2247 | 1/1 | 0.88 | 0.52 | 88,88,88,88 | 0 |
| 86 | OHX | A6 | 2058 | 7/7 | 0.88 | 0.24 | 196,196,196,196 | 7 |
| 87 | MG | A6 | 2109 | 1/1 | 0.88 | 0.33 | 54,54,54,54 | 0 |
| 87 | MG | A1 | 4113 | 1/1 | 0.88 | 0.33 | 70,70,70,70 | 0 |
| 86 | OHX | A5 | 3685 | 7/7 | 0.88 | 0.26 | 141,141,141,141 | 7 |
| 87 | MG | A6 | 2117 | 1/1 | 0.88 | 0.26 | 64,64,64,64 | 0 |
| 87 | MG | A5 | 4227 | 1/1 | 0.88 | 0.20 | 46,46,46,46 | 0 |
| 86 | OHX | A5 | 3791 | 7/7 | 0.88 | 0.23 | 175,175,175,175 | 7 |
| 87 | MG | A5 | 4058 | 1/1 | 0.88 | 0.21 | 59,59,59,59 | 0 |
| 86 | OHX | A1 | 3750 | 7/7 | 0.88 | 0.35 | 118,118,118,118 | 7 |
| 87 | MG | A1 | 3986 | 1/1 | 0.88 | 0.37 | 41,41,41,41 | 0 |
| 86 | OHX | A5 | 3793 | 7/7 | 0.88 | 0.22 | 158,158,158,158 | 7 |
| 87 | MG | A5 | 4413 | 1/1 | 0.88 | 0.14 | 80,80,80,80 | 0 |
| 86 | OHX | A2 | 2036 | 7/7 | 0.88 | 0.24 | 162,162,162,162 | 7 |
| 87 | MG | A2 | 2124 | 1/1 | 0.88 | 0.24 | 79,79,79,79 | 0 |
| 87 | MG | A7 | 234 | 1/1 | 0.88 | 0.31 | 90,90,90,90 | 0 |
| 86 | OHX | A5 | 3796 | 7/7 | 0.88 | 0.26 | 176,176,176,176 | 7 |
| 86 | OHX | A1 | 3755 | 7/7 | 0.88 | 0.33 | 135,135,135,135 | 7 |
| 86 | OHX | A1 | 3756 | 7/7 | 0.88 | 0.24 | 158,158,158,158 | 7 |
| 87 | MG | A1 | 3877 | 1/1 | 0.88 | 0.29 | 34,34,34,34 | 0 |
| 87 | MG | A1 | 3879 | 1/1 | 0.88 | 0.44 | 89,89,89,89 | 0 |
| 86 | OHX | A5 | 3719 | 7/7 | 0.88 | 0.24 | 180,180,180,180 | 7 |
| 87 | MG | A1 | 4231 | 1/1 | 0.88 | 0.83 | 82,82,82,82 | 0 |
| 86 | OHX | A5 | 3725 | 7/7 | 0.88 | 0.18 | 171,171,171,171 | 7 |
| 87 | MG | A8 | 232 | 1/1 | 0.88 | 0.16 | 43,43,43,43 | 0 |
| 87 | MG | A1 | 4442 | 1/1 | 0.88 | 0.48 | 91,91,91,91 | 0 |
| 87 | MG | A5 | 4430 | 1/1 | 0.88 | 0.31 | 95,95,95,95 | 0 |
| 87 | MG | A4 | 238 | 1/1 | 0.88 | 0.33 | 68,68,68,68 | 0 |
| 87 | MG | A2 | 2136 | 1/1 | 0.88 | 0.15 | 70,70,70,70 | 0 |
| 87 | MG | A4 | 241 | 1/1 | 0.88 | 0.73 | 60,60,60,60 | 0 |
| 86 | OHX | A5 | 3733 | 7/7 | 0.88 | 0.21 | 162,162,162,162 | 7 |
| 87 | MG | AE | 301 | 1/1 | 0.88 | 0.76 | 88,88,88,88 | 0 |
| 87 | MG | A6 | 2148 | 1/1 | 0.88 | 0.33 | 39,39,39,39 | 0 |
| 87 | MG | A5 | 4443 | 1/1 | 0.88 | 0.24 | 64,64,64,64 | 0 |
| 87 | MG | A2 | 2202 | 1/1 | 0.88 | 0.11 | 66,66,66,66 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | A5 | 4446 | 1/1 | 0.88 | 0.20 | 64,64,64,64 | 0 |
| 87 | MG | A5 | 4093 | 1/1 | 0.88 | 0.30 | 64,64,64,64 | 0 |
| 87 | MG | A1 | 4146 | 1/1 | 0.88 | 0.32 | 91,91,91,91 | 0 |
| 87 | MG | A1 | 3892 | 1/1 | 0.88 | 0.28 | 75,75,75,75 | 0 |
| 87 | MG | A6 | 2291 | 1/1 | 0.88 | 0.56 | 100,100,100,100 | 0 |
| 86 | OHX | A2 | 2017 | 7/7 | 0.88 | 0.12 | 186,186,186,186 | 7 |
| 87 | MG | A1 | 4245 | 1/1 | 0.88 | 0.21 | 73,73,73,73 | 0 |
| 87 | MG | A5 | 4457 | 1/1 | 0.88 | 0.25 | 78,78,78,78 | 0 |
| 86 | OHX | A4 | 211 | 7/7 | 0.88 | 0.33 | 108,108,108,108 | 7 |
| 86 | OHX | A1 | 3789 | 7/7 | 0.88 | 0.32 | 189,189,189,189 | 7 |
| 86 | OHX | A1 | 3790 | 7/7 | 0.88 | 0.18 | 164,164,164,164 | 7 |
| 87 | MG | A1 | 3901 | 1/1 | 0.88 | 0.32 | 74,74,74,74 | 0 |
| 87 | MG | A5 | 4468 | 1/1 | 0.88 | 0.79 | 73,73,73,73 | 0 |
| 87 | MG | A1 | 4251 | 1/1 | 0.88 | 0.23 | 71,71,71,71 | 0 |
| 87 | MG | AS | 201 | 1/1 | 0.88 | 0.11 | 105,105,105,105 | 0 |
| 87 | MG | A5 | 4288 | 1/1 | 0.88 | 0.78 | 49,49,49,49 | 0 |
| 86 | OHX | A1 | 3791 | 7/7 | 0.88 | 0.18 | 149,149,149,149 | 7 |
| 86 | OHX | A5 | 3753 | 7/7 | 0.88 | 0.12 | 207,207,207,207 | 7 |
| 86 | OHX | A5 | 3758 | 7/7 | 0.88 | 0.20 | 167,167,167,167 | 7 |
| 86 | OHX | A2 | 2039 | 7/7 | 0.88 | 0.36 | 157,157,157,157 | 7 |
| 87 | MG | A5 | 4296 | 1/1 | 0.88 | 0.41 | 54,54,54,54 | 0 |
| 87 | MG | DR | 202 | 1/1 | 0.88 | 0.99 | 67,67,67,67 | 0 |
| 87 | MG | A5 | 4125 | 1/1 | 0.88 | 0.14 | 67,67,67,67 | 0 |
| 87 | MG | DV | 202 | 1/1 | 0.88 | 0.40 | 35,35,35,35 | 0 |
| 86 | OHX | A2 | 2057 | 7/7 | 0.88 | 0.17 | 173,173,173,173 | 7 |
| 87 | MG | DW | 201 | 1/1 | 0.88 | 1.32 | 85,85,85,85 | 0 |
| 87 | MG | A5 | 4304 | 1/1 | 0.88 | 0.28 | 66,66,66,66 | 0 |
| 87 | MG | A5 | 4306 | 1/1 | 0.88 | 0.38 | 72,72,72,72 | 0 |
| 86 | OHX | A1 | 3794 | 7/7 | 0.88 | 0.29 | 150,150,150,150 | 7 |
| 87 | MG | BN | 303 | 1/1 | 0.88 | 0.94 | 72,72,72,72 | 0 |
| 87 | MG | A5 | 3921 | 1/1 | 0.88 | 0.25 | 82,82,82,82 | 0 |
| 87 | MG | A1 | 3406 | 1/1 | 0.88 | 0.18 | 67,67,67,67 | 0 |
| 87 | MG | A2 | 2216 | 1/1 | 0.88 | 0.12 | 63,63,63,63 | 0 |
| 87 | MG | A1 | 4361 | 1/1 | 0.88 | 1.09 | 126,126,126,126 | 0 |
| 86 | OHX | A8 | 213 | 7/7 | 0.88 | 0.21 | 146,146,146,146 | 7 |
| 86 | OHX | A5 | 3767 | 7/7 | 0.88 | 0.16 | 185,185,185,185 | 7 |
| 86 | OHX | A1 | 3766 | 7/7 | 0.88 | 0.42 | 135,135,135,135 | 7 |
| 86 | OHX | A2 | 2046 | 7/7 | 0.88 | 0.42 | 139,139,139,139 | 7 |
| 87 | MG | A1 | 3824 | 1/1 | 0.88 | 0.30 | 65,65,65,65 | 0 |
| 87 | MG | BP | 206 | 1/1 | 0.88 | 0.19 | 86,86,86,86 | 0 |
| 86 | OHX | A6 | 2025 | 7/7 | 0.88 | 0.14 | 161,161,161,161 | 7 |
| 87 | MG | A5 | 4505 | 1/1 | 0.88 | 1.86 | 71,71,71,71 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | A6 | 2198 | 1/1 | 0.88 | 0.17 | 49,49,49,49 | 0 |
| 86 | OHX | A6 | 2026 | 7/7 | 0.88 | 0.16 | 176,176,176,176 | 7 |
| 87 | MG | A1 | 4421 | 1/1 | 0.89 | 0.41 | 63,63,63,63 | 0 |
| 86 | OHX | BA | 301 | 7/7 | 0.89 | 0.47 | 217,217,217,217 | 7 |
| 87 | MG | A1 | 4315 | 1/1 | 0.89 | 0.78 | 62,62,62,62 | 0 |
| 87 | MG | A5 | 3991 | 1/1 | 0.89 | 0.28 | 46,46,46,46 | 0 |
| 87 | MG | A5 | 4178 | 1/1 | 0.89 | 0.26 | 83,83,83,83 | 0 |
| 87 | MG | A2 | 2088 | 1/1 | 0.89 | 0.33 | 59,59,59,59 | 0 |
| 87 | MG | A6 | 2239 | 1/1 | 0.89 | 0.23 | 82,82,82,82 | 0 |
| 87 | MG | A4 | 219 | 1/1 | 0.89 | 0.26 | 59,59,59,59 | 0 |
| 87 | MG | A2 | 2223 | 1/1 | 0.89 | 1.95 | 156,156,156,156 | 0 |
| 87 | MG | A4 | 221 | 1/1 | 0.89 | 0.28 | 43,43,43,43 | 0 |
| 86 | OHX | A1 | 3741 | 7/7 | 0.89 | 0.26 | 151,151,151,151 | 7 |
| 86 | OHX | A6 | 2067 | 7/7 | 0.89 | 0.24 | 136,136,136,136 | 7 |
| 87 | MG | A1 | 4322 | 1/1 | 0.89 | 0.26 | 74,74,74,74 | 0 |
| 86 | OHX | A5 | 3669 | 7/7 | 0.89 | 0.28 | 109,109,109,109 | 7 |
| 87 | MG | A5 | 4357 | 1/1 | 0.89 | 0.64 | 75,75,75,75 | 0 |
| 86 | OHX | A5 | 3671 | 7/7 | 0.89 | 0.21 | 171,171,171,171 | 7 |
| 87 | MG | A5 | 4193 | 1/1 | 0.89 | 0.28 | 43,43,43,43 | 0 |
| 86 | OHX | A5 | 3784 | 7/7 | 0.89 | 0.21 | 173,173,173,173 | 7 |
| 86 | OHX | A1 | 3744 | 7/7 | 0.89 | 0.49 | 205,205,205,205 | 7 |
| 87 | MG | A1 | 4043 | 1/1 | 0.89 | 0.37 | 62,62,62,62 | 0 |
| 87 | MG | A5 | 4366 | 1/1 | 0.89 | 0.43 | 65,65,65,65 | 0 |
| 86 | OHX | A2 | 2063 | 7/7 | 0.89 | 0.13 | 183,183,183,183 | 7 |
| 86 | OHX | A5 | 3787 | 7/7 | 0.89 | 0.22 | 195,195,195,195 | 7 |
| 87 | MG | A1 | 4240 | 1/1 | 0.89 | 0.23 | 59,59,59,59 | 0 |
| 87 | MG | A1 | 4049 | 1/1 | 0.89 | 0.17 | 59,59,59,59 | 0 |
| 87 | MG | A5 | 4553 | 1/1 | 0.89 | 1.10 | 73,73,73,73 | 0 |
| 87 | MG | A1 | 3833 | 1/1 | 0.89 | 0.34 | 49,49,49,49 | 0 |
| 86 | OHX | A1 | 3748 | 7/7 | 0.89 | 0.20 | 163,163,163,163 | 7 |
| 86 | OHX | A1 | 3797 | 7/7 | 0.89 | 0.17 | 171,171,171,171 | 7 |
| 87 | MG | A4 | 243 | 1/1 | 0.89 | 0.20 | 48,48,48,48 | 0 |
| 87 | MG | A6 | 2266 | 1/1 | 0.89 | 0.61 | 106,106,106,106 | 0 |
| 86 | OHX | A5 | 3707 | 7/7 | 0.89 | 0.47 | 135,135,135,135 | 7 |
| 86 | OHX | A1 | 3687 | 7/7 | 0.89 | 0.35 | 182,182,182,182 | 7 |
| 87 | MG | A5 | 4215 | 1/1 | 0.89 | 0.26 | 52,52,52,52 | 0 |
| 86 | OHX | A6 | 2075 | 7/7 | 0.89 | 0.13 | 194,194,194,194 | 7 |
| 87 | MG | A2 | 2183 | 1/1 | 0.89 | 0.22 | 49,49,49,49 | 0 |
| 87 | MG | A5 | 4046 | 1/1 | 0.89 | 0.16 | 39,39,39,39 | 0 |
| 87 | MG | A1 | 3842 | 1/1 | 0.89 | 0.40 | 77,77,77,77 | 0 |
| 86 | OHX | Bj | 103 | 7/7 | 0.89 | 0.44 | 138,138,138,138 | 7 |
| 87 | MG | A1 | 4070 | 1/1 | 0.89 | 0.30 | 76,76,76,76 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | A5 | 4391 | 1/1 | 0.89 | 0.60 | 57,57,57,57 | 0 |
| 87 | MG | A1 | 4254 | 1/1 | 0.89 | 0.26 | 72,72,72,72 | 0 |
| 86 | OHX | A5 | 3727 | 7/7 | 0.89 | 0.19 | 167,167,167,167 | 7 |
| 87 | MG | A5 | 3861 | 1/1 | 0.89 | 0.21 | 65,65,65,65 | 0 |
| 87 | MG | A1 | 4348 | 1/1 | 0.89 | 0.16 | 73,73,73,73 | 0 |
| 86 | OHX | A6 | 2078 | 7/7 | 0.89 | 0.15 | 185,185,185,185 | 7 |
| 87 | MG | A5 | 4065 | 1/1 | 0.89 | 0.25 | 68,68,68,68 | 0 |
| 87 | MG | A2 | 2246 | 1/1 | 0.89 | 0.12 | 100,100,100,100 | 0 |
| 87 | MG | A6 | 2165 | 1/1 | 0.89 | 0.38 | 51,51,51,51 | 0 |
| 86 | OHX | A6 | 1991 | 7/7 | 0.89 | 0.23 | 149,149,149,149 | 7 |
| 87 | MG | A5 | 4407 | 1/1 | 0.89 | 0.12 | 95,95,95,95 | 0 |
| 87 | MG | A2 | 2126 | 1/1 | 0.89 | 0.32 | 54,54,54,54 | 0 |
| 87 | MG | A5 | 3878 | 1/1 | 0.89 | 0.25 | 56,56,56,56 | 0 |
| 87 | MG | A5 | 4411 | 1/1 | 0.89 | 0.29 | 94,94,94,94 | 0 |
| 87 | MG | A1 | 4171 | 1/1 | 0.89 | 0.18 | 79,79,79,79 | 0 |
| 86 | OHX | A1 | 3803 | 7/7 | 0.89 | 0.17 | 196,196,196,196 | 7 |
| 86 | OHX | A5 | 3741 | 7/7 | 0.89 | 0.14 | 185,185,185,185 | 7 |
| 87 | MG | A2 | 2252 | 1/1 | 0.89 | 0.21 | 89,89,89,89 | 0 |
| 86 | OHX | A6 | 2085 | 7/7 | 0.89 | 0.51 | 188,188,188,188 | 7 |
| 86 | OHX | A2 | 2086 | 7/7 | 0.89 | 0.61 | 156,156,156,156 | 7 |
| 87 | MG | A6 | 2297 | 1/1 | 0.89 | 0.86 | 68,68,68,68 | 0 |
| 87 | MG | A7 | 236 | 1/1 | 0.89 | 0.39 | 102,102,102,102 | 0 |
| 87 | MG | A1 | 3859 | 1/1 | 0.89 | 0.40 | 78,78,78,78 | 0 |
| 87 | MG | A1 | 3861 | 1/1 | 0.89 | 0.25 | 34,34,34,34 | 0 |
| 87 | MG | A1 | 3956 | 1/1 | 0.89 | 0.32 | 45,45,45,45 | 0 |
| 87 | MG | A2 | 2134 | 1/1 | 0.89 | 0.17 | 74,74,74,74 | 0 |
| 87 | MG | A6 | 2307 | 1/1 | 0.89 | 0.54 | 94,94,94,94 | 0 |
| 87 | MG | A1 | 3864 | 1/1 | 0.89 | 0.20 | 46,46,46,46 | 0 |
| 87 | MG | BO | 208 | 1/1 | 0.89 | 0.23 | 75,75,75,75 | 0 |
| 87 | MG | A5 | 4092 | 1/1 | 0.89 | 0.31 | 82,82,82,82 | 0 |
| 86 | OHX | A1 | 3607 | 7/7 | 0.89 | 0.15 | 204,204,204,204 | 7 |
| 87 | MG | A5 | 3905 | 1/1 | 0.89 | 0.27 | 75,75,75,75 | 0 |
| 86 | OHX | A1 | 3782 | 7/7 | 0.89 | 0.25 | 186,186,186,186 | 7 |
| 87 | MG | A1 | 3970 | 1/1 | 0.89 | 0.33 | 69,69,69,69 | 0 |
| 87 | MG | A5 | 4098 | 1/1 | 0.89 | 0.14 | 55,55,55,55 | 0 |
| 87 | MG | A5 | 4444 | 1/1 | 0.89 | 0.42 | 66,66,66,66 | 0 |
| 87 | MG | A1 | 3972 | 1/1 | 0.89 | 0.42 | 45,45,45,45 | 0 |
| 87 | MG | A1 | 4280 | 1/1 | 0.89 | 0.11 | 51,51,51,51 | 0 |
| 86 | OHX | A2 | 2064 | 7/7 | 0.89 | 0.31 | 169,169,169,169 | 7 |
| 86 | OHX | A5 | 3760 | 7/7 | 0.89 | 0.11 | 202,202,202,202 | 7 |
| 86 | OHX | A6 | 2091 | 7/7 | 0.89 | 0.28 | 165,165,165,165 | 7 |
| 86 | OHX | A6 | 2039 | 7/7 | 0.89 | 0.17 | 168,168,168,168 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | A5 | 4278 | 1/1 | 0.89 | 0.88 | 82,82,82,82 | 0 |
| 87 | MG | A2 | 2204 | 1/1 | 0.89 | 1.48 | 109,109,109,109 | 0 |
| 86 | OHX | A1 | 3784 | 7/7 | 0.89 | 0.23 | 169,169,169,169 | 7 |
| 87 | MG | A1 | 4389 | 1/1 | 0.89 | 0.61 | 46,46,46,46 | 0 |
| 87 | MG | A5 | 4116 | 1/1 | 0.89 | 0.36 | 56,56,56,56 | 0 |
| 87 | MG | A5 | 4290 | 1/1 | 0.89 | 0.48 | 47,47,47,47 | 0 |
| 86 | OHX | A6 | 2045 | 7/7 | 0.89 | 0.30 | 124,124,124,124 | 7 |
| 87 | MG | A5 | 4467 | 1/1 | 0.89 | 0.14 | 70,70,70,70 | 0 |
| 87 | MG | BT | 202 | 1/1 | 0.89 | 0.65 | 89,89,89,89 | 0 |
| 86 | OHX | A6 | 2046 | 7/7 | 0.89 | 0.19 | 204,204,204,204 | 7 |
| 87 | MG | A1 | 3883 | 1/1 | 0.89 | 0.36 | 37,37,37,37 | 0 |
| 87 | MG | A5 | 4295 | 1/1 | 0.89 | 0.19 | 61,61,61,61 | 0 |
| 87 | MG | A1 | 4114 | 1/1 | 0.89 | 0.42 | 71,71,71,71 | 0 |
| 87 | MG | A5 | 3928 | 1/1 | 0.89 | 0.32 | 90,90,90,90 | 0 |
| 87 | MG | DO | 206 | 1/1 | 0.89 | 0.73 | 55,55,55,55 | 0 |
| 87 | MG | A1 | 4202 | 1/1 | 0.89 | 0.21 | 67,67,67,67 | 0 |
| 87 | MG | A5 | 4302 | 1/1 | 0.89 | 0.19 | 72,72,72,72 | 0 |
| 87 | MG | DP | 203 | 1/1 | 0.89 | 0.38 | 37,37,37,37 | 0 |
| 87 | MG | A1 | 4205 | 1/1 | 0.89 | 0.13 | 63,63,63,63 | 0 |
| 86 | OHX | A1 | 3704 | 7/7 | 0.89 | 0.15 | 176,176,176,176 | 7 |
| 87 | MG | A5 | 3937 | 1/1 | 0.89 | 0.34 | 69,69,69,69 | 0 |
| 86 | OHX | CB | 301 | 7/7 | 0.89 | 0.18 | 162,162,162,162 | 7 |
| 87 | MG | DS | 203 | 1/1 | 0.89 | 0.33 | 65,65,65,65 | 0 |
| 87 | MG | DS | 204 | 1/1 | 0.89 | 0.72 | 63,63,63,63 | 0 |
| 87 | MG | A1 | 4117 | 1/1 | 0.89 | 0.27 | 80,80,80,80 | 0 |
| 87 | MG | A5 | 3942 | 1/1 | 0.89 | 0.33 | 38,38,38,38 | 0 |
| 87 | MG | A1 | 3993 | 1/1 | 0.89 | 0.29 | 52,52,52,52 | 0 |
| 87 | MG | A3 | 219 | 1/1 | 0.89 | 0.35 | 40,40,40,40 | 0 |
| 87 | MG | A5 | 4142 | 1/1 | 0.89 | 0.23 | 91,91,91,91 | 0 |
| 86 | OHX | A1 | 3813 | 7/7 | 0.89 | 0.17 | 201,201,201,201 | 7 |
| 86 | OHX | A2 | 2029 | 7/7 | 0.89 | 0.34 | 150,150,150,150 | 7 |
| 87 | MG | Bj | 105 | 1/1 | 0.89 | 0.87 | 64,64,64,64 | 0 |
| 87 | MG | CI | 302 | 1/1 | 0.89 | 0.27 | 63,63,63,63 | 0 |
| 86 | OHX | A1 | 3762 | 7/7 | 0.89 | 0.32 | 144,144,144,144 | 7 |
| 86 | OHX | A3 | 210 | 7/7 | 0.89 | 0.19 | 175,175,175,175 | 7 |
| 87 | MG | CL | 203 | 1/1 | 0.89 | 0.22 | 61,61,61,61 | 0 |
| 87 | MG | A1 | 4305 | 1/1 | 0.89 | 0.30 | 65,65,65,65 | 0 |
| 87 | MG | A1 | 4128 | 1/1 | 0.89 | 0.28 | 63,63,63,63 | 0 |
| 87 | MG | CQ | 201 | 1/1 | 0.89 | 0.14 | 75,75,75,75 | 0 |
| 87 | MG | A1 | 4414 | 1/1 | 0.89 | 0.23 | 90,90,90,90 | 0 |
| 86 | OHX | A2 | 2041 | 7/7 | 0.89 | 0.15 | 184,184,184,184 | 7 |
| 86 | OHX | DQ | 201 | 7/7 | 0.89 | 0.26 | 147,147,147,147 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87 | MG | A5 | 4165 | 1/1 | 0.89 | 0.13 | 73,73,73,73 | 0 |
| 87 | MG | A5 | 3976 | 1/1 | 0.89 | 0.23 | 43,43,43,43 | 0 |
| 87 | MG | A5 | 3977 | 1/1 | 0.89 | 0.36 | 69,69,69,69 | 0 |
| 86 | OHX | A2 | 2004 | 7/7 | 0.89 | 0.19 | 164,164,164,164 | 7 |
| 87 | MG | A5 | 3873 | 1/1 | 0.90 | 0.34 | 60,60,60,60 | 0 |
| 87 | MG | A2 | 2248 | 1/1 | 0.90 | 0.26 | 69,69,69,69 | 0 |
| 87 | MG | A5 | 4055 | 1/1 | 0.90 | 0.22 | 81,81,81,81 | 0 |
| 86 | OHX | A1 | 3722 | 7/7 | 0.90 | 0.22 | 150,150,150,150 | 7 |
| 87 | MG | A5 | 4367 | 1/1 | 0.90 | 0.59 | 74,74,74,74 | 0 |
| 87 | MG | BL | 204 | 1/1 | 0.90 | 0.84 | 72,72,72,72 | 0 |
| 86 | OHX | A5 | 3721 | 7/7 | 0.90 | 0.20 | 167,167,167,167 | 7 |
| 87 | MG | A5 | 3882 | 1/1 | 0.90 | 0.06 | 74,74,74,74 | 0 |
| 87 | MG | A5 | 4063 | 1/1 | 0.90 | 0.23 | 52,52,52,52 | 0 |
| 86 | OHX | A6 | 2042 | 7/7 | 0.90 | 0.20 | 169,169,169,169 | 7 |
| 87 | MG | A1 | 3860 | 1/1 | 0.90 | 0.24 | 59,59,59,59 | 0 |
| 87 | MG | A1 | 4090 | 1/1 | 0.90 | 0.30 | 78,78,78,78 | 0 |
| 87 | MG | A5 | 4069 | 1/1 | 0.90 | 0.20 | 88,88,88,88 | 0 |
| 87 | MG | A5 | 4221 | 1/1 | 0.90 | 0.61 | 88,88,88,88 | 0 |
| 86 | OHX | A1 | 3749 | 7/7 | 0.90 | 0.14 | 177,177,177,177 | 7 |
| 86 | OHX | A5 | 3728 | 7/7 | 0.90 | 0.40 | 131,131,131,131 | 7 |
| 86 | OHX | A1 | 3670 | 7/7 | 0.90 | 0.19 | 152,152,152,152 | 7 |
| 86 | OHX | A2 | 1988 | 7/7 | 0.90 | 0.18 | 189,189,189,189 | 7 |
| 86 | OHX | A1 | 3787 | 7/7 | 0.90 | 0.20 | 173,173,173,173 | 7 |
| 86 | OHX | A3 | 212 | 7/7 | 0.90 | 0.35 | 159,159,159,159 | 7 |
| 87 | MG | BP | 205 | 1/1 | 0.90 | 0.24 | 53,53,53,53 | 0 |
| 86 | OHX | A5 | 3744 | 7/7 | 0.90 | 0.26 | 140,140,140,140 | 7 |
| 86 | OHX | A5 | 3801 | 7/7 | 0.90 | 0.28 | 156,156,156,156 | 7 |
| 87 | MG | A1 | 3980 | 1/1 | 0.90 | 0.31 | 38,38,38,38 | 0 |
| 87 | MG | BP | 209 | 1/1 | 0.90 | 0.26 | 59,59,59,59 | 0 |
| 86 | OHX | A1 | 3727 | 7/7 | 0.90 | 0.29 | 146,146,146,146 | 7 |
| 86 | OHX | A2 | 2021 | 7/7 | 0.90 | 0.27 | 158,158,158,158 | 7 |
| 87 | MG | A1 | 4295 | 1/1 | 0.90 | 0.19 | 62,62,62,62 | 0 |
| 86 | OHX | A5 | 3751 | 7/7 | 0.90 | 0.22 | 148,148,148,148 | 7 |
| 87 | MG | A1 | 3878 | 1/1 | 0.90 | 0.28 | 45,45,45,45 | 0 |
| 86 | OHX | A6 | 2053 | 7/7 | 0.90 | 0.20 | 123,123,123,123 | 7 |
| 86 | OHX | A4 | 215 | 7/7 | 0.90 | 0.20 | 175,175,175,175 | 7 |
| 87 | MG | A5 | 4404 | 1/1 | 0.90 | 0.83 | 54,54,54,54 | 0 |
| 87 | MG | BS | 201 | 1/1 | 0.90 | 0.46 | 64,64,64,64 | 0 |
| 87 | MG | A1 | 4210 | 1/1 | 0.90 | 0.62 | 44,44,44,44 | 0 |
| 87 | MG | A1 | 4506 | 1/1 | 0.90 | 0.22 | 77,77,77,77 | 0 |
| 86 | OHX | A1 | 3689 | 7/7 | 0.90 | 0.28 | 99,99,99,99 | 7 |
| 87 | MG | AL | 202 | 1/1 | 0.90 | 0.97 | 78,78,78,78 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86 | OHX | A1 | 3730 | 7/7 | 0.90 | 0.19 | 135,135,135,135 | 7 |
| 87 | MG | A1 | 4406 | 1/1 | 0.90 | 0.60 | 69,69,69,69 | 0 |
| 87 | MG | Ba | 202 | 1/1 | 0.90 | 0.54 | 63,63,63,63 | 0 |
| 87 | MG | A5 | 4259 | 1/1 | 0.90 | 0.27 | 56,56,56,56 | 0 |
| 87 | MG | A2 | 2138 | 1/1 | 0.90 | 0.13 | 56,56,56,56 | 0 |
| 87 | MG | A1 | 4216 | 1/1 | 0.90 | 0.21 | 93,93,93,93 | 0 |
| 86 | OHX | A2 | 2053 | 7/7 | 0.90 | 0.23 | 173,173,173,173 | 7 |
| 87 | MG | A1 | 4123 | 1/1 | 0.90 | 0.31 | 77,77,77,77 | 0 |
| 87 | MG | A5 | 4113 | 1/1 | 0.90 | 0.17 | 39,39,39,39 | 0 |
| 87 | MG | CF | 301 | 1/1 | 0.90 | 0.44 | 87,87,87,87 | 0 |
| 87 | MG | A1 | 4008 | 1/1 | 0.90 | 0.34 | 36,36,36,36 | 0 |
| 87 | MG | A7 | 231 | 1/1 | 0.90 | 0.25 | 87,87,87,87 | 0 |
| 86 | OHX | A1 | 3691 | 7/7 | 0.90 | 0.28 | 175,175,175,175 | 7 |
| 86 | OHX | A5 | 3821 | 7/7 | 0.90 | 0.18 | 223,223,223,223 | 7 |
| 86 | OHX | A6 | 2063 | 7/7 | 0.90 | 0.21 | 176,176,176,176 | 7 |
| 87 | MG | Ad | 103 | 1/1 | 0.90 | 0.14 | 67,67,67,67 | 0 |
| 86 | OHX | A5 | 3766 | 7/7 | 0.90 | 0.13 | 173,173,173,173 | 7 |
| 87 | MG | A2 | 2213 | 1/1 | 0.90 | 0.21 | 107,107,107,107 | 0 |
| 87 | MG | A5 | 4127 | 1/1 | 0.90 | 0.30 | 68,68,68,68 | 0 |
| 87 | MG | A1 | 4320 | 1/1 | 0.90 | 0.25 | 59,59,59,59 | 0 |
| 87 | MG | A8 | 224 | 1/1 | 0.90 | 0.20 | 67,67,67,67 | 0 |
| 87 | MG | A8 | 226 | 1/1 | 0.90 | 0.22 | 62,62,62,62 | 0 |
| 87 | MG | A1 | 4026 | 1/1 | 0.90 | 0.38 | 42,42,42,42 | 0 |
| 87 | MG | A5 | 4286 | 1/1 | 0.90 | 0.31 | 58,58,58,58 | 0 |
| 87 | MG | A5 | 3953 | 1/1 | 0.90 | 0.47 | 69,69,69,69 | 0 |
| 87 | MG | A1 | 4136 | 1/1 | 0.90 | 0.24 | 53,53,53,53 | 0 |
| 87 | MG | A5 | 3957 | 1/1 | 0.90 | 0.44 | 43,43,43,43 | 0 |
| 86 | OHX | A7 | 212 | 7/7 | 0.90 | 0.51 | 165,165,165,165 | 7 |
| 86 | OHX | A2 | 2073 | 7/7 | 0.90 | 0.25 | 147,147,147,147 | 7 |
| 86 | OHX | A2 | 1998 | 7/7 | 0.90 | 0.26 | 135,135,135,135 | 7 |
| 86 | OHX | A5 | 3585 | 7/7 | 0.90 | 0.21 | 163,163,163,163 | 7 |
| 86 | OHX | A5 | 3591 | 7/7 | 0.90 | 0.23 | 209,209,209,209 | 7 |
| 86 | OHX | A5 | 3623 | 7/7 | 0.90 | 0.21 | 156,156,156,156 | 7 |
| 87 | MG | A5 | 4143 | 1/1 | 0.90 | 0.16 | 70,70,70,70 | 0 |
| 87 | MG | DB | 407 | 1/1 | 0.90 | 0.79 | 72,72,72,72 | 0 |
| 86 | OHX | DB | 402 | 7/7 | 0.90 | 0.19 | 145,145,145,145 | 7 |
| 87 | MG | A5 | 4147 | 1/1 | 0.90 | 0.14 | 63,63,63,63 | 0 |
| 86 | OHX | A1 | 3639 | 7/7 | 0.90 | 0.19 | 145,145,145,145 | 7 |
| 87 | MG | A2 | 2157 | 1/1 | 0.90 | 0.28 | 82,82,82,82 | 0 |
| 86 | OHX | A5 | 3656 | 7/7 | 0.90 | 0.20 | 169,169,169,169 | 7 |
| 87 | MG | A5 | 4470 | 1/1 | 0.90 | 0.15 | 76,76,76,76 | 0 |
| 86 | OHX | A1 | 3771 | 7/7 | 0.90 | 0.26 | 174,174,174,174 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | A5 | 3411 | 1/1 | 0.90 | 0.22 | 82,82,82,82 | 0 |
| 86 | OHX | A1 | 3739 | 7/7 | 0.90 | 0.20 | 185,185,185,185 | 7 |
| 87 | MG | A2 | 2228 | 1/1 | 0.90 | 0.13 | 85,85,85,85 | 0 |
| 87 | MG | A1 | 3835 | 1/1 | 0.90 | 0.18 | 41,41,41,41 | 0 |
| 87 | MG | A5 | 3990 | 1/1 | 0.90 | 0.44 | 68,68,68,68 | 0 |
| 87 | MG | A5 | 4160 | 1/1 | 0.90 | 0.15 | 53,53,53,53 | 0 |
| 86 | OHX | AP | 201 | 7/7 | 0.90 | 0.16 | 196,196,196,196 | 7 |
| 86 | OHX | A2 | 2066 | 7/7 | 0.90 | 0.32 | 164,164,164,164 | 7 |
| 87 | MG | A5 | 4163 | 1/1 | 0.90 | 0.22 | 58,58,58,58 | 0 |
| 86 | OHX | A5 | 3683 | 7/7 | 0.90 | 0.24 | 119,119,119,119 | 7 |
| 87 | MG | A1 | 3924 | 1/1 | 0.90 | 0.30 | 57,57,57,57 | 0 |
| 87 | MG | DO | 203 | 1/1 | 0.90 | 0.27 | 58,58,58,58 | 0 |
| 87 | MG | A5 | 4487 | 1/1 | 0.90 | 1.23 | 76,76,76,76 | 0 |
| 87 | MG | A1 | 4065 | 1/1 | 0.90 | 0.24 | 47,47,47,47 | 0 |
| 87 | MG | A5 | 3837 | 1/1 | 0.90 | 0.33 | 58,58,58,58 | 0 |
| 87 | MG | A1 | 4067 | 1/1 | 0.90 | 0.15 | 66,66,66,66 | 0 |
| 87 | MG | A4 | 246 | 1/1 | 0.90 | 0.88 | 91,91,91,91 | 0 |
| 87 | MG | A4 | 247 | 1/1 | 0.90 | 0.68 | 56,56,56,56 | 0 |
| 87 | MG | A5 | 4008 | 1/1 | 0.90 | 0.36 | 42,42,42,42 | 0 |
| 86 | OHX | A1 | 3776 | 7/7 | 0.90 | 0.34 | 123,123,123,123 | 7 |
| 87 | MG | DS | 202 | 1/1 | 0.90 | 0.19 | 75,75,75,75 | 0 |
| 86 | OHX | A1 | 3554 | 7/7 | 0.90 | 0.20 | 159,159,159,159 | 7 |
| 87 | MG | BA | 303 | 1/1 | 0.90 | 0.25 | 30,30,30,30 | 0 |
| 87 | MG | BA | 304 | 1/1 | 0.90 | 0.20 | 62,62,62,62 | 0 |
| 87 | MG | A2 | 2093 | 1/1 | 0.90 | 0.25 | 47,47,47,47 | 0 |
| 87 | MG | A1 | 3931 | 1/1 | 0.90 | 0.26 | 40,40,40,40 | 0 |
| 86 | OHX | A6 | 2079 | 7/7 | 0.90 | 0.17 | 161,161,161,161 | 7 |
| 87 | MG | A5 | 4343 | 1/1 | 0.90 | 0.55 | 56,56,56,56 | 0 |
| 87 | MG | A6 | 2143 | 1/1 | 0.90 | 0.35 | 45,45,45,45 | 0 |
| 86 | OHX | A5 | 3783 | 7/7 | 0.90 | 0.25 | 154,154,154,154 | 7 |
| 87 | MG | A5 | 4346 | 1/1 | 0.90 | 0.23 | 89,89,89,89 | 0 |
| 87 | MG | A2 | 2096 | 1/1 | 0.90 | 0.29 | 76,76,76,76 | 0 |
| 87 | MG | A5 | 4512 | 1/1 | 0.90 | 0.29 | 56,56,56,56 | 0 |
| 87 | MG | A1 | 4173 | 1/1 | 0.90 | 0.14 | 45,45,45,45 | 0 |
| 87 | MG | A1 | 4076 | 1/1 | 0.90 | 0.29 | 64,64,64,64 | 0 |
| 87 | MG | A5 | 4350 | 1/1 | 0.90 | 0.95 | 58,58,58,58 | 0 |
| 87 | MG | A6 | 2151 | 1/1 | 0.90 | 0.47 | 64,64,64,64 | 0 |
| 87 | MG | BF | 4101 | 1/1 | 0.90 | 0.24 | 64,64,64,64 | 0 |
| 87 | MG | Dn | 101 | 1/1 | 0.90 | 0.40 | 84,84,84,84 | 0 |
| 86 | OHX | A6 | 2081 | 7/7 | 0.90 | 0.12 | 201,201,201,201 | 7 |
| 86 | OHX | A6 | 2031 | 6/7 | 0.90 | 0.12 | 195,195,195,195 | 6 |
| 86 | OHX | A1 | 3746 | 7/7 | 0.90 | 0.30 | 142,142,142,142 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87 | MG | A6 | 2163 | 1/1 | 0.90 | 0.34 | 58,58,58,58 | 0 |
| 86 | OHX | A5 | 3712 | 7/7 | 0.90 | 0.25 | 149,149,149,149 | 7 |
| 87 | MG | A2 | 2103 | 1/1 | 0.90 | 0.35 | 58,58,58,58 | 0 |
| 87 | MG | A2 | 2105 | 1/1 | 0.90 | 0.28 | 55,55,55,55 | 0 |
| 87 | MG | A5 | 3949 | 1/1 | 0.91 | 0.25 | 37,37,37,37 | 0 |
| 87 | MG | A1 | 4358 | 1/1 | 0.91 | 0.41 | 86,86,86,86 | 0 |
| 86 | OHX | A1 | 3752 | 7/7 | 0.91 | 0.10 | 207,207,207,207 | 7 |
| 87 | MG | A5 | 3954 | 1/1 | 0.91 | 0.37 | 46,46,46,46 | 0 |
| 87 | MG | A1 | 4157 | 1/1 | 0.91 | 0.29 | 87,87,87,87 | 0 |
| 87 | MG | A2 | 2128 | 1/1 | 0.91 | 0.38 | 62,62,62,62 | 0 |
| 86 | OHX | A5 | 3797 | 7/7 | 0.91 | 0.23 | 130,130,130,130 | 7 |
| 87 | MG | A5 | 3959 | 1/1 | 0.91 | 0.40 | 61,61,61,61 | 0 |
| 87 | MG | A5 | 4519 | 1/1 | 0.91 | 0.10 | 63,63,63,63 | 0 |
| 87 | MG | A1 | 3913 | 1/1 | 0.91 | 0.32 | 86,86,86,86 | 0 |
| 87 | MG | A1 | 4056 | 1/1 | 0.91 | 0.23 | 61,61,61,61 | 0 |
| 86 | OHX | A2 | 2048 | 7/7 | 0.91 | 0.15 | 155,155,155,155 | 7 |
| 86 | OHX | A6 | 2093 | 7/7 | 0.91 | 0.20 | 149,149,149,149 | 7 |
| 86 | OHX | A6 | 2048 | 7/7 | 0.91 | 0.24 | 169,169,169,169 | 7 |
| 86 | OHX | A1 | 3688 | 7/7 | 0.91 | 0.13 | 181,181,181,181 | 7 |
| 87 | MG | BP | 212 | 1/1 | 0.91 | 0.28 | 93,93,93,93 | 0 |
| 86 | OHX | A2 | 2044 | 7/7 | 0.91 | 0.16 | 162,162,162,162 | 7 |
| 86 | OHX | A5 | 3805 | 7/7 | 0.91 | 0.15 | 172,172,172,172 | 7 |
| 87 | MG | A1 | 4494 | 1/1 | 0.91 | 0.35 | 87,87,87,87 | 0 |
| 86 | OHX | A5 | 3736 | 7/7 | 0.91 | 0.30 | 143,143,143,143 | 7 |
| 87 | MG | A1 | 3829 | 1/1 | 0.91 | 0.37 | 55,55,55,55 | 0 |
| 86 | OHX | A2 | 2045 | 7/7 | 0.91 | 0.14 | 164,164,164,164 | 7 |
| 87 | MG | A1 | 3923 | 1/1 | 0.91 | 0.24 | 44,44,44,44 | 0 |
| 86 | OHX | A5 | 3742 | 7/7 | 0.91 | 0.31 | 143,143,143,143 | 7 |
| 87 | MG | A1 | 3832 | 1/1 | 0.91 | 0.19 | 65,65,65,65 | 0 |
| 87 | MG | A1 | 3927 | 1/1 | 0.91 | 0.20 | 31,31,31,31 | 0 |
| 86 | OHX | A1 | 3660 | 7/7 | 0.91 | 0.27 | 137,137,137,137 | 7 |
| 86 | OHX | A5 | 3746 | 7/7 | 0.91 | 0.23 | 151,151,151,151 | 7 |
| 87 | MG | A5 | 4183 | 1/1 | 0.91 | 0.15 | 76,76,76,76 | 0 |
| 87 | MG | A5 | 4184 | 1/1 | 0.91 | 0.29 | 55,55,55,55 | 0 |
| 87 | MG | A6 | 2219 | 1/1 | 0.91 | 0.20 | 50,50,50,50 | 0 |
| 87 | MG | BY | 201 | 1/1 | 0.91 | 0.24 | 56,56,56,56 | 0 |
| 87 | MG | A1 | 4505 | 1/1 | 0.91 | 0.89 | 145,145,145,145 | 0 |
| 86 | OHX | A5 | 3747 | 7/7 | 0.91 | 0.20 | 160,160,160,160 | 7 |
| 86 | OHX | A4 | 213 | 7/7 | 0.91 | 0.14 | 164,164,164,164 | 7 |
| 87 | MG | Ba | 204 | 1/1 | 0.91 | 0.69 | 74,74,74,74 | 0 |
| 86 | OHX | A6 | 2056 | 7/7 | 0.91 | 0.12 | 178,178,178,178 | 7 |
| 87 | MG | A5 | 4013 | 1/1 | 0.91 | 0.35 | 44,44,44,44 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86 | OHX | A1 | 3731 | 7/7 | 0.91 | 0.23 | 119,119,119,119 | 7 |
| 87 | MG | A5 | 4197 | 1/1 | 0.91 | 0.39 | 84,84,84,84 | 0 |
| 87 | MG | A5 | 4564 | 1/1 | 0.91 | 0.31 | 79,79,79,79 | 0 |
| 87 | MG | A5 | 4373 | 1/1 | 0.91 | 0.41 | 74,74,74,74 | 0 |
| 87 | MG | A3 | 218 | 1/1 | 0.91 | 0.30 | 46,46,46,46 | 0 |
| 87 | MG | A5 | 3830 | 1/1 | 0.91 | 0.19 | 39,39,39,39 | 0 |
| 86 | OHX | A2 | 1960 | 7/7 | 0.91 | 0.14 | 173,173,173,173 | 7 |
| 86 | OHX | A2 | 2081 | 7/7 | 0.91 | 0.16 | 199,199,199,199 | 7 |
| 86 | OHX | A5 | 3754 | 7/7 | 0.91 | 0.23 | 147,147,147,147 | 7 |
| 87 | MG | A2 | 2153 | 1/1 | 0.91 | 0.21 | 72,72,72,72 | 0 |
| 87 | MG | A1 | 4191 | 1/1 | 0.91 | 0.17 | 58,58,58,58 | 0 |
| 86 | OHX | A5 | 3756 | 7/7 | 0.91 | 0.26 | 158,158,158,158 | 7 |
| 87 | MG | A3 | 225 | 1/1 | 0.91 | 0.34 | 61,61,61,61 | 0 |
| 86 | OHX | A8 | 212 | 7/7 | 0.91 | 0.19 | 172,172,172,172 | 7 |
| 87 | MG | Bj | 110 | 1/1 | 0.91 | 0.76 | 94,94,94,94 | 0 |
| 87 | MG | A5 | 4386 | 1/1 | 0.91 | 0.23 | 65,65,65,65 | 0 |
| 86 | OHX | A5 | 3403 | 7/7 | 0.91 | 0.19 | 171,171,171,171 | 7 |
| 86 | OHX | A1 | 3702 | 7/7 | 0.91 | 0.18 | 141,141,141,141 | 7 |
| 86 | OHX | A5 | 3406 | 7/7 | 0.91 | 0.13 | 170,170,170,170 | 7 |
| 86 | OHX | A5 | 3407 | 7/7 | 0.91 | 0.14 | 196,196,196,196 | 7 |
| 87 | MG | A1 | 3963 | 1/1 | 0.91 | 0.22 | 56,56,56,56 | 0 |
| 87 | MG | A1 | 4096 | 1/1 | 0.91 | 0.23 | 80,80,80,80 | 0 |
| 86 | OHX | A8 | 220 | 7/7 | 0.91 | 0.23 | 111,111,111,111 | 7 |
| 86 | OHX | A5 | 3764 | 7/7 | 0.91 | 0.26 | 120,120,120,120 | 7 |
| 87 | MG | A5 | 4396 | 1/1 | 0.91 | 0.23 | 71,71,71,71 | 0 |
| 87 | MG | A5 | 4051 | 1/1 | 0.91 | 0.15 | 77,77,77,77 | 0 |
| 87 | MG | A4 | 218 | 1/1 | 0.91 | 0.33 | 59,59,59,59 | 0 |
| 87 | MG | A1 | 4416 | 1/1 | 0.91 | 1.11 | 57,57,57,57 | 0 |
| 87 | MG | A1 | 4418 | 1/1 | 0.91 | 0.48 | 48,48,48,48 | 0 |
| 87 | MG | A2 | 2165 | 1/1 | 0.91 | 0.27 | 78,78,78,78 | 0 |
| 87 | MG | A6 | 2112 | 1/1 | 0.91 | 0.33 | 64,64,64,64 | 0 |
| 87 | MG | A5 | 4406 | 1/1 | 0.91 | 0.65 | 75,75,75,75 | 0 |
| 87 | MG | A6 | 2115 | 1/1 | 0.91 | 0.37 | 47,47,47,47 | 0 |
| 87 | MG | A5 | 4408 | 1/1 | 0.91 | 0.40 | 65,65,65,65 | 0 |
| 86 | OHX | A1 | 3795 | 7/7 | 0.91 | 0.43 | 195,195,195,195 | 7 |
| 87 | MG | A1 | 3858 | 1/1 | 0.91 | 0.33 | 64,64,64,64 | 0 |
| 87 | MG | A1 | 4106 | 1/1 | 0.91 | 0.33 | 69,69,69,69 | 0 |
| 87 | MG | A1 | 4308 | 1/1 | 0.91 | 0.75 | 59,59,59,59 | 0 |
| 87 | MG | A1 | 3973 | 1/1 | 0.91 | 0.34 | 37,37,37,37 | 0 |
| 87 | MG | A5 | 4238 | 1/1 | 0.91 | 0.50 | 44,44,44,44 | 0 |
| 87 | MG | A5 | 4239 | 1/1 | 0.91 | 0.31 | 44,44,44,44 | 0 |
| 86 | OHX | DJ | 201 | 7/7 | 0.91 | 0.14 | 185,185,185,185 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | A1 | 4426 | 1/1 | 0.91 | 0.87 | 82,82,82,82 | 0 |
| 86 | OHX | A6 | 2066 | 7/7 | 0.91 | 0.24 | 119,119,119,119 | 7 |
| 87 | MG | A5 | 3877 | 1/1 | 0.91 | 0.32 | 60,60,60,60 | 0 |
| 86 | OHX | A2 | 2024 | 7/7 | 0.91 | 0.24 | 174,174,174,174 | 7 |
| 86 | OHX | A1 | 3707 | 7/7 | 0.91 | 0.20 | 135,135,135,135 | 7 |
| 87 | MG | A8 | 238 | 1/1 | 0.91 | 0.32 | 93,93,93,93 | 0 |
| 87 | MG | A6 | 2131 | 1/1 | 0.91 | 0.30 | 46,46,46,46 | 0 |
| 87 | MG | A1 | 3979 | 1/1 | 0.91 | 0.41 | 52,52,52,52 | 0 |
| 87 | MG | A2 | 2171 | 1/1 | 0.91 | 0.29 | 89,89,89,89 | 0 |
| 86 | OHX | A1 | 3798 | 7/7 | 0.91 | 0.71 | 226,226,226,226 | 7 |
| 87 | MG | A1 | 3983 | 1/1 | 0.91 | 0.13 | 65,65,65,65 | 0 |
| 86 | OHX | A1 | 3674 | 7/7 | 0.91 | 0.19 | 159,159,159,159 | 7 |
| 87 | MG | A1 | 4439 | 1/1 | 0.91 | 0.38 | 88,88,88,88 | 0 |
| 86 | OHX | A1 | 3800 | 7/7 | 0.91 | 0.21 | 188,188,188,188 | 7 |
| 86 | OHX | A5 | 3662 | 7/7 | 0.91 | 0.24 | 148,148,148,148 | 7 |
| 87 | MG | A5 | 3892 | 1/1 | 0.91 | 0.20 | 45,45,45,45 | 0 |
| 87 | MG | A6 | 2289 | 1/1 | 0.91 | 0.24 | 96,96,96,96 | 0 |
| 87 | MG | A1 | 4225 | 1/1 | 0.91 | 0.27 | 67,67,67,67 | 0 |
| 87 | MG | A6 | 2142 | 1/1 | 0.91 | 0.34 | 46,46,46,46 | 0 |
| 86 | OHX | A6 | 2008 | 7/7 | 0.91 | 0.17 | 176,176,176,176 | 7 |
| 86 | OHX | A1 | 3677 | 7/7 | 0.91 | 0.27 | 115,115,115,115 | 7 |
| 87 | MG | DF | 301 | 1/1 | 0.91 | 0.19 | 75,75,75,75 | 0 |
| 87 | MG | A5 | 4266 | 1/1 | 0.91 | 0.28 | 72,72,72,72 | 0 |
| 87 | MG | DF | 304 | 1/1 | 0.91 | 0.61 | 57,57,57,57 | 0 |
| 87 | MG | A5 | 3900 | 1/1 | 0.91 | 0.24 | 63,63,63,63 | 0 |
| 87 | MG | A6 | 2295 | 1/1 | 0.91 | 0.15 | 79,79,79,79 | 0 |
| 86 | OHX | A1 | 3711 | 7/7 | 0.91 | 0.17 | 155,155,155,155 | 7 |
| 87 | MG | A5 | 4456 | 1/1 | 0.91 | 0.31 | 79,79,79,79 | 0 |
| 86 | OHX | A5 | 3673 | 7/7 | 0.91 | 0.23 | 144,144,144,144 | 7 |
| 86 | OHX | A5 | 3674 | 7/7 | 0.91 | 0.26 | 100,100,100,100 | 7 |
| 87 | MG | A5 | 3910 | 1/1 | 0.91 | 0.32 | 57,57,57,57 | 0 |
| 87 | MG | DN | 301 | 1/1 | 0.91 | 0.24 | 77,77,77,77 | 0 |
| 87 | MG | A5 | 4102 | 1/1 | 0.91 | 0.40 | 71,71,71,71 | 0 |
| 87 | MG | DO | 205 | 1/1 | 0.91 | 0.51 | 52,52,52,52 | 0 |
| 87 | MG | A5 | 4103 | 1/1 | 0.91 | 0.33 | 74,74,74,74 | 0 |
| 87 | MG | A6 | 2149 | 1/1 | 0.91 | 0.38 | 49,49,49,49 | 0 |
| 87 | MG | A6 | 2303 | 1/1 | 0.91 | 0.33 | 60,60,60,60 | 0 |
| 87 | MG | DO | 209 | 1/1 | 0.91 | 0.79 | 62,62,62,62 | 0 |
| 87 | MG | A5 | 4469 | 1/1 | 0.91 | 0.17 | 70,70,70,70 | 0 |
| 87 | MG | A5 | 4109 | 1/1 | 0.91 | 0.29 | 88,88,88,88 | 0 |
| 87 | MG | A5 | 3913 | 1/1 | 0.91 | 0.12 | 68,68,68,68 | 0 |
| 86 | OHX | A5 | 3680 | 7/7 | 0.91 | 0.30 | 134,134,134,134 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86 | OHX | A1 | 3678 | 7/7 | 0.91 | 0.16 | 186,186,186,186 | 7 |
| 87 | MG | BC | 402 | 1/1 | 0.91 | 0.28 | 54,54,54,54 | 0 |
| 86 | OHX | A1 | 3806 | 7/7 | 0.91 | 0.25 | 198,198,198,198 | 7 |
| 87 | MG | BC | 405 | 1/1 | 0.91 | 0.56 | 49,49,49,49 | 0 |
| 86 | OHX | A1 | 3807 | 7/7 | 0.91 | 0.17 | 167,167,167,167 | 7 |
| 87 | MG | BC | 407 | 1/1 | 0.91 | 0.57 | 58,58,58,58 | 0 |
| 86 | OHX | A1 | 3721 | 7/7 | 0.91 | 0.17 | 153,153,153,153 | 7 |
| 86 | OHX | A5 | 3696 | 7/7 | 0.91 | 0.18 | 167,167,167,167 | 7 |
| 86 | OHX | AN | 201 | 7/7 | 0.91 | 0.16 | 192,192,192,192 | 7 |
| 87 | MG | A1 | 3890 | 1/1 | 0.91 | 0.34 | 61,61,61,61 | 0 |
| 87 | MG | Da | 201 | 1/1 | 0.91 | 0.28 | 54,54,54,54 | 0 |
| 87 | MG | Da | 202 | 1/1 | 0.91 | 0.49 | 84,84,84,84 | 0 |
| 87 | MG | A5 | 4305 | 1/1 | 0.91 | 0.74 | 88,88,88,88 | 0 |
| 86 | OHX | A5 | 3700 | 7/7 | 0.91 | 0.39 | 146,146,146,146 | 7 |
| 86 | OHX | A5 | 3704 | 7/7 | 0.91 | 0.21 | 141,141,141,141 | 7 |
| 87 | MG | A1 | 4030 | 1/1 | 0.91 | 0.19 | 37,37,37,37 | 0 |
| 86 | OHX | A6 | 2041 | 7/7 | 0.91 | 0.26 | 145,145,145,145 | 7 |
| 87 | MG | A1 | 4345 | 1/1 | 0.91 | 0.18 | 73,73,73,73 | 0 |
| 86 | OHX | A5 | 3709 | 7/7 | 0.91 | 0.13 | 171,171,171,171 | 7 |
| 86 | OHX | A1 | 3781 | 7/7 | 0.91 | 0.28 | 122,122,122,122 | 7 |
| 87 | MG | A5 | 3939 | 1/1 | 0.91 | 0.39 | 42,42,42,42 | 0 |
| 87 | MG | Dj | 101 | 1/1 | 0.91 | 0.25 | 38,38,38,38 | 0 |
| 87 | MG | Dj | 102 | 1/1 | 0.91 | 1.24 | 74,74,74,74 | 0 |
| 87 | MG | A2 | 2116 | 1/1 | 0.91 | 0.36 | 59,59,59,59 | 0 |
| 87 | MG | A2 | 2120 | 1/1 | 0.91 | 0.35 | 73,73,73,73 | 0 |
| 86 | OHX | A1 | 3684 | 7/7 | 0.91 | 0.15 | 143,143,143,143 | 7 |
| 86 | OHX | A6 | 2088 | 7/7 | 0.91 | 0.23 | 160,160,160,160 | 7 |
| 86 | OHX | A1 | 3724 | 7/7 | 0.91 | 0.24 | 144,144,144,144 | 7 |
| 87 | MG | A2 | 2205 | 1/1 | 0.91 | 0.13 | 83,83,83,83 | 0 |
| 87 | MG | A5 | 4148 | 1/1 | 0.91 | 0.26 | 75,75,75,75 | 0 |
| 87 | MG | A5 | 4325 | 1/1 | 0.91 | 0.99 | 57,57,57,57 | 0 |
| 87 | MG | A5 | 4321 | 1/1 | 0.92 | 0.22 | 77,77,77,77 | 0 |
| 86 | OHX | A1 | 3705 | 7/7 | 0.92 | 0.14 | 164,164,164,164 | 7 |
| 87 | MG | BQ | 204 | 1/1 | 0.92 | 1.35 | 99,99,99,99 | 0 |
| 87 | MG | A5 | 4144 | 1/1 | 0.92 | 0.71 | 75,75,75,75 | 0 |
| 87 | MG | A1 | 3944 | 1/1 | 0.92 | 0.45 | 45,45,45,45 | 0 |
| 87 | MG | A6 | 2339 | 1/1 | 0.92 | 0.20 | 64,64,64,64 | 0 |
| 87 | MG | A1 | 4272 | 1/1 | 0.92 | 0.24 | 53,53,53,53 | 0 |
| 87 | MG | A1 | 4377 | 1/1 | 0.92 | 0.76 | 54,54,54,54 | 0 |
| 87 | MG | A2 | 2090 | 1/1 | 0.92 | 0.28 | 53,53,53,53 | 0 |
| 87 | MG | A5 | 4521 | 1/1 | 0.92 | 0.71 | 68,68,68,68 | 0 |
| 87 | MG | A1 | 4075 | 1/1 | 0.92 | 0.24 | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86 | OHX | A6 | 2084 | 7/7 | 0.92 | 0.15 | 196,196,196,196 | 7 |
| 87 | MG | A1 | 3947 | 1/1 | 0.92 | 0.42 | 42,42,42,42 | 0 |
| 86 | OHX | A2 | 1947 | 7/7 | 0.92 | 0.17 | 157,157,157,157 | 7 |
| 86 | OHX | A5 | 3689 | 7/7 | 0.92 | 0.20 | 134,134,134,134 | 7 |
| 86 | OHX | A1 | 3777 | 7/7 | 0.92 | 0.26 | 137,137,137,137 | 7 |
| 87 | MG | A5 | 4158 | 1/1 | 0.92 | 0.27 | 62,62,62,62 | 0 |
| 86 | OHX | A1 | 3740 | 7/7 | 0.92 | 0.30 | 107,107,107,107 | 7 |
| 86 | OHX | A1 | 3811 | 7/7 | 0.92 | 0.32 | 183,183,183,183 | 7 |
| 87 | MG | A1 | 4394 | 1/1 | 0.92 | 0.79 | 58,58,58,58 | 0 |
| 86 | OHX | A6 | 2044 | 7/7 | 0.92 | 0.14 | 178,178,178,178 | 7 |
| 86 | OHX | A1 | 3548 | 7/7 | 0.92 | 0.20 | 136,136,136,136 | 7 |
| 86 | OHX | A1 | 3780 | 7/7 | 0.92 | 0.26 | 136,136,136,136 | 7 |
| 87 | MG | A2 | 2180 | 1/1 | 0.92 | 0.12 | 101,101,101,101 | 0 |
| 87 | MG | A5 | 3979 | 1/1 | 0.92 | 0.44 | 61,61,61,61 | 0 |
| 87 | MG | A5 | 3980 | 1/1 | 0.92 | 0.35 | 58,58,58,58 | 0 |
| 86 | OHX | A1 | 3742 | 7/7 | 0.92 | 0.31 | 140,140,140,140 | 7 |
| 87 | MG | A5 | 3985 | 1/1 | 0.92 | 0.45 | 51,51,51,51 | 0 |
| 87 | MG | A1 | 3971 | 1/1 | 0.92 | 0.34 | 35,35,35,35 | 0 |
| 86 | OHX | A5 | 3710 | 7/7 | 0.92 | 0.18 | 132,132,132,132 | 7 |
| 87 | MG | A6 | 2223 | 1/1 | 0.92 | 0.20 | 75,75,75,75 | 0 |
| 86 | OHX | A5 | 3788 | 7/7 | 0.92 | 0.29 | 141,141,141,141 | 7 |
| 87 | MG | Ch | 301 | 1/1 | 0.92 | 0.18 | 44,44,44,44 | 0 |
| 87 | MG | A2 | 2184 | 1/1 | 0.92 | 0.25 | 109,109,109,109 | 0 |
| 87 | MG | A5 | 4555 | 1/1 | 0.92 | 0.68 | 63,63,63,63 | 0 |
| 87 | MG | A5 | 3409 | 1/1 | 0.92 | 0.30 | 45,45,45,45 | 0 |
| 87 | MG | A1 | 4294 | 1/1 | 0.92 | 0.21 | 78,78,78,78 | 0 |
| 86 | OHX | A2 | 2059 | 7/7 | 0.92 | 0.11 | 183,183,183,183 | 7 |
| 87 | MG | A1 | 4196 | 1/1 | 0.92 | 0.22 | 71,71,71,71 | 0 |
| 87 | MG | A1 | 4409 | 1/1 | 0.92 | 1.01 | 58,58,58,58 | 0 |
| 86 | OHX | A6 | 2049 | 7/7 | 0.92 | 0.14 | 175,175,175,175 | 7 |
| 87 | MG | A5 | 4003 | 1/1 | 0.92 | 0.36 | 46,46,46,46 | 0 |
| 87 | MG | A1 | 4099 | 1/1 | 0.92 | 0.26 | 71,71,71,71 | 0 |
| 87 | MG | A5 | 4190 | 1/1 | 0.92 | 0.71 | 58,58,58,58 | 0 |
| 87 | MG | A1 | 4412 | 1/1 | 0.92 | 0.32 | 104,104,104,104 | 0 |
| 87 | MG | A1 | 4100 | 1/1 | 0.92 | 0.14 | 34,34,34,34 | 0 |
| 86 | OHX | A3 | 209 | 7/7 | 0.92 | 0.16 | 180,180,180,180 | 7 |
| 86 | OHX | A1 | 3676 | 7/7 | 0.92 | 0.22 | 148,148,148,148 | 7 |
| 87 | MG | A6 | 2241 | 1/1 | 0.92 | 0.81 | 112,112,112,112 | 0 |
| 87 | MG | A5 | 4574 | 1/1 | 0.92 | 0.34 | 74,74,74,74 | 0 |
| 87 | MG | A5 | 3836 | 1/1 | 0.92 | 0.34 | 66,66,66,66 | 0 |
| 87 | MG | A2 | 2189 | 1/1 | 0.92 | 0.21 | 55,55,55,55 | 0 |
| 87 | MG | A1 | 4203 | 1/1 | 0.92 | 0.29 | 69,69,69,69 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86 | OHX | A5 | 3724 | 7/7 | 0.92 | 0.26 | 124,124,124,124 | 7 |
| 87 | MG | A1 | 3982 | 1/1 | 0.92 | 0.41 | 43,43,43,43 | 0 |
| 86 | OHX | A2 | 2012 | 7/7 | 0.92 | 0.15 | 180,180,180,180 | 7 |
| 87 | MG | A6 | 2108 | 1/1 | 0.92 | 0.27 | 52,52,52,52 | 0 |
| 87 | MG | A5 | 4034 | 1/1 | 0.92 | 0.16 | 46,46,46,46 | 0 |
| 86 | OHX | A1 | 3716 | 7/7 | 0.92 | 0.26 | 113,113,113,113 | 7 |
| 87 | MG | A1 | 4211 | 1/1 | 0.92 | 0.34 | 102,102,102,102 | 0 |
| 87 | MG | A1 | 3985 | 1/1 | 0.92 | 0.42 | 51,51,51,51 | 0 |
| 86 | OHX | A1 | 3719 | 7/7 | 0.92 | 0.18 | 154,154,154,154 | 7 |
| 87 | MG | A7 | 223 | 1/1 | 0.92 | 0.23 | 69,69,69,69 | 0 |
| 87 | MG | A5 | 4213 | 1/1 | 0.92 | 0.44 | 52,52,52,52 | 0 |
| 87 | MG | A1 | 4311 | 1/1 | 0.92 | 0.23 | 92,92,92,92 | 0 |
| 86 | OHX | A5 | 3731 | 7/7 | 0.92 | 0.13 | 138,138,138,138 | 7 |
| 86 | OHX | A5 | 3732 | 7/7 | 0.92 | 0.29 | 209,209,209,209 | 7 |
| 87 | MG | A5 | 4044 | 1/1 | 0.92 | 0.22 | 35,35,35,35 | 0 |
| 86 | OHX | A1 | 3569 | 7/7 | 0.92 | 0.17 | 144,144,144,144 | 7 |
| 87 | MG | AL | 203 | 1/1 | 0.92 | 0.63 | 80,80,80,80 | 0 |
| 87 | MG | A5 | 4048 | 1/1 | 0.92 | 0.11 | 34,34,34,34 | 0 |
| 87 | MG | A1 | 4218 | 1/1 | 0.92 | 0.18 | 69,69,69,69 | 0 |
| 87 | MG | A6 | 2124 | 1/1 | 0.92 | 0.29 | 55,55,55,55 | 0 |
| 87 | MG | A4 | 239 | 1/1 | 0.92 | 0.89 | 70,70,70,70 | 0 |
| 87 | MG | A5 | 4403 | 1/1 | 0.92 | 0.40 | 81,81,81,81 | 0 |
| 86 | OHX | CJ | 201 | 7/7 | 0.92 | 0.28 | 105,105,105,105 | 7 |
| 86 | OHX | A1 | 3751 | 7/7 | 0.92 | 0.14 | 189,189,189,189 | 7 |
| 87 | MG | A6 | 2269 | 1/1 | 0.92 | 0.52 | 60,60,60,60 | 0 |
| 86 | OHX | A1 | 3574 | 7/7 | 0.92 | 0.25 | 189,189,189,189 | 7 |
| 87 | MG | A5 | 3868 | 1/1 | 0.92 | 0.21 | 44,44,44,44 | 0 |
| 87 | MG | A6 | 2130 | 1/1 | 0.92 | 0.38 | 74,74,74,74 | 0 |
| 86 | OHX | A1 | 3683 | 7/7 | 0.92 | 0.20 | 159,159,159,159 | 7 |
| 87 | MG | A5 | 4062 | 1/1 | 0.92 | 0.28 | 37,37,37,37 | 0 |
| 86 | OHX | A1 | 3754 | 7/7 | 0.92 | 0.24 | 159,159,159,159 | 7 |
| 87 | MG | A5 | 4064 | 1/1 | 0.92 | 0.17 | 30,30,30,30 | 0 |
| 86 | OHX | A2 | 2015 | 7/7 | 0.92 | 0.20 | 138,138,138,138 | 7 |
| 87 | MG | A1 | 4126 | 1/1 | 0.92 | 0.26 | 84,84,84,84 | 0 |
| 87 | MG | A5 | 3876 | 1/1 | 0.92 | 0.22 | 66,66,66,66 | 0 |
| 86 | OHX | A6 | 2065 | 7/7 | 0.92 | 0.19 | 156,156,156,156 | 7 |
| 87 | MG | A5 | 4071 | 1/1 | 0.92 | 0.23 | 79,79,79,79 | 0 |
| 86 | OHX | A1 | 3686 | 7/7 | 0.92 | 0.13 | 204,204,204,204 | 7 |
| 86 | OHX | A5 | 3551 | 7/7 | 0.92 | 0.17 | 142,142,142,142 | 7 |
| 87 | MG | A1 | 4449 | 1/1 | 0.92 | 0.14 | 98,98,98,98 | 0 |
| 86 | OHX | A2 | 1983 | 7/7 | 0.92 | 0.14 | 166,166,166,166 | 7 |
| 86 | OHX | A2 | 2018 | 7/7 | 0.92 | 0.15 | 176,176,176,176 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87 | MG | DB | 409 | 1/1 | 0.92 | 0.62 | 56,56,56,56 | 0 |
| 87 | MG | DB | 411 | 1/1 | 0.92 | 1.23 | 61,61,61,61 | 0 |
| 87 | MG | A1 | 4022 | 1/1 | 0.92 | 0.28 | 40,40,40,40 | 0 |
| 86 | OHX | A5 | 3605 | 7/7 | 0.92 | 0.27 | 112,112,112,112 | 7 |
| 87 | MG | A1 | 4027 | 1/1 | 0.92 | 0.44 | 65,65,65,65 | 0 |
| 87 | MG | BC | 404 | 1/1 | 0.92 | 1.23 | 67,67,67,67 | 0 |
| 87 | MG | DC | 403 | 1/1 | 0.92 | 0.41 | 65,65,65,65 | 0 |
| 87 | MG | A1 | 4235 | 1/1 | 0.92 | 0.27 | 62,62,62,62 | 0 |
| 87 | MG | A1 | 4457 | 1/1 | 0.92 | 0.21 | 97,97,97,97 | 0 |
| 86 | OHX | A5 | 3621 | 7/7 | 0.92 | 0.23 | 123,123,123,123 | 7 |
| 87 | MG | A5 | 3894 | 1/1 | 0.92 | 0.39 | 67,67,67,67 | 0 |
| 87 | MG | DD | 304 | 1/1 | 0.92 | 0.22 | 71,71,71,71 | 0 |
| 86 | OHX | A2 | 2001 | 7/7 | 0.92 | 0.19 | 140,140,140,140 | 7 |
| 87 | MG | A6 | 2152 | 1/1 | 0.92 | 0.44 | 64,64,64,64 | 0 |
| 87 | MG | DF | 302 | 1/1 | 0.92 | 0.59 | 48,48,48,48 | 0 |
| 86 | OHX | A5 | 3633 | 7/7 | 0.92 | 0.26 | 126,126,126,126 | 7 |
| 86 | OHX | A5 | 3637 | 7/7 | 0.92 | 0.17 | 178,178,178,178 | 7 |
| 86 | OHX | A5 | 3642 | 7/7 | 0.92 | 0.21 | 118,118,118,118 | 7 |
| 87 | MG | A6 | 2301 | 1/1 | 0.92 | 0.54 | 116,116,116,116 | 0 |
| 87 | MG | A5 | 3901 | 1/1 | 0.92 | 0.28 | 85,85,85,85 | 0 |
| 87 | MG | A5 | 4269 | 1/1 | 0.92 | 0.25 | 66,66,66,66 | 0 |
| 86 | OHX | A5 | 3644 | 7/7 | 0.92 | 0.29 | 135,135,135,135 | 7 |
| 87 | MG | A5 | 4096 | 1/1 | 0.92 | 0.33 | 72,72,72,72 | 0 |
| 87 | MG | A5 | 3903 | 1/1 | 0.92 | 0.24 | 34,34,34,34 | 0 |
| 87 | MG | A5 | 4274 | 1/1 | 0.92 | 0.09 | 51,51,51,51 | 0 |
| 87 | MG | A1 | 4243 | 1/1 | 0.92 | 0.51 | 61,61,61,61 | 0 |
| 87 | MG | A5 | 4461 | 1/1 | 0.92 | 0.26 | 62,62,62,62 | 0 |
| 86 | OHX | A6 | 1977 | 7/7 | 0.92 | 0.19 | 128,128,128,128 | 7 |
| 87 | MG | A2 | 2218 | 1/1 | 0.92 | 0.25 | 63,63,63,63 | 0 |
| 87 | MG | A5 | 3909 | 1/1 | 0.92 | 0.42 | 70,70,70,70 | 0 |
| 87 | MG | A5 | 4282 | 1/1 | 0.92 | 0.40 | 52,52,52,52 | 0 |
| 86 | OHX | A8 | 216 | 7/7 | 0.92 | 0.12 | 198,198,198,198 | 7 |
| 87 | MG | A1 | 4471 | 1/1 | 0.92 | 0.17 | 88,88,88,88 | 0 |
| 87 | MG | A2 | 2151 | 1/1 | 0.92 | 0.15 | 49,49,49,49 | 0 |
| 87 | MG | A5 | 4287 | 1/1 | 0.92 | 0.31 | 101,101,101,101 | 0 |
| 87 | MG | A5 | 4107 | 1/1 | 0.92 | 0.14 | 66,66,66,66 | 0 |
| 86 | OHX | A1 | 3623 | 7/7 | 0.92 | 0.22 | 147,147,147,147 | 7 |
| 87 | MG | A6 | 2172 | 1/1 | 0.92 | 0.31 | 66,66,66,66 | 0 |
| 87 | MG | A6 | 2313 | 1/1 | 0.92 | 1.07 | 78,78,78,78 | 0 |
| 87 | MG | DT | 201 | 1/1 | 0.92 | 0.53 | 63,63,63,63 | 0 |
| 86 | OHX | A2 | 2055 | 7/7 | 0.92 | 0.28 | 116,116,116,116 | 7 |
| 87 | MG | A1 | 4476 | 1/1 | 0.92 | 0.44 | 68,68,68,68 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87 | MG | A1 | 3834 | 1/1 | 0.92 | 0.10 | 44,44,44,44 | 0 |
| 86 | OHX | A1 | 3645 | 7/7 | 0.92 | 0.27 | 102,102,102,102 | 7 |
| 87 | MG | A5 | 4484 | 1/1 | 0.92 | 0.94 | 89,89,89,89 | 0 |
| 87 | MG | A1 | 4054 | 1/1 | 0.92 | 0.38 | 65,65,65,65 | 0 |
| 87 | MG | A5 | 4298 | 1/1 | 0.92 | 0.12 | 106,106,106,106 | 0 |
| 87 | MG | A1 | 4055 | 1/1 | 0.92 | 0.21 | 58,58,58,58 | 0 |
| 86 | OHX | A1 | 3733 | 7/7 | 0.92 | 0.33 | 125,125,125,125 | 7 |
| 86 | OHX | A6 | 2024 | 7/7 | 0.92 | 0.15 | 156,156,156,156 | 7 |
| 86 | OHX | DG | 301 | 7/7 | 0.92 | 0.50 | 226,226,226,226 | 7 |
| 86 | OHX | A2 | 2034 | 7/7 | 0.92 | 0.16 | 173,173,173,173 | 7 |
| 87 | MG | A2 | 2229 | 1/1 | 0.92 | 0.10 | 60,60,60,60 | 0 |
| 87 | MG | A6 | 2325 | 1/1 | 0.92 | 0.64 | 106,106,106,106 | 0 |
| 87 | MG | Df | 202 | 1/1 | 0.92 | 0.34 | 81,81,81,81 | 0 |
| 87 | MG | A5 | 4494 | 1/1 | 0.92 | 0.40 | 111,111,111,111 | 0 |
| 86 | OHX | A6 | 2080 | 7/7 | 0.92 | 0.30 | 167,167,167,167 | 7 |
| 87 | MG | Dg | 202 | 1/1 | 0.92 | 0.15 | 50,50,50,50 | 0 |
| 87 | MG | A5 | 4310 | 1/1 | 0.92 | 0.57 | 69,69,69,69 | 0 |
| 86 | OHX | A2 | 2068 | 7/7 | 0.92 | 0.38 | 177,177,177,177 | 7 |
| 87 | MG | A6 | 2191 | 1/1 | 0.92 | 0.34 | 84,84,84,84 | 0 |
| 87 | MG | Dm | 201 | 1/1 | 0.92 | 0.27 | 75,75,75,75 | 0 |
| 87 | MG | A1 | 3933 | 1/1 | 0.92 | 0.47 | 53,53,53,53 | 0 |
| 87 | MG | Dp | 101 | 1/1 | 0.92 | 0.17 | 54,54,54,54 | 0 |
| 87 | MG | A5 | 4500 | 1/1 | 0.92 | 0.23 | 82,82,82,82 | 0 |
| 87 | MG | A6 | 2331 | 1/1 | 0.92 | 0.15 | 79,79,79,79 | 0 |
| 87 | MG | A5 | 4316 | 1/1 | 0.92 | 0.45 | 57,57,57,57 | 0 |
| 86 | OHX | A5 | 3675 | 7/7 | 0.92 | 0.22 | 132,132,132,132 | 7 |
| 87 | MG | A2 | 2162 | 1/1 | 0.92 | 0.44 | 84,84,84,84 | 0 |
| 86 | OHX | A5 | 3676 | 7/7 | 0.92 | 0.17 | 155,155,155,155 | 7 |
| 86 | OHX | A1 | 3407 | 7/7 | 0.92 | 0.29 | 138,138,138,138 | 7 |
| 87 | MG | A5 | 4516 | 1/1 | 0.93 | 0.92 | 74,74,74,74 | 0 |
| 86 | OHX | A1 | 3785 | 7/7 | 0.93 | 0.42 | 183,183,183,183 | 7 |
| 87 | MG | A5 | 4328 | 1/1 | 0.93 | 0.66 | 72,72,72,72 | 0 |
| 87 | MG | A1 | 3899 | 1/1 | 0.93 | 0.22 | 57,57,57,57 | 0 |
| 87 | MG | A2 | 2192 | 1/1 | 0.93 | 0.31 | 66,66,66,66 | 0 |
| 87 | MG | A5 | 3970 | 1/1 | 0.93 | 0.50 | 60,60,60,60 | 0 |
| 86 | OHX | A6 | 2009 | 7/7 | 0.93 | 0.20 | 136,136,136,136 | 7 |
| 87 | MG | A5 | 3973 | 1/1 | 0.93 | 0.37 | 38,38,38,38 | 0 |
| 86 | OHX | A5 | 3518 | 7/7 | 0.93 | 0.18 | 159,159,159,159 | 7 |
| 87 | MG | A1 | 4371 | 1/1 | 0.93 | 0.61 | 63,63,63,63 | 0 |
| 87 | MG | A1 | 4032 | 1/1 | 0.93 | 0.18 | 46,46,46,46 | 0 |
| 87 | MG | A1 | 3904 | 1/1 | 0.93 | 0.28 | 43,43,43,43 | 0 |
| 87 | MG | A5 | 4339 | 1/1 | 0.93 | 0.17 | 66,66,66,66 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | BV | 204 | 1/1 | 0.93 | 0.37 | 40,40,40,40 | 0 |
| 86 | OHX | A2 | 2030 | 7/7 | 0.93 | 0.37 | 155,155,155,155 | 7 |
| 86 | OHX | A5 | 3730 | 7/7 | 0.93 | 0.22 | 97,97,97,97 | 7 |
| 87 | MG | A1 | 4036 | 1/1 | 0.93 | 0.30 | 71,71,71,71 | 0 |
| 87 | MG | A5 | 3987 | 1/1 | 0.93 | 0.41 | 59,59,59,59 | 0 |
| 87 | MG | A2 | 2118 | 1/1 | 0.93 | 0.32 | 47,47,47,47 | 0 |
| 86 | OHX | A6 | 2017 | 7/7 | 0.93 | 0.21 | 132,132,132,132 | 7 |
| 87 | MG | A1 | 4040 | 1/1 | 0.93 | 0.11 | 40,40,40,40 | 0 |
| 87 | MG | A1 | 4265 | 1/1 | 0.93 | 0.33 | 74,74,74,74 | 0 |
| 87 | MG | A1 | 3911 | 1/1 | 0.93 | 0.18 | 58,58,58,58 | 0 |
| 87 | MG | A5 | 4175 | 1/1 | 0.93 | 0.21 | 114,114,114,114 | 0 |
| 87 | MG | A1 | 4386 | 1/1 | 0.93 | 0.70 | 78,78,78,78 | 0 |
| 86 | OHX | A6 | 2018 | 7/7 | 0.93 | 0.20 | 153,153,153,153 | 7 |
| 86 | OHX | A6 | 2070 | 7/7 | 0.93 | 0.17 | 139,139,139,139 | 7 |
| 87 | MG | A5 | 3996 | 1/1 | 0.93 | 0.48 | 46,46,46,46 | 0 |
| 87 | MG | A5 | 3997 | 1/1 | 0.93 | 0.46 | 43,43,43,43 | 0 |
| 87 | MG | A3 | 215 | 1/1 | 0.93 | 0.32 | 77,77,77,77 | 0 |
| 87 | MG | A1 | 4044 | 1/1 | 0.93 | 0.27 | 44,44,44,44 | 0 |
| 87 | MG | A5 | 3832 | 1/1 | 0.93 | 0.10 | 35,35,35,35 | 0 |
| 87 | MG | A5 | 4361 | 1/1 | 0.93 | 0.23 | 92,92,92,92 | 0 |
| 87 | MG | A1 | 4045 | 1/1 | 0.93 | 0.17 | 55,55,55,55 | 0 |
| 87 | MG | A1 | 4046 | 1/1 | 0.93 | 0.41 | 50,50,50,50 | 0 |
| 87 | MG | A5 | 4007 | 1/1 | 0.93 | 0.37 | 47,47,47,47 | 0 |
| 87 | MG | A6 | 2237 | 1/1 | 0.93 | 0.18 | 96,96,96,96 | 0 |
| 86 | OHX | A6 | 2022 | 7/7 | 0.93 | 0.14 | 145,145,145,145 | 7 |
| 87 | MG | A5 | 4368 | 1/1 | 0.93 | 0.28 | 75,75,75,75 | 0 |
| 87 | MG | A2 | 2125 | 1/1 | 0.93 | 0.47 | 61,61,61,61 | 0 |
| 87 | MG | Bj | 109 | 1/1 | 0.93 | 0.26 | 122,122,122,122 | 0 |
| 87 | MG | A5 | 4019 | 1/1 | 0.93 | 0.48 | 48,48,48,48 | 0 |
| 86 | OHX | A5 | 3612 | 7/7 | 0.93 | 0.19 | 147,147,147,147 | 7 |
| 87 | MG | A5 | 4195 | 1/1 | 0.93 | 0.31 | 72,72,72,72 | 0 |
| 86 | OHX | A5 | 3804 | 7/7 | 0.93 | 0.16 | 162,162,162,162 | 7 |
| 87 | MG | A5 | 4573 | 1/1 | 0.93 | 0.74 | 56,56,56,56 | 0 |
| 87 | MG | A1 | 4052 | 1/1 | 0.93 | 0.26 | 71,71,71,71 | 0 |
| 86 | OHX | A5 | 3615 | 7/7 | 0.93 | 0.19 | 147,147,147,147 | 7 |
| 86 | OHX | A5 | 3806 | 7/7 | 0.93 | 0.23 | 120,120,120,120 | 7 |
| 87 | MG | A5 | 4200 | 1/1 | 0.93 | 0.53 | 70,70,70,70 | 0 |
| 87 | MG | A1 | 3823 | 1/1 | 0.93 | 0.29 | 60,60,60,60 | 0 |
| 86 | OHX | A1 | 3641 | 7/7 | 0.93 | 0.24 | 137,137,137,137 | 7 |
| 86 | OHX | A5 | 3622 | 7/7 | 0.93 | 0.18 | 136,136,136,136 | 7 |
| 86 | OHX | A1 | 3685 | 7/7 | 0.93 | 0.15 | 150,150,150,150 | 7 |
| 86 | OHX | A5 | 3745 | 7/7 | 0.93 | 0.24 | 131,131,131,131 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86 | OHX | A5 | 3815 | 7/7 | 0.93 | 0.26 | 221,221,221,221 | 7 |
| 87 | MG | A5 | 4037 | 1/1 | 0.93 | 0.36 | 67,67,67,67 | 0 |
| 87 | MG | A7 | 220 | 1/1 | 0.93 | 0.22 | 61,61,61,61 | 0 |
| 86 | OHX | A5 | 3624 | 7/7 | 0.93 | 0.27 | 82,82,82,82 | 7 |
| 87 | MG | A5 | 3855 | 1/1 | 0.93 | 0.40 | 55,55,55,55 | 0 |
| 86 | OHX | A1 | 3763 | 7/7 | 0.93 | 0.36 | 157,157,157,157 | 7 |
| 87 | MG | A5 | 4041 | 1/1 | 0.93 | 0.23 | 47,47,47,47 | 0 |
| 87 | MG | A7 | 225 | 1/1 | 0.93 | 0.36 | 45,45,45,45 | 0 |
| 87 | MG | A1 | 4066 | 1/1 | 0.93 | 0.25 | 53,53,53,53 | 0 |
| 86 | OHX | A2 | 2003 | 7/7 | 0.93 | 0.23 | 147,147,147,147 | 7 |
| 86 | OHX | A6 | 2028 | 7/7 | 0.93 | 0.26 | 136,136,136,136 | 7 |
| 86 | OHX | A1 | 3720 | 7/7 | 0.93 | 0.20 | 139,139,139,139 | 7 |
| 87 | MG | A4 | 227 | 1/1 | 0.93 | 0.10 | 53,53,53,53 | 0 |
| 86 | OHX | A5 | 3646 | 7/7 | 0.93 | 0.20 | 135,135,135,135 | 7 |
| 87 | MG | A7 | 232 | 1/1 | 0.93 | 0.20 | 91,91,91,91 | 0 |
| 87 | MG | A5 | 3864 | 1/1 | 0.93 | 0.35 | 63,63,63,63 | 0 |
| 87 | MG | A2 | 2143 | 1/1 | 0.93 | 0.23 | 82,82,82,82 | 0 |
| 86 | OHX | A6 | 2032 | 7/7 | 0.93 | 0.16 | 143,143,143,143 | 7 |
| 86 | OHX | A7 | 210 | 7/7 | 0.93 | 0.24 | 114,114,114,114 | 7 |
| 87 | MG | A7 | 238 | 1/1 | 0.93 | 0.46 | 95,95,95,95 | 0 |
| 87 | MG | A2 | 2146 | 1/1 | 0.93 | 0.27 | 71,71,71,71 | 0 |
| 87 | MG | A6 | 2125 | 1/1 | 0.93 | 0.21 | 47,47,47,47 | 0 |
| 86 | OHX | A5 | 3648 | 7/7 | 0.93 | 0.25 | 111,111,111,111 | 7 |
| 87 | MG | A8 | 222 | 1/1 | 0.93 | 0.36 | 47,47,47,47 | 0 |
| 87 | MG | A5 | 4057 | 1/1 | 0.93 | 0.41 | 82,82,82,82 | 0 |
| 86 | OHX | A5 | 3650 | 7/7 | 0.93 | 0.22 | 133,133,133,133 | 7 |
| 87 | MG | A8 | 225 | 1/1 | 0.93 | 0.29 | 58,58,58,58 | 0 |
| 87 | MG | A6 | 2274 | 1/1 | 0.93 | 0.14 | 95,95,95,95 | 0 |
| 86 | OHX | A8 | 211 | 7/7 | 0.93 | 0.23 | 135,135,135,135 | 7 |
| 87 | MG | A5 | 4232 | 1/1 | 0.93 | 0.80 | 53,53,53,53 | 0 |
| 87 | MG | A5 | 4061 | 1/1 | 0.93 | 0.23 | 83,83,83,83 | 0 |
| 87 | MG | A1 | 3845 | 1/1 | 0.93 | 0.16 | 70,70,70,70 | 0 |
| 86 | OHX | A5 | 3651 | 7/7 | 0.93 | 0.28 | 137,137,137,137 | 7 |
| 86 | OHX | A6 | 2034 | 7/7 | 0.93 | 0.20 | 137,137,137,137 | 7 |
| 87 | MG | A5 | 4240 | 1/1 | 0.93 | 0.96 | 77,77,77,77 | 0 |
| 87 | MG | A1 | 4429 | 1/1 | 0.93 | 0.32 | 54,54,54,54 | 0 |
| 86 | OHX | A5 | 3657 | 7/7 | 0.93 | 0.28 | 83,83,83,83 | 7 |
| 86 | OHX | A6 | 2036 | 7/7 | 0.93 | 0.24 | 122,122,122,122 | 7 |
| 86 | OHX | A2 | 1997 | 7/7 | 0.93 | 0.28 | 121,121,121,121 | 7 |
| 87 | MG | A1 | 3957 | 1/1 | 0.93 | 0.45 | 50,50,50,50 | 0 |
| 87 | MG | DB | 403 | 1/1 | 0.93 | 0.40 | 36,36,36,36 | 0 |
| 87 | MG | A1 | 3958 | 1/1 | 0.93 | 0.30 | 45,45,45,45 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | A5 | 4249 | 1/1 | 0.93 | 0.41 | 40,40,40,40 | 0 |
| 87 | MG | A5 | 3889 | 1/1 | 0.93 | 0.40 | 86,86,86,86 | 0 |
| 87 | MG | A5 | 4074 | 1/1 | 0.93 | 0.17 | 51,51,51,51 | 0 |
| 86 | OHX | A1 | 3769 | 7/7 | 0.93 | 0.19 | 142,142,142,142 | 7 |
| 87 | MG | A6 | 2139 | 1/1 | 0.93 | 0.34 | 72,72,72,72 | 0 |
| 87 | MG | A1 | 4204 | 1/1 | 0.93 | 0.22 | 59,59,59,59 | 0 |
| 87 | MG | A5 | 4439 | 1/1 | 0.93 | 0.17 | 56,56,56,56 | 0 |
| 87 | MG | A1 | 3961 | 1/1 | 0.93 | 0.33 | 33,33,33,33 | 0 |
| 86 | OHX | A8 | 219 | 7/7 | 0.93 | 0.22 | 166,166,166,166 | 7 |
| 87 | MG | A5 | 4442 | 1/1 | 0.93 | 0.49 | 76,76,76,76 | 0 |
| 87 | MG | A1 | 4441 | 1/1 | 0.93 | 0.81 | 61,61,61,61 | 0 |
| 87 | MG | A5 | 4082 | 1/1 | 0.93 | 0.31 | 46,46,46,46 | 0 |
| 87 | MG | A1 | 3964 | 1/1 | 0.93 | 0.39 | 50,50,50,50 | 0 |
| 87 | MG | DD | 303 | 1/1 | 0.93 | 0.62 | 67,67,67,67 | 0 |
| 87 | MG | BA | 305 | 1/1 | 0.93 | 0.49 | 61,61,61,61 | 0 |
| 86 | OHX | A2 | 2258 | 7/7 | 0.93 | 0.17 | 162,162,162,162 | 7 |
| 87 | MG | A5 | 4448 | 1/1 | 0.93 | 0.66 | 64,64,64,64 | 0 |
| 86 | OHX | A1 | 3743 | 7/7 | 0.93 | 0.37 | 148,148,148,148 | 7 |
| 87 | MG | A5 | 4450 | 1/1 | 0.93 | 0.27 | 73,73,73,73 | 0 |
| 86 | OHX | DC | 402 | 7/7 | 0.93 | 0.27 | 145,145,145,145 | 7 |
| 87 | MG | BB | 405 | 1/1 | 0.93 | 0.62 | 51,51,51,51 | 0 |
| 86 | OHX | A5 | 3672 | 7/7 | 0.93 | 0.24 | 142,142,142,142 | 7 |
| 87 | MG | A5 | 4454 | 1/1 | 0.93 | 0.57 | 68,68,68,68 | 0 |
| 87 | MG | A6 | 2153 | 1/1 | 0.93 | 0.39 | 54,54,54,54 | 0 |
| 86 | OHX | A1 | 3662 | 7/7 | 0.93 | 0.30 | 119,119,119,119 | 7 |
| 87 | MG | A6 | 2155 | 1/1 | 0.93 | 0.31 | 41,41,41,41 | 0 |
| 87 | MG | A2 | 2164 | 1/1 | 0.93 | 0.16 | 74,74,74,74 | 0 |
| 86 | OHX | DI | 302 | 7/7 | 0.93 | 0.25 | 160,160,160,160 | 7 |
| 86 | OHX | A2 | 2071 | 7/7 | 0.93 | 0.27 | 162,162,162,162 | 7 |
| 87 | MG | A5 | 4462 | 1/1 | 0.93 | 0.64 | 83,83,83,83 | 0 |
| 87 | MG | A6 | 2311 | 1/1 | 0.93 | 0.59 | 76,76,76,76 | 0 |
| 87 | MG | A6 | 2161 | 1/1 | 0.93 | 0.40 | 55,55,55,55 | 0 |
| 86 | OHX | A1 | 3725 | 7/7 | 0.93 | 0.21 | 191,191,191,191 | 7 |
| 87 | MG | A1 | 4328 | 1/1 | 0.93 | 1.25 | 76,76,76,76 | 0 |
| 86 | OHX | A2 | 2027 | 7/7 | 0.93 | 0.16 | 166,166,166,166 | 7 |
| 86 | OHX | A5 | 3773 | 7/7 | 0.93 | 0.19 | 141,141,141,141 | 7 |
| 87 | MG | DP | 205 | 1/1 | 0.93 | 0.20 | 56,56,56,56 | 0 |
| 87 | MG | A5 | 4284 | 1/1 | 0.93 | 0.18 | 69,69,69,69 | 0 |
| 87 | MG | DP | 208 | 1/1 | 0.93 | 0.29 | 42,42,42,42 | 0 |
| 86 | OHX | BD | 301 | 7/7 | 0.93 | 0.25 | 138,138,138,138 | 7 |
| 86 | OHX | A2 | 1954 | 7/7 | 0.93 | 0.23 | 162,162,162,162 | 7 |
| 86 | OHX | A2 | 2038 | 7/7 | 0.93 | 0.18 | 195,195,195,195 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86 | OHX | A1 | 3675 | 7/7 | 0.93 | 0.14 | 169,169,169,169 | 7 |
| 86 | OHX | A1 | 3609 | 7/7 | 0.93 | 0.22 | 122,122,122,122 | 7 |
| 87 | MG | A5 | 3924 | 1/1 | 0.93 | 0.35 | 39,39,39,39 | 0 |
| 87 | MG | DT | 202 | 1/1 | 0.93 | 1.35 | 89,89,89,89 | 0 |
| 87 | MG | A2 | 2176 | 1/1 | 0.93 | 0.35 | 64,64,64,64 | 0 |
| 87 | MG | A6 | 2176 | 1/1 | 0.93 | 0.47 | 67,67,67,67 | 0 |
| 86 | OHX | A2 | 1946 | 7/7 | 0.93 | 0.17 | 156,156,156,156 | 7 |
| 86 | OHX | A1 | 3619 | 7/7 | 0.93 | 0.30 | 128,128,128,128 | 7 |
| 87 | MG | A1 | 4466 | 1/1 | 0.93 | 0.17 | 80,80,80,80 | 0 |
| 87 | MG | A1 | 3881 | 1/1 | 0.93 | 0.23 | 39,39,39,39 | 0 |
| 86 | OHX | A6 | 1970 | 7/7 | 0.93 | 0.15 | 160,160,160,160 | 7 |
| 87 | MG | A5 | 4119 | 1/1 | 0.93 | 0.27 | 65,65,65,65 | 0 |
| 86 | OHX | A1 | 3680 | 7/7 | 0.93 | 0.25 | 127,127,127,127 | 7 |
| 87 | MG | A1 | 4120 | 1/1 | 0.93 | 0.17 | 26,26,26,26 | 0 |
| 86 | OHX | A6 | 1984 | 7/7 | 0.93 | 0.14 | 174,174,174,174 | 7 |
| 87 | MG | A1 | 4234 | 1/1 | 0.93 | 0.35 | 82,82,82,82 | 0 |
| 86 | OHX | A6 | 1988 | 7/7 | 0.93 | 0.22 | 138,138,138,138 | 7 |
| 87 | MG | BO | 207 | 1/1 | 0.93 | 0.66 | 56,56,56,56 | 0 |
| 86 | OHX | A1 | 3524 | 7/7 | 0.93 | 0.20 | 139,139,139,139 | 7 |
| 86 | OHX | CP | 201 | 7/7 | 0.93 | 0.14 | 177,177,177,177 | 7 |
| 86 | OHX | A6 | 1999 | 7/7 | 0.93 | 0.21 | 140,140,140,140 | 7 |
| 87 | MG | A5 | 3948 | 1/1 | 0.93 | 0.29 | 28,28,28,28 | 0 |
| 87 | MG | A1 | 4006 | 1/1 | 0.93 | 0.36 | 42,42,42,42 | 0 |
| 86 | OHX | Cg | 401 | 7/7 | 0.93 | 0.14 | 182,182,182,182 | 7 |
| 87 | MG | A1 | 4010 | 1/1 | 0.93 | 0.40 | 61,61,61,61 | 0 |
| 87 | MG | Dl | 101 | 1/1 | 0.93 | 0.47 | 112,112,112,112 | 0 |
| 87 | MG | A1 | 4482 | 1/1 | 0.93 | 0.16 | 129,129,129,129 | 0 |
| 87 | MG | A2 | 2104 | 1/1 | 0.93 | 0.28 | 63,63,63,63 | 0 |
| 87 | MG | Do | 202 | 1/1 | 0.93 | 0.44 | 50,50,50,50 | 0 |
| 87 | MG | A5 | 3956 | 1/1 | 0.93 | 0.30 | 39,39,39,39 | 0 |
| 87 | MG | A1 | 3893 | 1/1 | 0.93 | 0.19 | 26,26,26,26 | 0 |
| 86 | OHX | A5 | 3716 | 7/7 | 0.93 | 0.42 | 115,115,115,115 | 7 |
| 86 | OHX | A6 | 2062 | 7/7 | 0.93 | 0.24 | 163,163,163,163 | 7 |
| 86 | OHX | A6 | 2003 | 7/7 | 0.93 | 0.20 | 177,177,177,177 | 7 |
| 87 | MG | A1 | 4139 | 1/1 | 0.93 | 0.18 | 56,56,56,56 | 0 |
| 87 | MG | A5 | 3963 | 1/1 | 0.93 | 0.37 | 44,44,44,44 | 0 |
| 87 | MG | A1 | 4019 | 1/1 | 0.93 | 0.42 | 42,42,42,42 | 0 |
| 86 | OHX | A2 | 2006 | 7/7 | 0.94 | 0.15 | 162,162,162,162 | 7 |
| 86 | OHX | A6 | 2064 | 7/7 | 0.94 | 0.12 | 164,164,164,164 | 7 |
| 87 | MG | A6 | 2208 | 1/1 | 0.94 | 0.11 | 56,56,56,56 | 0 |
| 86 | OHX | A5 | 3653 | 7/7 | 0.94 | 0.25 | 130,130,130,130 | 7 |
| 87 | MG | A1 | 4102 | 1/1 | 0.94 | 0.11 | 61,61,61,61 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | A5 | 4068 | 1/1 | 0.94 | 0.23 | 72,72,72,72 | 0 |
| 87 | MG | A1 | 3936 | 1/1 | 0.94 | 0.33 | 34,34,34,34 | 0 |
| 87 | MG | A5 | 4070 | 1/1 | 0.94 | 0.33 | 56,56,56,56 | 0 |
| 86 | OHX | A1 | 3608 | 7/7 | 0.94 | 0.19 | 160,160,160,160 | 7 |
| 87 | MG | A1 | 3938 | 1/1 | 0.94 | 0.29 | 48,48,48,48 | 0 |
| 86 | OHX | BP | 202 | 7/7 | 0.94 | 0.14 | 139,139,139,139 | 7 |
| 87 | MG | A1 | 4107 | 1/1 | 0.94 | 0.18 | 74,74,74,74 | 0 |
| 87 | MG | A5 | 4507 | 1/1 | 0.94 | 0.93 | 92,92,92,92 | 0 |
| 86 | OHX | A2 | 2035 | 7/7 | 0.94 | 0.26 | 120,120,120,120 | 7 |
| 87 | MG | A5 | 4289 | 1/1 | 0.94 | 0.42 | 112,112,112,112 | 0 |
| 87 | MG | BN | 302 | 1/1 | 0.94 | 0.28 | 44,44,44,44 | 0 |
| 86 | OHX | A5 | 3659 | 7/7 | 0.94 | 0.26 | 106,106,106,106 | 7 |
| 86 | OHX | A5 | 3661 | 7/7 | 0.94 | 0.17 | 134,134,134,134 | 7 |
| 87 | MG | A2 | 2150 | 1/1 | 0.94 | 0.15 | 102,102,102,102 | 0 |
| 86 | OHX | A1 | 3615 | 7/7 | 0.94 | 0.20 | 139,139,139,139 | 7 |
| 86 | OHX | A5 | 3663 | 7/7 | 0.94 | 0.25 | 136,136,136,136 | 7 |
| 87 | MG | A1 | 3948 | 1/1 | 0.94 | 0.40 | 55,55,55,55 | 0 |
| 87 | MG | A1 | 4266 | 1/1 | 0.94 | 0.18 | 70,70,70,70 | 0 |
| 87 | MG | A6 | 2226 | 1/1 | 0.94 | 0.22 | 68,68,68,68 | 0 |
| 86 | OHX | A6 | 1962 | 7/7 | 0.94 | 0.18 | 126,126,126,126 | 7 |
| 87 | MG | A1 | 3951 | 1/1 | 0.94 | 0.43 | 46,46,46,46 | 0 |
| 87 | MG | A5 | 4303 | 1/1 | 0.94 | 0.60 | 57,57,57,57 | 0 |
| 86 | OHX | A5 | 3666 | 7/7 | 0.94 | 0.28 | 127,127,127,127 | 7 |
| 87 | MG | A5 | 4525 | 1/1 | 0.94 | 0.70 | 66,66,66,66 | 0 |
| 87 | MG | Aa | 201 | 1/1 | 0.94 | 0.58 | 82,82,82,82 | 0 |
| 86 | OHX | A5 | 3667 | 7/7 | 0.94 | 0.34 | 100,100,100,100 | 7 |
| 86 | OHX | A5 | 3668 | 7/7 | 0.94 | 0.20 | 163,163,163,163 | 7 |
| 86 | OHX | AI | 301 | 7/7 | 0.94 | 0.13 | 156,156,156,156 | 7 |
| 87 | MG | A1 | 4124 | 1/1 | 0.94 | 0.23 | 53,53,53,53 | 0 |
| 86 | OHX | A1 | 3618 | 7/7 | 0.94 | 0.13 | 158,158,158,158 | 7 |
| 86 | OHX | A6 | 2072 | 7/7 | 0.94 | 0.32 | 133,133,133,133 | 7 |
| 87 | MG | A5 | 4535 | 1/1 | 0.94 | 0.17 | 68,68,68,68 | 0 |
| 87 | MG | A5 | 3886 | 1/1 | 0.94 | 0.28 | 43,43,43,43 | 0 |
| 86 | OHX | A6 | 1978 | 7/7 | 0.94 | 0.18 | 146,146,146,146 | 7 |
| 86 | OHX | A6 | 1982 | 7/7 | 0.94 | 0.20 | 123,123,123,123 | 7 |
| 86 | OHX | A2 | 1931 | 7/7 | 0.94 | 0.19 | 143,143,143,143 | 7 |
| 87 | MG | A1 | 4446 | 1/1 | 0.94 | 0.19 | 62,62,62,62 | 0 |
| 87 | MG | A1 | 4131 | 1/1 | 0.94 | 0.15 | 75,75,75,75 | 0 |
| 86 | OHX | A2 | 2049 | 7/7 | 0.94 | 0.16 | 140,140,140,140 | 7 |
| 86 | OHX | A5 | 3678 | 7/7 | 0.94 | 0.23 | 111,111,111,111 | 7 |
| 86 | OHX | A5 | 3679 | 7/7 | 0.94 | 0.15 | 174,174,174,174 | 7 |
| 86 | OHX | A6 | 1989 | 7/7 | 0.94 | 0.19 | 122,122,122,122 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | A1 | 4287 | 1/1 | 0.94 | 0.27 | 61,61,61,61 | 0 |
| 86 | OHX | A6 | 1990 | 7/7 | 0.94 | 0.17 | 177,177,177,177 | 7 |
| 86 | OHX | A1 | 3627 | 7/7 | 0.94 | 0.18 | 130,130,130,130 | 7 |
| 87 | MG | A1 | 4138 | 1/1 | 0.94 | 0.30 | 62,62,62,62 | 0 |
| 87 | MG | A5 | 4112 | 1/1 | 0.94 | 0.23 | 65,65,65,65 | 0 |
| 87 | MG | BV | 203 | 1/1 | 0.94 | 0.27 | 63,63,63,63 | 0 |
| 86 | OHX | A5 | 3686 | 7/7 | 0.94 | 0.19 | 121,121,121,121 | 7 |
| 87 | MG | A1 | 3975 | 1/1 | 0.94 | 0.32 | 67,67,67,67 | 0 |
| 87 | MG | A5 | 4331 | 1/1 | 0.94 | 0.19 | 104,104,104,104 | 0 |
| 86 | OHX | A6 | 1994 | 7/7 | 0.94 | 0.19 | 133,133,133,133 | 7 |
| 86 | OHX | A6 | 1996 | 7/7 | 0.94 | 0.16 | 148,148,148,148 | 7 |
| 87 | MG | A6 | 2263 | 1/1 | 0.94 | 0.20 | 89,89,89,89 | 0 |
| 87 | MG | A5 | 3908 | 1/1 | 0.94 | 0.28 | 37,37,37,37 | 0 |
| 87 | MG | A5 | 4122 | 1/1 | 0.94 | 0.31 | 52,52,52,52 | 0 |
| 87 | MG | A5 | 4123 | 1/1 | 0.94 | 0.12 | 39,39,39,39 | 0 |
| 86 | OHX | A5 | 3690 | 7/7 | 0.94 | 0.21 | 130,130,130,130 | 7 |
| 86 | OHX | A5 | 3691 | 7/7 | 0.94 | 0.18 | 155,155,155,155 | 7 |
| 86 | OHX | A1 | 3692 | 7/7 | 0.94 | 0.21 | 124,124,124,124 | 7 |
| 86 | OHX | A5 | 3694 | 7/7 | 0.94 | 0.23 | 127,127,127,127 | 7 |
| 87 | MG | Ba | 206 | 1/1 | 0.94 | 0.28 | 61,61,61,61 | 0 |
| 86 | OHX | A5 | 3695 | 7/7 | 0.94 | 0.20 | 158,158,158,158 | 7 |
| 86 | OHX | A1 | 3695 | 7/7 | 0.94 | 0.13 | 163,163,163,163 | 7 |
| 86 | OHX | A1 | 3696 | 7/7 | 0.94 | 0.25 | 143,143,143,143 | 7 |
| 86 | OHX | A1 | 3747 | 7/7 | 0.94 | 0.34 | 118,118,118,118 | 7 |
| 86 | OHX | A5 | 3702 | 7/7 | 0.94 | 0.24 | 121,121,121,121 | 7 |
| 86 | OHX | A5 | 3703 | 7/7 | 0.94 | 0.21 | 123,123,123,123 | 7 |
| 86 | OHX | A6 | 2010 | 7/7 | 0.94 | 0.13 | 181,181,181,181 | 7 |
| 86 | OHX | A5 | 3705 | 7/7 | 0.94 | 0.17 | 152,152,152,152 | 7 |
| 86 | OHX | A8 | 206 | 7/7 | 0.94 | 0.19 | 136,136,136,136 | 7 |
| 87 | MG | A7 | 216 | 1/1 | 0.94 | 0.37 | 78,78,78,78 | 0 |
| 87 | MG | A5 | 4140 | 1/1 | 0.94 | 0.16 | 56,56,56,56 | 0 |
| 86 | OHX | A5 | 3706 | 7/7 | 0.94 | 0.18 | 139,139,139,139 | 7 |
| 86 | OHX | A1 | 3628 | 7/7 | 0.94 | 0.18 | 154,154,154,154 | 7 |
| 87 | MG | A1 | 4160 | 1/1 | 0.94 | 0.24 | 70,70,70,70 | 0 |
| 87 | MG | A5 | 4145 | 1/1 | 0.94 | 0.18 | 57,57,57,57 | 0 |
| 86 | OHX | A5 | 3708 | 7/7 | 0.94 | 0.17 | 141,141,141,141 | 7 |
| 87 | MG | A1 | 3999 | 1/1 | 0.94 | 0.34 | 37,37,37,37 | 0 |
| 86 | OHX | A6 | 2015 | 7/7 | 0.94 | 0.22 | 159,159,159,159 | 7 |
| 87 | MG | A1 | 4003 | 1/1 | 0.94 | 0.46 | 48,48,48,48 | 0 |
| 86 | OHX | A1 | 3699 | 7/7 | 0.94 | 0.25 | 107,107,107,107 | 7 |
| 87 | MG | A5 | 3935 | 1/1 | 0.94 | 0.29 | 51,51,51,51 | 0 |
| 87 | MG | A5 | 3936 | 1/1 | 0.94 | 0.42 | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86 | OHX | A1 | 3629 | 7/7 | 0.94 | 0.18 | 128,128,128,128 | 7 |
| 87 | MG | A6 | 2102 | 1/1 | 0.94 | 0.22 | 63,63,63,63 | 0 |
| 87 | MG | A1 | 4168 | 1/1 | 0.94 | 0.16 | 44,44,44,44 | 0 |
| 86 | OHX | A6 | 2021 | 7/7 | 0.94 | 0.21 | 131,131,131,131 | 7 |
| 86 | OHX | A5 | 3713 | 7/7 | 0.94 | 0.23 | 122,122,122,122 | 7 |
| 86 | OHX | A5 | 3715 | 7/7 | 0.94 | 0.23 | 100,100,100,100 | 7 |
| 86 | OHX | A1 | 3701 | 7/7 | 0.94 | 0.38 | 112,112,112,112 | 7 |
| 87 | MG | A6 | 2298 | 1/1 | 0.94 | 0.09 | 77,77,77,77 | 0 |
| 87 | MG | A1 | 3856 | 1/1 | 0.94 | 0.28 | 38,38,38,38 | 0 |
| 87 | MG | A6 | 2300 | 1/1 | 0.94 | 0.55 | 56,56,56,56 | 0 |
| 86 | OHX | A5 | 3717 | 7/7 | 0.94 | 0.50 | 108,108,108,108 | 7 |
| 87 | MG | A5 | 3950 | 1/1 | 0.94 | 0.43 | 38,38,38,38 | 0 |
| 87 | MG | A1 | 4018 | 1/1 | 0.94 | 0.42 | 38,38,38,38 | 0 |
| 87 | MG | A6 | 2114 | 1/1 | 0.94 | 0.36 | 61,61,61,61 | 0 |
| 87 | MG | A6 | 2304 | 1/1 | 0.94 | 0.10 | 81,81,81,81 | 0 |
| 86 | OHX | A5 | 3718 | 7/7 | 0.94 | 0.14 | 157,157,157,157 | 7 |
| 86 | OHX | A1 | 3635 | 7/7 | 0.94 | 0.29 | 84,84,84,84 | 7 |
| 87 | MG | A8 | 227 | 1/1 | 0.94 | 0.19 | 65,65,65,65 | 0 |
| 86 | OHX | DH | 201 | 7/7 | 0.94 | 0.14 | 142,142,142,142 | 7 |
| 87 | MG | A1 | 4025 | 1/1 | 0.94 | 0.45 | 39,39,39,39 | 0 |
| 87 | MG | A8 | 230 | 1/1 | 0.94 | 0.55 | 68,68,68,68 | 0 |
| 86 | OHX | DI | 301 | 7/7 | 0.94 | 0.20 | 118,118,118,118 | 7 |
| 87 | MG | A5 | 4388 | 1/1 | 0.94 | 0.46 | 47,47,47,47 | 0 |
| 87 | MG | A1 | 3862 | 1/1 | 0.94 | 0.23 | 76,76,76,76 | 0 |
| 86 | OHX | A6 | 2096 | 7/7 | 0.94 | 0.19 | 156,156,156,156 | 7 |
| 87 | MG | A6 | 2123 | 1/1 | 0.94 | 0.35 | 51,51,51,51 | 0 |
| 87 | MG | A1 | 4031 | 1/1 | 0.94 | 0.22 | 32,32,32,32 | 0 |
| 87 | MG | A1 | 4185 | 1/1 | 0.94 | 0.24 | 65,65,65,65 | 0 |
| 87 | MG | A8 | 239 | 1/1 | 0.94 | 0.12 | 93,93,93,93 | 0 |
| 86 | OHX | A5 | 3723 | 7/7 | 0.94 | 0.18 | 180,180,180,180 | 7 |
| 87 | MG | A5 | 3967 | 1/1 | 0.94 | 0.36 | 57,57,57,57 | 0 |
| 87 | MG | A5 | 4185 | 1/1 | 0.94 | 0.76 | 49,49,49,49 | 0 |
| 86 | OHX | A1 | 3802 | 7/7 | 0.94 | 0.40 | 146,146,146,146 | 7 |
| 87 | MG | A5 | 4398 | 1/1 | 0.94 | 0.20 | 54,54,54,54 | 0 |
| 87 | MG | DB | 405 | 1/1 | 0.94 | 0.80 | 62,62,62,62 | 0 |
| 86 | OHX | A1 | 3636 | 7/7 | 0.94 | 0.16 | 148,148,148,148 | 7 |
| 86 | OHX | A5 | 3726 | 7/7 | 0.94 | 0.16 | 135,135,135,135 | 7 |
| 86 | OHX | A1 | 3403 | 7/7 | 0.94 | 0.14 | 169,169,169,169 | 7 |
| 86 | OHX | A6 | 2100 | 7/7 | 0.94 | 0.32 | 206,206,206,206 | 7 |
| 86 | OHX | A5 | 3729 | 7/7 | 0.94 | 0.19 | 165,165,165,165 | 7 |
| 87 | MG | A3 | 216 | 1/1 | 0.94 | 0.16 | 67,67,67,67 | 0 |
| 87 | MG | A1 | 4039 | 1/1 | 0.94 | 0.37 | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87 | MG | A1 | 4346 | 1/1 | 0.94 | 0.32 | 53,53,53,53 | 0 |
| 87 | MG | A5 | 3981 | 1/1 | 0.94 | 0.42 | 79,79,79,79 | 0 |
| 86 | OHX | A2 | 2078 | 7/7 | 0.94 | 0.27 | 169,169,169,169 | 7 |
| 86 | OHX | A6 | 2029 | 7/7 | 0.94 | 0.23 | 141,141,141,141 | 7 |
| 86 | OHX | A6 | 2030 | 7/7 | 0.94 | 0.11 | 170,170,170,170 | 7 |
| 87 | MG | DC | 407 | 1/1 | 0.94 | 0.73 | 75,75,75,75 | 0 |
| 87 | MG | A5 | 4412 | 1/1 | 0.94 | 0.33 | 104,104,104,104 | 0 |
| 86 | OHX | A1 | 3453 | 7/7 | 0.94 | 0.31 | 134,134,134,134 | 0 |
| 86 | OHX | A1 | 3651 | 7/7 | 0.94 | 0.19 | 131,131,131,131 | 7 |
| 87 | MG | A5 | 4201 | 1/1 | 0.94 | 0.16 | 49,49,49,49 | 0 |
| 87 | MG | DD | 308 | 1/1 | 0.94 | 1.18 | 70,70,70,70 | 0 |
| 86 | OHX | A1 | 3652 | 7/7 | 0.94 | 0.26 | 115,115,115,115 | 7 |
| 87 | MG | A1 | 4355 | 1/1 | 0.94 | 0.25 | 53,53,53,53 | 0 |
| 87 | MG | A5 | 4204 | 1/1 | 0.94 | 0.12 | 56,56,56,56 | 0 |
| 86 | OHX | A6 | 2035 | 7/7 | 0.94 | 0.20 | 129,129,129,129 | 7 |
| 86 | OHX | A1 | 3761 | 7/7 | 0.94 | 0.11 | 173,173,173,173 | 7 |
| 87 | MG | A1 | 3885 | 1/1 | 0.94 | 0.27 | 61,61,61,61 | 0 |
| 86 | OHX | A2 | 2014 | 7/7 | 0.94 | 0.25 | 166,166,166,166 | 7 |
| 87 | MG | A2 | 2220 | 1/1 | 0.94 | 0.15 | 111,111,111,111 | 0 |
| 86 | OHX | A1 | 3714 | 7/7 | 0.94 | 0.23 | 118,118,118,118 | 7 |
| 87 | MG | DL | 201 | 1/1 | 0.94 | 1.06 | 94,94,94,94 | 0 |
| 87 | MG | A2 | 2100 | 1/1 | 0.94 | 0.25 | 67,67,67,67 | 0 |
| 87 | MG | A1 | 4208 | 1/1 | 0.94 | 0.63 | 58,58,58,58 | 0 |
| 87 | MG | A5 | 3999 | 1/1 | 0.94 | 0.25 | 32,32,32,32 | 0 |
| 87 | MG | A5 | 4433 | 1/1 | 0.94 | 0.14 | 83,83,83,83 | 0 |
| 86 | OHX | A1 | 3657 | 7/7 | 0.94 | 0.15 | 166,166,166,166 | 7 |
| 86 | OHX | A2 | 1987 | 7/7 | 0.94 | 0.20 | 147,147,147,147 | 7 |
| 87 | MG | A1 | 4366 | 1/1 | 0.94 | 0.28 | 86,86,86,86 | 0 |
| 86 | OHX | A2 | 2002 | 7/7 | 0.94 | 0.11 | 169,169,169,169 | 7 |
| 86 | OHX | A5 | 3521 | 7/7 | 0.94 | 0.21 | 150,150,150,150 | 7 |
| 87 | MG | DP | 202 | 1/1 | 0.94 | 0.20 | 56,56,56,56 | 0 |
| 87 | MG | A1 | 3895 | 1/1 | 0.94 | 0.22 | 92,92,92,92 | 0 |
| 87 | MG | A2 | 2107 | 1/1 | 0.94 | 0.45 | 66,66,66,66 | 0 |
| 86 | OHX | A1 | 3549 | 7/7 | 0.94 | 0.25 | 139,139,139,139 | 7 |
| 86 | OHX | A5 | 3541 | 7/7 | 0.94 | 0.23 | 113,113,113,113 | 7 |
| 87 | MG | A5 | 4015 | 1/1 | 0.94 | 0.41 | 45,45,45,45 | 0 |
| 87 | MG | A5 | 4017 | 1/1 | 0.94 | 0.43 | 62,62,62,62 | 0 |
| 87 | MG | A5 | 4018 | 1/1 | 0.94 | 0.41 | 40,40,40,40 | 0 |
| 86 | OHX | A2 | 2040 | 7/7 | 0.94 | 0.12 | 171,171,171,171 | 7 |
| 87 | MG | A2 | 2112 | 1/1 | 0.94 | 0.38 | 95,95,95,95 | 0 |
| 86 | OHX | A5 | 3557 | 7/7 | 0.94 | 0.16 | 154,154,154,154 | 7 |
| 86 | OHX | A5 | 3572 | 7/7 | 0.94 | 0.19 | 145,145,145,145 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87 | MG | A1 | 4381 | 1/1 | 0.94 | 0.66 | 65,65,65,65 | 0 |
| 87 | MG | A2 | 2234 | 1/1 | 0.94 | 0.26 | 94,94,94,94 | 0 |
| 86 | OHX | A5 | 3755 | 7/7 | 0.94 | 0.17 | 174,174,174,174 | 7 |
| 87 | MG | A6 | 2174 | 1/1 | 0.94 | 0.18 | 50,50,50,50 | 0 |
| 87 | MG | A5 | 4031 | 1/1 | 0.94 | 0.45 | 39,39,39,39 | 0 |
| 86 | OHX | A1 | 3667 | 7/7 | 0.94 | 0.29 | 92,92,92,92 | 7 |
| 87 | MG | A2 | 2117 | 1/1 | 0.94 | 0.37 | 80,80,80,80 | 0 |
| 86 | OHX | A3 | 211 | 7/7 | 0.94 | 0.23 | 137,137,137,137 | 7 |
| 86 | OHX | A1 | 3668 | 7/7 | 0.94 | 0.18 | 151,151,151,151 | 7 |
| 87 | MG | A1 | 4388 | 1/1 | 0.94 | 0.51 | 78,78,78,78 | 0 |
| 86 | OHX | A5 | 3761 | 7/7 | 0.94 | 0.16 | 146,146,146,146 | 7 |
| 86 | OHX | A5 | 3609 | 7/7 | 0.94 | 0.14 | 153,153,153,153 | 7 |
| 86 | OHX | A5 | 3611 | 7/7 | 0.94 | 0.25 | 115,115,115,115 | 7 |
| 86 | OHX | A2 | 1966 | 7/7 | 0.94 | 0.23 | 101,101,101,101 | 7 |
| 87 | MG | A1 | 4393 | 1/1 | 0.94 | 0.72 | 78,78,78,78 | 0 |
| 86 | OHX | A4 | 209 | 7/7 | 0.94 | 0.15 | 153,153,153,153 | 7 |
| 87 | MG | A6 | 2188 | 1/1 | 0.94 | 0.21 | 38,38,38,38 | 0 |
| 86 | OHX | A1 | 3566 | 7/7 | 0.94 | 0.19 | 122,122,122,122 | 7 |
| 86 | OHX | A4 | 212 | 7/7 | 0.94 | 0.26 | 118,118,118,118 | 7 |
| 87 | MG | A1 | 4397 | 1/1 | 0.94 | 0.20 | 80,80,80,80 | 0 |
| 86 | OHX | A2 | 2056 | 7/7 | 0.94 | 0.23 | 130,130,130,130 | 7 |
| 86 | OHX | A2 | 2043 | 7/7 | 0.94 | 0.12 | 192,192,192,192 | 7 |
| 86 | OHX | A5 | 3630 | 7/7 | 0.94 | 0.21 | 128,128,128,128 | 7 |
| 87 | MG | A5 | 4052 | 1/1 | 0.94 | 0.21 | 46,46,46,46 | 0 |
| 86 | OHX | A6 | 2055 | 7/7 | 0.94 | 0.29 | 131,131,131,131 | 7 |
| 86 | OHX | A5 | 3634 | 7/7 | 0.94 | 0.17 | 130,130,130,130 | 7 |
| 86 | OHX | A1 | 3586 | 7/7 | 0.94 | 0.18 | 117,117,117,117 | 7 |
| 86 | OHX | BB | 401 | 7/7 | 0.94 | 0.19 | 111,111,111,111 | 7 |
| 86 | OHX | A2 | 1979 | 7/7 | 0.94 | 0.21 | 121,121,121,121 | 7 |
| 86 | OHX | A1 | 3679 | 7/7 | 0.94 | 0.27 | 114,114,114,114 | 7 |
| 86 | OHX | A2 | 2020 | 7/7 | 0.94 | 0.20 | 118,118,118,118 | 7 |
| 87 | MG | A6 | 2203 | 1/1 | 0.94 | 0.39 | 63,63,63,63 | 0 |
| 87 | MG | A1 | 3930 | 1/1 | 0.94 | 0.34 | 38,38,38,38 | 0 |
| 86 | OHX | A1 | 3606 | 7/7 | 0.94 | 0.17 | 132,132,132,132 | 7 |
| 87 | MG | A5 | 4523 | 1/1 | 0.95 | 0.30 | 65,65,65,65 | 0 |
| 86 | OHX | A2 | 2011 | 7/7 | 0.95 | 0.16 | 154,154,154,154 | 7 |
| 86 | OHX | A5 | 3560 | 7/7 | 0.95 | 0.23 | 106,106,106,106 | 7 |
| 87 | MG | A6 | 2183 | 1/1 | 0.95 | 0.26 | 64,64,64,64 | 0 |
| 87 | MG | A5 | 4150 | 1/1 | 0.95 | 0.61 | 68,68,68,68 | 0 |
| 86 | OHX | A5 | 3571 | 7/7 | 0.95 | 0.19 | 143,143,143,143 | 7 |
| 86 | OHX | A1 | 3713 | 7/7 | 0.95 | 0.24 | 101,101,101,101 | 7 |
| 87 | MG | A1 | 4051 | 1/1 | 0.95 | 0.36 | 71,71,71,71 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86 | OHX | A5 | 3583 | 7/7 | 0.95 | 0.17 | 137,137,137,137 | 7 |
| 86 | OHX | A5 | 3714 | 7/7 | 0.95 | 0.21 | 126,126,126,126 | 7 |
| 87 | MG | A5 | 3978 | 1/1 | 0.95 | 0.28 | 29,29,29,29 | 0 |
| 86 | OHX | A5 | 3584 | 7/7 | 0.95 | 0.22 | 119,119,119,119 | 7 |
| 86 | OHX | A5 | 3820 | 7/7 | 0.95 | 0.39 | 80,80,80,80 | 7 |
| 86 | OHX | A6 | 2059 | 7/7 | 0.95 | 0.15 | 153,153,153,153 | 7 |
| 86 | OHX | A6 | 1986 | 7/7 | 0.95 | 0.14 | 165,165,165,165 | 7 |
| 87 | MG | A1 | 4186 | 1/1 | 0.95 | 0.19 | 75,75,75,75 | 0 |
| 86 | OHX | A5 | 3593 | 7/7 | 0.95 | 0.15 | 134,134,134,134 | 7 |
| 87 | MG | BN | 307 | 1/1 | 0.95 | 0.80 | 58,58,58,58 | 0 |
| 86 | OHX | A7 | 207 | 7/7 | 0.95 | 0.17 | 145,145,145,145 | 7 |
| 87 | MG | A1 | 3926 | 1/1 | 0.95 | 0.29 | 55,55,55,55 | 0 |
| 87 | MG | A1 | 4062 | 1/1 | 0.95 | 0.32 | 72,72,72,72 | 0 |
| 87 | MG | A5 | 4167 | 1/1 | 0.95 | 0.24 | 71,71,71,71 | 0 |
| 86 | OHX | A7 | 209 | 7/7 | 0.95 | 0.20 | 115,115,115,115 | 7 |
| 87 | MG | A5 | 4550 | 1/1 | 0.95 | 1.13 | 83,83,83,83 | 0 |
| 86 | OHX | A5 | 3594 | 7/7 | 0.95 | 0.18 | 131,131,131,131 | 7 |
| 86 | OHX | A7 | 211 | 7/7 | 0.95 | 0.21 | 117,117,117,117 | 7 |
| 86 | OHX | A5 | 3595 | 7/7 | 0.95 | 0.19 | 125,125,125,125 | 7 |
| 87 | MG | A5 | 4173 | 1/1 | 0.95 | 0.30 | 67,67,67,67 | 0 |
| 86 | OHX | A5 | 3722 | 7/7 | 0.95 | 0.14 | 164,164,164,164 | 7 |
| 87 | MG | A5 | 4358 | 1/1 | 0.95 | 0.59 | 54,54,54,54 | 0 |
| 86 | OHX | A5 | 3602 | 7/7 | 0.95 | 0.24 | 109,109,109,109 | 7 |
| 86 | OHX | A2 | 1982 | 7/7 | 0.95 | 0.19 | 125,125,125,125 | 7 |
| 86 | OHX | A5 | 3607 | 7/7 | 0.95 | 0.23 | 142,142,142,142 | 7 |
| 87 | MG | A5 | 4362 | 1/1 | 0.95 | 0.34 | 60,60,60,60 | 0 |
| 86 | OHX | A1 | 3673 | 7/7 | 0.95 | 0.22 | 154,154,154,154 | 7 |
| 87 | MG | BP | 210 | 1/1 | 0.95 | 0.57 | 46,46,46,46 | 0 |
| 87 | MG | A5 | 4001 | 1/1 | 0.95 | 0.40 | 48,48,48,48 | 0 |
| 86 | OHX | A1 | 3760 | 7/7 | 0.95 | 0.18 | 136,136,136,136 | 7 |
| 86 | OHX | A1 | 3519 | 7/7 | 0.95 | 0.17 | 137,137,137,137 | 7 |
| 87 | MG | A1 | 4469 | 1/1 | 0.95 | 0.44 | 66,66,66,66 | 0 |
| 87 | MG | A5 | 4006 | 1/1 | 0.95 | 0.38 | 40,40,40,40 | 0 |
| 86 | OHX | A5 | 3614 | 7/7 | 0.95 | 0.22 | 120,120,120,120 | 7 |
| 87 | MG | A1 | 3941 | 1/1 | 0.95 | 0.35 | 52,52,52,52 | 0 |
| 86 | OHX | A1 | 3520 | 7/7 | 0.95 | 0.18 | 129,129,129,129 | 7 |
| 86 | OHX | A5 | 3620 | 7/7 | 0.95 | 0.20 | 113,113,113,113 | 7 |
| 87 | MG | A6 | 2217 | 1/1 | 0.95 | 0.75 | 87,87,87,87 | 0 |
| 86 | OHX | A2 | 2000 | 7/7 | 0.95 | 0.20 | 140,140,140,140 | 7 |
| 87 | MG | A5 | 4376 | 1/1 | 0.95 | 0.87 | 67,67,67,67 | 0 |
| 87 | MG | A5 | 4016 | 1/1 | 0.95 | 0.30 | 42,42,42,42 | 0 |
| 86 | OHX | DA | 302 | 7/7 | 0.95 | 0.32 | 157,157,157,157 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86 | OHX | A6 | 1998 | 7/7 | 0.95 | 0.14 | 147,147,147,147 | 7 |
| 87 | MG | A1 | 4209 | 1/1 | 0.95 | 0.17 | 76,76,76,76 | 0 |
| 87 | MG | A5 | 4020 | 1/1 | 0.95 | 0.43 | 33,33,33,33 | 0 |
| 87 | MG | A1 | 4083 | 1/1 | 0.95 | 0.19 | 44,44,44,44 | 0 |
| 86 | OHX | DC | 401 | 7/7 | 0.95 | 0.16 | 148,148,148,148 | 7 |
| 86 | OHX | A1 | 3539 | 7/7 | 0.95 | 0.21 | 103,103,103,103 | 7 |
| 87 | MG | A5 | 3843 | 1/1 | 0.95 | 0.25 | 50,50,50,50 | 0 |
| 87 | MG | A5 | 4025 | 1/1 | 0.95 | 0.32 | 38,38,38,38 | 0 |
| 86 | OHX | A1 | 3542 | 7/7 | 0.95 | 0.19 | 159,159,159,159 | 7 |
| 86 | OHX | A5 | 3626 | 7/7 | 0.95 | 0.18 | 147,147,147,147 | 7 |
| 86 | OHX | A5 | 3740 | 7/7 | 0.95 | 0.21 | 155,155,155,155 | 7 |
| 87 | MG | A5 | 4029 | 1/1 | 0.95 | 0.40 | 44,44,44,44 | 0 |
| 87 | MG | A5 | 4030 | 1/1 | 0.95 | 0.45 | 39,39,39,39 | 0 |
| 86 | OHX | A5 | 3628 | 7/7 | 0.95 | 0.18 | 129,129,129,129 | 7 |
| 87 | MG | A1 | 3954 | 1/1 | 0.95 | 0.24 | 45,45,45,45 | 0 |
| 86 | OHX | A5 | 3629 | 7/7 | 0.95 | 0.25 | 100,100,100,100 | 7 |
| 86 | OHX | A5 | 3743 | 7/7 | 0.95 | 0.24 | 167,167,167,167 | 7 |
| 87 | MG | A6 | 2234 | 1/1 | 0.95 | 0.17 | 92,92,92,92 | 0 |
| 86 | OHX | A6 | 2004 | 7/7 | 0.95 | 0.19 | 105,105,105,105 | 7 |
| 86 | OHX | A6 | 2005 | 7/7 | 0.95 | 0.18 | 145,145,145,145 | 7 |
| 86 | OHX | A6 | 2007 | 7/7 | 0.95 | 0.12 | 164,164,164,164 | 7 |
| 87 | MG | A5 | 4400 | 1/1 | 0.95 | 0.30 | 86,86,86,86 | 0 |
| 87 | MG | A7 | 237 | 1/1 | 0.95 | 0.43 | 69,69,69,69 | 0 |
| 87 | MG | A1 | 4098 | 1/1 | 0.95 | 0.19 | 54,54,54,54 | 0 |
| 86 | OHX | A1 | 3767 | 7/7 | 0.95 | 0.19 | 158,158,158,158 | 7 |
| 86 | OHX | A5 | 3638 | 7/7 | 0.95 | 0.18 | 135,135,135,135 | 7 |
| 86 | OHX | A5 | 3749 | 7/7 | 0.95 | 0.13 | 178,178,178,178 | 7 |
| 87 | MG | Be | 202 | 1/1 | 0.95 | 0.44 | 67,67,67,67 | 0 |
| 87 | MG | Bf | 202 | 1/1 | 0.95 | 0.51 | 69,69,69,69 | 0 |
| 87 | MG | A1 | 3967 | 1/1 | 0.95 | 0.42 | 40,40,40,40 | 0 |
| 87 | MG | A5 | 3865 | 1/1 | 0.95 | 0.28 | 37,37,37,37 | 0 |
| 86 | OHX | A5 | 3639 | 7/7 | 0.95 | 0.16 | 157,157,157,157 | 7 |
| 86 | OHX | A2 | 1956 | 7/7 | 0.95 | 0.18 | 128,128,128,128 | 7 |
| 87 | MG | A5 | 3869 | 1/1 | 0.95 | 0.37 | 58,58,58,58 | 0 |
| 86 | OHX | A5 | 3643 | 7/7 | 0.95 | 0.14 | 150,150,150,150 | 7 |
| 86 | OHX | A1 | 3624 | 7/7 | 0.95 | 0.26 | 137,137,137,137 | 7 |
| 86 | OHX | A5 | 3645 | 7/7 | 0.95 | 0.20 | 141,141,141,141 | 7 |
| 87 | MG | A6 | 2251 | 1/1 | 0.95 | 0.55 | 73,73,73,73 | 0 |
| 87 | MG | A5 | 4416 | 1/1 | 0.95 | 0.54 | 48,48,48,48 | 0 |
| 87 | MG | A5 | 4417 | 1/1 | 0.95 | 0.66 | 50,50,50,50 | 0 |
| 87 | MG | A5 | 3874 | 1/1 | 0.95 | 0.31 | 32,32,32,32 | 0 |
| 86 | OHX | A2 | 2016 | 7/7 | 0.95 | 0.15 | 156,156,156,156 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86 | OHX | A6 | 2014 | 7/7 | 0.95 | 0.16 | 144,144,144,144 | 7 |
| 87 | MG | A1 | 4367 | 1/1 | 0.95 | 0.18 | 69,69,69,69 | 0 |
| 87 | MG | A5 | 4236 | 1/1 | 0.95 | 0.14 | 19,19,19,19 | 0 |
| 87 | MG | A5 | 4237 | 1/1 | 0.95 | 0.21 | 51,51,51,51 | 0 |
| 86 | OHX | A1 | 3682 | 7/7 | 0.95 | 0.13 | 145,145,145,145 | 7 |
| 87 | MG | A6 | 2256 | 1/1 | 0.95 | 0.19 | 73,73,73,73 | 0 |
| 87 | MG | A1 | 4111 | 1/1 | 0.95 | 0.26 | 65,65,65,65 | 0 |
| 87 | MG | A5 | 4429 | 1/1 | 0.95 | 0.17 | 58,58,58,58 | 0 |
| 87 | MG | DB | 406 | 1/1 | 0.95 | 0.63 | 47,47,47,47 | 0 |
| 86 | OHX | A1 | 3550 | 7/7 | 0.95 | 0.18 | 130,130,130,130 | 7 |
| 87 | MG | A6 | 2260 | 1/1 | 0.95 | 0.24 | 62,62,62,62 | 0 |
| 86 | OHX | A3 | 207 | 7/7 | 0.95 | 0.15 | 167,167,167,167 | 7 |
| 86 | OHX | A2 | 2031 | 7/7 | 0.95 | 0.13 | 140,140,140,140 | 7 |
| 86 | OHX | A1 | 3633 | 7/7 | 0.95 | 0.22 | 101,101,101,101 | 7 |
| 87 | MG | A3 | 217 | 1/1 | 0.95 | 0.41 | 56,56,56,56 | 0 |
| 87 | MG | A5 | 4436 | 1/1 | 0.95 | 0.76 | 90,90,90,90 | 0 |
| 86 | OHX | A1 | 3634 | 7/7 | 0.95 | 0.15 | 133,133,133,133 | 7 |
| 86 | OHX | A1 | 3557 | 7/7 | 0.95 | 0.18 | 121,121,121,121 | 7 |
| 86 | OHX | A1 | 3558 | 7/7 | 0.95 | 0.17 | 139,139,139,139 | 7 |
| 86 | OHX | A1 | 3638 | 7/7 | 0.95 | 0.16 | 141,141,141,141 | 7 |
| 87 | MG | A1 | 4380 | 1/1 | 0.95 | 0.21 | 95,95,95,95 | 0 |
| 86 | OHX | A2 | 1968 | 7/7 | 0.95 | 0.18 | 134,134,134,134 | 7 |
| 86 | OHX | A2 | 1965 | 7/7 | 0.95 | 0.20 | 138,138,138,138 | 7 |
| 86 | OHX | A2 | 1995 | 7/7 | 0.95 | 0.13 | 171,171,171,171 | 7 |
| 86 | OHX | A4 | 214 | 7/7 | 0.95 | 0.15 | 167,167,167,167 | 7 |
| 86 | OHX | A6 | 2092 | 7/7 | 0.95 | 0.38 | 182,182,182,182 | 7 |
| 86 | OHX | A1 | 3694 | 7/7 | 0.95 | 0.21 | 131,131,131,131 | 7 |
| 86 | OHX | A6 | 2033 | 7/7 | 0.95 | 0.31 | 133,133,133,133 | 7 |
| 86 | OHX | A5 | 3670 | 7/7 | 0.95 | 0.22 | 109,109,109,109 | 7 |
| 87 | MG | A6 | 2279 | 1/1 | 0.95 | 0.23 | 81,81,81,81 | 0 |
| 87 | MG | A6 | 2120 | 1/1 | 0.95 | 0.38 | 51,51,51,51 | 0 |
| 87 | MG | A1 | 3872 | 1/1 | 0.95 | 0.28 | 37,37,37,37 | 0 |
| 87 | MG | A1 | 4130 | 1/1 | 0.95 | 0.28 | 69,69,69,69 | 0 |
| 86 | OHX | A1 | 3646 | 7/7 | 0.95 | 0.21 | 110,110,110,110 | 7 |
| 87 | MG | A1 | 3997 | 1/1 | 0.95 | 0.35 | 40,40,40,40 | 0 |
| 86 | OHX | A1 | 3573 | 7/7 | 0.95 | 0.18 | 120,120,120,120 | 7 |
| 87 | MG | A5 | 4271 | 1/1 | 0.95 | 0.82 | 68,68,68,68 | 0 |
| 86 | OHX | A2 | 1980 | 7/7 | 0.95 | 0.15 | 152,152,152,152 | 7 |
| 87 | MG | A2 | 2121 | 1/1 | 0.95 | 0.37 | 61,61,61,61 | 0 |
| 87 | MG | A1 | 4262 | 1/1 | 0.95 | 0.21 | 70,70,70,70 | 0 |
| 87 | MG | A5 | 4275 | 1/1 | 0.95 | 0.43 | 63,63,63,63 | 0 |
| 87 | MG | A5 | 4466 | 1/1 | 0.95 | 0.23 | 79,79,79,79 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | A4 | 222 | 1/1 | 0.95 | 0.37 | 43,43,43,43 | 0 |
| 87 | MG | A4 | 224 | 1/1 | 0.95 | 0.18 | 30,30,30,30 | 0 |
| 87 | MG | A4 | 225 | 1/1 | 0.95 | 0.38 | 65,65,65,65 | 0 |
| 87 | MG | A1 | 4004 | 1/1 | 0.95 | 0.42 | 57,57,57,57 | 0 |
| 86 | OHX | BC | 401 | 7/7 | 0.95 | 0.21 | 130,130,130,130 | 7 |
| 86 | OHX | A6 | 2038 | 7/7 | 0.95 | 0.18 | 169,169,169,169 | 7 |
| 87 | MG | A1 | 4009 | 1/1 | 0.95 | 0.44 | 51,51,51,51 | 0 |
| 86 | OHX | A2 | 2009 | 7/7 | 0.95 | 0.11 | 144,144,144,144 | 7 |
| 86 | OHX | A6 | 2040 | 7/7 | 0.95 | 0.24 | 87,87,87,87 | 7 |
| 86 | OHX | CG | 301 | 7/7 | 0.95 | 0.13 | 147,147,147,147 | 7 |
| 87 | MG | A2 | 2127 | 1/1 | 0.95 | 0.33 | 49,49,49,49 | 0 |
| 86 | OHX | A1 | 3590 | 7/7 | 0.95 | 0.14 | 135,135,135,135 | 7 |
| 86 | OHX | A5 | 3681 | 7/7 | 0.95 | 0.31 | 112,112,112,112 | 7 |
| 87 | MG | A1 | 4017 | 1/1 | 0.95 | 0.40 | 48,48,48,48 | 0 |
| 86 | OHX | A1 | 3658 | 7/7 | 0.95 | 0.19 | 118,118,118,118 | 7 |
| 87 | MG | A2 | 2131 | 1/1 | 0.95 | 0.19 | 65,65,65,65 | 0 |
| 87 | MG | A5 | 3932 | 1/1 | 0.95 | 0.31 | 34,34,34,34 | 0 |
| 86 | OHX | A5 | 3684 | 7/7 | 0.95 | 0.20 | 122,122,122,122 | 7 |
| 86 | OHX | A1 | 3659 | 7/7 | 0.95 | 0.16 | 156,156,156,156 | 7 |
| 87 | MG | A1 | 4152 | 1/1 | 0.95 | 0.19 | 34,34,34,34 | 0 |
| 86 | OHX | CL | 201 | 7/7 | 0.95 | 0.17 | 134,134,134,134 | 7 |
| 86 | OHX | Ag | 401 | 7/7 | 0.95 | 0.14 | 167,167,167,167 | 7 |
| 86 | OHX | A1 | 3661 | 7/7 | 0.95 | 0.23 | 118,118,118,118 | 7 |
| 86 | OHX | A1 | 3706 | 7/7 | 0.95 | 0.16 | 135,135,135,135 | 7 |
| 86 | OHX | CS | 201 | 7/7 | 0.95 | 0.18 | 129,129,129,129 | 7 |
| 86 | OHX | A1 | 3600 | 7/7 | 0.95 | 0.22 | 100,100,100,100 | 7 |
| 87 | MG | A1 | 4286 | 1/1 | 0.95 | 0.84 | 57,57,57,57 | 0 |
| 86 | OHX | A6 | 1947 | 7/7 | 0.95 | 0.17 | 134,134,134,134 | 7 |
| 86 | OHX | A5 | 3404 | 7/7 | 0.95 | 0.24 | 111,111,111,111 | 7 |
| 86 | OHX | A6 | 1955 | 7/7 | 0.95 | 0.15 | 153,153,153,153 | 7 |
| 87 | MG | A6 | 2162 | 1/1 | 0.95 | 0.49 | 63,63,63,63 | 0 |
| 87 | MG | A5 | 4128 | 1/1 | 0.95 | 0.16 | 66,66,66,66 | 0 |
| 86 | OHX | A6 | 1961 | 7/7 | 0.95 | 0.24 | 132,132,132,132 | 7 |
| 87 | MG | A5 | 4313 | 1/1 | 0.95 | 0.47 | 66,66,66,66 | 0 |
| 86 | OHX | A1 | 3601 | 7/7 | 0.95 | 0.15 | 184,184,184,184 | 7 |
| 87 | MG | A1 | 4428 | 1/1 | 0.95 | 0.80 | 58,58,58,58 | 0 |
| 86 | OHX | A5 | 3488 | 7/7 | 0.95 | 0.18 | 125,125,125,125 | 0 |
| 87 | MG | A6 | 2167 | 1/1 | 0.95 | 0.30 | 46,46,46,46 | 0 |
| 87 | MG | BB | 406 | 1/1 | 0.95 | 0.64 | 59,59,59,59 | 0 |
| 86 | OHX | A2 | 2022 | 7/7 | 0.95 | 0.17 | 138,138,138,138 | 7 |
| 86 | OHX | A5 | 3803 | 7/7 | 0.95 | 0.23 | 107,107,107,107 | 7 |
| 86 | OHX | A1 | 3710 | 7/7 | 0.95 | 0.18 | 122,122,122,122 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86 | OHX | A2 | 2010 | 7/7 | 0.95 | 0.22 | 119,119,119,119 | 7 |
| 87 | MG | A1 | 4434 | 1/1 | 0.95 | 1.00 | 55,55,55,55 | 0 |
| 87 | MG | Dp | 103 | 1/1 | 0.95 | 0.33 | 72,72,72,72 | 0 |
| 87 | MG | A5 | 4141 | 1/1 | 0.95 | 0.11 | 66,66,66,66 | 0 |
| 87 | MG | A1 | 4435 | 1/1 | 0.95 | 0.20 | 105,105,105,105 | 0 |
| 87 | MG | A1 | 3910 | 1/1 | 0.95 | 0.33 | 58,58,58,58 | 0 |
| 86 | OHX | A6 | 1979 | 7/7 | 0.95 | 0.18 | 116,116,116,116 | 7 |
| 86 | OHX | A5 | 3547 | 7/7 | 0.95 | 0.24 | 104,104,104,104 | 7 |
| 86 | OHX | A6 | 1981 | 7/7 | 0.95 | 0.21 | 110,110,110,110 | 7 |
| 87 | MG | A1 | 3939 | 1/1 | 0.96 | 0.32 | 32,32,32,32 | 0 |
| 86 | OHX | A2 | 2023 | 7/7 | 0.96 | 0.14 | 136,136,136,136 | 7 |
| 87 | MG | A1 | 4091 | 1/1 | 0.96 | 0.29 | 65,65,65,65 | 0 |
| 86 | OHX | A2 | 2005 | 7/7 | 0.96 | 0.15 | 134,134,134,134 | 7 |
| 87 | MG | A6 | 2144 | 1/1 | 0.96 | 0.36 | 51,51,51,51 | 0 |
| 86 | OHX | A5 | 3664 | 7/7 | 0.96 | 0.29 | 106,106,106,106 | 7 |
| 87 | MG | A1 | 4094 | 1/1 | 0.96 | 0.21 | 34,34,34,34 | 0 |
| 86 | OHX | A2 | 2067 | 7/7 | 0.96 | 0.25 | 108,108,108,108 | 7 |
| 86 | OHX | A2 | 1986 | 7/7 | 0.96 | 0.17 | 124,124,124,124 | 7 |
| 87 | MG | A5 | 4532 | 1/1 | 0.96 | 0.44 | 95,95,95,95 | 0 |
| 86 | OHX | A2 | 2026 | 7/7 | 0.96 | 0.14 | 140,140,140,140 | 7 |
| 86 | OHX | A1 | 3577 | 7/7 | 0.96 | 0.16 | 122,122,122,122 | 7 |
| 86 | OHX | A1 | 3579 | 7/7 | 0.96 | 0.23 | 97,97,97,97 | 7 |
| 86 | OHX | A6 | 2012 | 7/7 | 0.96 | 0.14 | 149,149,149,149 | 7 |
| 87 | MG | A1 | 3949 | 1/1 | 0.96 | 0.32 | 43,43,43,43 | 0 |
| 87 | MG | Ad | 104 | 1/1 | 0.96 | 0.23 | 65,65,65,65 | 0 |
| 87 | MG | A5 | 4539 | 1/1 | 0.96 | 0.76 | 77,77,77,77 | 0 |
| 87 | MG | A5 | 4342 | 1/1 | 0.96 | 0.21 | 50,50,50,50 | 0 |
| 86 | OHX | A1 | 3801 | 7/7 | 0.96 | 0.32 | 125,125,125,125 | 7 |
| 86 | OHX | A1 | 3665 | 7/7 | 0.96 | 0.24 | 104,104,104,104 | 7 |
| 86 | OHX | A1 | 3580 | 7/7 | 0.96 | 0.17 | 149,149,149,149 | 7 |
| 86 | OHX | A6 | 2016 | 7/7 | 0.96 | 0.16 | 124,124,124,124 | 7 |
| 87 | MG | A1 | 3955 | 1/1 | 0.96 | 0.39 | 42,42,42,42 | 0 |
| 86 | OHX | A1 | 3582 | 7/7 | 0.96 | 0.23 | 92,92,92,92 | 7 |
| 86 | OHX | A1 | 3583 | 7/7 | 0.96 | 0.17 | 147,147,147,147 | 7 |
| 87 | MG | A5 | 4548 | 1/1 | 0.96 | 0.63 | 74,74,74,74 | 0 |
| 86 | OHX | A6 | 2019 | 7/7 | 0.96 | 0.18 | 127,127,127,127 | 7 |
| 86 | OHX | A1 | 3669 | 7/7 | 0.96 | 0.15 | 130,130,130,130 | 7 |
| 87 | MG | A5 | 4551 | 1/1 | 0.96 | 0.24 | 62,62,62,62 | 0 |
| 86 | OHX | A1 | 3585 | 7/7 | 0.96 | 0.16 | 122,122,122,122 | 7 |
| 86 | OHX | A2 | 2008 | 7/7 | 0.96 | 0.17 | 135,135,135,135 | 7 |
| 86 | OHX | A5 | 3682 | 7/7 | 0.96 | 0.17 | 110,110,110,110 | 7 |
| 87 | MG | A6 | 2170 | 1/1 | 0.96 | 0.21 | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | A1 | 4413 | 1/1 | 0.96 | 0.24 | 106,106,106,106 | 0 |
| 87 | MG | CB | 302 | 1/1 | 0.96 | 0.16 | 93,93,93,93 | 0 |
| 86 | OHX | A1 | 3587 | 7/7 | 0.96 | 0.14 | 147,147,147,147 | 7 |
| 86 | OHX | A1 | 3589 | 7/7 | 0.96 | 0.24 | 97,97,97,97 | 7 |
| 86 | OHX | Ad | 101 | 7/7 | 0.96 | 0.17 | 130,130,130,130 | 7 |
| 87 | MG | CG | 303 | 1/1 | 0.96 | 0.30 | 54,54,54,54 | 0 |
| 86 | OHX | CY | 202 | 7/7 | 0.96 | 0.15 | 130,130,130,130 | 7 |
| 86 | OHX | A5 | 3687 | 7/7 | 0.96 | 0.21 | 109,109,109,109 | 7 |
| 86 | OHX | A5 | 3814 | 7/7 | 0.96 | 0.19 | 114,114,114,114 | 7 |
| 86 | OHX | A1 | 3592 | 7/7 | 0.96 | 0.20 | 108,108,108,108 | 7 |
| 86 | OHX | A5 | 3402 | 7/7 | 0.96 | 0.19 | 116,116,116,116 | 7 |
| 86 | OHX | A1 | 3593 | 7/7 | 0.96 | 0.18 | 113,113,113,113 | 7 |
| 86 | OHX | A1 | 3596 | 7/7 | 0.96 | 0.20 | 120,120,120,120 | 7 |
| 87 | MG | A2 | 2174 | 1/1 | 0.96 | 0.21 | 53,53,53,53 | 0 |
| 86 | OHX | A5 | 3692 | 7/7 | 0.96 | 0.15 | 170,170,170,170 | 7 |
| 86 | OHX | A2 | 1932 | 7/7 | 0.96 | 0.18 | 117,117,117,117 | 7 |
| 86 | OHX | A3 | 206 | 7/7 | 0.96 | 0.14 | 140,140,140,140 | 7 |
| 86 | OHX | A1 | 3402 | 7/7 | 0.96 | 0.20 | 130,130,130,130 | 7 |
| 86 | OHX | A5 | 3472 | 7/7 | 0.96 | 0.23 | 105,105,105,105 | 0 |
| 86 | OHX | A5 | 3697 | 7/7 | 0.96 | 0.14 | 167,167,167,167 | 7 |
| 86 | OHX | A3 | 208 | 7/7 | 0.96 | 0.19 | 126,126,126,126 | 7 |
| 86 | OHX | A5 | 3493 | 7/7 | 0.96 | 0.20 | 102,102,102,102 | 7 |
| 86 | OHX | A5 | 3513 | 7/7 | 0.96 | 0.19 | 115,115,115,115 | 7 |
| 86 | OHX | A2 | 1934 | 7/7 | 0.96 | 0.18 | 123,123,123,123 | 7 |
| 86 | OHX | A1 | 3602 | 7/7 | 0.96 | 0.22 | 99,99,99,99 | 7 |
| 87 | MG | A5 | 4005 | 1/1 | 0.96 | 0.36 | 31,31,31,31 | 0 |
| 87 | MG | Ch | 302 | 1/1 | 0.96 | 0.18 | 53,53,53,53 | 0 |
| 87 | MG | BL | 205 | 1/1 | 0.96 | 0.59 | 62,62,62,62 | 0 |
| 87 | MG | A1 | 3988 | 1/1 | 0.96 | 0.34 | 67,67,67,67 | 0 |
| 87 | MG | A5 | 4010 | 1/1 | 0.96 | 0.43 | 50,50,50,50 | 0 |
| 86 | OHX | A2 | 1989 | 7/7 | 0.96 | 0.17 | 131,131,131,131 | 7 |
| 87 | MG | A1 | 4140 | 1/1 | 0.96 | 0.32 | 56,56,56,56 | 0 |
| 86 | OHX | A5 | 3538 | 7/7 | 0.96 | 0.19 | 104,104,104,104 | 7 |
| 87 | MG | A5 | 3825 | 1/1 | 0.96 | 0.16 | 29,29,29,29 | 0 |
| 86 | OHX | A5 | 3540 | 7/7 | 0.96 | 0.19 | 119,119,119,119 | 7 |
| 87 | MG | A1 | 3992 | 1/1 | 0.96 | 0.31 | 41,41,41,41 | 0 |
| 87 | MG | A5 | 3828 | 1/1 | 0.96 | 0.10 | 34,34,34,34 | 0 |
| 86 | OHX | A2 | 2052 | 7/7 | 0.96 | 0.24 | 117,117,117,117 | 7 |
| 87 | MG | BO | 203 | 1/1 | 0.96 | 0.77 | 74,74,74,74 | 0 |
| 87 | MG | BO | 204 | 1/1 | 0.96 | 0.37 | 53,53,53,53 | 0 |
| 86 | OHX | A8 | 214 | 7/7 | 0.96 | 0.16 | 125,125,125,125 | 7 |
| 86 | OHX | A5 | 3544 | 7/7 | 0.96 | 0.21 | 97,97,97,97 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87 | MG | A5 | 4209 | 1/1 | 0.96 | 0.40 | 53,53,53,53 | 0 |
| 86 | OHX | A1 | 3506 | 7/7 | 0.96 | 0.19 | 103,103,103,103 | 7 |
| 86 | OHX | A2 | 1992 | 7/7 | 0.96 | 0.15 | 123,123,123,123 | 7 |
| 86 | OHX | A1 | 3518 | 7/7 | 0.96 | 0.17 | 140,140,140,140 | 7 |
| 86 | OHX | A1 | 3757 | 7/7 | 0.96 | 0.27 | 73,73,73,73 | 7 |
| 87 | MG | BP | 204 | 1/1 | 0.96 | 0.34 | 51,51,51,51 | 0 |
| 86 | OHX | A5 | 3566 | 7/7 | 0.96 | 0.23 | 99,99,99,99 | 7 |
| 86 | OHX | A5 | 3568 | 7/7 | 0.96 | 0.20 | 103,103,103,103 | 7 |
| 87 | MG | A1 | 4007 | 1/1 | 0.96 | 0.22 | 29,29,29,29 | 0 |
| 86 | OHX | A1 | 3610 | 7/7 | 0.96 | 0.20 | 121,121,121,121 | 7 |
| 86 | OHX | A2 | 2013 | 7/7 | 0.96 | 0.19 | 116,116,116,116 | 7 |
| 87 | MG | A5 | 3846 | 1/1 | 0.96 | 0.17 | 37,37,37,37 | 0 |
| 87 | MG | A1 | 3865 | 1/1 | 0.96 | 0.10 | 31,31,31,31 | 0 |
| 87 | MG | A1 | 3866 | 1/1 | 0.96 | 0.11 | 87,87,87,87 | 0 |
| 87 | MG | A1 | 3867 | 1/1 | 0.96 | 0.31 | 61,61,61,61 | 0 |
| 86 | OHX | A5 | 3577 | 7/7 | 0.96 | 0.18 | 128,128,128,128 | 7 |
| 86 | OHX | A2 | 1937 | 7/7 | 0.96 | 0.20 | 122,122,122,122 | 7 |
| 87 | MG | BQ | 203 | 1/1 | 0.96 | 0.87 | 63,63,63,63 | 0 |
| 87 | MG | A1 | 4461 | 1/1 | 0.96 | 0.12 | 86,86,86,86 | 0 |
| 86 | OHX | A5 | 3720 | 7/7 | 0.96 | 0.17 | 101,101,101,101 | 7 |
| 86 | OHX | A2 | 1969 | 7/7 | 0.96 | 0.15 | 144,144,144,144 | 7 |
| 86 | OHX | A1 | 3536 | 7/7 | 0.96 | 0.16 | 136,136,136,136 | 7 |
| 87 | MG | A5 | 4421 | 1/1 | 0.96 | 0.60 | 55,55,55,55 | 0 |
| 86 | OHX | A5 | 3588 | 7/7 | 0.96 | 0.23 | 106,106,106,106 | 7 |
| 87 | MG | A6 | 2229 | 1/1 | 0.96 | 0.23 | 65,65,65,65 | 0 |
| 87 | MG | A6 | 2230 | 1/1 | 0.96 | 0.13 | 86,86,86,86 | 0 |
| 87 | MG | DA | 304 | 1/1 | 0.96 | 0.74 | 69,69,69,69 | 0 |
| 87 | MG | A1 | 4020 | 1/1 | 0.96 | 0.34 | 52,52,52,52 | 0 |
| 87 | MG | A1 | 4312 | 1/1 | 0.96 | 0.70 | 60,60,60,60 | 0 |
| 87 | MG | A1 | 4166 | 1/1 | 0.96 | 0.32 | 74,74,74,74 | 0 |
| 87 | MG | A5 | 3863 | 1/1 | 0.96 | 0.28 | 51,51,51,51 | 0 |
| 86 | OHX | A5 | 3589 | 7/7 | 0.96 | 0.20 | 93,93,93,93 | 7 |
| 86 | OHX | A1 | 3620 | 7/7 | 0.96 | 0.16 | 139,139,139,139 | 7 |
| 87 | MG | A5 | 3866 | 1/1 | 0.96 | 0.30 | 51,51,51,51 | 0 |
| 87 | MG | A1 | 4023 | 1/1 | 0.96 | 0.42 | 42,42,42,42 | 0 |
| 87 | MG | A1 | 4024 | 1/1 | 0.96 | 0.40 | 40,40,40,40 | 0 |
| 86 | OHX | A1 | 3764 | 7/7 | 0.96 | 0.15 | 159,159,159,159 | 7 |
| 86 | OHX | A1 | 3621 | 7/7 | 0.96 | 0.18 | 119,119,119,119 | 7 |
| 87 | MG | BY | 202 | 1/1 | 0.96 | 0.44 | 85,85,85,85 | 0 |
| 87 | MG | A5 | 4438 | 1/1 | 0.96 | 0.43 | 58,58,58,58 | 0 |
| 87 | MG | A5 | 4248 | 1/1 | 0.96 | 0.23 | 99,99,99,99 | 0 |
| 86 | OHX | A2 | 1973 | 7/7 | 0.96 | 0.18 | 136,136,136,136 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87 | MG | A1 | 4029 | 1/1 | 0.96 | 0.18 | 29,29,29,29 | 0 |
| 87 | MG | A1 | 3880 | 1/1 | 0.96 | 0.31 | 42,42,42,42 | 0 |
| 86 | OHX | DV | 201 | 7/7 | 0.96 | 0.16 | 126,126,126,126 | 7 |
| 86 | OHX | A1 | 3541 | 7/7 | 0.96 | 0.23 | 109,109,109,109 | 7 |
| 86 | OHX | A5 | 3603 | 7/7 | 0.96 | 0.25 | 107,107,107,107 | 7 |
| 86 | OHX | A5 | 3604 | 7/7 | 0.96 | 0.20 | 113,113,113,113 | 7 |
| 87 | MG | DD | 305 | 1/1 | 0.96 | 0.21 | 74,74,74,74 | 0 |
| 86 | OHX | A2 | 1999 | 7/7 | 0.96 | 0.13 | 168,168,168,168 | 7 |
| 87 | MG | A1 | 3886 | 1/1 | 0.96 | 0.35 | 72,72,72,72 | 0 |
| 87 | MG | A5 | 3881 | 1/1 | 0.96 | 0.29 | 60,60,60,60 | 0 |
| 86 | OHX | A1 | 3544 | 7/7 | 0.96 | 0.20 | 96,96,96,96 | 7 |
| 86 | OHX | A5 | 3608 | 7/7 | 0.96 | 0.15 | 125,125,125,125 | 7 |
| 86 | OHX | A1 | 3546 | 7/7 | 0.96 | 0.19 | 106,106,106,106 | 7 |
| 86 | OHX | A5 | 3610 | 7/7 | 0.96 | 0.14 | 161,161,161,161 | 7 |
| 86 | OHX | A1 | 3630 | 7/7 | 0.96 | 0.16 | 119,119,119,119 | 7 |
| 86 | OHX | Bj | 101 | 7/7 | 0.96 | 0.18 | 100,100,100,100 | 7 |
| 86 | OHX | A5 | 3613 | 7/7 | 0.96 | 0.17 | 137,137,137,137 | 7 |
| 86 | OHX | A1 | 3632 | 7/7 | 0.96 | 0.10 | 170,170,170,170 | 7 |
| 87 | MG | A5 | 4268 | 1/1 | 0.96 | 0.40 | 96,96,96,96 | 0 |
| 87 | MG | A5 | 4080 | 1/1 | 0.96 | 0.35 | 71,71,71,71 | 0 |
| 86 | OHX | A6 | 1939 | 7/7 | 0.96 | 0.17 | 134,134,134,134 | 0 |
| 86 | OHX | A5 | 3618 | 7/7 | 0.96 | 0.24 | 101,101,101,101 | 7 |
| 86 | OHX | A1 | 3547 | 7/7 | 0.96 | 0.19 | 99,99,99,99 | 7 |
| 87 | MG | DO | 204 | 1/1 | 0.96 | 0.63 | 57,57,57,57 | 0 |
| 87 | MG | A5 | 3893 | 1/1 | 0.96 | 0.30 | 73,73,73,73 | 0 |
| 86 | OHX | A2 | 1943 | 7/7 | 0.96 | 0.22 | 123,123,123,123 | 7 |
| 86 | OHX | A2 | 1959 | 7/7 | 0.96 | 0.15 | 147,147,147,147 | 7 |
| 87 | MG | A2 | 2106 | 1/1 | 0.96 | 0.36 | 57,57,57,57 | 0 |
| 86 | OHX | A2 | 1945 | 7/7 | 0.96 | 0.14 | 140,140,140,140 | 7 |
| 86 | OHX | A6 | 1963 | 7/7 | 0.96 | 0.18 | 103,103,103,103 | 7 |
| 86 | OHX | A6 | 1967 | 7/7 | 0.96 | 0.17 | 112,112,112,112 | 7 |
| 87 | MG | A5 | 4280 | 1/1 | 0.96 | 0.84 | 49,49,49,49 | 0 |
| 87 | MG | A1 | 4350 | 1/1 | 0.96 | 0.93 | 76,76,76,76 | 0 |
| 87 | MG | DP | 206 | 1/1 | 0.96 | 0.88 | 55,55,55,55 | 0 |
| 87 | MG | A5 | 4474 | 1/1 | 0.96 | 0.73 | 44,44,44,44 | 0 |
| 86 | OHX | A5 | 3627 | 7/7 | 0.96 | 0.24 | 80,80,80,80 | 7 |
| 86 | OHX | A1 | 3552 | 7/7 | 0.96 | 0.20 | 115,115,115,115 | 7 |
| 86 | OHX | A6 | 1973 | 7/7 | 0.96 | 0.20 | 87,87,87,87 | 7 |
| 87 | MG | DS | 201 | 1/1 | 0.96 | 0.21 | 61,61,61,61 | 0 |
| 86 | OHX | A6 | 1974 | 7/7 | 0.96 | 0.19 | 116,116,116,116 | 7 |
| 87 | MG | A6 | 2107 | 1/1 | 0.96 | 0.41 | 52,52,52,52 | 0 |
| 86 | OHX | A5 | 3631 | 7/7 | 0.96 | 0.24 | 89,89,89,89 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86 | OHX | A6 | 1976 | 7/7 | 0.96 | 0.28 | 105,105,105,105 | 7 |
| 86 | OHX | A2 | 1961 | 7/7 | 0.96 | 0.15 | 150,150,150,150 | 7 |
| 86 | OHX | A5 | 3635 | 7/7 | 0.96 | 0.14 | 147,147,147,147 | 7 |
| 87 | MG | A6 | 2113 | 1/1 | 0.96 | 0.26 | 48,48,48,48 | 0 |
| 86 | OHX | A1 | 3640 | 7/7 | 0.96 | 0.16 | 153,153,153,153 | 7 |
| 87 | MG | A2 | 2244 | 1/1 | 0.96 | 0.14 | 99,99,99,99 | 0 |
| 87 | MG | A6 | 2283 | 1/1 | 0.96 | 0.21 | 75,75,75,75 | 0 |
| 87 | MG | A5 | 4105 | 1/1 | 0.96 | 0.28 | 68,68,68,68 | 0 |
| 86 | OHX | A2 | 2042 | 7/7 | 0.96 | 0.13 | 155,155,155,155 | 7 |
| 86 | OHX | A6 | 1980 | 7/7 | 0.96 | 0.22 | 133,133,133,133 | 7 |
| 87 | MG | A6 | 2286 | 1/1 | 0.96 | 0.29 | 75,75,75,75 | 0 |
| 86 | OHX | A5 | 3640 | 7/7 | 0.96 | 0.15 | 147,147,147,147 | 7 |
| 87 | MG | A5 | 3919 | 1/1 | 0.96 | 0.24 | 66,66,66,66 | 0 |
| 86 | OHX | A5 | 3641 | 7/7 | 0.96 | 0.18 | 127,127,127,127 | 7 |
| 86 | OHX | A1 | 3643 | 7/7 | 0.96 | 0.16 | 153,153,153,153 | 7 |
| 86 | OHX | A1 | 3715 | 7/7 | 0.96 | 0.18 | 120,120,120,120 | 7 |
| 86 | OHX | A2 | 1984 | 7/7 | 0.96 | 0.18 | 108,108,108,108 | 7 |
| 86 | OHX | A1 | 3717 | 7/7 | 0.96 | 0.19 | 141,141,141,141 | 7 |
| 86 | OHX | A1 | 3560 | 7/7 | 0.96 | 0.18 | 116,116,116,116 | 7 |
| 86 | OHX | A1 | 3647 | 7/7 | 0.96 | 0.16 | 129,129,129,129 | 7 |
| 87 | MG | A5 | 4120 | 1/1 | 0.96 | 0.39 | 49,49,49,49 | 0 |
| 86 | OHX | A1 | 3649 | 7/7 | 0.96 | 0.16 | 167,167,167,167 | 7 |
| 86 | OHX | A5 | 3649 | 7/7 | 0.96 | 0.20 | 129,129,129,129 | 7 |
| 87 | MG | Dj | 103 | 1/1 | 0.96 | 1.50 | 65,65,65,65 | 0 |
| 86 | OHX | A1 | 3650 | 7/7 | 0.96 | 0.31 | 120,120,120,120 | 7 |
| 87 | MG | A5 | 3930 | 1/1 | 0.96 | 0.18 | 29,29,29,29 | 0 |
| 86 | OHX | A1 | 3561 | 7/7 | 0.96 | 0.20 | 110,110,110,110 | 7 |
| 86 | OHX | A1 | 3562 | 7/7 | 0.96 | 0.17 | 143,143,143,143 | 7 |
| 87 | MG | A1 | 4081 | 1/1 | 0.96 | 0.14 | 56,56,56,56 | 0 |
| 86 | OHX | A5 | 3654 | 7/7 | 0.96 | 0.17 | 116,116,116,116 | 7 |
| 86 | OHX | A5 | 3655 | 7/7 | 0.96 | 0.27 | 124,124,124,124 | 7 |
| 86 | OHX | A6 | 1997 | 7/7 | 0.96 | 0.19 | 125,125,125,125 | 7 |
| 88 | ZN | Aa | 202 | 1/1 | 0.96 | 0.11 | 92,92,92,92 | 0 |
| 86 | OHX | A1 | 3563 | 7/7 | 0.96 | 0.17 | 131,131,131,131 | 7 |
| 86 | OHX | A1 | 3656 | 7/7 | 0.96 | 0.19 | 114,114,114,114 | 7 |
| 87 | MG | A4 | 223 | 1/1 | 0.96 | 0.43 | 44,44,44,44 | 0 |
| 86 | OHX | A6 | 2000 | 7/7 | 0.96 | 0.19 | 128,128,128,128 | 7 |
| 86 | OHX | A6 | 2001 | 7/7 | 0.96 | 0.17 | 149,149,149,149 | 7 |
| 86 | OHX | A7 | 203 | 7/7 | 0.97 | 0.22 | 105,105,105,105 | 7 |
| 86 | OHX | A6 | 1954 | 7/7 | 0.97 | 0.13 | 141,141,141,141 | 7 |
| 86 | OHX | A5 | 3652 | 7/7 | 0.97 | 0.17 | 150,150,150,150 | 7 |
| 86 | OHX | A1 | 3530 | 7/7 | 0.97 | 0.17 | 125,125,125,125 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86 | OHX | A6 | 1958 | 7/7 | 0.97 | 0.16 | 133,133,133,133 | 7 |
| 87 | MG | A5 | 4047 | 1/1 | 0.97 | 0.25 | 57,57,57,57 | 0 |
| 86 | OHX | A6 | 1959 | 7/7 | 0.97 | 0.21 | 107,107,107,107 | 7 |
| 87 | MG | A1 | 4330 | 1/1 | 0.97 | 0.16 | 82,82,82,82 | 0 |
| 86 | OHX | A1 | 3531 | 7/7 | 0.97 | 0.15 | 140,140,140,140 | 7 |
| 86 | OHX | A8 | 204 | 7/7 | 0.97 | 0.20 | 101,101,101,101 | 7 |
| 86 | OHX | A1 | 3532 | 7/7 | 0.97 | 0.20 | 87,87,87,87 | 7 |
| 86 | OHX | A8 | 209 | 7/7 | 0.97 | 0.18 | 130,130,130,130 | 7 |
| 86 | OHX | A8 | 210 | 7/7 | 0.97 | 0.17 | 133,133,133,133 | 7 |
| 87 | MG | A5 | 4504 | 1/1 | 0.97 | 0.45 | 84,84,84,84 | 0 |
| 86 | OHX | A1 | 3534 | 7/7 | 0.97 | 0.19 | 106,106,106,106 | 7 |
| 86 | OHX | A6 | 1964 | 7/7 | 0.97 | 0.18 | 132,132,132,132 | 7 |
| 87 | MG | A6 | 2177 | 1/1 | 0.97 | 0.23 | 79,79,79,79 | 0 |
| 86 | OHX | A5 | 3660 | 7/7 | 0.97 | 0.22 | 108,108,108,108 | 7 |
| 86 | OHX | A6 | 1965 | 7/7 | 0.97 | 0.15 | 123,123,123,123 | 7 |
| 87 | MG | A5 | 4281 | 1/1 | 0.97 | 0.49 | 56,56,56,56 | 0 |
| 87 | MG | A1 | 3962 | 1/1 | 0.97 | 0.41 | 61,61,61,61 | 0 |
| 87 | MG | A5 | 3842 | 1/1 | 0.97 | 0.08 | 34,34,34,34 | 0 |
| 86 | OHX | A6 | 1966 | 7/7 | 0.97 | 0.20 | 92,92,92,92 | 7 |
| 87 | MG | A5 | 3844 | 1/1 | 0.97 | 0.18 | 59,59,59,59 | 0 |
| 86 | OHX | A2 | 1976 | 7/7 | 0.97 | 0.15 | 139,139,139,139 | 7 |
| 86 | OHX | A6 | 1968 | 7/7 | 0.97 | 0.16 | 101,101,101,101 | 7 |
| 87 | MG | A1 | 3966 | 1/1 | 0.97 | 0.46 | 60,60,60,60 | 0 |
| 86 | OHX | A1 | 3612 | 7/7 | 0.97 | 0.15 | 146,146,146,146 | 7 |
| 86 | OHX | A6 | 1972 | 7/7 | 0.97 | 0.20 | 109,109,109,109 | 7 |
| 86 | OHX | A1 | 3613 | 7/7 | 0.97 | 0.23 | 98,98,98,98 | 7 |
| 86 | OHX | A1 | 3614 | 7/7 | 0.97 | 0.19 | 112,112,112,112 | 7 |
| 87 | MG | A1 | 4349 | 1/1 | 0.97 | 0.37 | 119,119,119,119 | 0 |
| 86 | OHX | A1 | 3693 | 7/7 | 0.97 | 0.20 | 100,100,100,100 | 7 |
| 86 | OHX | A1 | 3538 | 7/7 | 0.97 | 0.20 | 105,105,105,105 | 7 |
| 86 | OHX | A2 | 1977 | 7/7 | 0.97 | 0.12 | 174,174,174,174 | 7 |
| 86 | OHX | A1 | 3617 | 7/7 | 0.97 | 0.14 | 144,144,144,144 | 7 |
| 87 | MG | A5 | 4528 | 1/1 | 0.97 | 0.28 | 97,97,97,97 | 0 |
| 86 | OHX | A1 | 3540 | 7/7 | 0.97 | 0.14 | 141,141,141,141 | 7 |
| 87 | MG | A5 | 4299 | 1/1 | 0.97 | 0.30 | 80,80,80,80 | 0 |
| 86 | OHX | A1 | 3698 | 7/7 | 0.97 | 0.17 | 105,105,105,105 | 7 |
| 87 | MG | A5 | 4301 | 1/1 | 0.97 | 0.06 | 71,71,71,71 | 0 |
| 86 | OHX | A2 | 1939 | 7/7 | 0.97 | 0.15 | 144,144,144,144 | 7 |
| 86 | OHX | A2 | 2007 | 7/7 | 0.97 | 0.21 | 146,146,146,146 | 7 |
| 86 | OHX | A6 | 1985 | 7/7 | 0.97 | 0.18 | 114,114,114,114 | 7 |
| 86 | OHX | A1 | 3543 | 7/7 | 0.97 | 0.15 | 137,137,137,137 | 7 |
| 87 | MG | A4 | 244 | 1/1 | 0.97 | 0.20 | 61,61,61,61 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86 | OHX | A6 | 1987 | 7/7 | 0.97 | 0.18 | 113,113,113,113 | 7 |
| 86 | OHX | A2 | 1955 | 7/7 | 0.97 | 0.17 | 123,123,123,123 | 7 |
| 86 | OHX | A1 | 3703 | 7/7 | 0.97 | 0.20 | 93,93,93,93 | 7 |
| 87 | MG | A4 | 248 | 1/1 | 0.97 | 0.34 | 114,114,114,114 | 0 |
| 87 | MG | A1 | 4172 | 1/1 | 0.97 | 0.22 | 54,54,54,54 | 0 |
| 86 | OHX | A2 | 1940 | 7/7 | 0.97 | 0.18 | 100,100,100,100 | 7 |
| 86 | OHX | A1 | 3625 | 7/7 | 0.97 | 0.21 | 92,92,92,92 | 7 |
| 86 | OHX | A6 | 1992 | 7/7 | 0.97 | 0.14 | 125,125,125,125 | 7 |
| 87 | MG | A2 | 2089 | 1/1 | 0.97 | 0.32 | 49,49,49,49 | 0 |
| 86 | OHX | A6 | 1993 | 7/7 | 0.97 | 0.17 | 129,129,129,129 | 7 |
| 86 | OHX | A1 | 3626 | 7/7 | 0.97 | 0.15 | 162,162,162,162 | 7 |
| 86 | OHX | A6 | 1995 | 7/7 | 0.97 | 0.12 | 143,143,143,143 | 7 |
| 86 | OHX | A2 | 1958 | 7/7 | 0.97 | 0.16 | 139,139,139,139 | 7 |
| 86 | OHX | A2 | 1921 | 7/7 | 0.97 | 0.19 | 113,113,113,113 | 7 |
| 86 | OHX | A5 | 3401 | 7/7 | 0.97 | 0.19 | 102,102,102,102 | 0 |
| 86 | OHX | A2 | 1985 | 7/7 | 0.97 | 0.14 | 144,144,144,144 | 7 |
| 86 | OHX | A2 | 1944 | 7/7 | 0.97 | 0.17 | 109,109,109,109 | 7 |
| 87 | MG | A1 | 3996 | 1/1 | 0.97 | 0.46 | 48,48,48,48 | 0 |
| 86 | OHX | A1 | 3631 | 7/7 | 0.97 | 0.14 | 141,141,141,141 | 7 |
| 87 | MG | A1 | 4378 | 1/1 | 0.97 | 0.62 | 51,51,51,51 | 0 |
| 86 | OHX | A2 | 1928 | 7/7 | 0.97 | 0.17 | 126,126,126,126 | 7 |
| 87 | MG | A5 | 4559 | 1/1 | 0.97 | 0.27 | 74,74,74,74 | 0 |
| 86 | OHX | A6 | 2002 | 7/7 | 0.97 | 0.21 | 96,96,96,96 | 7 |
| 87 | MG | A1 | 4002 | 1/1 | 0.97 | 0.33 | 37,37,37,37 | 0 |
| 87 | MG | A5 | 4106 | 1/1 | 0.97 | 0.25 | 41,41,41,41 | 0 |
| 86 | OHX | AL | 201 | 7/7 | 0.97 | 0.17 | 119,119,119,119 | 7 |
| 86 | OHX | A5 | 3441 | 7/7 | 0.97 | 0.24 | 96,96,96,96 | 0 |
| 87 | MG | A1 | 4005 | 1/1 | 0.97 | 0.36 | 42,42,42,42 | 0 |
| 87 | MG | BI | 306 | 1/1 | 0.97 | 0.18 | 32,32,32,32 | 0 |
| 86 | OHX | A5 | 3699 | 7/7 | 0.97 | 0.29 | 107,107,107,107 | 7 |
| 87 | MG | BI | 308 | 1/1 | 0.97 | 0.16 | 57,57,57,57 | 0 |
| 86 | OHX | A1 | 3555 | 7/7 | 0.97 | 0.17 | 125,125,125,125 | 7 |
| 86 | OHX | A1 | 3556 | 7/7 | 0.97 | 0.18 | 128,128,128,128 | 7 |
| 86 | OHX | A6 | 2006 | 7/7 | 0.97 | 0.20 | 87,87,87,87 | 7 |
| 86 | OHX | A5 | 3502 | 7/7 | 0.97 | 0.18 | 141,141,141,141 | 0 |
| 87 | MG | A5 | 4117 | 1/1 | 0.97 | 0.09 | 49,49,49,49 | 0 |
| 87 | MG | A2 | 2109 | 1/1 | 0.97 | 0.34 | 56,56,56,56 | 0 |
| 86 | OHX | A5 | 3510 | 7/7 | 0.97 | 0.21 | 90,90,90,90 | 7 |
| 87 | MG | A1 | 4013 | 1/1 | 0.97 | 0.29 | 47,47,47,47 | 0 |
| 86 | OHX | A2 | 1962 | 7/7 | 0.97 | 0.16 | 136,136,136,136 | 7 |
| 86 | OHX | A5 | 3515 | 7/7 | 0.97 | 0.16 | 121,121,121,121 | 7 |
| 86 | OHX | A1 | 3637 | 7/7 | 0.97 | 0.12 | 146,146,146,146 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | A1 | 3828 | 1/1 | 0.97 | 0.28 | 43,43,43,43 | 0 |
| 87 | MG | A5 | 3904 | 1/1 | 0.97 | 0.19 | 60,60,60,60 | 0 |
| 86 | OHX | A2 | 1963 | 7/7 | 0.97 | 0.14 | 129,129,129,129 | 7 |
| 86 | OHX | A5 | 3522 | 7/7 | 0.97 | 0.17 | 123,123,123,123 | 7 |
| 87 | MG | A1 | 4400 | 1/1 | 0.97 | 0.14 | 70,70,70,70 | 0 |
| 86 | OHX | A5 | 3528 | 7/7 | 0.97 | 0.16 | 163,163,163,163 | 0 |
| 86 | OHX | A5 | 3529 | 7/7 | 0.97 | 0.20 | 93,93,93,93 | 7 |
| 86 | OHX | A1 | 3559 | 7/7 | 0.97 | 0.17 | 116,116,116,116 | 7 |
| 86 | OHX | A5 | 3533 | 7/7 | 0.97 | 0.16 | 118,118,118,118 | 7 |
| 87 | MG | A5 | 4133 | 1/1 | 0.97 | 0.31 | 54,54,54,54 | 0 |
| 86 | OHX | A5 | 3536 | 7/7 | 0.97 | 0.20 | 97,97,97,97 | 7 |
| 86 | OHX | A6 | 2011 | 7/7 | 0.97 | 0.19 | 120,120,120,120 | 7 |
| 86 | OHX | A2 | 1990 | 7/7 | 0.97 | 0.17 | 105,105,105,105 | 7 |
| 86 | OHX | A2 | 1935 | 7/7 | 0.97 | 0.18 | 120,120,120,120 | 7 |
| 87 | MG | A1 | 4028 | 1/1 | 0.97 | 0.41 | 28,28,28,28 | 0 |
| 86 | OHX | A5 | 3542 | 7/7 | 0.97 | 0.23 | 103,103,103,103 | 7 |
| 86 | OHX | A5 | 3543 | 7/7 | 0.97 | 0.21 | 109,109,109,109 | 7 |
| 86 | OHX | A1 | 3642 | 7/7 | 0.97 | 0.11 | 139,139,139,139 | 7 |
| 86 | OHX | A5 | 3546 | 7/7 | 0.97 | 0.16 | 132,132,132,132 | 7 |
| 87 | MG | A1 | 3843 | 1/1 | 0.97 | 0.30 | 46,46,46,46 | 0 |
| 86 | OHX | A1 | 3401 | 7/7 | 0.97 | 0.16 | 121,121,121,121 | 7 |
| 86 | OHX | A5 | 3548 | 7/7 | 0.97 | 0.18 | 134,134,134,134 | 7 |
| 86 | OHX | A5 | 3549 | 7/7 | 0.97 | 0.20 | 107,107,107,107 | 7 |
| 86 | OHX | A5 | 3550 | 7/7 | 0.97 | 0.21 | 119,119,119,119 | 7 |
| 86 | OHX | A1 | 3644 | 7/7 | 0.97 | 0.15 | 139,139,139,139 | 7 |
| 87 | MG | A1 | 3849 | 1/1 | 0.97 | 0.38 | 56,56,56,56 | 0 |
| 86 | OHX | A5 | 3555 | 7/7 | 0.97 | 0.14 | 152,152,152,152 | 0 |
| 87 | MG | A6 | 2268 | 1/1 | 0.97 | 0.28 | 68,68,68,68 | 0 |
| 86 | OHX | A5 | 3556 | 7/7 | 0.97 | 0.19 | 111,111,111,111 | 7 |
| 87 | MG | A5 | 3931 | 1/1 | 0.97 | 0.33 | 35,35,35,35 | 0 |
| 86 | OHX | A2 | 1993 | 7/7 | 0.97 | 0.11 | 159,159,159,159 | 7 |
| 86 | OHX | A2 | 1994 | 7/7 | 0.97 | 0.16 | 118,118,118,118 | 7 |
| 86 | OHX | A5 | 3561 | 7/7 | 0.97 | 0.17 | 121,121,121,121 | 7 |
| 86 | OHX | A5 | 3562 | 7/7 | 0.97 | 0.20 | 104,104,104,104 | 7 |
| 86 | OHX | A5 | 3563 | 7/7 | 0.97 | 0.19 | 98,98,98,98 | 7 |
| 86 | OHX | A5 | 3564 | 7/7 | 0.97 | 0.13 | 143,143,143,143 | 7 |
| 86 | OHX | A5 | 3565 | 7/7 | 0.97 | 0.19 | 105,105,105,105 | 7 |
| 86 | OHX | A5 | 3738 | 7/7 | 0.97 | 0.20 | 101,101,101,101 | 7 |
| 87 | MG | A1 | 4237 | 1/1 | 0.97 | 0.19 | 46,46,46,46 | 0 |
| 86 | OHX | A5 | 3739 | 7/7 | 0.97 | 0.23 | 105,105,105,105 | 7 |
| 86 | OHX | A2 | 1915 | 7/7 | 0.97 | 0.17 | 109,109,109,109 | 7 |
| 86 | OHX | A5 | 3567 | 7/7 | 0.97 | 0.20 | 106,106,106,106 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86 | OHX | A6 | 2020 | 7/7 | 0.97 | 0.20 | 88,88,88,88 | 7 |
| 87 | MG | A5 | 3946 | 1/1 | 0.97 | 0.41 | 41,41,41,41 | 0 |
| 86 | OHX | A1 | 3648 | 7/7 | 0.97 | 0.15 | 102,102,102,102 | 7 |
| 86 | OHX | A1 | 3447 | 7/7 | 0.97 | 0.21 | 98,98,98,98 | 0 |
| 86 | OHX | A5 | 3574 | 7/7 | 0.97 | 0.17 | 154,154,154,154 | 7 |
| 86 | OHX | A5 | 3575 | 7/7 | 0.97 | 0.23 | 81,81,81,81 | 7 |
| 87 | MG | A1 | 4246 | 1/1 | 0.97 | 0.27 | 80,80,80,80 | 0 |
| 87 | MG | A5 | 3952 | 1/1 | 0.97 | 0.42 | 43,43,43,43 | 0 |
| 86 | OHX | A5 | 3576 | 7/7 | 0.97 | 0.22 | 124,124,124,124 | 7 |
| 86 | OHX | A1 | 3570 | 7/7 | 0.97 | 0.18 | 100,100,100,100 | 7 |
| 86 | OHX | A5 | 3579 | 7/7 | 0.97 | 0.18 | 105,105,105,105 | 7 |
| 86 | OHX | A5 | 3580 | 7/7 | 0.97 | 0.16 | 121,121,121,121 | 7 |
| 87 | MG | DB | 410 | 1/1 | 0.97 | 0.52 | 54,54,54,54 | 0 |
| 86 | OHX | A5 | 3581 | 7/7 | 0.97 | 0.15 | 148,148,148,148 | 7 |
| 86 | OHX | A1 | 3572 | 7/7 | 0.97 | 0.18 | 114,114,114,114 | 7 |
| 86 | OHX | A2 | 1967 | 7/7 | 0.97 | 0.16 | 120,120,120,120 | 7 |
| 86 | OHX | A1 | 3654 | 7/7 | 0.97 | 0.12 | 149,149,149,149 | 7 |
| 86 | OHX | A5 | 3586 | 7/7 | 0.97 | 0.19 | 112,112,112,112 | 7 |
| 87 | MG | A5 | 3962 | 1/1 | 0.97 | 0.36 | 41,41,41,41 | 0 |
| 86 | OHX | A5 | 3587 | 7/7 | 0.97 | 0.22 | 96,96,96,96 | 7 |
| 86 | OHX | A5 | 3757 | 7/7 | 0.97 | 0.10 | 192,192,192,192 | 7 |
| 86 | OHX | A6 | 2027 | 7/7 | 0.97 | 0.12 | 189,189,189,189 | 7 |
| 86 | OHX | A1 | 3735 | 7/7 | 0.97 | 0.24 | 83,83,83,83 | 7 |
| 86 | OHX | A5 | 3590 | 7/7 | 0.97 | 0.21 | 114,114,114,114 | 7 |
| 87 | MG | A1 | 4456 | 1/1 | 0.97 | 0.39 | 76,76,76,76 | 0 |
| 87 | MG | A5 | 3969 | 1/1 | 0.97 | 0.41 | 37,37,37,37 | 0 |
| 86 | OHX | A1 | 3816 | 7/7 | 0.97 | 0.10 | 150,150,150,150 | 7 |
| 86 | OHX | A3 | 201 | 7/7 | 0.97 | 0.19 | 109,109,109,109 | 0 |
| 87 | MG | A5 | 3972 | 1/1 | 0.97 | 0.29 | 55,55,55,55 | 0 |
| 87 | MG | A5 | 4418 | 1/1 | 0.97 | 0.22 | 91,91,91,91 | 0 |
| 86 | OHX | A3 | 205 | 7/7 | 0.97 | 0.17 | 113,113,113,113 | 7 |
| 86 | OHX | A1 | 3472 | 7/7 | 0.97 | 0.18 | 109,109,109,109 | 7 |
| 87 | MG | A5 | 3975 | 1/1 | 0.97 | 0.44 | 41,41,41,41 | 0 |
| 86 | OHX | A5 | 3596 | 7/7 | 0.97 | 0.25 | 84,84,84,84 | 7 |
| 86 | OHX | A5 | 3597 | 7/7 | 0.97 | 0.19 | 95,95,95,95 | 7 |
| 86 | OHX | A5 | 3598 | 7/7 | 0.97 | 0.13 | 143,143,143,143 | 7 |
| 86 | OHX | A5 | 3599 | 7/7 | 0.97 | 0.17 | 120,120,120,120 | 7 |
| 86 | OHX | A5 | 3600 | 7/7 | 0.97 | 0.12 | 133,133,133,133 | 7 |
| 86 | OHX | A1 | 3575 | 7/7 | 0.97 | 0.15 | 120,120,120,120 | 7 |
| 86 | OHX | A1 | 3476 | 7/7 | 0.97 | 0.20 | 129,129,129,129 | 0 |
| 86 | OHX | A1 | 3578 | 7/7 | 0.97 | 0.20 | 112,112,112,112 | 7 |
| 86 | OHX | A1 | 3479 | 7/7 | 0.97 | 0.19 | 117,117,117,117 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | DO | 202 | 1/1 | 0.97 | 0.64 | 61,61,61,61 | 0 |
| 87 | MG | A6 | 2110 | 1/1 | 0.97 | 0.26 | 65,65,65,65 | 0 |
| 86 | OHX | A5 | 3606 | 7/7 | 0.97 | 0.18 | 130,130,130,130 | 7 |
| 86 | OHX | A1 | 3484 | 7/7 | 0.97 | 0.19 | 126,126,126,126 | 0 |
| 86 | OHX | A1 | 3490 | 7/7 | 0.97 | 0.19 | 126,126,126,126 | 0 |
| 86 | OHX | A1 | 3493 | 7/7 | 0.97 | 0.16 | 148,148,148,148 | 0 |
| 86 | OHX | A4 | 206 | 7/7 | 0.97 | 0.17 | 104,104,104,104 | 7 |
| 87 | MG | A5 | 4437 | 1/1 | 0.97 | 0.28 | 86,86,86,86 | 0 |
| 87 | MG | A1 | 4475 | 1/1 | 0.97 | 0.78 | 64,64,64,64 | 0 |
| 87 | MG | A1 | 4279 | 1/1 | 0.97 | 0.74 | 54,54,54,54 | 0 |
| 86 | OHX | A4 | 207 | 7/7 | 0.97 | 0.17 | 129,129,129,129 | 7 |
| 86 | OHX | A4 | 208 | 7/7 | 0.97 | 0.22 | 90,90,90,90 | 7 |
| 87 | MG | A6 | 2327 | 1/1 | 0.97 | 0.14 | 108,108,108,108 | 0 |
| 86 | OHX | A1 | 3663 | 7/7 | 0.97 | 0.30 | 126,126,126,126 | 7 |
| 86 | OHX | A4 | 210 | 7/7 | 0.97 | 0.11 | 131,131,131,131 | 7 |
| 86 | OHX | A1 | 3494 | 7/7 | 0.97 | 0.17 | 133,133,133,133 | 0 |
| 86 | OHX | A5 | 3616 | 7/7 | 0.97 | 0.21 | 102,102,102,102 | 7 |
| 86 | OHX | A5 | 3617 | 7/7 | 0.97 | 0.12 | 154,154,154,154 | 7 |
| 86 | OHX | A1 | 3497 | 7/7 | 0.97 | 0.27 | 100,100,100,100 | 7 |
| 86 | OHX | A5 | 3619 | 7/7 | 0.97 | 0.20 | 119,119,119,119 | 7 |
| 86 | OHX | A1 | 3501 | 7/7 | 0.97 | 0.19 | 94,94,94,94 | 7 |
| 87 | MG | A2 | 2195 | 1/1 | 0.97 | 0.24 | 90,90,90,90 | 0 |
| 86 | OHX | A1 | 3588 | 7/7 | 0.97 | 0.20 | 104,104,104,104 | 7 |
| 86 | OHX | A1 | 3503 | 7/7 | 0.97 | 0.17 | 111,111,111,111 | 7 |
| 86 | OHX | A1 | 3504 | 7/7 | 0.97 | 0.20 | 105,105,105,105 | 7 |
| 87 | MG | DV | 203 | 1/1 | 0.97 | 0.24 | 65,65,65,65 | 0 |
| 86 | OHX | A2 | 1949 | 7/7 | 0.97 | 0.15 | 135,135,135,135 | 7 |
| 86 | OHX | A5 | 3625 | 7/7 | 0.97 | 0.17 | 117,117,117,117 | 7 |
| 86 | OHX | A1 | 3672 | 7/7 | 0.97 | 0.23 | 99,99,99,99 | 7 |
| 86 | OHX | A1 | 3511 | 7/7 | 0.97 | 0.17 | 154,154,154,154 | 0 |
| 86 | OHX | A1 | 3594 | 7/7 | 0.97 | 0.13 | 144,144,144,144 | 7 |
| 87 | MG | A5 | 4460 | 1/1 | 0.97 | 0.71 | 74,74,74,74 | 0 |
| 86 | OHX | A1 | 3595 | 7/7 | 0.97 | 0.22 | 120,120,120,120 | 7 |
| 86 | OHX | A2 | 1952 | 7/7 | 0.97 | 0.14 | 127,127,127,127 | 7 |
| 86 | OHX | A1 | 3597 | 7/7 | 0.97 | 0.18 | 123,123,123,123 | 7 |
| 86 | OHX | A5 | 3632 | 7/7 | 0.97 | 0.20 | 106,106,106,106 | 7 |
| 87 | MG | A5 | 4465 | 1/1 | 0.97 | 0.40 | 62,62,62,62 | 0 |
| 86 | OHX | A1 | 3598 | 7/7 | 0.97 | 0.15 | 139,139,139,139 | 7 |
| 87 | MG | A5 | 4242 | 1/1 | 0.97 | 0.56 | 65,65,65,65 | 0 |
| 86 | OHX | A2 | 1970 | 7/7 | 0.97 | 0.14 | 138,138,138,138 | 7 |
| 87 | MG | Df | 204 | 1/1 | 0.97 | 0.54 | 61,61,61,61 | 0 |
| 86 | OHX | A2 | 1953 | 7/7 | 0.97 | 0.20 | 120,120,120,120 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86 | OHX | A5 | 3636 | 7/7 | 0.97 | 0.15 | 111,111,111,111 | 7 |
| 86 | OHX | A2 | 1974 | 7/7 | 0.97 | 0.12 | 170,170,170,170 | 7 |
| 86 | OHX | Bj | 102 | 7/7 | 0.97 | 0.21 | 102,102,102,102 | 7 |
| 86 | OHX | A2 | 1975 | 7/7 | 0.97 | 0.14 | 141,141,141,141 | 7 |
| 86 | OHX | A5 | 3812 | 7/7 | 0.97 | 0.13 | 135,135,135,135 | 7 |
| 87 | MG | A5 | 4475 | 1/1 | 0.97 | 0.79 | 127,127,127,127 | 0 |
| 86 | OHX | A6 | 1927 | 7/7 | 0.97 | 0.17 | 129,129,129,129 | 0 |
| 86 | OHX | A6 | 1929 | 7/7 | 0.97 | 0.17 | 128,128,128,128 | 0 |
| 87 | MG | A5 | 4252 | 1/1 | 0.97 | 0.23 | 68,68,68,68 | 0 |
| 86 | OHX | A6 | 1933 | 7/7 | 0.97 | 0.20 | 104,104,104,104 | 7 |
| 86 | OHX | A6 | 1934 | 7/7 | 0.97 | 0.21 | 105,105,105,105 | 7 |
| 86 | OHX | A6 | 1936 | 7/7 | 0.97 | 0.20 | 100,100,100,100 | 7 |
| 86 | OHX | A1 | 3527 | 7/7 | 0.97 | 0.22 | 94,94,94,94 | 7 |
| 86 | OHX | A6 | 1940 | 7/7 | 0.97 | 0.15 | 129,129,129,129 | 7 |
| 86 | OHX | A6 | 1941 | 7/7 | 0.97 | 0.17 | 112,112,112,112 | 7 |
| 88 | ZN | Ad | 105 | 1/1 | 0.97 | 0.18 | 83,83,83,83 | 0 |
| 88 | ZN | Bm | 202 | 1/1 | 0.97 | 0.18 | 56,56,56,56 | 0 |
| 86 | OHX | A6 | 1942 | 7/7 | 0.97 | 0.19 | 114,114,114,114 | 7 |
| 87 | MG | A6 | 2159 | 1/1 | 0.97 | 0.23 | 33,33,33,33 | 0 |
| 88 | ZN | Cd | 103 | 1/1 | 0.97 | 0.17 | 71,71,71,71 | 0 |
| 86 | OHX | A1 | 3605 | 7/7 | 0.97 | 0.13 | 166,166,166,166 | 7 |
| 86 | OHX | A6 | 1951 | 7/7 | 0.97 | 0.17 | 115,115,115,115 | 7 |
| 88 | ZN | Dp | 104 | 1/1 | 0.97 | 0.15 | 79,79,79,79 | 0 |
| 86 | OHX | A5 | 3578 | 7/7 | 0.98 | 0.11 | 159,159,159,159 | 7 |
| 86 | OHX | A6 | 1943 | 7/7 | 0.98 | 0.18 | 106,106,106,106 | 7 |
| 87 | MG | A1 | 3905 | 1/1 | 0.98 | 0.16 | 19,19,19,19 | 0 |
| 87 | MG | A1 | 4318 | 1/1 | 0.98 | 0.43 | 66,66,66,66 | 0 |
| 87 | MG | A5 | 4509 | 1/1 | 0.98 | 0.92 | 134,134,134,134 | 0 |
| 86 | OHX | A6 | 1944 | 7/7 | 0.98 | 0.15 | 115,115,115,115 | 7 |
| 86 | OHX | A2 | 1927 | 7/7 | 0.98 | 0.17 | 115,115,115,115 | 7 |
| 86 | OHX | A5 | 3759 | 7/7 | 0.98 | 0.20 | 80,80,80,80 | 7 |
| 86 | OHX | A5 | 3582 | 7/7 | 0.98 | 0.20 | 95,95,95,95 | 7 |
| 86 | OHX | A6 | 1948 | 7/7 | 0.98 | 0.17 | 114,114,114,114 | 7 |
| 86 | OHX | A6 | 1949 | 7/7 | 0.98 | 0.17 | 102,102,102,102 | 7 |
| 86 | OHX | A6 | 1950 | 7/7 | 0.98 | 0.14 | 140,140,140,140 | 0 |
| 86 | OHX | A1 | 3454 | 7/7 | 0.98 | 0.18 | 106,106,106,106 | 7 |
| 86 | OHX | A6 | 1952 | 7/7 | 0.98 | 0.15 | 123,123,123,123 | 7 |
| 87 | MG | A1 | 4121 | 1/1 | 0.98 | 0.12 | 74,74,74,74 | 0 |
| 86 | OHX | A6 | 1953 | 7/7 | 0.98 | 0.12 | 136,136,136,136 | 7 |
| 86 | OHX | A1 | 3622 | 7/7 | 0.98 | 0.21 | 112,112,112,112 | 7 |
| 86 | OHX | A1 | 3458 | 7/7 | 0.98 | 0.17 | 111,111,111,111 | 7 |
| 86 | OHX | A6 | 1956 | 7/7 | 0.98 | 0.16 | 130,130,130,130 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86 | OHX | A5 | 3592 | 7/7 | 0.98 | 0.20 | 102,102,102,102 | 7 |
| 86 | OHX | A6 | 1957 | 7/7 | 0.98 | 0.14 | 144,144,144,144 | 7 |
| 86 | OHX | A1 | 3545 | 7/7 | 0.98 | 0.19 | 78,78,78,78 | 7 |
| 86 | OHX | A1 | 3459 | 7/7 | 0.98 | 0.21 | 86,86,86,86 | 7 |
| 86 | OHX | A6 | 1960 | 7/7 | 0.98 | 0.15 | 120,120,120,120 | 7 |
| 86 | OHX | A1 | 3460 | 7/7 | 0.98 | 0.18 | 111,111,111,111 | 0 |
| 87 | MG | A6 | 2199 | 1/1 | 0.98 | 0.28 | 62,62,62,62 | 0 |
| 86 | OHX | A1 | 3462 | 7/7 | 0.98 | 0.20 | 91,91,91,91 | 7 |
| 86 | OHX | A1 | 3463 | 7/7 | 0.98 | 0.15 | 110,110,110,110 | 7 |
| 86 | OHX | A1 | 3469 | 7/7 | 0.98 | 0.18 | 122,122,122,122 | 0 |
| 86 | OHX | A5 | 3601 | 7/7 | 0.98 | 0.18 | 96,96,96,96 | 7 |
| 86 | OHX | A1 | 3551 | 7/7 | 0.98 | 0.18 | 100,100,100,100 | 7 |
| 86 | OHX | A6 | 2076 | 7/7 | 0.98 | 0.24 | 90,90,90,90 | 7 |
| 86 | OHX | A1 | 3470 | 7/7 | 0.98 | 0.18 | 96,96,96,96 | 7 |
| 86 | OHX | A1 | 3553 | 7/7 | 0.98 | 0.23 | 110,110,110,110 | 7 |
| 86 | OHX | A1 | 3471 | 7/7 | 0.98 | 0.17 | 107,107,107,107 | 7 |
| 86 | OHX | A6 | 1969 | 7/7 | 0.98 | 0.21 | 90,90,90,90 | 7 |
| 86 | OHX | A2 | 1991 | 7/7 | 0.98 | 0.14 | 113,113,113,113 | 7 |
| 86 | OHX | A6 | 1971 | 7/7 | 0.98 | 0.14 | 108,108,108,108 | 7 |
| 86 | OHX | A1 | 3473 | 7/7 | 0.98 | 0.21 | 85,85,85,85 | 7 |
| 86 | OHX | A1 | 3475 | 7/7 | 0.98 | 0.20 | 98,98,98,98 | 7 |
| 86 | OHX | A2 | 1908 | 7/7 | 0.98 | 0.20 | 115,115,115,115 | 0 |
| 86 | OHX | A6 | 1975 | 7/7 | 0.98 | 0.17 | 106,106,106,106 | 7 |
| 86 | OHX | A1 | 3477 | 7/7 | 0.98 | 0.21 | 83,83,83,83 | 7 |
| 86 | OHX | A1 | 3718 | 7/7 | 0.98 | 0.19 | 94,94,94,94 | 7 |
| 86 | OHX | A1 | 3478 | 7/7 | 0.98 | 0.17 | 112,112,112,112 | 7 |
| 86 | OHX | A5 | 3795 | 7/7 | 0.98 | 0.27 | 117,117,117,117 | 7 |
| 86 | OHX | A2 | 1930 | 7/7 | 0.98 | 0.16 | 120,120,120,120 | 7 |
| 86 | OHX | A1 | 3482 | 7/7 | 0.98 | 0.17 | 106,106,106,106 | 7 |
| 86 | OHX | A1 | 3483 | 7/7 | 0.98 | 0.20 | 103,103,103,103 | 7 |
| 86 | OHX | A2 | 1909 | 7/7 | 0.98 | 0.19 | 93,93,93,93 | 7 |
| 86 | OHX | A6 | 1983 | 7/7 | 0.98 | 0.17 | 133,133,133,133 | 7 |
| 86 | OHX | A1 | 3565 | 7/7 | 0.98 | 0.14 | 127,127,127,127 | 7 |
| 86 | OHX | A1 | 3487 | 7/7 | 0.98 | 0.21 | 94,94,94,94 | 7 |
| 86 | OHX | A1 | 3568 | 7/7 | 0.98 | 0.14 | 133,133,133,133 | 7 |
| 86 | OHX | A1 | 3489 | 7/7 | 0.98 | 0.20 | 90,90,90,90 | 7 |
| 86 | OHX | A2 | 1948 | 7/7 | 0.98 | 0.17 | 108,108,108,108 | 7 |
| 86 | OHX | A1 | 3571 | 7/7 | 0.98 | 0.16 | 119,119,119,119 | 7 |
| 86 | OHX | A2 | 1996 | 7/7 | 0.98 | 0.20 | 113,113,113,113 | 7 |
| 86 | OHX | A5 | 3809 | 7/7 | 0.98 | 0.23 | 91,91,91,91 | 7 |
| 87 | MG | A1 | 3959 | 1/1 | 0.98 | 0.43 | 43,43,43,43 | 0 |
| 87 | MG | A5 | 4566 | 1/1 | 0.98 | 0.46 | 74,74,74,74 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86 | OHX | A2 | 1911 | 7/7 | 0.98 | 0.21 | 124,124,124,124 | 0 |
| 86 | OHX | A2 | 1971 | 7/7 | 0.98 | 0.14 | 110,110,110,110 | 7 |
| 86 | OHX | A1 | 3653 | 7/7 | 0.98 | 0.12 | 153,153,153,153 | 7 |
| 86 | OHX | A1 | 3498 | 7/7 | 0.98 | 0.23 | 89,89,89,89 | 7 |
| 86 | OHX | A1 | 3576 | 7/7 | 0.98 | 0.18 | 83,83,83,83 | 7 |
| 86 | OHX | A1 | 3500 | 7/7 | 0.98 | 0.18 | 87,87,87,87 | 7 |
| 86 | OHX | A3 | 202 | 7/7 | 0.98 | 0.16 | 103,103,103,103 | 7 |
| 86 | OHX | A3 | 203 | 7/7 | 0.98 | 0.16 | 118,118,118,118 | 7 |
| 86 | OHX | A2 | 1972 | 7/7 | 0.98 | 0.17 | 138,138,138,138 | 7 |
| 86 | OHX | CY | 201 | 7/7 | 0.98 | 0.17 | 121,121,121,121 | 7 |
| 86 | OHX | A1 | 3502 | 7/7 | 0.98 | 0.19 | 78,78,78,78 | 7 |
| 87 | MG | A5 | 4578 | 1/1 | 0.98 | 0.26 | 74,74,74,74 | 0 |
| 86 | OHX | Cd | 101 | 7/7 | 0.98 | 0.18 | 135,135,135,135 | 7 |
| 86 | OHX | A2 | 1950 | 7/7 | 0.98 | 0.13 | 122,122,122,122 | 7 |
| 86 | OHX | A1 | 3581 | 7/7 | 0.98 | 0.23 | 73,73,73,73 | 7 |
| 87 | MG | A7 | 214 | 1/1 | 0.98 | 0.47 | 55,55,55,55 | 0 |
| 86 | OHX | A7 | 202 | 7/7 | 0.98 | 0.21 | 81,81,81,81 | 7 |
| 86 | OHX | A2 | 1951 | 7/7 | 0.98 | 0.13 | 126,126,126,126 | 7 |
| 86 | OHX | A7 | 206 | 7/7 | 0.98 | 0.17 | 115,115,115,115 | 7 |
| 86 | OHX | A1 | 3505 | 7/7 | 0.98 | 0.17 | 124,124,124,124 | 7 |
| 86 | OHX | A7 | 208 | 7/7 | 0.98 | 0.18 | 105,105,105,105 | 7 |
| 86 | OHX | A1 | 3584 | 7/7 | 0.98 | 0.20 | 88,88,88,88 | 7 |
| 86 | OHX | A2 | 1933 | 7/7 | 0.98 | 0.17 | 109,109,109,109 | 7 |
| 86 | OHX | A1 | 3508 | 7/7 | 0.98 | 0.19 | 93,93,93,93 | 7 |
| 87 | MG | A6 | 2257 | 1/1 | 0.98 | 0.26 | 65,65,65,65 | 0 |
| 86 | OHX | A4 | 203 | 7/7 | 0.98 | 0.19 | 93,93,93,93 | 7 |
| 86 | OHX | A4 | 204 | 7/7 | 0.98 | 0.17 | 122,122,122,122 | 7 |
| 86 | OHX | A8 | 203 | 7/7 | 0.98 | 0.15 | 111,111,111,111 | 7 |
| 86 | OHX | A5 | 3446 | 7/7 | 0.98 | 0.20 | 82,82,82,82 | 0 |
| 86 | OHX | A8 | 205 | 7/7 | 0.98 | 0.14 | 107,107,107,107 | 7 |
| 86 | OHX | A5 | 3447 | 7/7 | 0.98 | 0.22 | 107,107,107,107 | 0 |
| 86 | OHX | A8 | 207 | 7/7 | 0.98 | 0.16 | 126,126,126,126 | 7 |
| 86 | OHX | A8 | 208 | 7/7 | 0.98 | 0.19 | 115,115,115,115 | 7 |
| 86 | OHX | A5 | 3455 | 7/7 | 0.98 | 0.20 | 100,100,100,100 | 0 |
| 86 | OHX | A5 | 3456 | 7/7 | 0.98 | 0.18 | 85,85,85,85 | 7 |
| 86 | OHX | A5 | 3459 | 7/7 | 0.98 | 0.20 | 100,100,100,100 | 0 |
| 86 | OHX | A5 | 3462 | 7/7 | 0.98 | 0.19 | 102,102,102,102 | 0 |
| 86 | OHX | A5 | 3463 | 7/7 | 0.98 | 0.22 | 130,130,130,130 | 0 |
| 86 | OHX | A5 | 3464 | 7/7 | 0.98 | 0.17 | 98,98,98,98 | 7 |
| 86 | OHX | A5 | 3465 | 7/7 | 0.98 | 0.20 | 91,91,91,91 | 7 |
| 87 | MG | A5 | 3940 | 1/1 | 0.98 | 0.41 | 39,39,39,39 | 0 |
| 86 | OHX | A5 | 3467 | 7/7 | 0.98 | 0.20 | 104,104,104,104 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87 | MG | A1 | 3998 | 1/1 | 0.98 | 0.24 | 28,28,28,28 | 0 |
| 86 | OHX | A4 | 205 | 7/7 | 0.98 | 0.16 | 122,122,122,122 | 7 |
| 87 | MG | A1 | 4000 | 1/1 | 0.98 | 0.19 | 18,18,18,18 | 0 |
| 86 | OHX | A5 | 3476 | 7/7 | 0.98 | 0.17 | 103,103,103,103 | 7 |
| 86 | OHX | A5 | 3477 | 7/7 | 0.98 | 0.16 | 108,108,108,108 | 7 |
| 86 | OHX | A5 | 3480 | 7/7 | 0.98 | 0.17 | 101,101,101,101 | 7 |
| 86 | OHX | A5 | 3481 | 7/7 | 0.98 | 0.18 | 92,92,92,92 | 7 |
| 86 | OHX | DB | 401 | 7/7 | 0.98 | 0.20 | 98,98,98,98 | 7 |
| 86 | OHX | A5 | 3482 | 7/7 | 0.98 | 0.22 | 85,85,85,85 | 7 |
| 86 | OHX | A5 | 3483 | 7/7 | 0.98 | 0.18 | 103,103,103,103 | 7 |
| 87 | MG | A5 | 4170 | 1/1 | 0.98 | 0.55 | 69,69,69,69 | 0 |
| 86 | OHX | A5 | 3487 | 7/7 | 0.98 | 0.18 | 94,94,94,94 | 7 |
| 86 | OHX | A1 | 3509 | 7/7 | 0.98 | 0.18 | 98,98,98,98 | 7 |
| 86 | OHX | A5 | 3489 | 7/7 | 0.98 | 0.20 | 88,88,88,88 | 7 |
| 86 | OHX | A5 | 3490 | 7/7 | 0.98 | 0.16 | 113,113,113,113 | 7 |
| 87 | MG | A8 | 236 | 1/1 | 0.98 | 0.19 | 75,75,75,75 | 0 |
| 86 | OHX | A5 | 3491 | 7/7 | 0.98 | 0.18 | 106,106,106,106 | 7 |
| 87 | MG | A5 | 4176 | 1/1 | 0.98 | 0.19 | 89,89,89,89 | 0 |
| 86 | OHX | A1 | 3510 | 7/7 | 0.98 | 0.22 | 92,92,92,92 | 7 |
| 86 | OHX | A5 | 3494 | 7/7 | 0.98 | 0.18 | 97,97,97,97 | 7 |
| 86 | OHX | A5 | 3495 | 7/7 | 0.98 | 0.20 | 92,92,92,92 | 7 |
| 87 | MG | A6 | 2292 | 1/1 | 0.98 | 0.24 | 75,75,75,75 | 0 |
| 86 | OHX | DO | 201 | 7/7 | 0.98 | 0.20 | 93,93,93,93 | 7 |
| 86 | OHX | A5 | 3496 | 7/7 | 0.98 | 0.20 | 73,73,73,73 | 7 |
| 86 | OHX | A5 | 3498 | 7/7 | 0.98 | 0.21 | 89,89,89,89 | 7 |
| 86 | OHX | A5 | 3677 | 7/7 | 0.98 | 0.18 | 113,113,113,113 | 7 |
| 86 | OHX | A5 | 3499 | 7/7 | 0.98 | 0.20 | 84,84,84,84 | 7 |
| 86 | OHX | De | 201 | 7/7 | 0.98 | 0.21 | 91,91,91,91 | 7 |
| 86 | OHX | Df | 201 | 7/7 | 0.98 | 0.18 | 99,99,99,99 | 7 |
| 86 | OHX | A5 | 3500 | 7/7 | 0.98 | 0.18 | 88,88,88,88 | 7 |
| 86 | OHX | Dh | 201 | 7/7 | 0.98 | 0.17 | 129,129,129,129 | 7 |
| 87 | MG | A1 | 3820 | 1/1 | 0.98 | 0.28 | 47,47,47,47 | 0 |
| 86 | OHX | Dj | 104 | 7/7 | 0.98 | 0.18 | 105,105,105,105 | 7 |
| 86 | OHX | Do | 201 | 7/7 | 0.98 | 0.22 | 89,89,89,89 | 7 |
| 86 | OHX | A5 | 3501 | 7/7 | 0.98 | 0.17 | 106,106,106,106 | 7 |
| 86 | OHX | A2 | 1912 | 7/7 | 0.98 | 0.19 | 115,115,115,115 | 0 |
| 86 | OHX | A5 | 3503 | 7/7 | 0.98 | 0.20 | 97,97,97,97 | 7 |
| 86 | OHX | A5 | 3504 | 7/7 | 0.98 | 0.18 | 101,101,101,101 | 7 |
| 87 | MG | A1 | 3827 | 1/1 | 0.98 | 0.28 | 47,47,47,47 | 0 |
| 86 | OHX | A5 | 3505 | 7/7 | 0.98 | 0.16 | 94,94,94,94 | 7 |
| 86 | OHX | A5 | 3506 | 7/7 | 0.98 | 0.19 | 102,102,102,102 | 7 |
| 86 | OHX | A5 | 3507 | 7/7 | 0.98 | 0.20 | 75,75,75,75 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86 | OHX | A5 | 3508 | 7/7 | 0.98 | 0.17 | 119,119,119,119 | 7 |
| 86 | OHX | A5 | 3509 | 7/7 | 0.98 | 0.19 | 97,97,97,97 | 7 |
| 87 | MG | A5 | 3983 | 1/1 | 0.98 | 0.41 | 47,47,47,47 | 0 |
| 87 | MG | DD | 306 | 1/1 | 0.98 | 0.42 | 77,77,77,77 | 0 |
| 87 | MG | A5 | 3984 | 1/1 | 0.98 | 0.47 | 56,56,56,56 | 0 |
| 86 | OHX | A2 | 1903 | 7/7 | 0.98 | 0.22 | 94,94,94,94 | 0 |
| 86 | OHX | A5 | 3512 | 7/7 | 0.98 | 0.16 | 111,111,111,111 | 7 |
| 86 | OHX | A1 | 3513 | 7/7 | 0.98 | 0.18 | 101,101,101,101 | 7 |
| 86 | OHX | A5 | 3514 | 7/7 | 0.98 | 0.22 | 90,90,90,90 | 7 |
| 86 | OHX | A1 | 3671 | 7/7 | 0.98 | 0.23 | 96,96,96,96 | 7 |
| 86 | OHX | A5 | 3516 | 7/7 | 0.98 | 0.20 | 89,89,89,89 | 7 |
| 86 | OHX | A5 | 3517 | 7/7 | 0.98 | 0.22 | 80,80,80,80 | 7 |
| 86 | OHX | A1 | 3514 | 7/7 | 0.98 | 0.20 | 99,99,99,99 | 7 |
| 86 | OHX | A5 | 3519 | 7/7 | 0.98 | 0.23 | 78,78,78,78 | 7 |
| 86 | OHX | A5 | 3520 | 7/7 | 0.98 | 0.20 | 113,113,113,113 | 7 |
| 86 | OHX | A1 | 3515 | 7/7 | 0.98 | 0.17 | 115,115,115,115 | 7 |
| 86 | OHX | A1 | 3516 | 7/7 | 0.98 | 0.19 | 86,86,86,86 | 7 |
| 86 | OHX | A5 | 3701 | 7/7 | 0.98 | 0.23 | 57,57,57,57 | 7 |
| 86 | OHX | A5 | 3524 | 7/7 | 0.98 | 0.20 | 92,92,92,92 | 7 |
| 86 | OHX | A5 | 3525 | 7/7 | 0.98 | 0.18 | 112,112,112,112 | 7 |
| 86 | OHX | A5 | 3526 | 7/7 | 0.98 | 0.19 | 85,85,85,85 | 7 |
| 86 | OHX | A5 | 3527 | 7/7 | 0.98 | 0.20 | 105,105,105,105 | 7 |
| 86 | OHX | A2 | 1978 | 7/7 | 0.98 | 0.18 | 108,108,108,108 | 7 |
| 86 | OHX | A2 | 2033 | 7/7 | 0.98 | 0.20 | 97,97,97,97 | 7 |
| 86 | OHX | A5 | 3531 | 7/7 | 0.98 | 0.19 | 106,106,106,106 | 7 |
| 86 | OHX | A2 | 1936 | 7/7 | 0.98 | 0.21 | 112,112,112,112 | 7 |
| 87 | MG | A2 | 2119 | 1/1 | 0.98 | 0.26 | 67,67,67,67 | 0 |
| 86 | OHX | A1 | 3521 | 7/7 | 0.98 | 0.23 | 84,84,84,84 | 7 |
| 86 | OHX | A5 | 3534 | 7/7 | 0.98 | 0.20 | 92,92,92,92 | 7 |
| 87 | MG | A5 | 4009 | 1/1 | 0.98 | 0.38 | 45,45,45,45 | 0 |
| 86 | OHX | A1 | 3523 | 7/7 | 0.98 | 0.17 | 111,111,111,111 | 7 |
| 87 | MG | A1 | 4064 | 1/1 | 0.98 | 0.29 | 69,69,69,69 | 0 |
| 87 | MG | A5 | 4012 | 1/1 | 0.98 | 0.42 | 43,43,43,43 | 0 |
| 86 | OHX | A5 | 3537 | 7/7 | 0.98 | 0.15 | 115,115,115,115 | 7 |
| 87 | MG | A5 | 4234 | 1/1 | 0.98 | 0.11 | 67,67,67,67 | 0 |
| 86 | OHX | A2 | 1916 | 7/7 | 0.98 | 0.17 | 110,110,110,110 | 7 |
| 86 | OHX | A5 | 3539 | 7/7 | 0.98 | 0.19 | 125,125,125,125 | 7 |
| 86 | OHX | BI | 301 | 7/7 | 0.98 | 0.20 | 94,94,94,94 | 7 |
| 86 | OHX | A1 | 3525 | 7/7 | 0.98 | 0.21 | 101,101,101,101 | 7 |
| 86 | OHX | A1 | 3603 | 7/7 | 0.98 | 0.17 | 136,136,136,136 | 7 |
| 86 | OHX | A2 | 1981 | 7/7 | 0.98 | 0.14 | 132,132,132,132 | 7 |
| 86 | OHX | BN | 301 | 7/7 | 0.98 | 0.19 | 116,116,116,116 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86 | OHX | A5 | 3545 | 7/7 | 0.98 | 0.17 | 133,133,133,133 | 7 |
| 86 | OHX | A1 | 3528 | 7/7 | 0.98 | 0.21 | 81,81,81,81 | 7 |
| 86 | OHX | A1 | 3529 | 7/7 | 0.98 | 0.23 | 77,77,77,77 | 7 |
| 86 | OHX | A2 | 1957 | 7/7 | 0.98 | 0.18 | 101,101,101,101 | 7 |
| 86 | OHX | Bf | 201 | 7/7 | 0.98 | 0.21 | 85,85,85,85 | 7 |
| 86 | OHX | A2 | 1938 | 7/7 | 0.98 | 0.15 | 111,111,111,111 | 7 |
| 86 | OHX | A2 | 1917 | 7/7 | 0.98 | 0.16 | 111,111,111,111 | 7 |
| 86 | OHX | A5 | 3552 | 7/7 | 0.98 | 0.16 | 138,138,138,138 | 7 |
| 86 | OHX | A5 | 3553 | 7/7 | 0.98 | 0.24 | 75,75,75,75 | 7 |
| 86 | OHX | A5 | 3554 | 7/7 | 0.98 | 0.20 | 130,130,130,130 | 7 |
| 86 | OHX | A1 | 3533 | 7/7 | 0.98 | 0.20 | 104,104,104,104 | 7 |
| 87 | MG | A5 | 4032 | 1/1 | 0.98 | 0.46 | 41,41,41,41 | 0 |
| 86 | OHX | Bo | 201 | 7/7 | 0.98 | 0.19 | 97,97,97,97 | 7 |
| 86 | OHX | A6 | 1909 | 7/7 | 0.98 | 0.19 | 84,84,84,84 | 0 |
| 87 | MG | A1 | 4500 | 1/1 | 0.98 | 0.26 | 106,106,106,106 | 0 |
| 87 | MG | A6 | 2150 | 1/1 | 0.98 | 0.41 | 48,48,48,48 | 0 |
| 86 | OHX | A5 | 3558 | 7/7 | 0.98 | 0.21 | 85,85,85,85 | 7 |
| 86 | OHX | A5 | 3559 | 7/7 | 0.98 | 0.15 | 109,109,109,109 | 7 |
| 87 | MG | A5 | 4481 | 1/1 | 0.98 | 0.68 | 60,60,60,60 | 0 |
| 86 | OHX | A6 | 1919 | 7/7 | 0.98 | 0.17 | 104,104,104,104 | 7 |
| 86 | OHX | A5 | 3737 | 7/7 | 0.98 | 0.21 | 75,75,75,75 | 7 |
| 86 | OHX | A6 | 1922 | 7/7 | 0.98 | 0.16 | 108,108,108,108 | 0 |
| 86 | OHX | A6 | 1925 | 7/7 | 0.98 | 0.16 | 112,112,112,112 | 7 |
| 86 | OHX | A1 | 3611 | 7/7 | 0.98 | 0.17 | 96,96,96,96 | 7 |
| 86 | OHX | A2 | 1918 | 7/7 | 0.98 | 0.18 | 99,99,99,99 | 7 |
| 86 | OHX | A6 | 1930 | 7/7 | 0.98 | 0.17 | 120,120,120,120 | 7 |
| 87 | MG | A6 | 2160 | 1/1 | 0.98 | 0.44 | 45,45,45,45 | 0 |
| 86 | OHX | A6 | 1932 | 7/7 | 0.98 | 0.16 | 109,109,109,109 | 7 |
| 86 | OHX | A1 | 3535 | 7/7 | 0.98 | 0.21 | 102,102,102,102 | 7 |
| 86 | OHX | A2 | 1941 | 7/7 | 0.98 | 0.17 | 117,117,117,117 | 7 |
| 86 | OHX | A5 | 3569 | 7/7 | 0.98 | 0.17 | 110,110,110,110 | 7 |
| 86 | OHX | A5 | 3570 | 7/7 | 0.98 | 0.24 | 97,97,97,97 | 7 |
| 86 | OHX | A6 | 1935 | 7/7 | 0.98 | 0.17 | 102,102,102,102 | 7 |
| 86 | OHX | A1 | 3537 | 7/7 | 0.98 | 0.17 | 119,119,119,119 | 7 |
| 86 | OHX | A5 | 3573 | 7/7 | 0.98 | 0.18 | 107,107,107,107 | 7 |
| 88 | ZN | Af | 202 | 1/1 | 0.98 | 0.12 | 113,113,113,113 | 0 |
| 86 | OHX | A2 | 1942 | 7/7 | 0.98 | 0.17 | 113,113,113,113 | 7 |
| 86 | OHX | A2 | 1907 | 7/7 | 0.98 | 0.20 | 104,104,104,104 | 7 |
| 88 | ZN | Bp | 501 | 1/1 | 0.98 | 0.13 | 68,68,68,68 | 0 |
| 87 | MG | A2 | 2163 | 1/1 | 0.98 | 0.18 | 80,80,80,80 | 0 |
| 87 | MG | A5 | 4501 | 1/1 | 0.98 | 0.87 | 56,56,56,56 | 0 |
| 87 | MG | A1 | 3900 | 1/1 | 0.98 | 0.16 | 78,78,78,78 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86 | OHX | A1 | 3442 | 7/7 | 0.98 | 0.19 | 95,95,95,95 | 0 |
| 86 | OHX | A2 | 1964 | 7/7 | 0.98 | 0.18 | 135,135,135,135 | 7 |
| 86 | OHX | A5 | 3416 | 7/7 | 0.99 | 0.24 | 68,68,68,68 | 0 |
| 86 | OHX | A5 | 3417 | 7/7 | 0.99 | 0.26 | 72,72,72,72 | 0 |
| 86 | OHX | A5 | 3418 | 7/7 | 0.99 | 0.26 | 77,77,77,77 | 0 |
| 87 | MG | A5 | 3824 | 1/1 | 0.99 | 0.28 | 37,37,37,37 | 0 |
| 86 | OHX | A5 | 3419 | 7/7 | 0.99 | 0.24 | 79,79,79,79 | 0 |
| 86 | OHX | A5 | 3420 | 7/7 | 0.99 | 0.23 | 74,74,74,74 | 0 |
| 86 | OHX | A5 | 3421 | 7/7 | 0.99 | 0.23 | 81,81,81,81 | 0 |
| 87 | MG | A5 | 4560 | 1/1 | 0.99 | 0.38 | 108,108,108,108 | 0 |
| 86 | OHX | A5 | 3422 | 7/7 | 0.99 | 0.22 | 75,75,75,75 | 0 |
| 86 | OHX | A5 | 3423 | 7/7 | 0.99 | 0.23 | 68,68,68,68 | 0 |
| 86 | OHX | A5 | 3424 | 7/7 | 0.99 | 0.25 | 86,86,86,86 | 0 |
| 86 | OHX | A5 | 3425 | 7/7 | 0.99 | 0.22 | 72,72,72,72 | 0 |
| 86 | OHX | A5 | 3426 | 7/7 | 0.99 | 0.19 | 67,67,67,67 | 0 |
| 86 | OHX | A5 | 3427 | 7/7 | 0.99 | 0.22 | 79,79,79,79 | 0 |
| 86 | OHX | A5 | 3428 | 7/7 | 0.99 | 0.23 | 88,88,88,88 | 0 |
| 86 | OHX | A5 | 3429 | 7/7 | 0.99 | 0.23 | 84,84,84,84 | 0 |
| 86 | OHX | A5 | 3431 | 7/7 | 0.99 | 0.20 | 83,83,83,83 | 0 |
| 86 | OHX | A5 | 3432 | 7/7 | 0.99 | 0.20 | 73,73,73,73 | 0 |
| 86 | OHX | A5 | 3433 | 7/7 | 0.99 | 0.20 | 81,81,81,81 | 0 |
| 86 | OHX | A5 | 3434 | 7/7 | 0.99 | 0.19 | 85,85,85,85 | 0 |
| 86 | OHX | A5 | 3435 | 7/7 | 0.99 | 0.17 | 70,70,70,70 | 0 |
| 86 | OHX | A5 | 3436 | 7/7 | 0.99 | 0.19 | 82,82,82,82 | 0 |
| 86 | OHX | A5 | 3437 | 7/7 | 0.99 | 0.19 | 83,83,83,83 | 0 |
| 86 | OHX | A5 | 3438 | 7/7 | 0.99 | 0.23 | 91,91,91,91 | 0 |
| 86 | OHX | A5 | 3439 | 7/7 | 0.99 | 0.19 | 81,81,81,81 | 0 |
| 86 | OHX | A6 | 1906 | 7/7 | 0.99 | 0.19 | 85,85,85,85 | 0 |
| 86 | OHX | A5 | 3442 | 7/7 | 0.99 | 0.18 | 85,85,85,85 | 0 |
| 86 | OHX | A5 | 3443 | 7/7 | 0.99 | 0.18 | 75,75,75,75 | 7 |
| 86 | OHX | A5 | 3444 | 7/7 | 0.99 | 0.18 | 74,74,74,74 | 7 |
| 87 | MG | A1 | 3873 | 1/1 | 0.99 | 0.38 | 62,62,62,62 | 0 |
| 86 | OHX | A5 | 3445 | 7/7 | 0.99 | 0.19 | 73,73,73,73 | 0 |
| 86 | OHX | A6 | 1907 | 7/7 | 0.99 | 0.22 | 91,91,91,91 | 0 |
| 86 | OHX | A6 | 1908 | 7/7 | 0.99 | 0.22 | 101,101,101,101 | 0 |
| 86 | OHX | A5 | 3448 | 7/7 | 0.99 | 0.19 | 93,93,93,93 | 0 |
| 86 | OHX | A5 | 3449 | 7/7 | 0.99 | 0.19 | 85,85,85,85 | 7 |
| 86 | OHX | A5 | 3451 | 7/7 | 0.99 | 0.18 | 81,81,81,81 | 7 |
| 86 | OHX | A5 | 3452 | 7/7 | 0.99 | 0.21 | 86,86,86,86 | 7 |
| 86 | OHX | A5 | 3453 | 7/7 | 0.99 | 0.18 | 102,102,102,102 | 0 |
| 87 | MG | A1 | 4417 | 1/1 | 0.99 | 0.34 | 94,94,94,94 | 0 |
| 86 | OHX | A5 | 3454 | 7/7 | 0.99 | 0.18 | 103,103,103,103 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86 | OHX | A1 | 3495 | 7/7 | 0.99 | 0.18 | 101,101,101,101 | 7 |
| 87 | MG | A1 | 4061 | 1/1 | 0.99 | 0.26 | 35,35,35,35 | 0 |
| 86 | OHX | A6 | 1910 | 7/7 | 0.99 | 0.17 | 84,84,84,84 | 0 |
| 86 | OHX | A5 | 3457 | 7/7 | 0.99 | 0.17 | 86,86,86,86 | 7 |
| 86 | OHX | A5 | 3458 | 7/7 | 0.99 | 0.19 | 91,91,91,91 | 0 |
| 86 | OHX | A6 | 1911 | 7/7 | 0.99 | 0.21 | 100,100,100,100 | 0 |
| 86 | OHX | A5 | 3460 | 7/7 | 0.99 | 0.19 | 80,80,80,80 | 7 |
| 86 | OHX | A5 | 3461 | 7/7 | 0.99 | 0.21 | 82,82,82,82 | 7 |
| 86 | OHX | A6 | 1912 | 7/7 | 0.99 | 0.18 | 96,96,96,96 | 0 |
| 86 | OHX | A6 | 1913 | 7/7 | 0.99 | 0.17 | 91,91,91,91 | 0 |
| 86 | OHX | A6 | 1914 | 7/7 | 0.99 | 0.17 | 111,111,111,111 | 0 |
| 86 | OHX | A6 | 1915 | 7/7 | 0.99 | 0.19 | 87,87,87,87 | 7 |
| 86 | OHX | A5 | 3466 | 7/7 | 0.99 | 0.20 | 120,120,120,120 | 0 |
| 86 | OHX | A6 | 1916 | 7/7 | 0.99 | 0.21 | 87,87,87,87 | 7 |
| 86 | OHX | A5 | 3468 | 7/7 | 0.99 | 0.20 | 75,75,75,75 | 7 |
| 86 | OHX | A5 | 3469 | 7/7 | 0.99 | 0.17 | 107,107,107,107 | 7 |
| 86 | OHX | A5 | 3470 | 7/7 | 0.99 | 0.15 | 118,118,118,118 | 0 |
| 86 | OHX | A5 | 3471 | 7/7 | 0.99 | 0.17 | 90,90,90,90 | 7 |
| 86 | OHX | A6 | 1917 | 7/7 | 0.99 | 0.19 | 100,100,100,100 | 7 |
| 86 | OHX | A5 | 3807 | 7/7 | 0.99 | 0.21 | 107,107,107,107 | 7 |
| 86 | OHX | A5 | 3473 | 7/7 | 0.99 | 0.20 | 82,82,82,82 | 7 |
| 86 | OHX | A5 | 3474 | 7/7 | 0.99 | 0.20 | 81,81,81,81 | 7 |
| 86 | OHX | A5 | 3475 | 7/7 | 0.99 | 0.18 | 95,95,95,95 | 7 |
| 86 | OHX | A6 | 1918 | 7/7 | 0.99 | 0.18 | 100,100,100,100 | 0 |
| 86 | OHX | A1 | 3567 | 7/7 | 0.99 | 0.19 | 88,88,88,88 | 7 |
| 87 | MG | A6 | 2248 | 1/1 | 0.99 | 0.15 | 75,75,75,75 | 0 |
| 86 | OHX | A5 | 3478 | 7/7 | 0.99 | 0.21 | 76,76,76,76 | 7 |
| 86 | OHX | A5 | 3479 | 7/7 | 0.99 | 0.17 | 110,110,110,110 | 0 |
| 86 | OHX | A6 | 1920 | 7/7 | 0.99 | 0.19 | 87,87,87,87 | 7 |
| 86 | OHX | A6 | 1921 | 7/7 | 0.99 | 0.19 | 92,92,92,92 | 7 |
| 86 | OHX | A1 | 3496 | 7/7 | 0.99 | 0.20 | 97,97,97,97 | 7 |
| 86 | OHX | A6 | 1923 | 7/7 | 0.99 | 0.18 | 76,76,76,76 | 7 |
| 86 | OHX | A5 | 3484 | 7/7 | 0.99 | 0.17 | 99,99,99,99 | 7 |
| 86 | OHX | A5 | 3485 | 7/7 | 0.99 | 0.18 | 85,85,85,85 | 7 |
| 86 | OHX | A5 | 3486 | 7/7 | 0.99 | 0.17 | 75,75,75,75 | 7 |
| 86 | OHX | A6 | 1924 | 7/7 | 0.99 | 0.17 | 83,83,83,83 | 7 |
| 86 | OHX | A1 | 3426 | 7/7 | 0.99 | 0.22 | 73,73,73,73 | 0 |
| 86 | OHX | A7 | 201 | 7/7 | 0.99 | 0.20 | 107,107,107,107 | 0 |
| 86 | OHX | A6 | 1926 | 7/7 | 0.99 | 0.19 | 82,82,82,82 | 7 |
| 86 | OHX | A1 | 3428 | 7/7 | 0.99 | 0.20 | 87,87,87,87 | 0 |
| 86 | OHX | A7 | 204 | 7/7 | 0.99 | 0.21 | 75,75,75,75 | 7 |
| 86 | OHX | A7 | 205 | 7/7 | 0.99 | 0.19 | 106,106,106,106 | 7 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86 | OHX | A6 | 1928 | 7/7 | 0.99 | 0.20 | 73,73,73,73 | 7 |
| 86 | OHX | A5 | 3492 | 7/7 | 0.99 | 0.21 | 89,89,89,89 | 7 |
| 86 | OHX | A1 | 3499 | 7/7 | 0.99 | 0.19 | 83,83,83,83 | 7 |
| 86 | OHX | A1 | 3429 | 7/7 | 0.99 | 0.20 | 87,87,87,87 | 0 |
| 86 | OHX | A6 | 1931 | 7/7 | 0.99 | 0.18 | 84,84,84,84 | 7 |
| 86 | OHX | A1 | 3432 | 7/7 | 0.99 | 0.20 | 90,90,90,90 | 0 |
| 86 | OHX | A5 | 3497 | 7/7 | 0.99 | 0.17 | 81,81,81,81 | 7 |
| 86 | OHX | A1 | 3433 | 7/7 | 0.99 | 0.19 | 85,85,85,85 | 0 |
| 86 | OHX | A8 | 202 | 7/7 | 0.99 | 0.23 | 77,77,77,77 | 0 |
| 86 | OHX | A1 | 3435 | 7/7 | 0.99 | 0.18 | 85,85,85,85 | 0 |
| 86 | OHX | A1 | 3437 | 7/7 | 0.99 | 0.21 | 74,74,74,74 | 7 |
| 86 | OHX | A1 | 3438 | 7/7 | 0.99 | 0.19 | 91,91,91,91 | 7 |
| 87 | MG | A1 | 3935 | 1/1 | 0.99 | 0.44 | 59,59,59,59 | 0 |
| 86 | OHX | A6 | 1937 | 7/7 | 0.99 | 0.18 | 96,96,96,96 | 7 |
| 86 | OHX | A6 | 1938 | 7/7 | 0.99 | 0.20 | 96,96,96,96 | 7 |
| 86 | OHX | A1 | 3439 | 7/7 | 0.99 | 0.19 | 81,81,81,81 | 7 |
| 86 | OHX | A1 | 3507 | 7/7 | 0.99 | 0.19 | 75,75,75,75 | 7 |
| 86 | OHX | A1 | 3440 | 7/7 | 0.99 | 0.17 | 86,86,86,86 | 0 |
| 86 | OHX | A1 | 3441 | 7/7 | 0.99 | 0.18 | 93,93,93,93 | 0 |
| 86 | OHX | A2 | 1920 | 7/7 | 0.99 | 0.16 | 115,115,115,115 | 7 |
| 86 | OHX | A1 | 3443 | 7/7 | 0.99 | 0.19 | 76,76,76,76 | 0 |
| 86 | OHX | A6 | 1945 | 7/7 | 0.99 | 0.13 | 148,148,148,148 | 0 |
| 86 | OHX | A5 | 3511 | 7/7 | 0.99 | 0.15 | 142,142,142,142 | 0 |
| 86 | OHX | A6 | 1946 | 7/7 | 0.99 | 0.17 | 105,105,105,105 | 7 |
| 86 | OHX | A1 | 3444 | 7/7 | 0.99 | 0.18 | 84,84,84,84 | 0 |
| 87 | MG | A2 | 2235 | 1/1 | 0.99 | 0.20 | 80,80,80,80 | 0 |
| 86 | OHX | A1 | 3445 | 7/7 | 0.99 | 0.17 | 81,81,81,81 | 0 |
| 86 | OHX | A1 | 3446 | 7/7 | 0.99 | 0.20 | 79,79,79,79 | 7 |
| 86 | OHX | A2 | 1902 | 7/7 | 0.99 | 0.20 | 102,102,102,102 | 0 |
| 86 | OHX | A1 | 3448 | 7/7 | 0.99 | 0.18 | 85,85,85,85 | 7 |
| 86 | OHX | A1 | 3517 | 7/7 | 0.99 | 0.15 | 99,99,99,99 | 7 |
| 86 | OHX | A1 | 3449 | 7/7 | 0.99 | 0.19 | 99,99,99,99 | 0 |
| 86 | OHX | A1 | 3591 | 7/7 | 0.99 | 0.18 | 95,95,95,95 | 7 |
| 86 | OHX | A1 | 3450 | 7/7 | 0.99 | 0.19 | 95,95,95,95 | 0 |
| 86 | OHX | A1 | 3451 | 7/7 | 0.99 | 0.17 | 105,105,105,105 | 0 |
| 87 | MG | A1 | 4314 | 1/1 | 0.99 | 0.21 | 78,78,78,78 | 0 |
| 86 | OHX | A5 | 3523 | 7/7 | 0.99 | 0.21 | 79,79,79,79 | 7 |
| 86 | OHX | A1 | 3452 | 7/7 | 0.99 | 0.17 | 81,81,81,81 | 7 |
| 86 | OHX | A1 | 3522 | 7/7 | 0.99 | 0.25 | 79,79,79,79 | 7 |
| 86 | OHX | A2 | 1922 | 7/7 | 0.99 | 0.17 | 99,99,99,99 | 7 |
| 86 | OHX | A2 | 1923 | 7/7 | 0.99 | 0.16 | 110,110,110,110 | 7 |
| 86 | OHX | A1 | 3455 | 7/7 | 0.99 | 0.17 | 100,100,100,100 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86 | OHX | A1 | 3526 | 7/7 | 0.99 | 0.17 | 126,126,126,126 | 7 |
| 86 | OHX | A5 | 3530 | 7/7 | 0.99 | 0.17 | 105,105,105,105 | 7 |
| 86 | OHX | A3 | 204 | 7/7 | 0.99 | 0.16 | 125,125,125,125 | 7 |
| 86 | OHX | A1 | 3456 | 7/7 | 0.99 | 0.18 | 100,100,100,100 | 7 |
| 86 | OHX | A1 | 3457 | 7/7 | 0.99 | 0.18 | 97,97,97,97 | 7 |
| 86 | OHX | Db | 101 | 7/7 | 0.99 | 0.20 | 86,86,86,86 | 0 |
| 86 | OHX | A2 | 1924 | 7/7 | 0.99 | 0.17 | 111,111,111,111 | 7 |
| 86 | OHX | A5 | 3535 | 7/7 | 0.99 | 0.19 | 77,77,77,77 | 7 |
| 86 | OHX | A2 | 1925 | 7/7 | 0.99 | 0.12 | 138,138,138,138 | 0 |
| 86 | OHX | A2 | 1926 | 7/7 | 0.99 | 0.14 | 112,112,112,112 | 7 |
| 86 | OHX | A1 | 3461 | 7/7 | 0.99 | 0.17 | 104,104,104,104 | 0 |
| 86 | OHX | A2 | 1913 | 7/7 | 0.99 | 0.18 | 129,129,129,129 | 0 |
| 86 | OHX | A2 | 1914 | 7/7 | 0.99 | 0.17 | 92,92,92,92 | 7 |
| 86 | OHX | A1 | 3464 | 7/7 | 0.99 | 0.19 | 88,88,88,88 | 7 |
| 86 | OHX | A4 | 201 | 7/7 | 0.99 | 0.25 | 77,77,77,77 | 0 |
| 86 | OHX | A4 | 202 | 7/7 | 0.99 | 0.22 | 80,80,80,80 | 0 |
| 86 | OHX | A1 | 3465 | 7/7 | 0.99 | 0.18 | 94,94,94,94 | 7 |
| 86 | OHX | A1 | 3466 | 7/7 | 0.99 | 0.18 | 90,90,90,90 | 7 |
| 86 | OHX | A1 | 3467 | 7/7 | 0.99 | 0.18 | 91,91,91,91 | 7 |
| 86 | OHX | A1 | 3468 | 7/7 | 0.99 | 0.20 | 74,74,74,74 | 7 |
| 86 | OHX | A2 | 1929 | 7/7 | 0.99 | 0.19 | 90,90,90,90 | 7 |
| 86 | OHX | A2 | 1901 | 7/7 | 0.99 | 0.22 | 95,95,95,95 | 0 |
| 86 | OHX | A2 | 1904 | 7/7 | 0.99 | 0.17 | 99,99,99,99 | 0 |
| 86 | OHX | A2 | 1910 | 7/7 | 0.99 | 0.18 | 104,104,104,104 | 0 |
| 86 | OHX | A2 | 1906 | 7/7 | 0.99 | 0.18 | 98,98,98,98 | 0 |
| 86 | OHX | A1 | 3474 | 7/7 | 0.99 | 0.18 | 92,92,92,92 | 7 |
| 87 | MG | A2 | 2102 | 1/1 | 0.99 | 0.33 | 60,60,60,60 | 0 |
| 86 | OHX | A2 | 1919 | 7/7 | 0.99 | 0.17 | 106,106,106,106 | 7 |
| 86 | OHX | A1 | 3408 | 7/7 | 0.99 | 0.26 | 66,66,66,66 | 0 |
| 86 | OHX | A1 | 3412 | 7/7 | 0.99 | 0.25 | 76,76,76,76 | 0 |
| 86 | OHX | A1 | 3414 | 7/7 | 0.99 | 0.24 | 77,77,77,77 | 0 |
| 86 | OHX | A1 | 3416 | 7/7 | 0.99 | 0.21 | 73,73,73,73 | 0 |
| 86 | OHX | A1 | 3480 | 7/7 | 0.99 | 0.21 | 96,96,96,96 | 7 |
| 86 | OHX | A1 | 3481 | 7/7 | 0.99 | 0.18 | 97,97,97,97 | 7 |
| 86 | OHX | A1 | 3417 | 7/7 | 0.99 | 0.24 | 82,82,82,82 | 0 |
| 86 | OHX | A1 | 3418 | 7/7 | 0.99 | 0.20 | 81,81,81,81 | 0 |
| 86 | OHX | A1 | 3419 | 7/7 | 0.99 | 0.20 | 76,76,76,76 | 0 |
| 86 | OHX | A1 | 3775 | 7/7 | 0.99 | 0.24 | 69,69,69,69 | 7 |
| 86 | OHX | A1 | 3485 | 7/7 | 0.99 | 0.16 | 113,113,113,113 | 7 |
| 86 | OHX | A1 | 3486 | 7/7 | 0.99 | 0.15 | 92,92,92,92 | 7 |
| 86 | OHX | BO | 201 | 7/7 | 0.99 | 0.18 | 97,97,97,97 | 7 |
| 86 | OHX | A1 | 3421 | 7/7 | 0.99 | 0.21 | 80,80,80,80 | 0 |

