# Full wwPDB EM Validation Report

Apr 16, 2024 – 05:40 pm BST

| | | |
|---|---|---|
| PDB ID | : | 6SKF |
| EMDB ID | : | EMD-10223 |
| Title | : | Cryo-EM Structure of T. kodakarensis 70S ribosome |
| Authors | : | Matzov, D.; Sas-Chen, A.; Thomas, J.M.; Santangelo, T.; Meier, J.L.; Schwartz, S.; Shalev-Benami, M. |
| Deposited on | : | 2019-08-15 |
| Resolution | : | 2.95 Å(reported) |

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

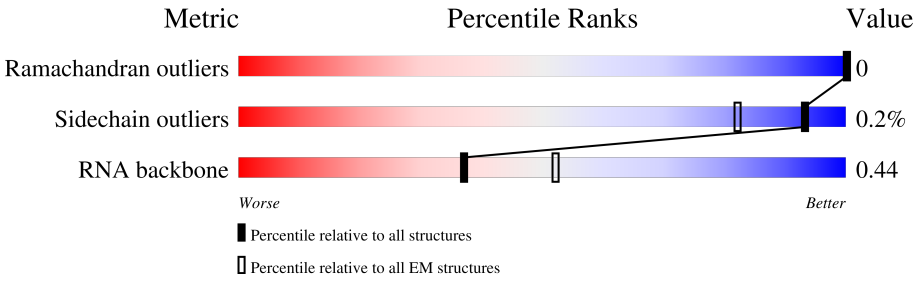
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev92 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.95 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) | EM structures (#Entries) |
|---|---|---|
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |
| RNA backbone | 4643 | 859 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | Aa | 1498 | 8% 72% 24% |
| 2 | Ab | 201 | 25% 98% |
| 3 | Ac | 209 | 71% 93% 7% |
| 4 | Ad | 200 | 29% 95% 5% |
| 5 | Ae | 180 | 16% 97% |
| 6 | Af | 243 | 15% 99% |
| 7 | Ag | 235 | 14% 95% 5% |
| 8 | Ah | 125 | 58% 98% |

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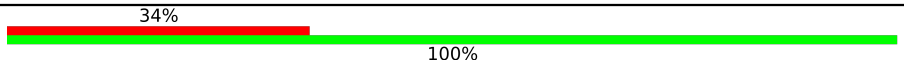
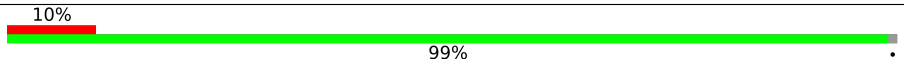
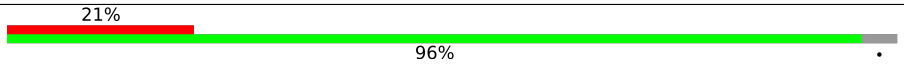
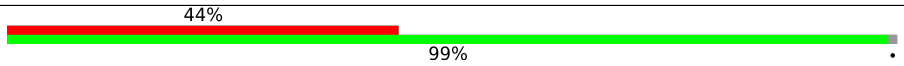
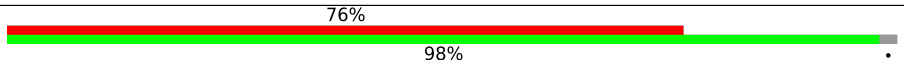
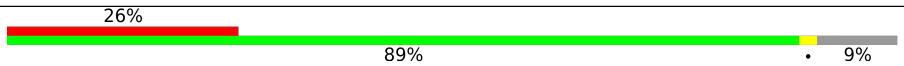
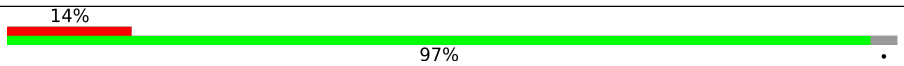
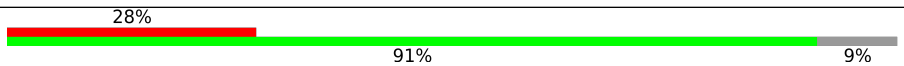
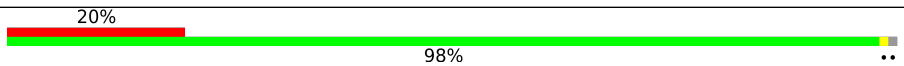
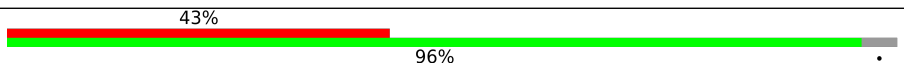
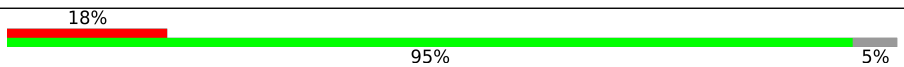
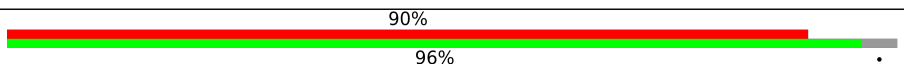
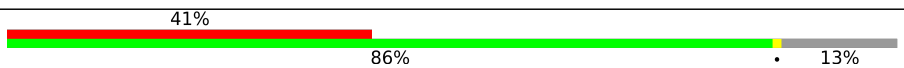
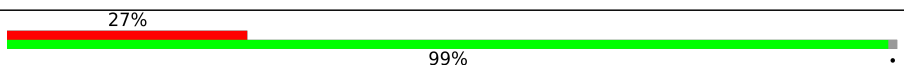
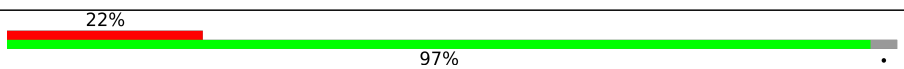
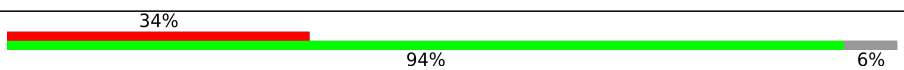
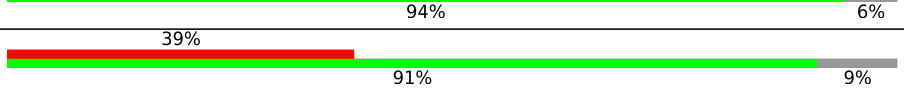
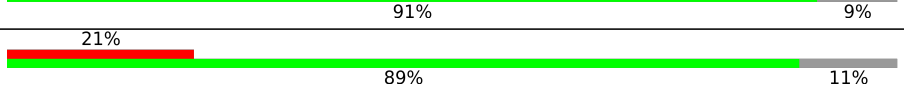
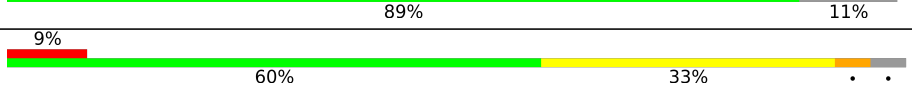
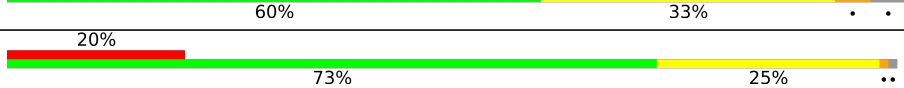
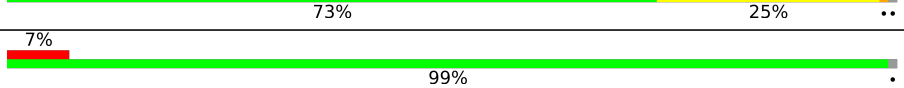
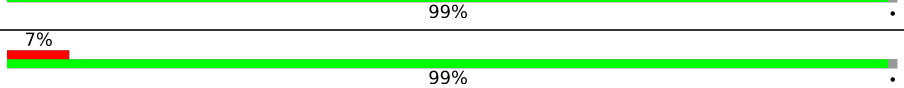
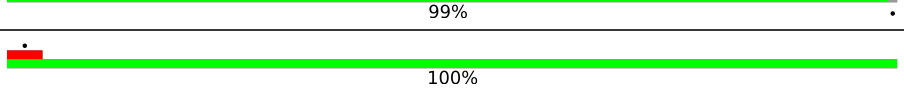
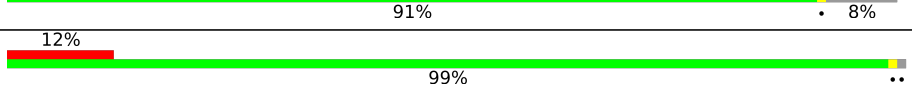
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 9 | Ai | 215 |   |
| 10 | Aj | 130 |   |
| 11 | Ak | 130 |   |
| 12 | Al | 135 |   |
| 13 | Am | 102 |   |
| 14 | An | 140 |   |
| 15 | Ao | 147 |   |
| 16 | Ap | 149 |   |
| 17 | Aq | 151 |   |
| 18 | Ar | 56 |   |
| 19 | As | 114 |   |
| 20 | At | 67 |   |
| 21 | Au | 133 |   |
| 22 | Av | 150 |   |
| 23 | Aw | 98 |   |
| 24 | Ax | 65 |   |
| 25 | Ay | 70 |   |
| 26 | Az | 62 |   |
| 27 | BA | 3037 |   |
| 28 | BB | 126 |   |
| 29 | BC | 239 |   |
| 30 | BD | 346 |   |
| 31 | BE | 255 |   |
| 32 | BF | 183 |   |
| 33 | BG | 184 |   |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 34 | BH | 123 | 36% 98% |
| 34 | BI | 123 | 98% 98% |
| 35 | BJ | 182 | 10% 92% 8% |
| 36 | BK | 142 | 100% |
| 37 | BL | 141 | 10% 99% |
| 38 | BM | 83 | 25% 96% |
| 38 | BN | 83 | 33% 96% |
| 39 | BO | 148 | 29% 99% |
| 40 | BP | 194 | 99% |
| 41 | BQ | 201 | 33% 82% 18% |
| 42 | BR | 121 | 98% |
| 43 | BS | 150 | 8% 97% |
| 44 | BT | 77 | 19% 96% |
| 45 | BU | 98 | 98% |
| 46 | BV | 156 | 97% |
| 47 | BW | 86 | 13% 99% |
| 48 | BX | 121 | 7% 99% |
| 49 | BY | 67 | 93% 7% |
| 50 | BZ | 66 | 27% 89% 9% |
| 51 | Ba | 155 | 5% 99% |
| 52 | Bb | 102 | 16% 94% 6% |
| 53 | Bc | 90 | 12% 99% |
| 54 | Bd | 125 | 6% 99% |
| 55 | Be | 90 | 7% 98% |
| 56 | Bg | 86 | 5% 97% |