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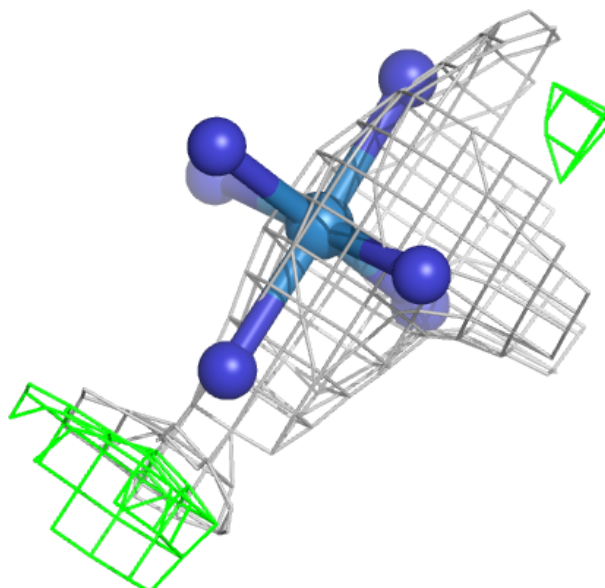
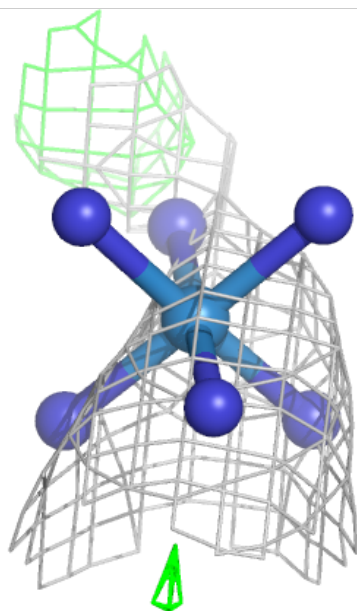
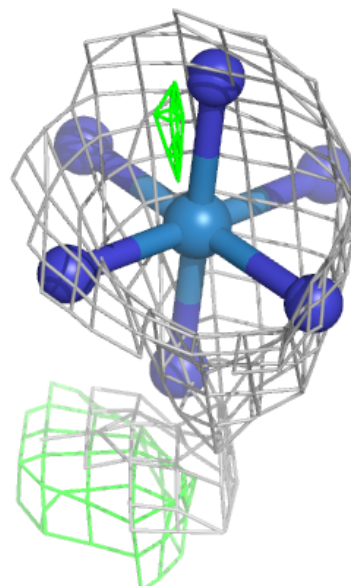
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 86 | OHX | A1 | 3488 | 7/7 | 0.99 | 0.18 | 109,109,109,109 | 7 |
| 86 | OHX | A1 | 3422 | 7/7 | 0.99 | 0.20 | 78,78,78,78 | 0 |
| 86 | OHX | BT | 201 | 7/7 | 0.99 | 0.21 | 78,78,78,78 | 0 |
| 86 | OHX | Bb | 101 | 7/7 | 0.99 | 0.20 | 77,77,77,77 | 0 |
| 86 | OHX | A1 | 3423 | 7/7 | 0.99 | 0.18 | 75,75,75,75 | 0 |
| 86 | OHX | A1 | 3491 | 7/7 | 0.99 | 0.19 | 90,90,90,90 | 7 |
| 86 | OHX | A1 | 3492 | 7/7 | 0.99 | 0.16 | 98,98,98,98 | 7 |
| 86 | OHX | A1 | 3424 | 7/7 | 0.99 | 0.18 | 81,81,81,81 | 0 |
| 86 | OHX | A1 | 3425 | 7/7 | 0.99 | 0.20 | 85,85,85,85 | 0 |
| 86 | OHX | A6 | 1901 | 7/7 | 0.99 | 0.24 | 78,78,78,78 | 0 |
| 88 | ZN | Bj | 111 | 1/1 | 0.99 | 0.17 | 44,44,44,44 | 0 |
| 86 | OHX | A6 | 1902 | 7/7 | 0.99 | 0.25 | 90,90,90,90 | 0 |
| 86 | OHX | A6 | 1903 | 7/7 | 0.99 | 0.22 | 84,84,84,84 | 0 |
| 86 | OHX | A6 | 1904 | 7/7 | 0.99 | 0.23 | 88,88,88,88 | 0 |
| 88 | ZN | Ca | 202 | 1/1 | 0.99 | 0.12 | 73,73,73,73 | 0 |
| 86 | OHX | A6 | 1905 | 7/7 | 0.99 | 0.20 | 88,88,88,88 | 0 |
| 86 | OHX | A5 | 3413 | 7/7 | 0.99 | 0.30 | 71,71,71,71 | 0 |
| 86 | OHX | A5 | 3414 | 7/7 | 0.99 | 0.27 | 69,69,69,69 | 0 |
| 88 | ZN | Dj | 105 | 1/1 | 0.99 | 0.17 | 48,48,48,48 | 0 |
| 87 | MG | A1 | 4379 | 1/1 | 0.99 | 0.21 | 70,70,70,70 | 0 |
| 86 | OHX | A5 | 3415 | 7/7 | 0.99 | 0.24 | 67,67,67,67 | 0 |
| 86 | OHX | A1 | 3415 | 7/7 | 1.00 | 0.19 | 68,68,68,68 | 0 |
| 86 | OHX | A1 | 3410 | 7/7 | 1.00 | 0.25 | 68,68,68,68 | 0 |
| 86 | OHX | A1 | 3434 | 7/7 | 1.00 | 0.17 | 72,72,72,72 | 7 |
| 86 | OHX | A1 | 3411 | 7/7 | 1.00 | 0.24 | 71,71,71,71 | 0 |
| 86 | OHX | A1 | 3436 | 7/7 | 1.00 | 0.18 | 69,69,69,69 | 7 |
| 86 | OHX | A5 | 3450 | 7/7 | 1.00 | 0.18 | 76,76,76,76 | 7 |
| 86 | OHX | A2 | 1905 | 7/7 | 1.00 | 0.19 | 88,88,88,88 | 0 |
| 86 | OHX | A1 | 3413 | 7/7 | 1.00 | 0.26 | 75,75,75,75 | 0 |
| 86 | OHX | A1 | 3427 | 7/7 | 1.00 | 0.19 | 86,86,86,86 | 0 |
| 86 | OHX | A1 | 3420 | 7/7 | 1.00 | 0.19 | 69,69,69,69 | 0 |
| 86 | OHX | A5 | 3440 | 7/7 | 1.00 | 0.21 | 63,63,63,63 | 7 |
| 86 | OHX | A1 | 3409 | 7/7 | 1.00 | 0.26 | 70,70,70,70 | 0 |
| 86 | OHX | A1 | 3430 | 7/7 | 1.00 | 0.20 | 93,93,93,93 | 0 |
| 88 | ZN | Dm | 202 | 1/1 | 1.00 | 0.19 | 41,41,41,41 | 0 |
| 86 | OHX | A1 | 3431 | 7/7 | 1.00 | 0.18 | 89,89,89,89 | 0 |
| 86 | OHX | A5 | 3430 | 7/7 | 1.00 | 0.18 | 80,80,80,80 | 0 |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

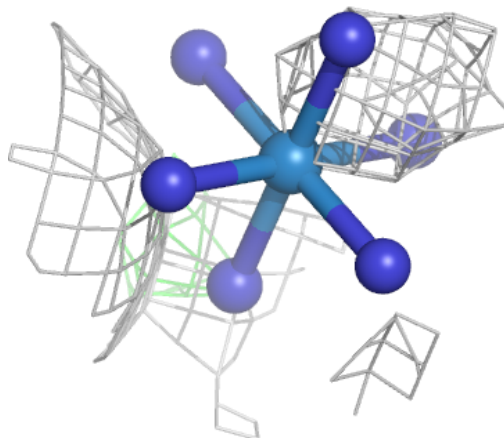
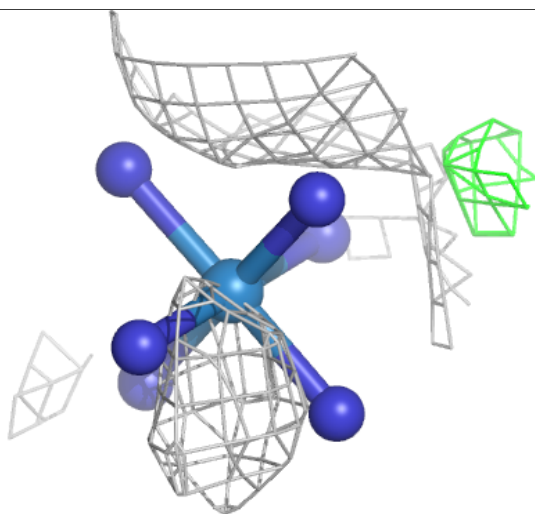
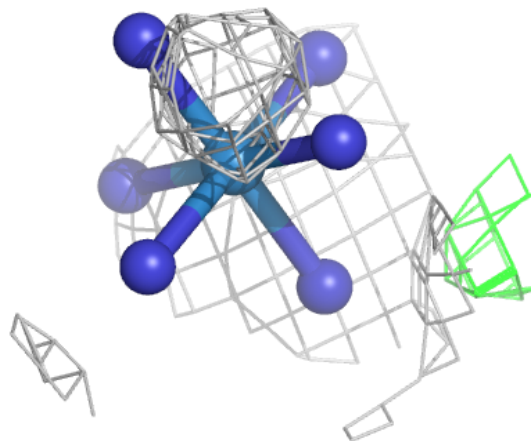
Electron density around OHX A6 2095:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