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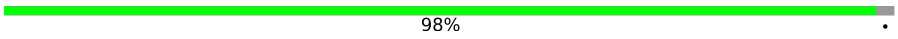
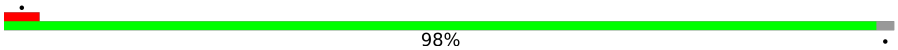
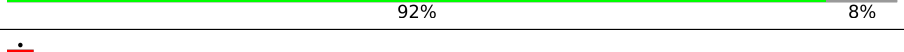
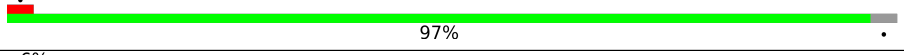
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 57 | Bh | 63 |   |
| 58 | Bi | 51 |   |
| 59 | Bj | 51 |   |
| 60 | Bk | 37 |   |
| 61 | Bl | 94 |   |

# 2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 161921 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 16S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 1 | Aa | 1463 | 31591 | 14101 | 5837 | 10190 | 1463 | 0 | 0 |

- Molecule 2 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | Ab | 196 | 1580 | 1021 | 272 | 284 | 3 | 0 | 0 |

- Molecule 3 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | Ac | 195 | 1524 | 973 | 277 | 271 | 3 | 0 | 0 |

- Molecule 4 is a protein called 30S ribosomal protein S3Ae.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | Ad | 190 | 1550 | 997 | 277 | 273 | 3 | 0 | 0 |

- Molecule 5 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | Ae | 174 | 1454 | 912 | 287 | 253 | 2 | 0 | 0 |

- Molecule 6 is a protein called 30S ribosomal protein S4e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | Af | 241 | 1945 | 1256 | 348 | 336 | 5 | 0 | 0 |

- Molecule 7 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | Ag | 223 | Total | C | N | O | S | 0 | 0 |
| | | | 1753 | 1107 | 327 | 312 | 7 | | |

- Molecule 8 is a protein called 30S ribosomal protein S6e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | Ah | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 952 | 599 | 179 | 172 | 2 | | |

- Molecule 9 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | Ai | 214 | Total | C | N | O | S | 0 | 0 |
| | | | 1715 | 1087 | 317 | 303 | 8 | | |

- Molecule 10 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | Aj | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1020 | 662 | 176 | 180 | 2 | | |

- Molecule 11 is a protein called 30S ribosomal protein S8e.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 11 | Ak | 125 | Total | C | N | O | 0 | 0 |
| | | | 982 | 615 | 198 | 169 | | |

- Molecule 12 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | Al | 133 | Total | C | N | O | S | 0 | 0 |
| | | | 1054 | 656 | 205 | 188 | 5 | | |

- Molecule 13 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | Am | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 803 | 498 | 154 | 148 | 3 | | |

- Molecule 14 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | An | 127 | Total | C | N | O | S | 0 | 0 |
| | | | 950 | 586 | 190 | 171 | 3 | | |

- Molecule 15 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | Ao | 143 | Total | C | N | O | S | 0 | 0 |
| | | | 1122 | 712 | 216 | 192 | 2 | | |

- Molecule 16 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | Ap | 135 | Total | C | N | O | S | 0 | 0 |
| | | | 1090 | 691 | 214 | 181 | 4 | | |

- Molecule 17 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | Aq | 149 | Total | C | N | O | S | 0 | 0 |
| | | | 1217 | 776 | 233 | 206 | 2 | | |

- Molecule 18 is a protein called 30S ribosomal protein S14 type Z.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | Ar | 54 | Total | C | N | O | S | 0 | 0 |
| | | | 447 | 284 | 92 | 65 | 6 | | |

- Molecule 19 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | As | 108 | Total | C | N | O | S | 0 | 0 |
| | | | 879 | 560 | 164 | 152 | 3 | | |

- Molecule 20 is a protein called 30S ribosomal protein S17e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | At | 64 | Total | C | N | O | S | 0 | 0 |
| | | | 538 | 338 | 103 | 95 | 2 | | |

- Molecule 21 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | Au | 116 | Total | C | N | O | S | 0 | 0 |
| | | | 952 | 608 | 175 | 163 | 6 | | |

- Molecule 22 is a protein called 30S ribosomal protein S19e.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 22 | Av | 149 | Total | C | N | O | 0 | 0 |
| | | | 1216 | 788 | 215 | 213 | | |

- Molecule 23 is a protein called 30S ribosomal protein S24e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 23 | Aw | 95 | Total | C | N | O | S | 0 | 0 |
| | | | 777 | 497 | 131 | 146 | 3 | | |

- Molecule 24 is a protein called 30S ribosomal protein S27e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 24 | Ax | 61 | Total | C | N | O | S | 0 | 0 |
| | | | 461 | 294 | 83 | 79 | 5 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| Ax | 64 | GLU | LEU | conflict | UNP Q5JE50 |

- Molecule 25 is a protein called 30S ribosomal protein S28e.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 25 | Ay | 64 | Total | C | N | O | 0 | 0 |
| | | | 499 | 307 | 99 | 93 | | |

- Molecule 26 is a protein called Predicted zinc-ribbon RNA-binding protein involved in translation.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 26 | Az | 55 | Total | C | N | O | S | 0 | 0 |
| | | | 426 | 269 | 74 | 75 | 8 | | |

- Molecule 27 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 27 | BA | 2929 | Total | C | N | O | P | S | 0 | 0 |
| | | | 63265 | 28239 | 11728 | 20367 | 2929 | 2 | | |

- Molecule 28 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | BB | 125 | Total | C | N | O | P | 0 | 0 |
| | | | 2678 | 1191 | 492 | 870 | 125 | | |

- Molecule 29 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 29 | BC | 237 | Total | C | N | O | S | 0 | 0 |
| | | | 1820 | 1150 | 356 | 311 | 3 | | |

- Molecule 30 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | BD | 344 | Total | C | N | O | S | 0 | 0 |
| | | | 2746 | 1765 | 505 | 469 | 7 | | |

- Molecule 31 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 31 | BE | 255 | Total | C | N | O | S | 0 | 0 |
| | | | 2026 | 1286 | 389 | 347 | 4 | | |

- Molecule 32 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 32 | BF | 169 | Total | C | N | O | S | 0 | 0 |
| | | | 1313 | 821 | 252 | 233 | 7 | | |

- Molecule 33 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 33 | BG | 183 | Total | C | N | O | S | 0 | 0 |
| | | | 1463 | 942 | 253 | 266 | 2 | | |

- Molecule 34 is a protein called 50S ribosomal protein L7Ae.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 34 | BH | 121 | Total | C | N | O | S | 0 | 0 |
| | | | 928 | 591 | 154 | 180 | 3 | | |
| 34 | BI | 121 | Total | C | N | O | S | 0 | 0 |
| | | | 928 | 591 | 154 | 180 | 3 | | |

- Molecule 35 is a protein called 50S ribosomal protein L10e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 35 | BJ | 168 | Total | C | N | O | S | 0 | 0 |
| | | | 1378 | 877 | 258 | 236 | 7 | | |

- Molecule 36 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 36 | BK | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1146 | 731 | 213 | 198 | 4 | | |

- Molecule 37 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 37 | BL | 140 | Total | C | N | O | S | 0 | 0 |
| | | | 1055 | 658 | 214 | 180 | 3 | | |