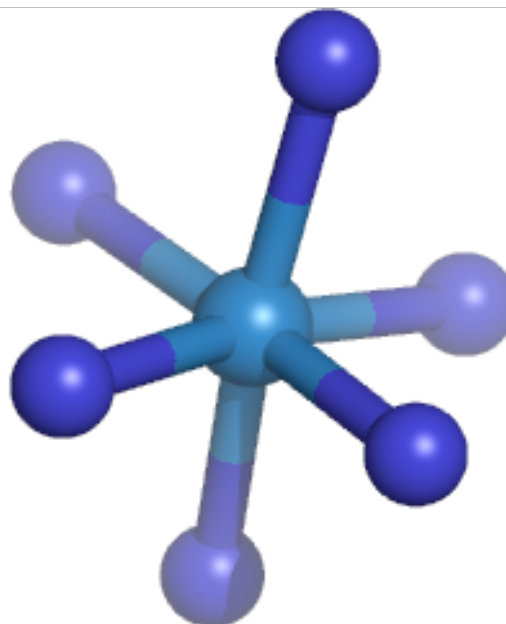
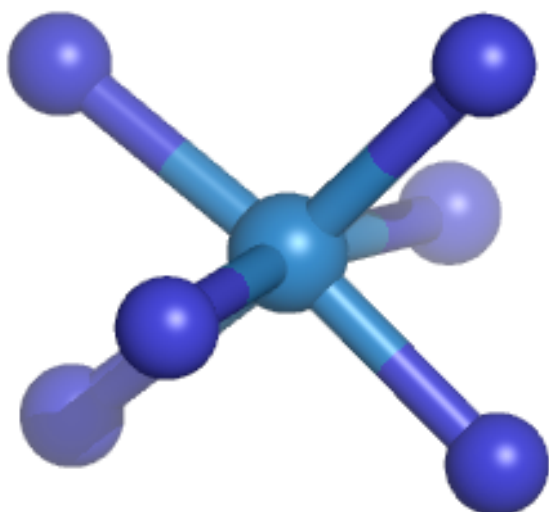
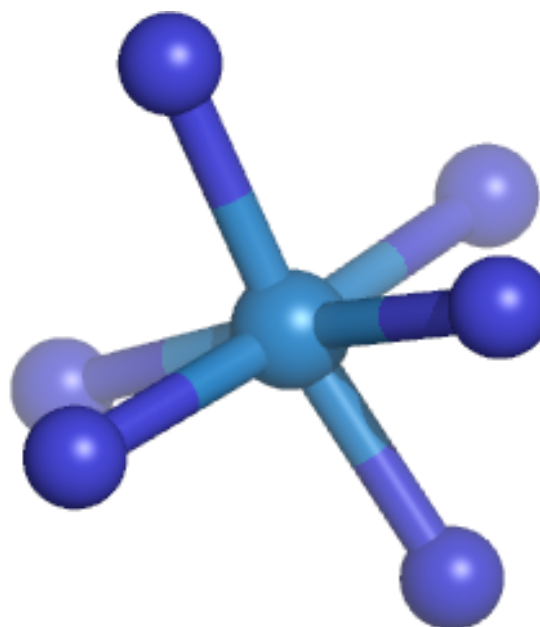
Electron density around OHX A6 2083:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