- Molecule 38 is a protein called 50S ribosomal protein L14e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 38 | BM | 81 | Total | C | N | O | S | 0 | 0 |
| | | | 610 | 382 | 119 | 108 | 1 | | |
| 38 | BN | 81 | Total | C | N | O | S | 0 | 0 |
| | | | 610 | 382 | 119 | 108 | 1 | | |

- Molecule 39 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 39 | BO | 148 | Total | C | N | O | S | 0 | 0 |
| | | | 1165 | 742 | 222 | 198 | 3 | | |

- Molecule 40 is a protein called 50S ribosomal protein L15e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 40 | BP | 193 | Total | C | N | O | S | 0 | 0 |
| | | | 1582 | 1010 | 316 | 250 | 6 | | |

- Molecule 41 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 41 | BQ | 164 | Total | C | N | O | S | 0 | 0 |
| | | | 1314 | 841 | 243 | 228 | 2 | | |

- Molecule 42 is a protein called 50S ribosomal protein L18e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 42 | BR | 120 | Total | C | N | O | S | 0 | 0 |
| | | | 959 | 601 | 187 | 169 | 2 | | |

- Molecule 43 is a protein called 50S ribosomal protein L19e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 43 | BS | 146 | Total | C | N | O | S | 0 | 0 |
| | | | 1200 | 753 | 246 | 194 | 7 | | |

- Molecule 44 is a protein called 50S ribosomal protein L18Ae.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 44 | BT | 74 | Total | C | N | O | 0 | 0 |
| | | | 624 | 399 | 113 | 112 | | |

- Molecule 45 is a protein called 50S ribosomal protein L21e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 45 | BU | 96 | Total | C | N | O | S | 0 | 0 |
| | | | 784 | 502 | 158 | 123 | 1 | | |

- Molecule 46 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 46 | BV | 154 | Total | C | N | O | S | 0 | 0 |
| | | | 1234 | 777 | 242 | 211 | 4 | | |

- Molecule 47 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 47 | BW | 85 | Total | C | N | O | S | 0 | 0 |
| | | | 683 | 438 | 119 | 123 | 3 | | |

- Molecule 48 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 48 | BX | 120 | Total | C | N | O | S | 0 | 0 |
| | | | 991 | 628 | 188 | 170 | 5 | | |

- Molecule 49 is a protein called 50S ribosomal protein L24e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 49 | BY | 62 | Total | C | N | O | S | 0 | 0 |
| | | | 524 | 334 | 99 | 85 | 6 | | |

- Molecule 50 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 50 | BZ | 60 | Total | C | N | O | S | 0 | 0 |
| | | | 506 | 314 | 98 | 90 | 4 | | |

- Molecule 51 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 51 | Ba | 154 | Total | C | N | O | S | 0 | 0 |
| | | | 1242 | 788 | 235 | 214 | 5 | | |

- Molecule 52 is a protein called 50S ribosomal protein L30e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 52 | Bb | 96 | Total | C | N | O | S | 0 | 0 |
| | | | 730 | 473 | 123 | 133 | 1 | | |

- Molecule 53 is a protein called 50S ribosomal protein L31e.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 53 | Bc | 89 | Total | C | N | O | 0 | 0 |
| | | | 721 | 463 | 140 | 118 | | |

- Molecule 54 is a protein called 50S ribosomal protein L32e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 54 | Bd | 124 | Total | C | N | O | S | 0 | 0 |
| | | | 1022 | 650 | 208 | 162 | 2 | | |

- Molecule 55 is a protein called 50S ribosomal protein L34e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 55 | Be | 89 | Total | C | N | O | S | 0 | 0 |
| | | | 728 | 454 | 155 | 110 | 9 | | |

- Molecule 56 is a protein called 50S ribosomal protein L37Ae.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 56 | Bg | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 630 | 392 | 132 | 101 | 5 | | |

- Molecule 57 is a protein called 50S ribosomal protein L37e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 57 | Bh | 62 | Total | C | N | O | S | 0 | 0 |
| | | | 512 | 314 | 118 | 75 | 5 | | |

- Molecule 58 is a protein called 50S ribosomal protein L39e.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 58 | Bi | 50 | Total | C | N | O | 0 | 0 |
| | | | 432 | 276 | 97 | 59 | | |

- Molecule 59 is a protein called 50S ribosomal protein L40e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 59 | Bj | 47 | Total | C | N | O | S | 0 | 0 |
| | | | 373 | 233 | 79 | 56 | 5 | | |

- Molecule 60 is a protein called LSU ribosomal protein L41E.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 60 | Bk | 36 | Total | C | N | O | S | 0 | 0 |
| | | | 345 | 218 | 86 | 39 | 2 | | |

- Molecule 61 is a protein called 50S ribosomal protein L44e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 61 | Bl | 93 | Total | C | N | O | S | 0 | 0 |
| | | | 778 | 494 | 160 | 119 | 5 | | |

- Molecule 62 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 62 | Ag | 1 | Total Zn<br>1 1 | 0 |
| 62 | Ar | 1 | Total Zn<br>1 1 | 0 |
| 62 | As | 1 | Total Zn<br>1 1 | 0 |
| 62 | Ax | 1 | Total Zn<br>1 1 | 0 |
| 62 | Az | 2 | Total Zn<br>2 2 | 0 |
| 62 | BY | 1 | Total Zn<br>1 1 | 0 |
| 62 | Be | 1 | Total Zn<br>1 1 | 0 |
| 62 | Bg | 1 | Total Zn<br>1 1 | 0 |
| 62 | Bh | 1 | Total Zn<br>1 1 | 0 |
| 62 | Bj | 1 | Total Zn<br>1 1 | 0 |
| 62 | Bl | 1 | Total Zn<br>1 1 | 0 |

- Molecule 63 is water.

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 63 | Aa | 714 | Total O<br>714 714 | 0 |
| 63 | Ab | 8 | Total O<br>8 8 | 0 |
| 63 | Ac | 10 | Total O<br>10 10 | 0 |
| 63 | Ad | 4 | Total O<br>4 4 | 0 |
| 63 | Ae | 13 | Total O<br>13 13 | 0 |
| 63 | Af | 14 | Total O<br>14 14 | 0 |
| 63 | Ag | 14 | Total O<br>14 14 | 0 |
| 63 | Ah | 2 | Total O<br>2 2 | 0 |
| 63 | Ai | 13 | Total O<br>13 13 | 0 |

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| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 63 | Aj | 12 | Total O<br>12 12 | 0 |
| 63 | Ak | 8 | Total O<br>8 8 | 0 |
| 63 | Al | 7 | Total O<br>7 7 | 0 |
| 63 | Am | 2 | Total O<br>2 2 | 0 |
| 63 | An | 8 | Total O<br>8 8 | 0 |
| 63 | Ao | 10 | Total O<br>10 10 | 0 |
| 63 | Ap | 11 | Total O<br>11 11 | 0 |
| 63 | Aq | 10 | Total O<br>10 10 | 0 |
| 63 | Ar | 2 | Total O<br>2 2 | 0 |
| 63 | As | 6 | Total O<br>6 6 | 0 |
| 63 | At | 1 | Total O<br>1 1 | 0 |
| 63 | Au | 4 | Total O<br>4 4 | 0 |
| 63 | Av | 13 | Total O<br>13 13 | 0 |
| 63 | Aw | 1 | Total O<br>1 1 | 0 |
| 63 | Ax | 3 | Total O<br>3 3 | 0 |
| 63 | Ay | 4 | Total O<br>4 4 | 0 |
| 63 | Az | 4 | Total O<br>4 4 | 0 |
| 63 | BA | 1226 | Total O<br>1226 1226 | 0 |
| 63 | BB | 19 | Total O<br>19 19 | 0 |
| 63 | BC | 19 | Total O<br>19 19 | 0 |
| 63 | BD | 24 | Total O<br>24 24 | 0 |

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| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 63 | BE | 11 | Total O<br>11 11 | 0 |
| 63 | BG | 6 | Total O<br>6 6 | 0 |
| 63 | BJ | 11 | Total O<br>11 11 | 0 |
| 63 | BK | 11 | Total O<br>11 11 | 0 |
| 63 | BL | 4 | Total O<br>4 4 | 0 |
| 63 | BM | 2 | Total O<br>2 2 | 0 |
| 63 | BN | 4 | Total O<br>4 4 | 0 |
| 63 | BO | 10 | Total O<br>10 10 | 0 |
| 63 | BP | 18 | Total O<br>18 18 | 0 |
| 63 | BQ | 7 | Total O<br>7 7 | 0 |
| 63 | BR | 8 | Total O<br>8 8 | 0 |
| 63 | BS | 7 | Total O<br>7 7 | 0 |
| 63 | BT | 3 | Total O<br>3 3 | 0 |
| 63 | BU | 7 | Total O<br>7 7 | 0 |
| 63 | BV | 7 | Total O<br>7 7 | 0 |
| 63 | BW | 4 | Total O<br>4 4 | 0 |
| 63 | BX | 6 | Total O<br>6 6 | 0 |
| 63 | BY | 3 | Total O<br>3 3 | 0 |
| 63 | BZ | 1 | Total O<br>1 1 | 0 |
| 63 | Ba | 10 | Total O<br>10 10 | 0 |
| 63 | Bb | 1 | Total O<br>1 1 | 0 |