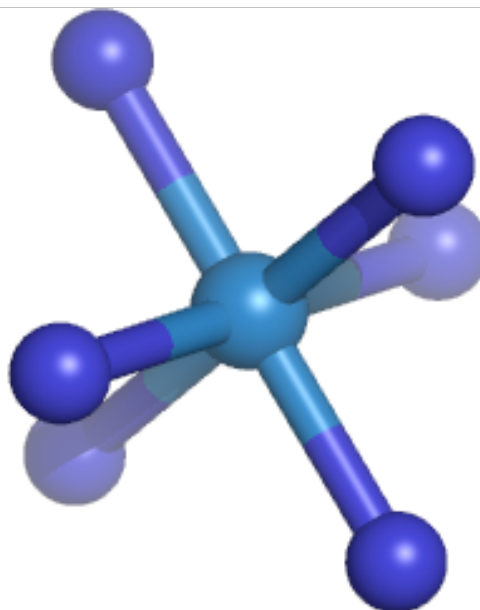
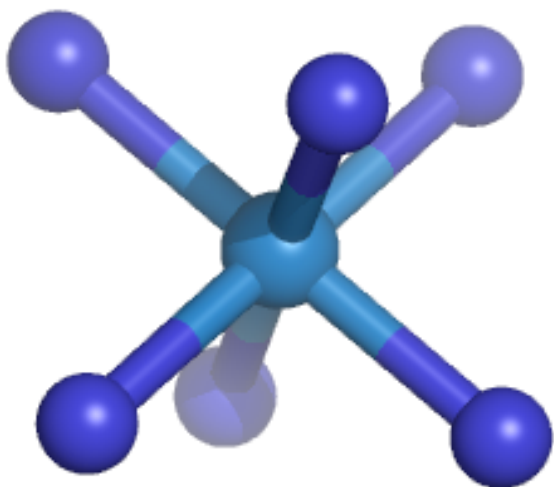
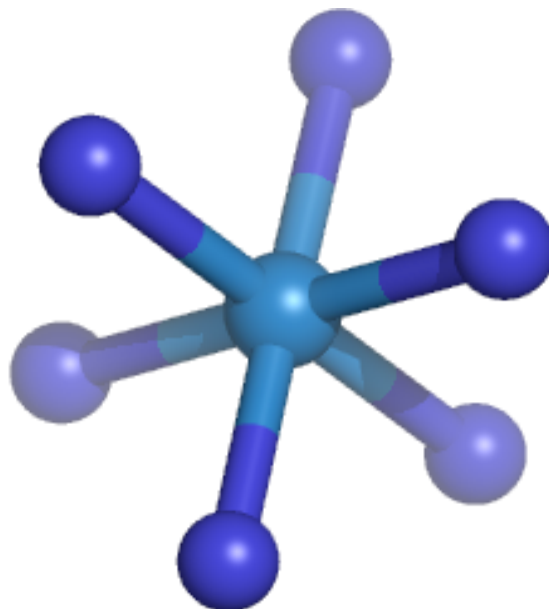
Electron density around OHX BI 303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



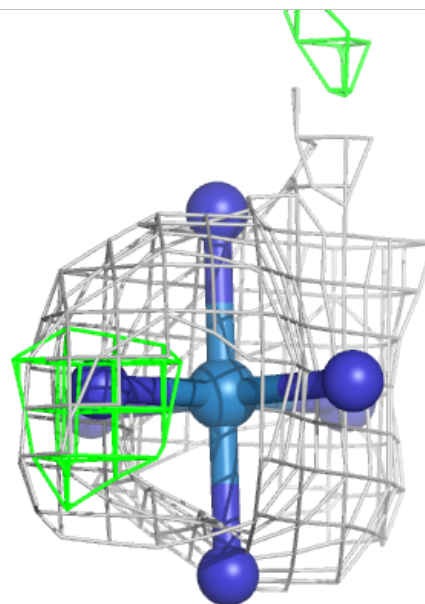
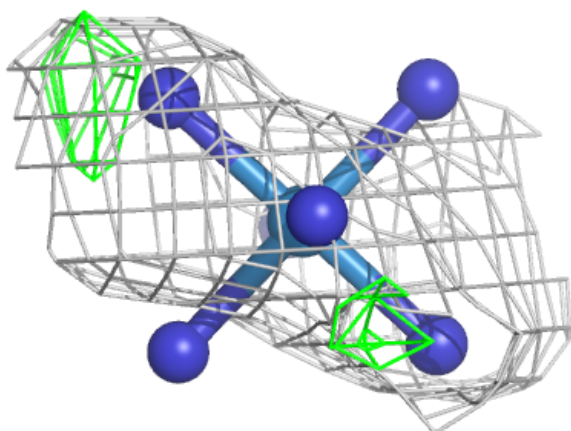
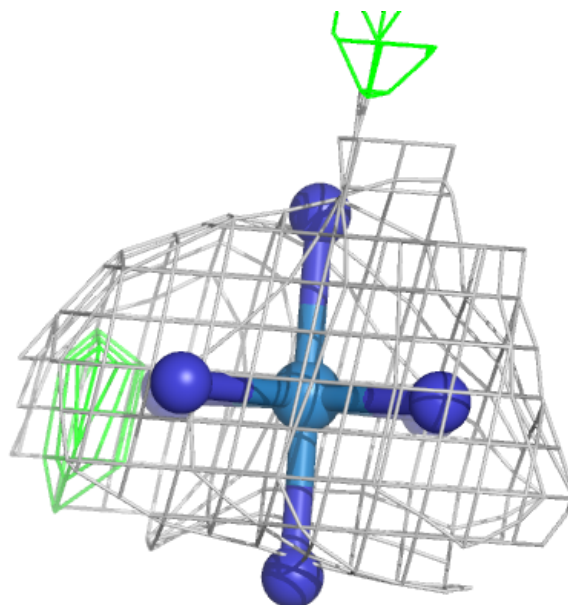
Electron density around OHX A1 3779:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



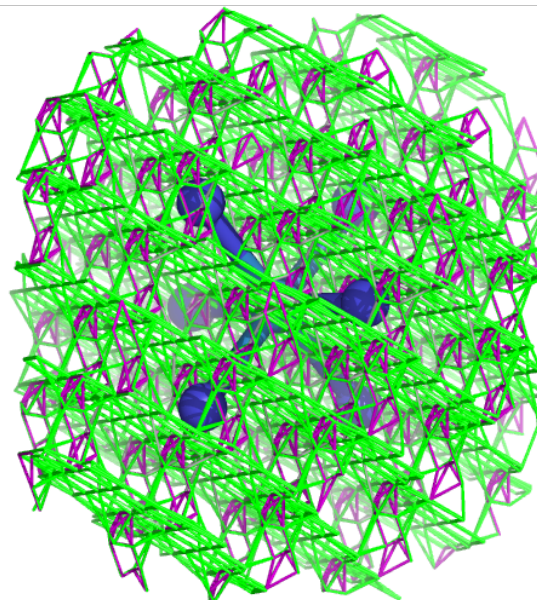
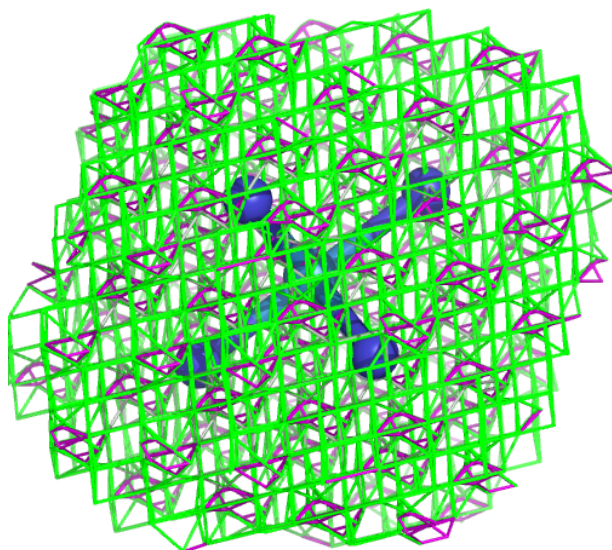
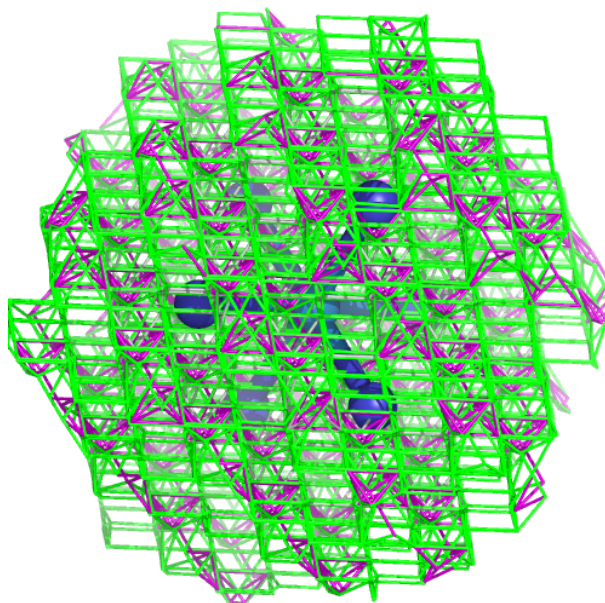
Electron density around OHX A5 3792:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



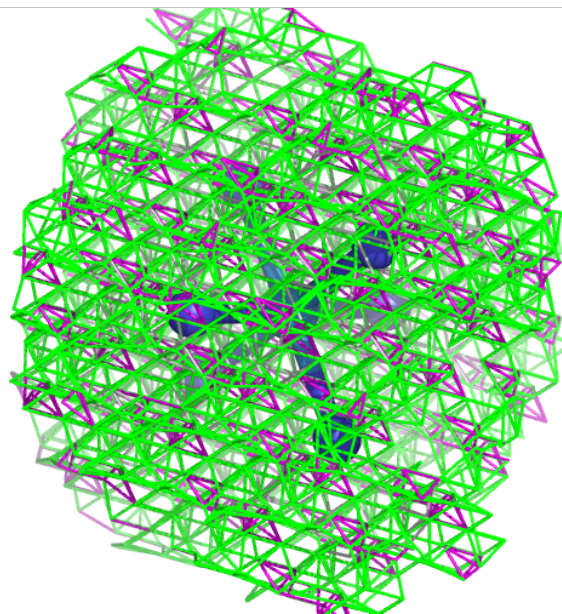
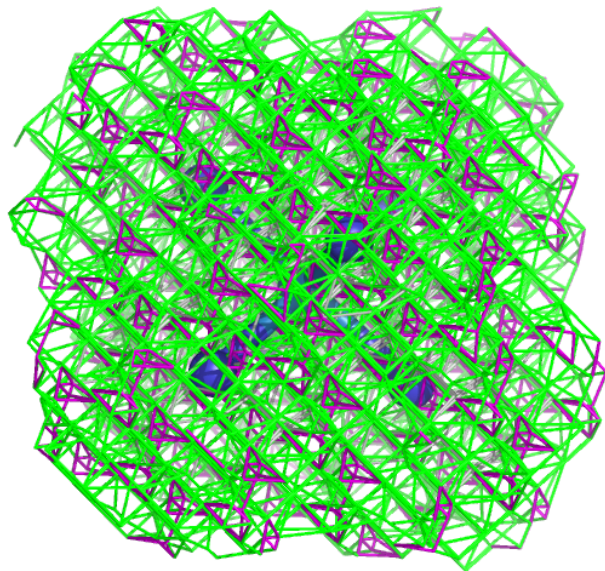
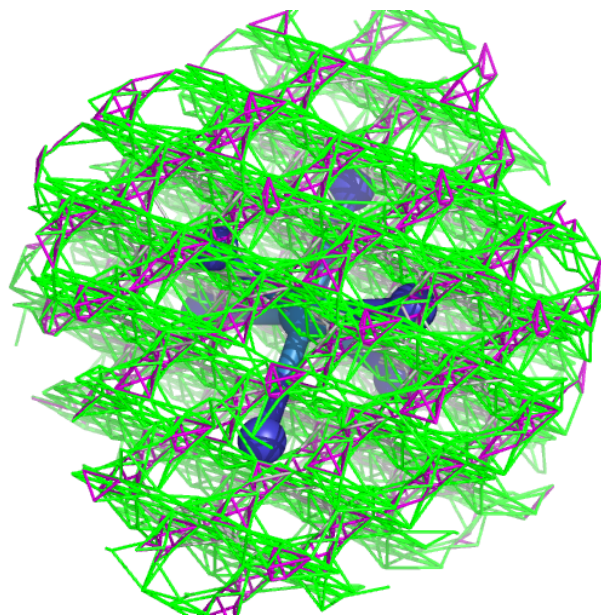
Electron density around OHX A1 3814:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



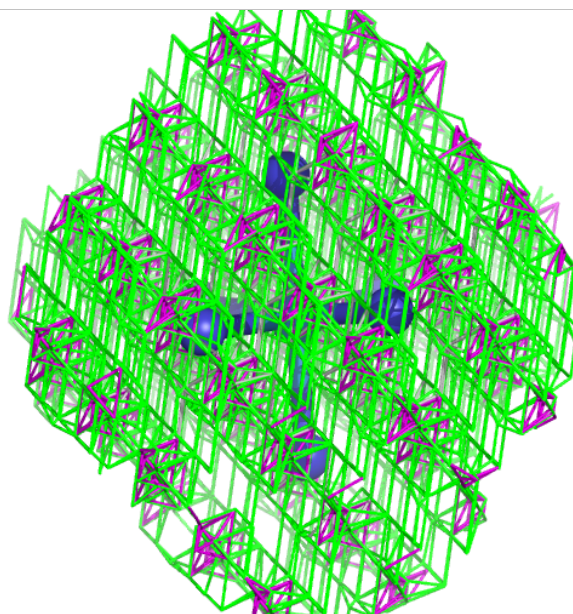
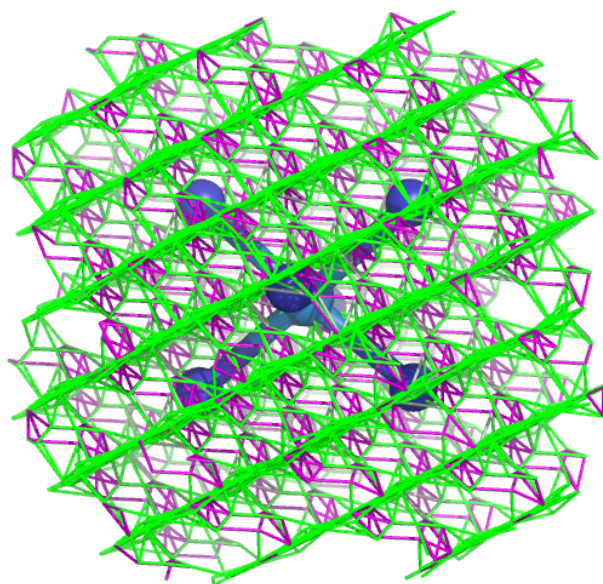
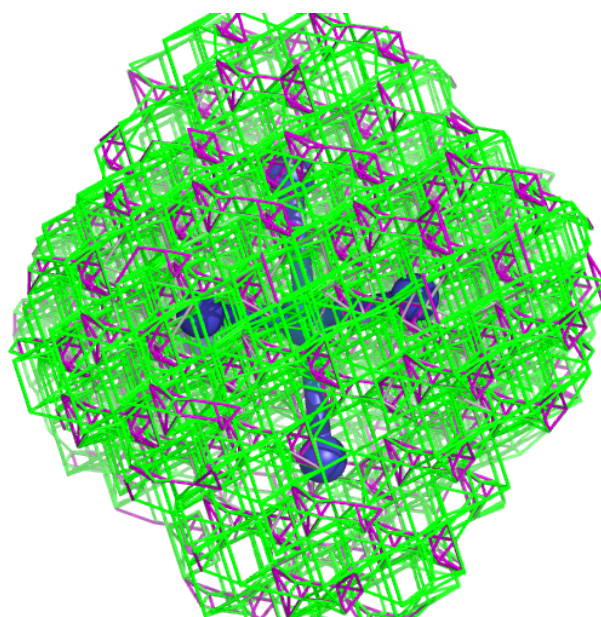
Electron density around OHX A5 3819:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



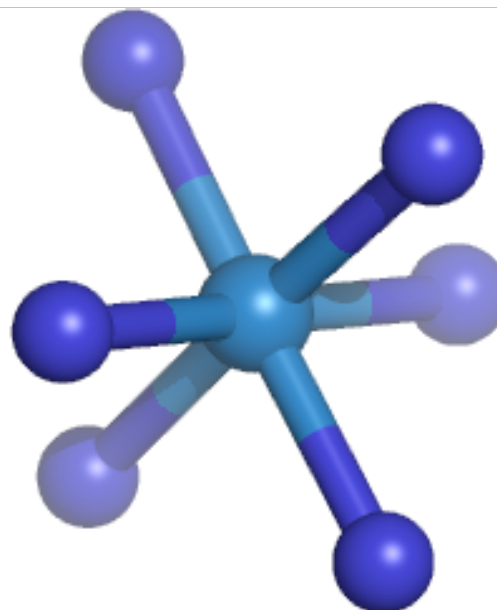
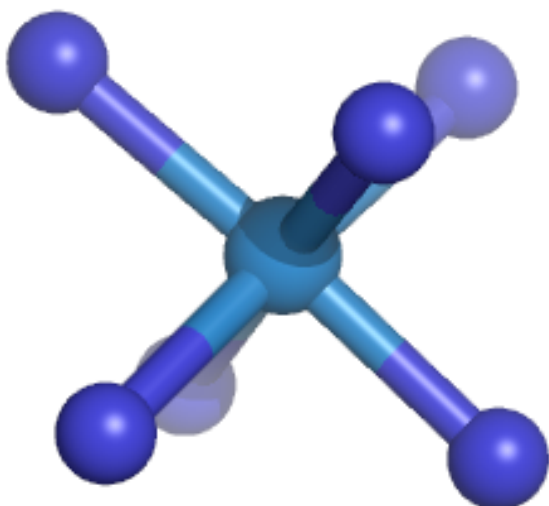
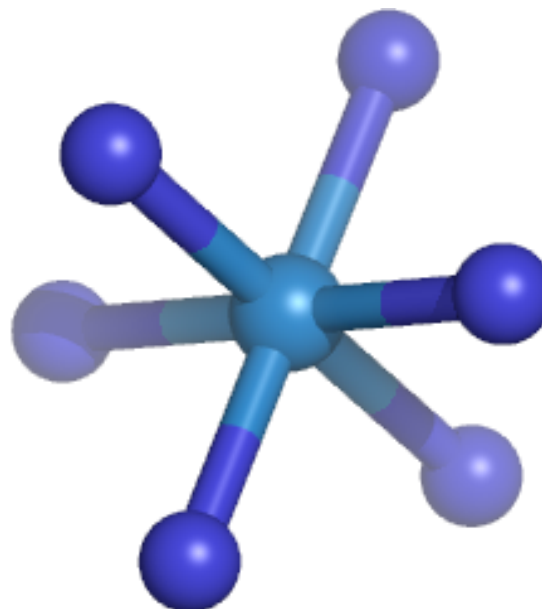
Electron density around OHX A1 3805:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



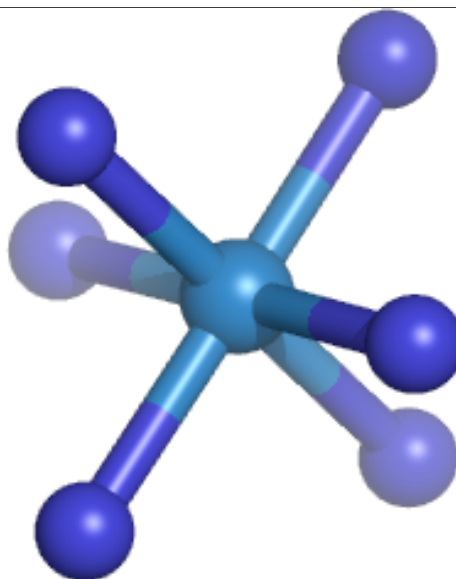
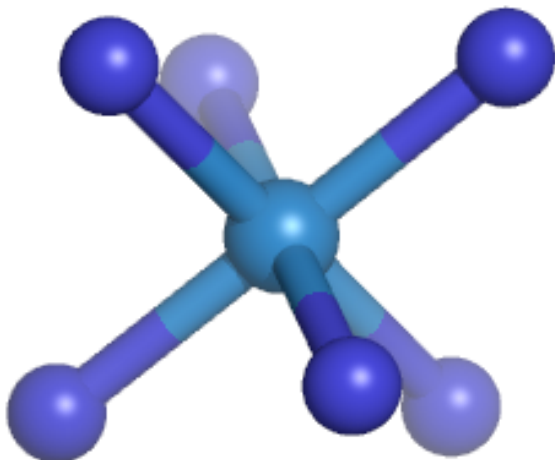
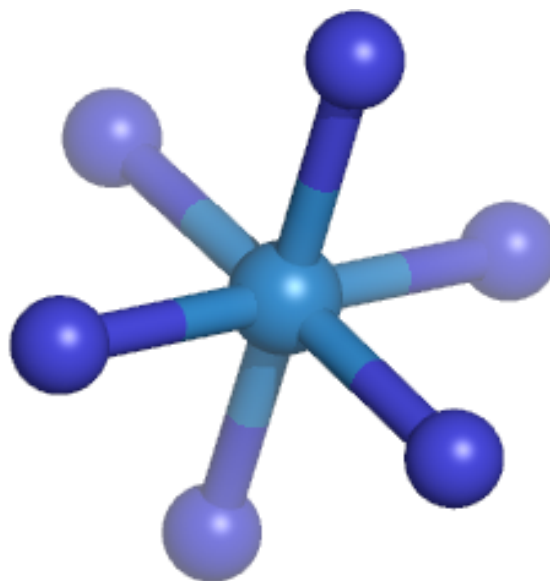
Electron density around OHX A1 3753:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



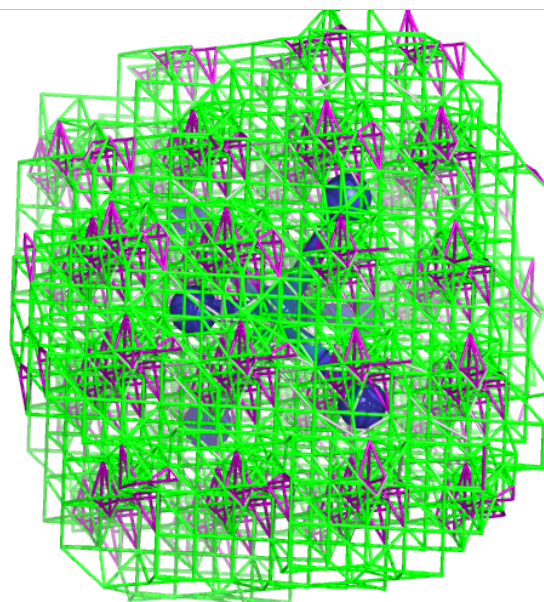
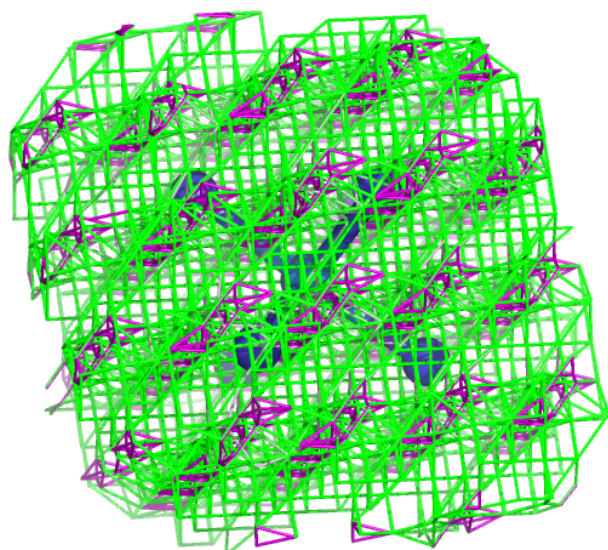
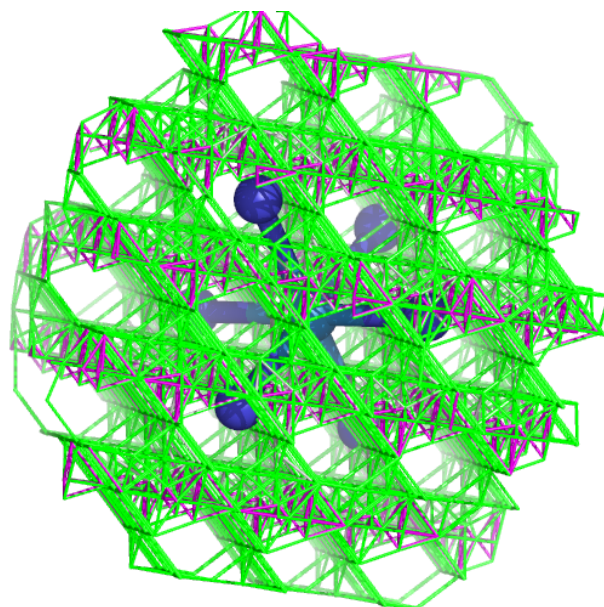
Electron density around OHX A1 3815:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



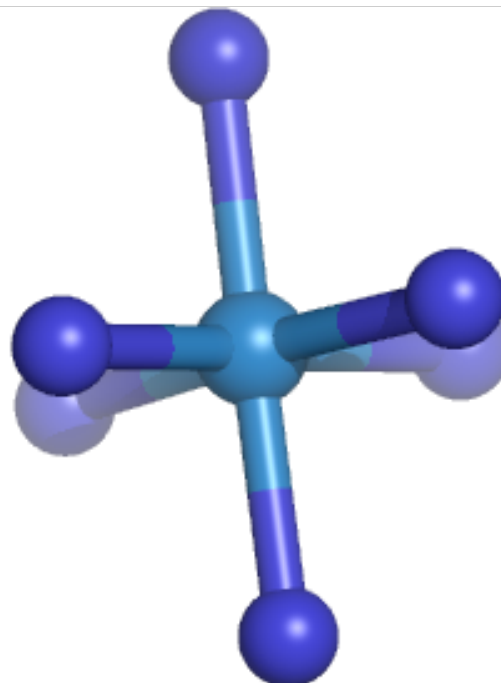
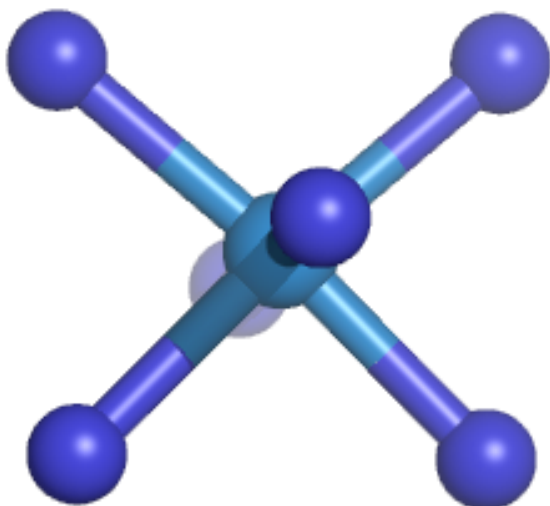
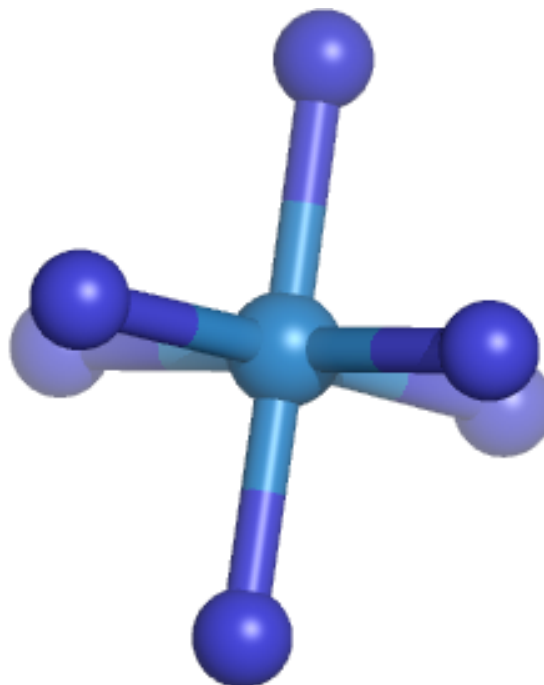
Electron density around OHX A8 218:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



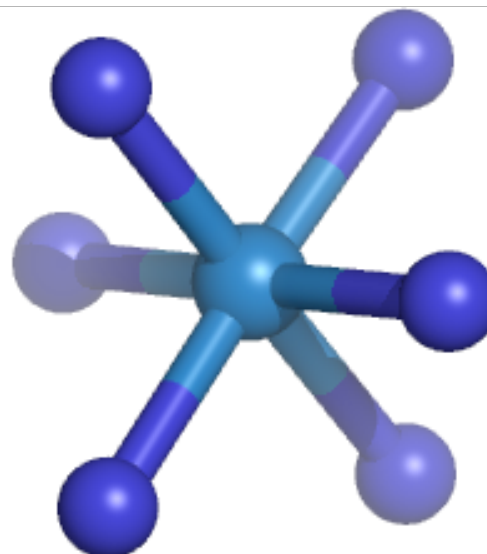
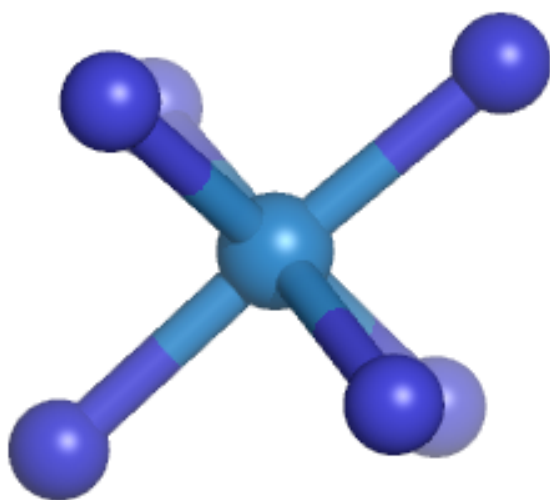
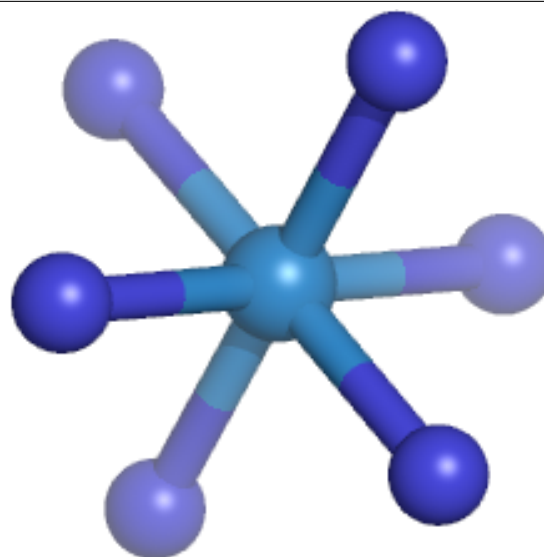
Electron density around OHX A6 2090:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



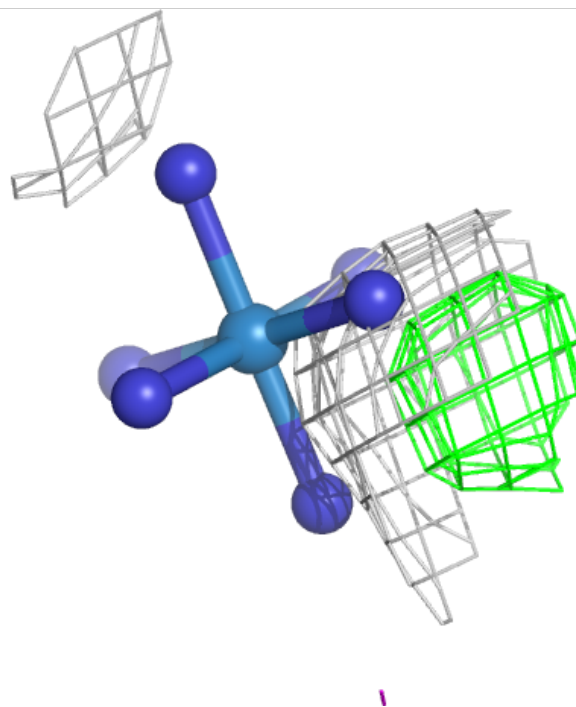
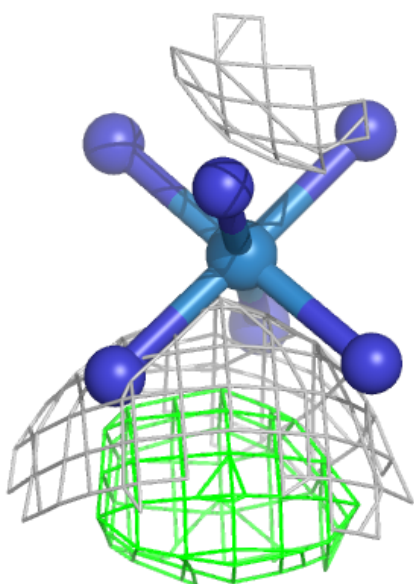
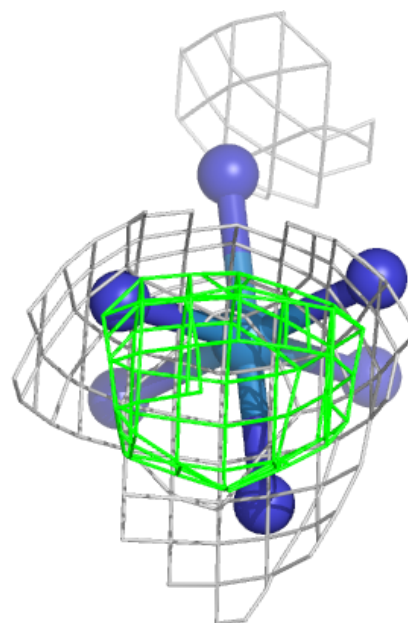
Electron density around OHX A5 3768:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



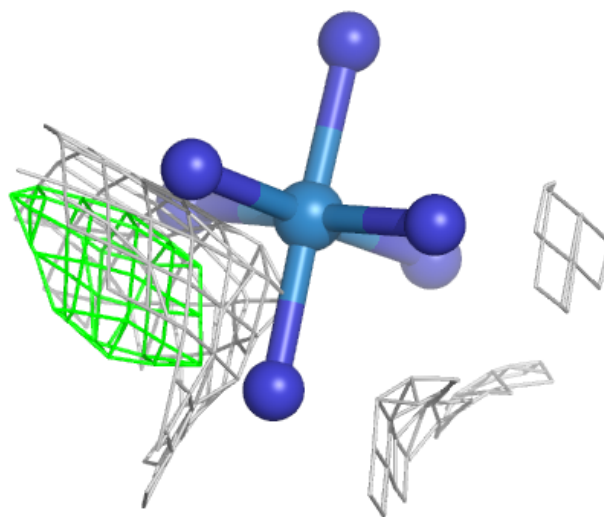
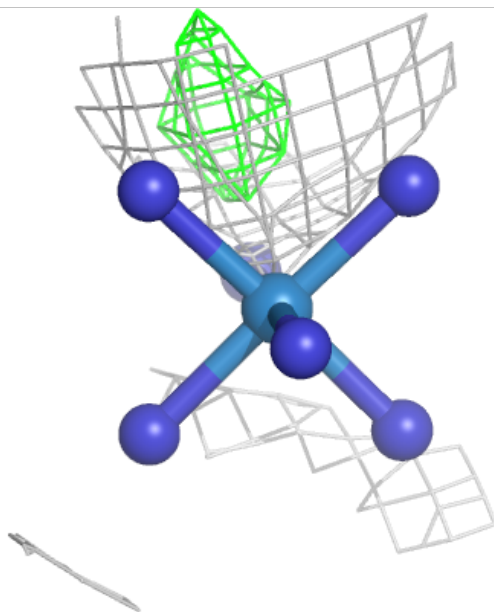
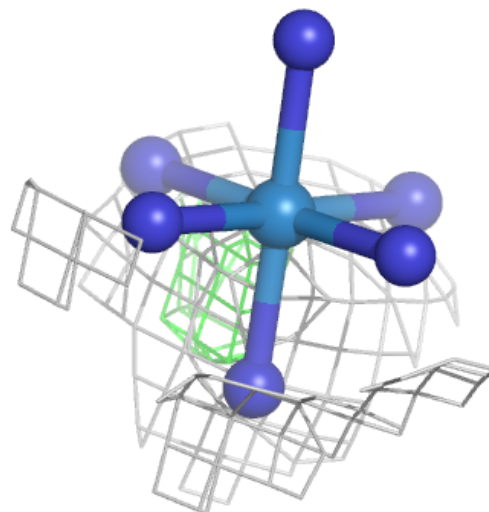
Electron density around OHX CP 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



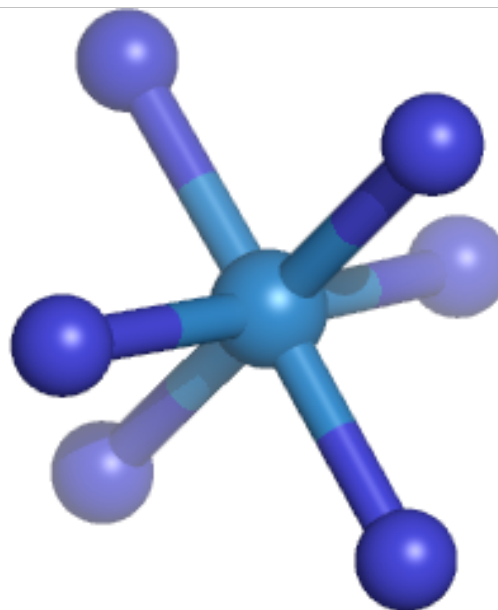
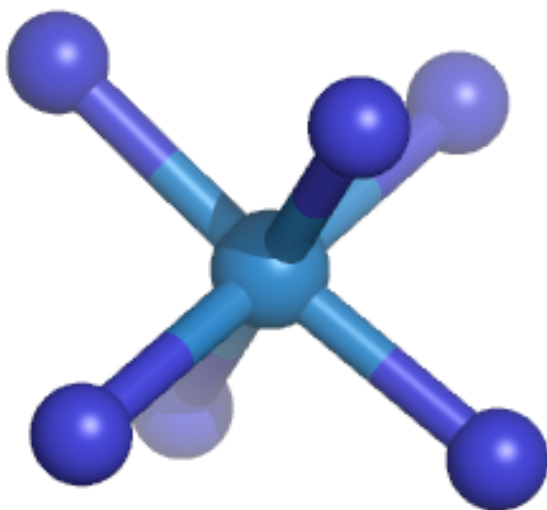
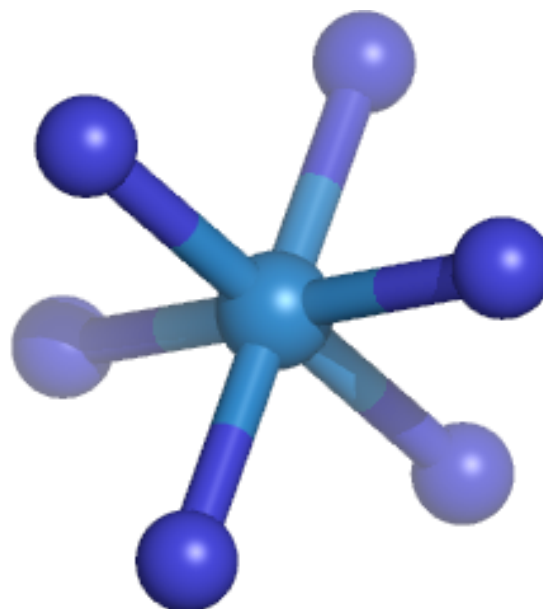
Electron density around OHX A6 2086:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



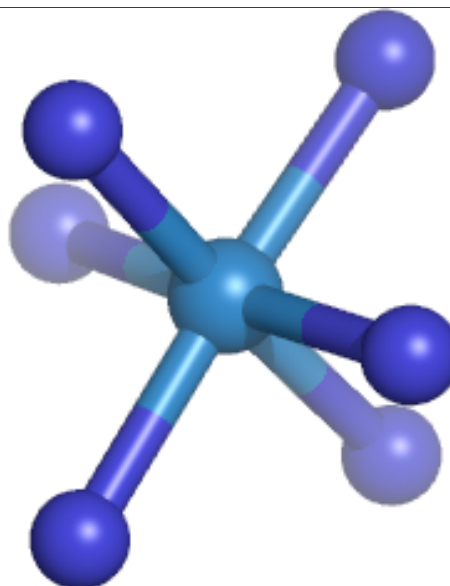
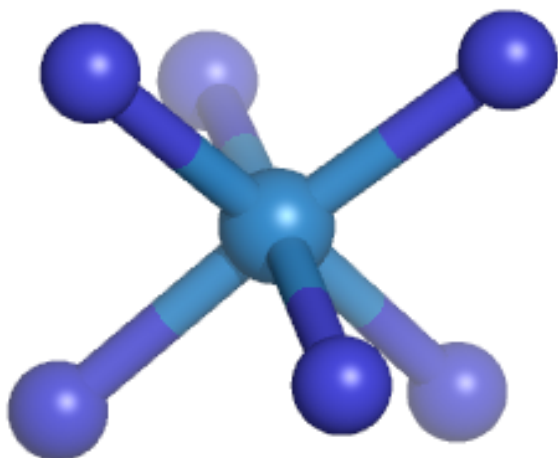
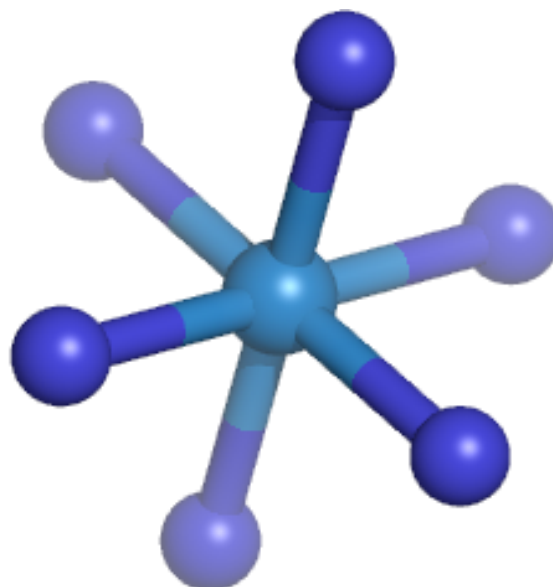
Electron density around OHX A2 2051:

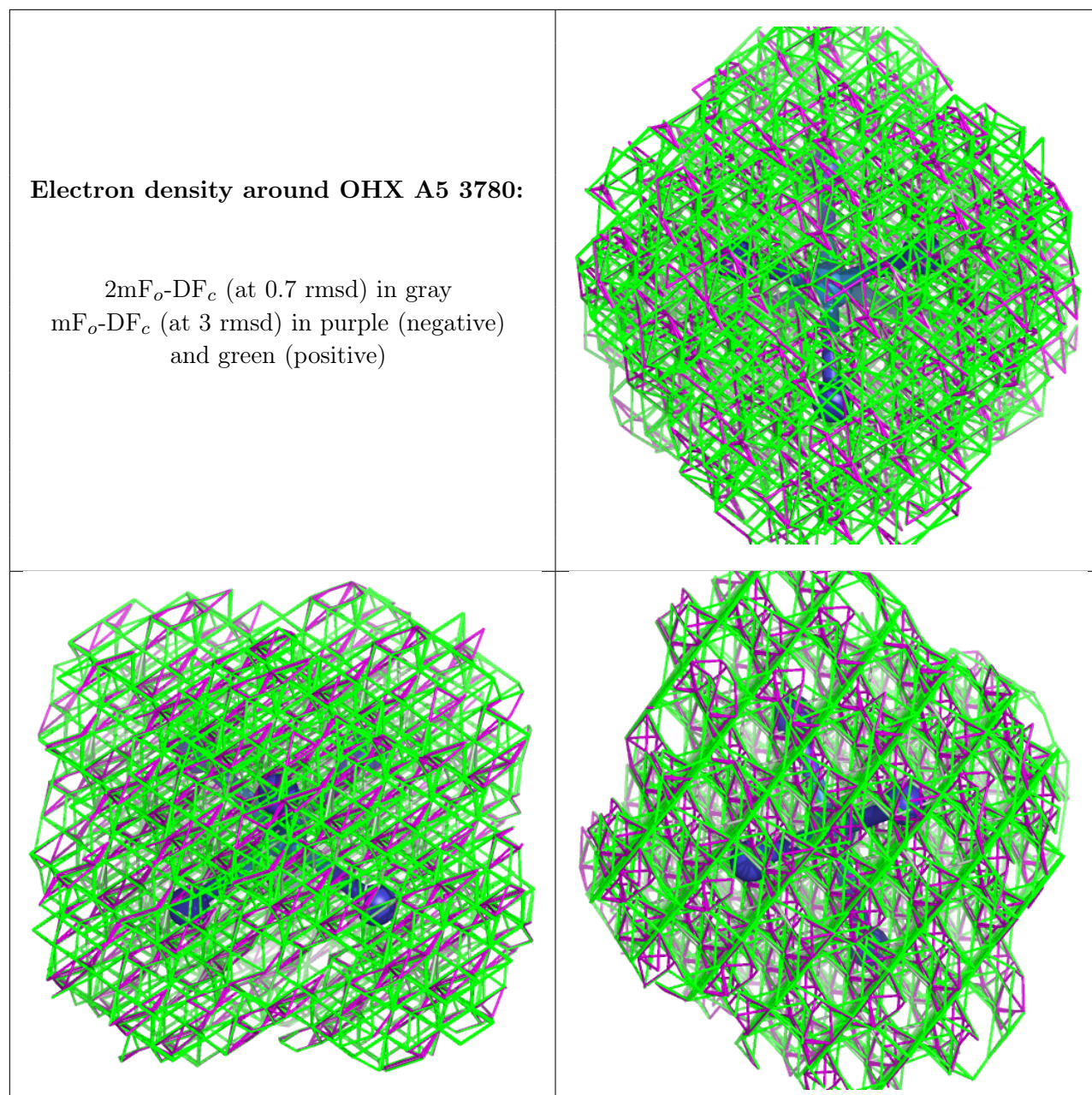
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OHX A5 3810:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.