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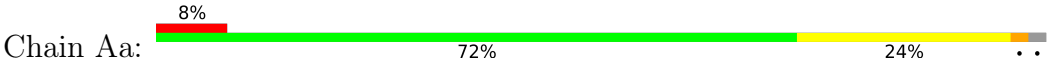
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 63 | Bc | 3 | Total O<br>3 3 | 0 |
| 63 | Bd | 5 | Total O<br>5 5 | 0 |
| 63 | Be | 3 | Total O<br>3 3 | 0 |
| 63 | Bg | 3 | Total O<br>3 3 | 0 |
| 63 | Bh | 11 | Total O<br>11 11 | 0 |
| 63 | Bi | 2 | Total O<br>2 2 | 0 |
| 63 | Bj | 2 | Total O<br>2 2 | 0 |
| 63 | Bk | 3 | Total O<br>3 3 | 0 |
| 63 | Bl | 8 | Total O<br>8 8 | 0 |

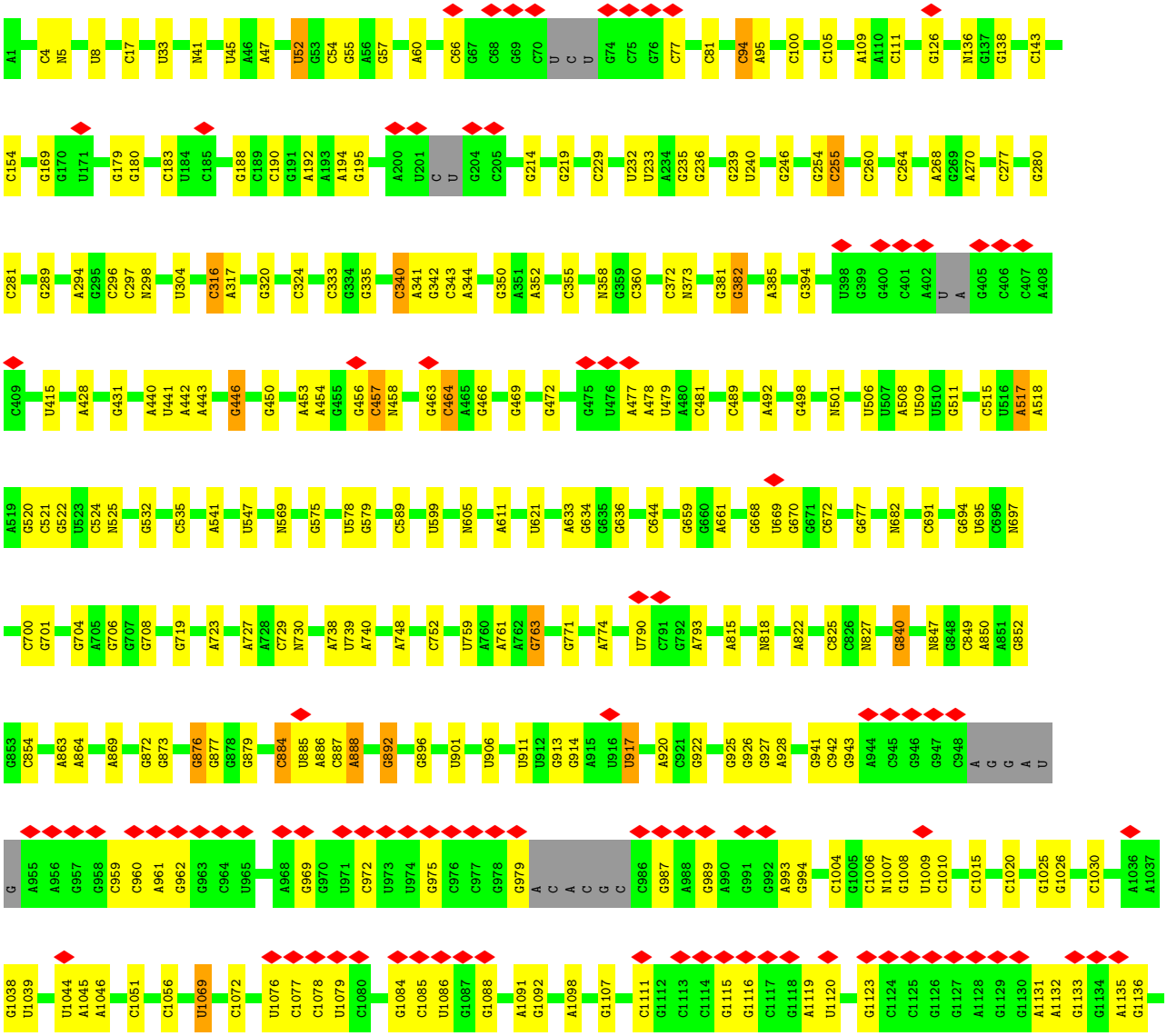
# 3 Residue-property plots (i)

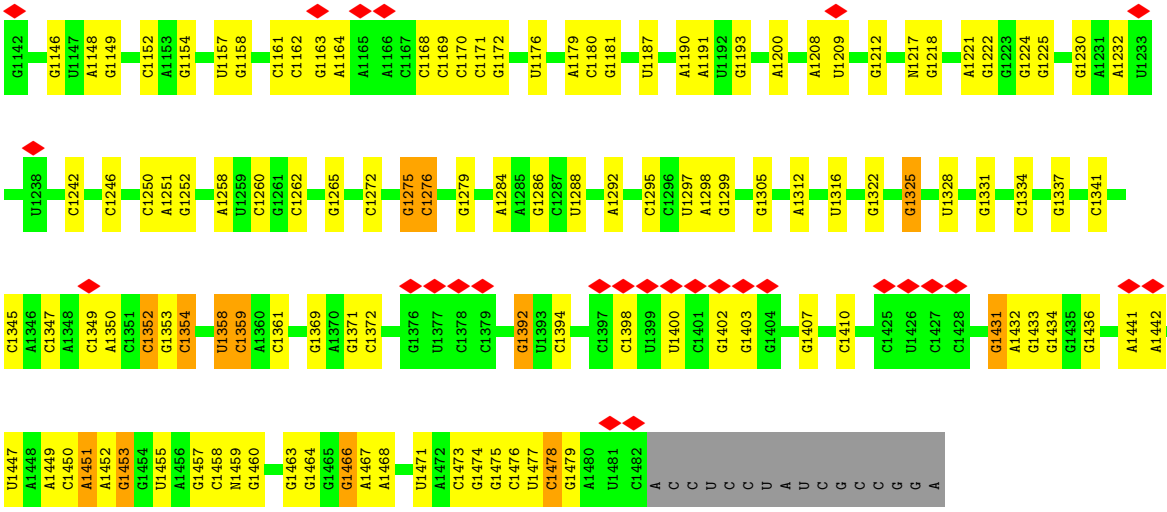
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: 16S rRNA

Chain Aa:

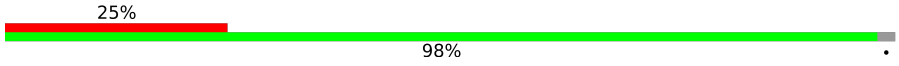


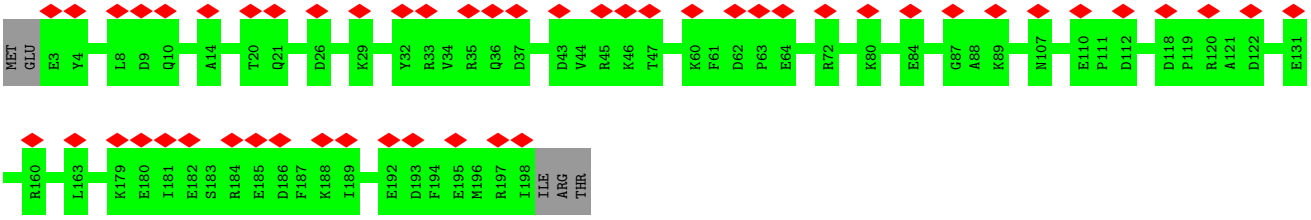






• Molecule 2: 30S ribosomal protein S2

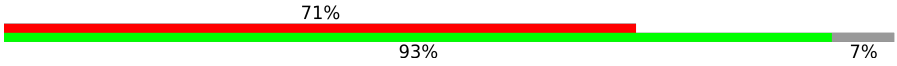
Chain Ab:

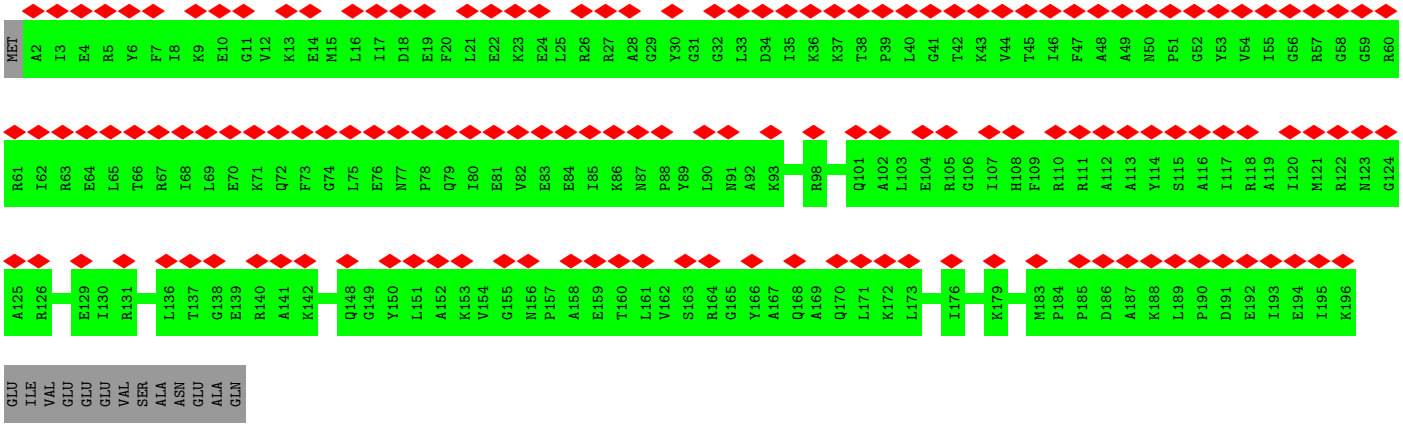



• Molecule 3: 30S ribosomal protein S3

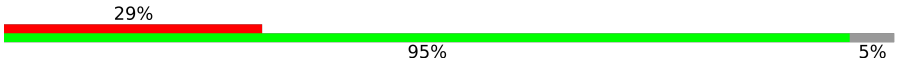
Chain Ac:

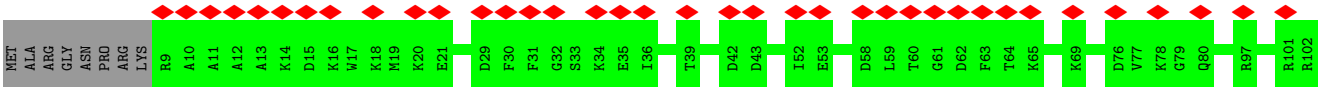


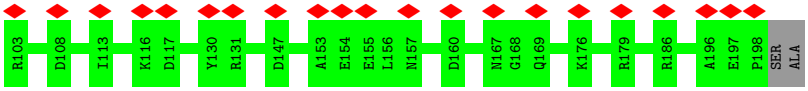




• Molecule 4: 30S ribosomal protein S3Ae

Chain Ad:

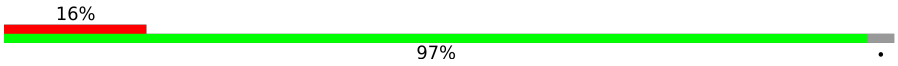


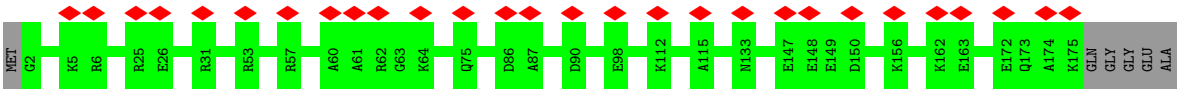






• Molecule 5: 30S ribosomal protein S4

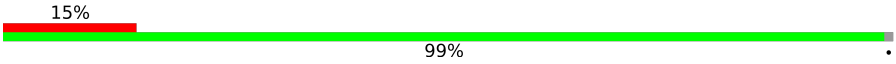
Chain Ae:

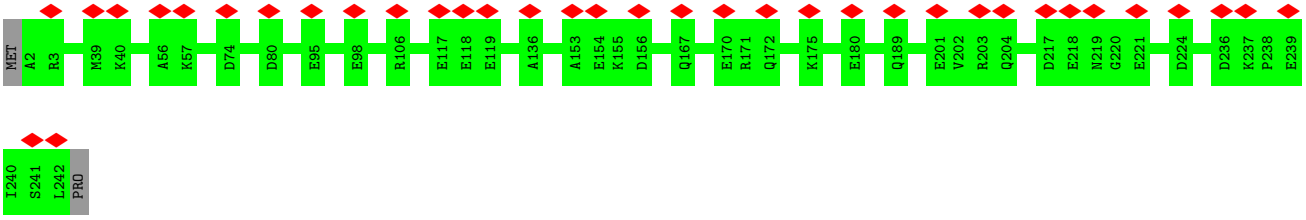



• Molecule 6: 30S ribosomal protein S4e

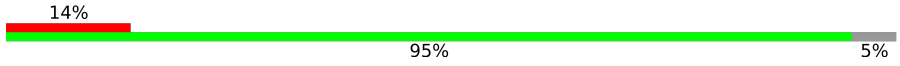
Chain Af:

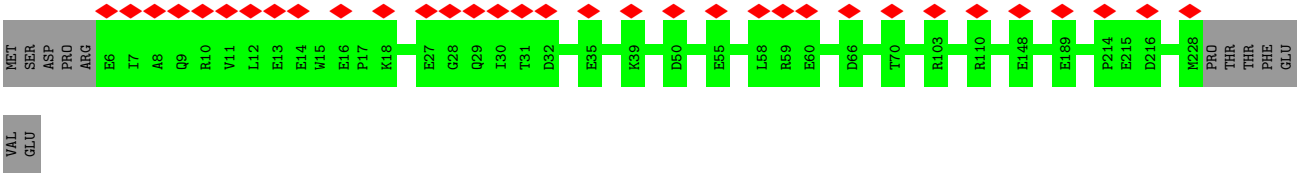



• Molecule 7: 30S ribosomal protein S5

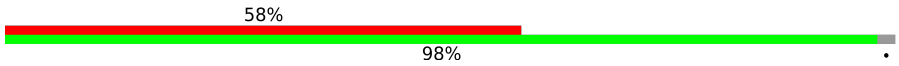
Chain Ag:

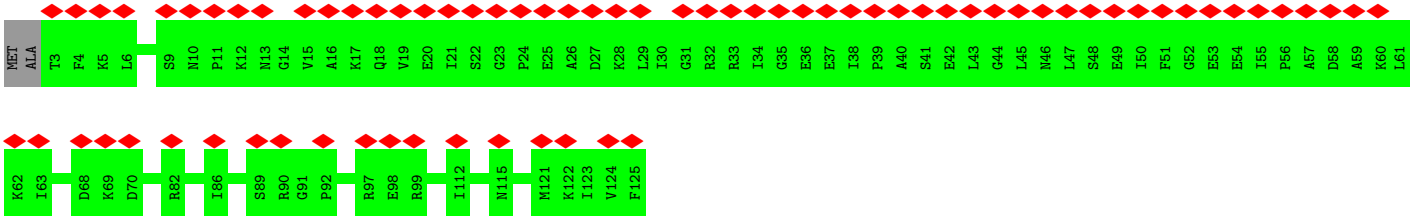



• Molecule 8: 30S ribosomal protein S6e

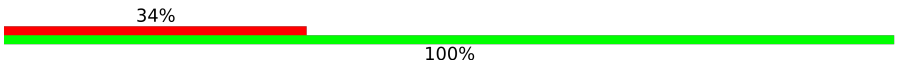
Chain Ah:

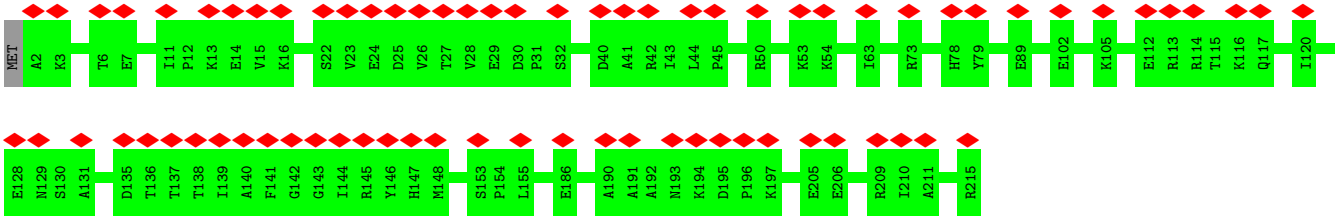


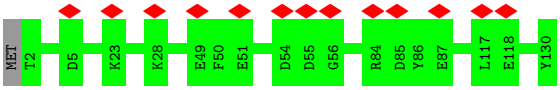

• Molecule 9: 30S ribosomal protein S7

Chain Ai:

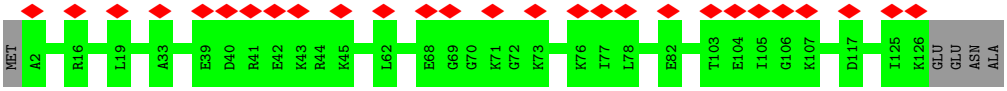




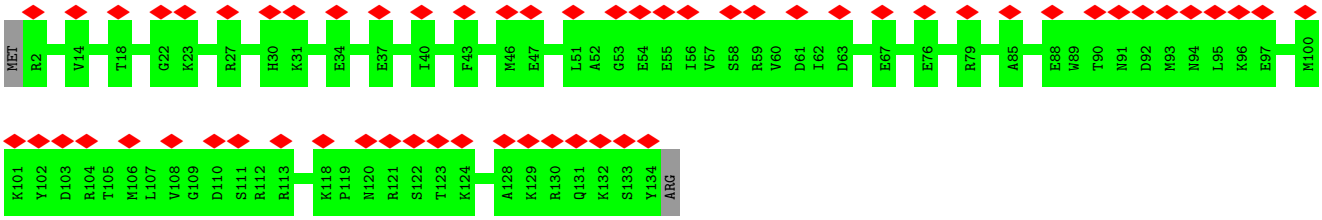

• Molecule 10: 30S ribosomal protein S8

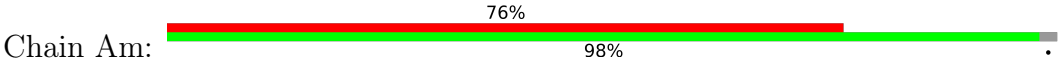

• Molecule 11: 30S ribosomal protein S8e

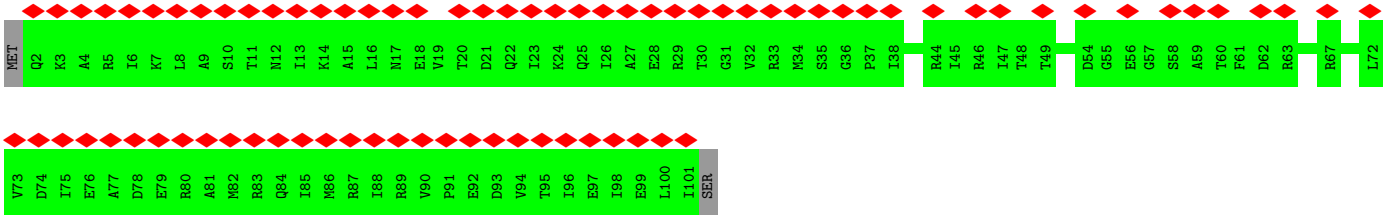




• Molecule 12: 30S ribosomal protein S9

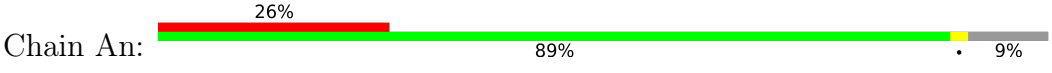



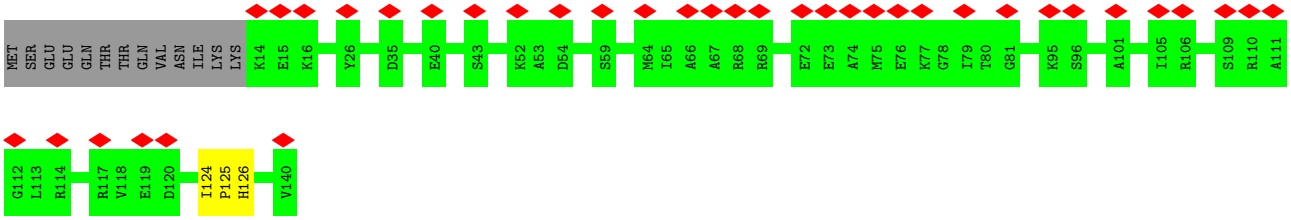

• Molecule 13: 30S ribosomal protein S10



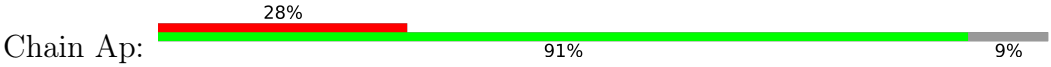

• Molecule 14: 30S ribosomal protein S11





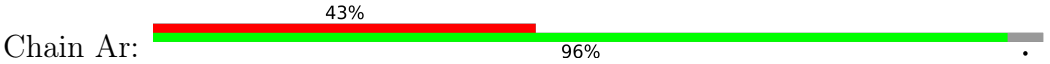

• Molecule 15: 30S ribosomal protein S12


• Molecule 16: 30S ribosomal protein S13




• Molecule 17: 30S ribosomal protein S15

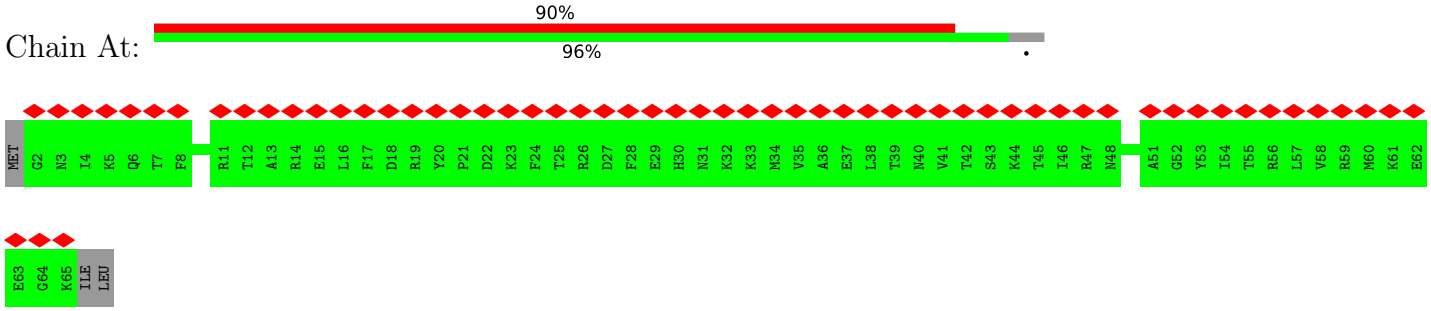

• Molecule 18: 30S ribosomal protein S14 type Z




• Molecule 19: 30S ribosomal protein S17

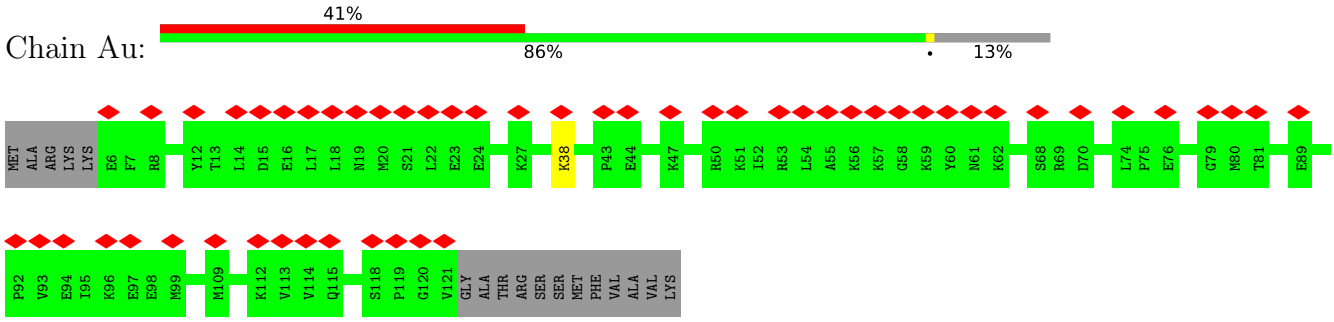

• Molecule 20: 30S ribosomal protein S17e

Chain At:



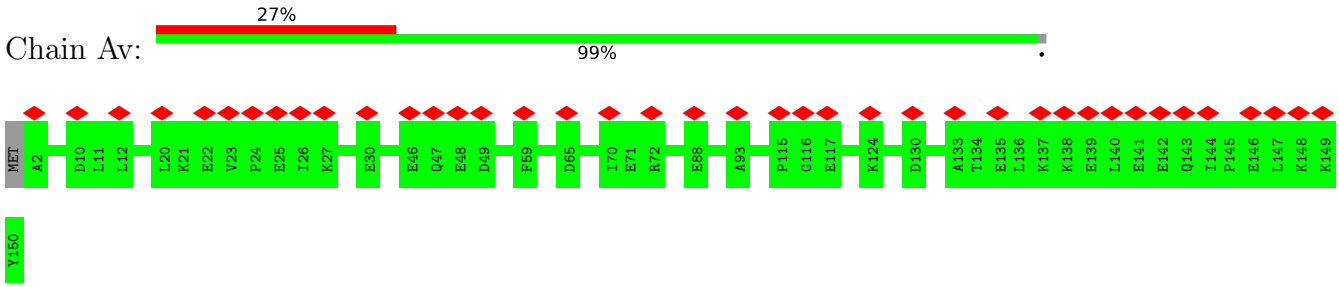

• Molecule 21: 30S ribosomal protein S19

Chain Au:



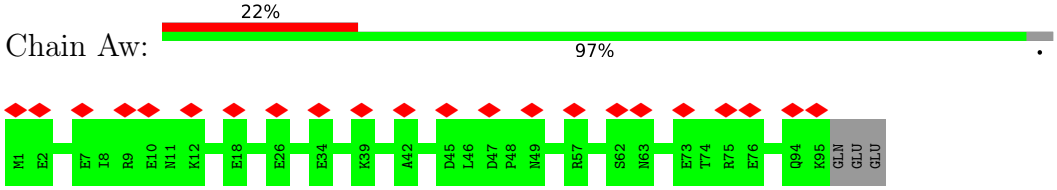

• Molecule 22: 30S ribosomal protein S19e

Chain Av:



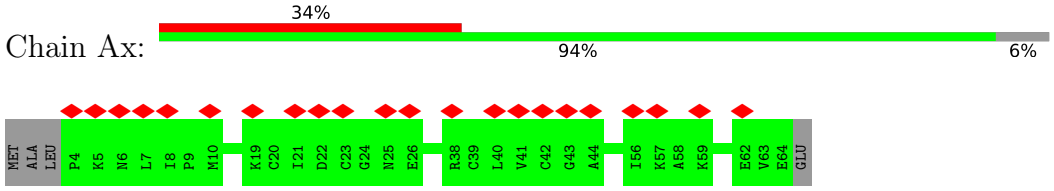

• Molecule 23: 30S ribosomal protein S24e

Chain Aw:



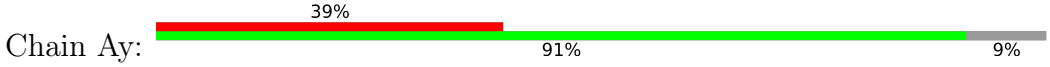

• Molecule 24: 30S ribosomal protein S27e

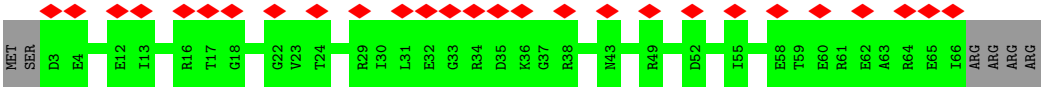
Chain Ax:




• Molecule 25: 30S ribosomal protein S28e

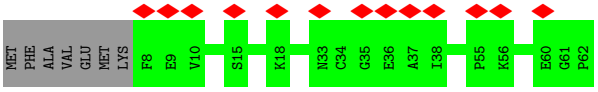
Chain Ay:





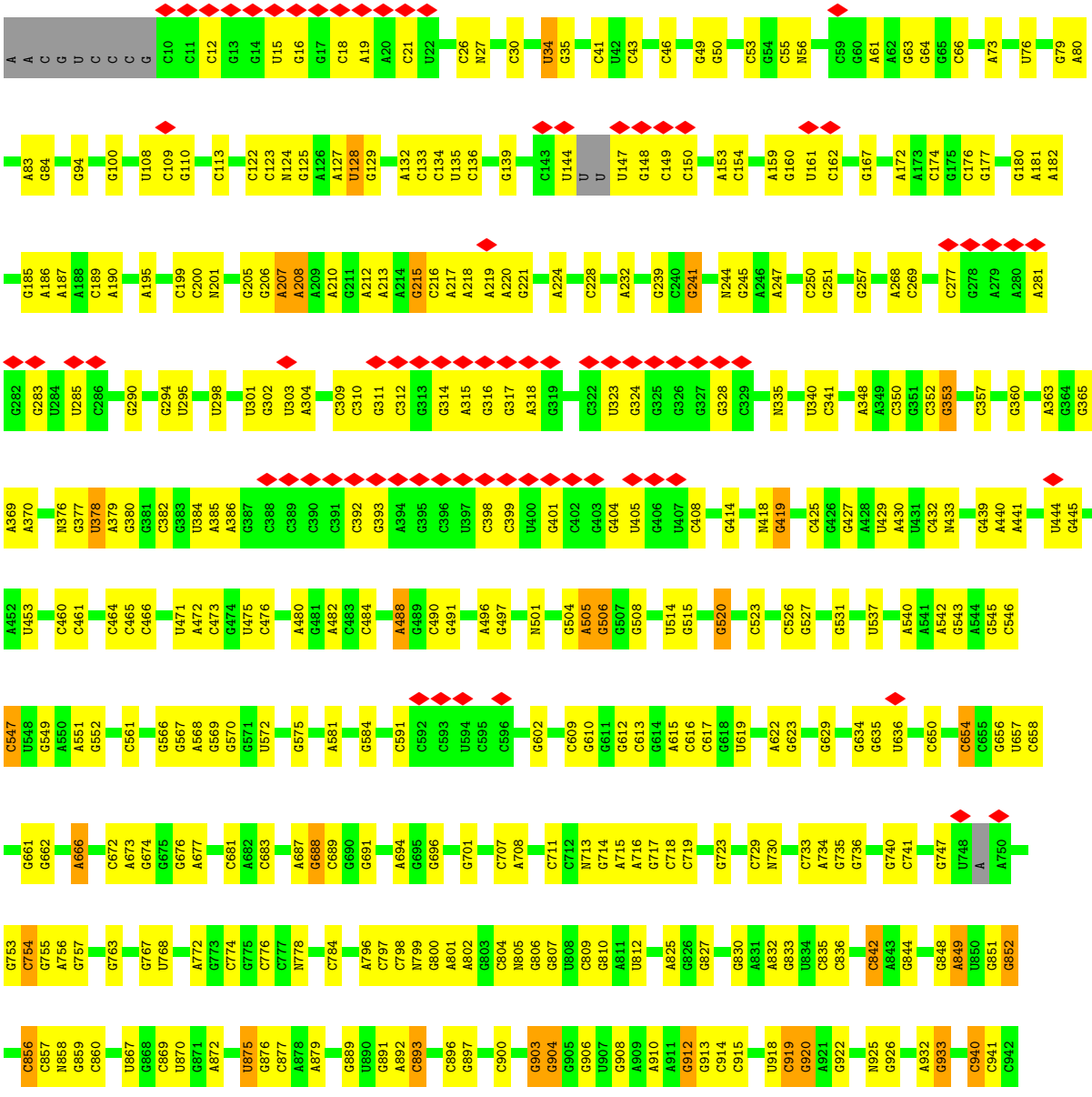
• Molecule 26: Predicted zinc-ribbon RNA-binding protein involved in translation

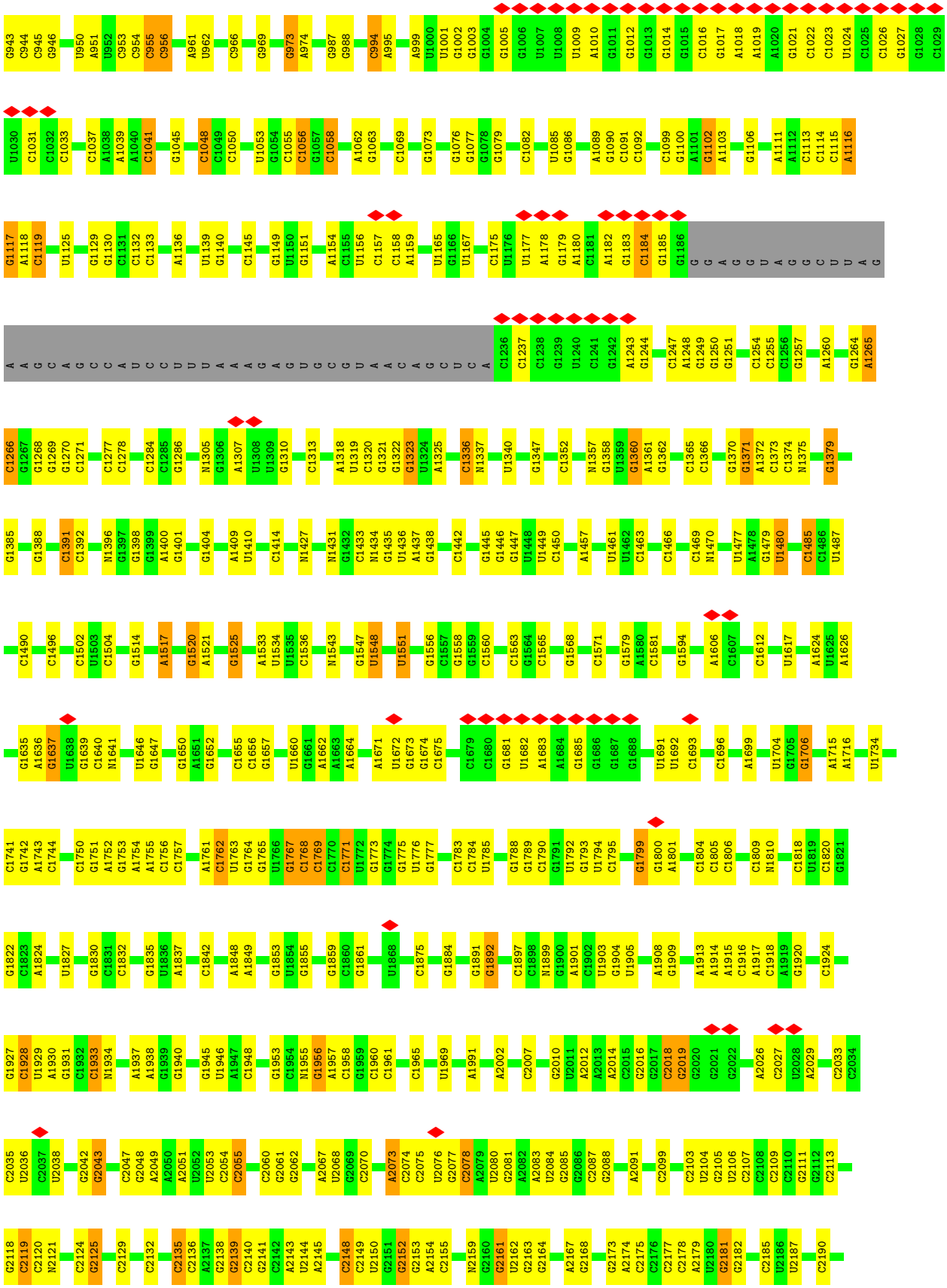
Chain Az:

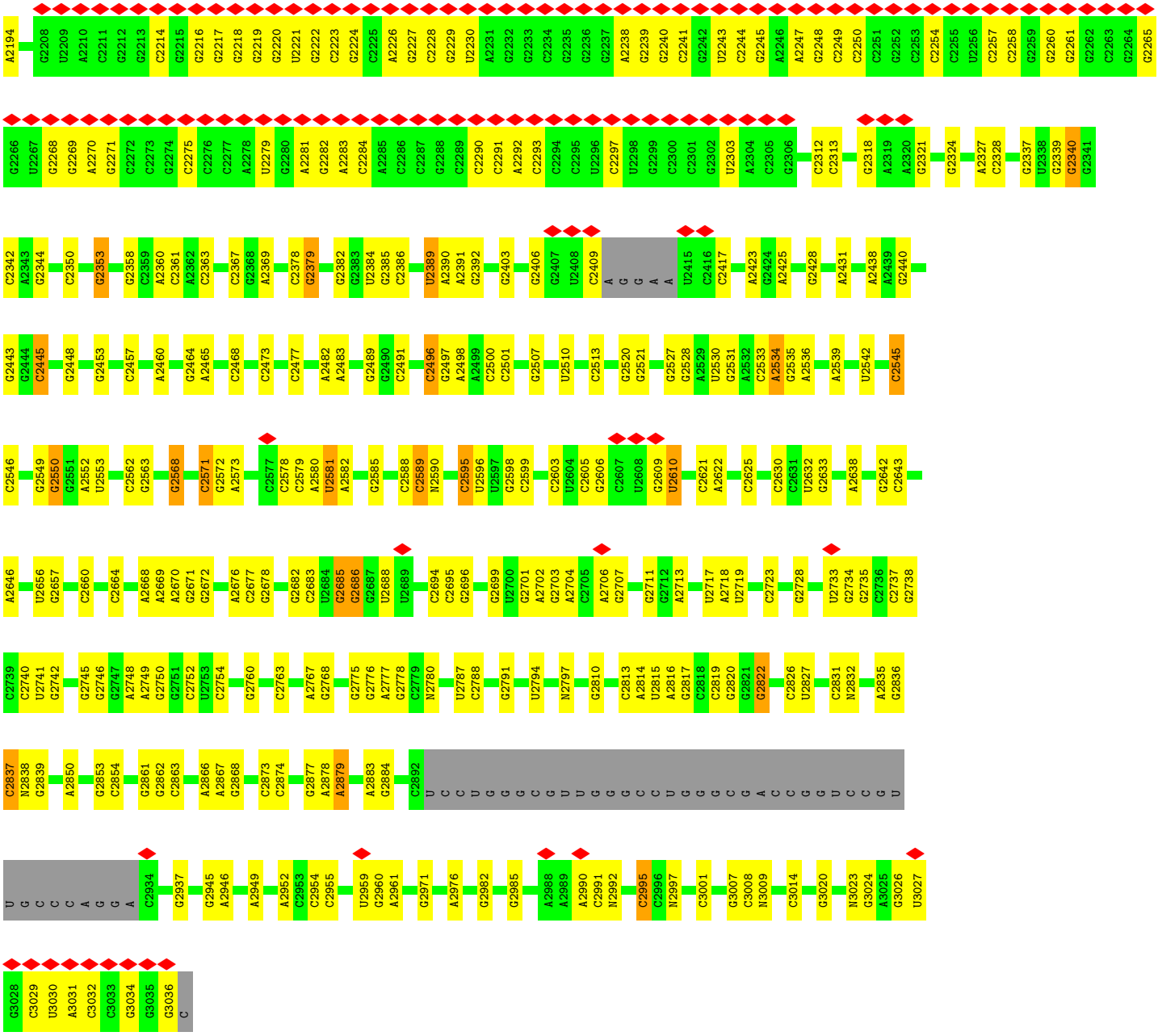



• Molecule 27: 23S rRNA

Chain BA:

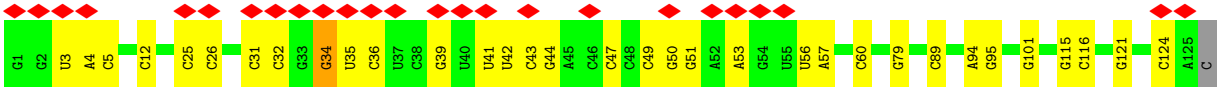







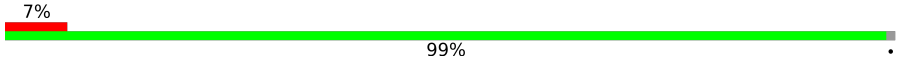
• Molecule 28: 5S rRNA

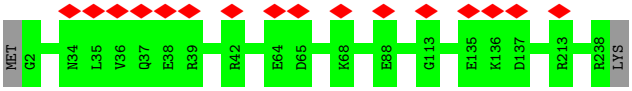
Chain BB:

• Molecule 29: 50S ribosomal protein L2

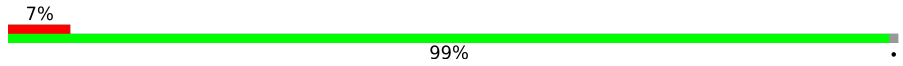
Chain BC:

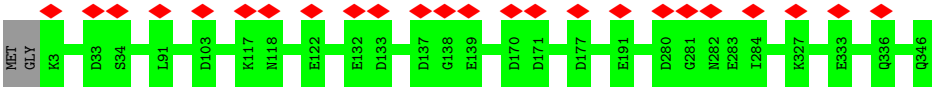





• Molecule 30: 50S ribosomal protein L3

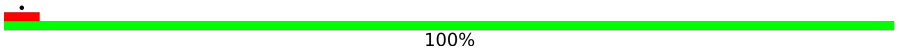
Chain BD:

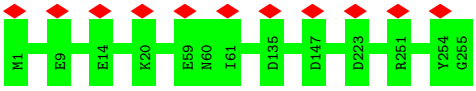



• Molecule 31: 50S ribosomal protein L4

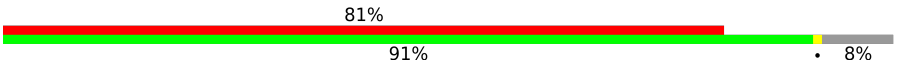
Chain BE:

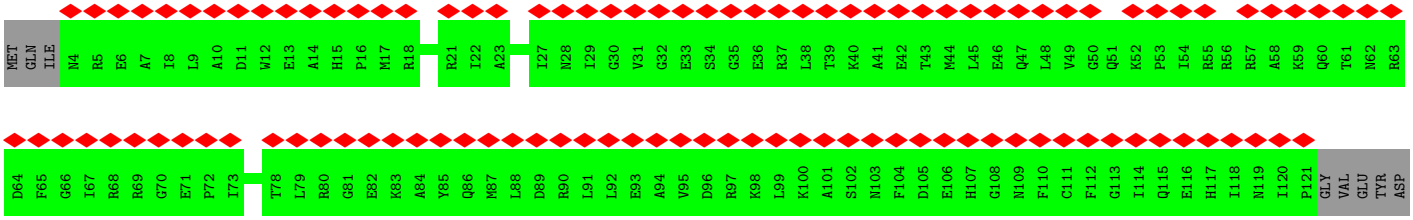



• Molecule 32: 50S ribosomal protein L5

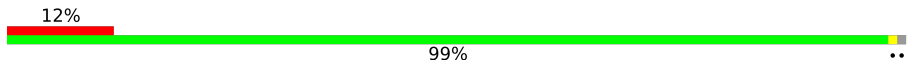
Chain BF:

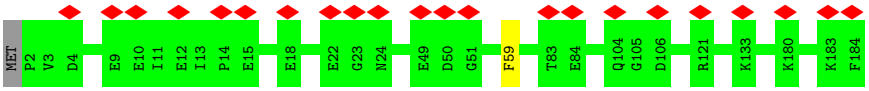



• Molecule 33: 50S ribosomal protein L6

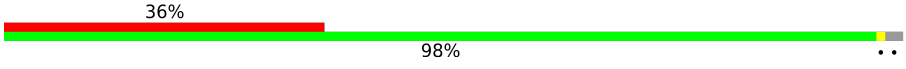
Chain BG:

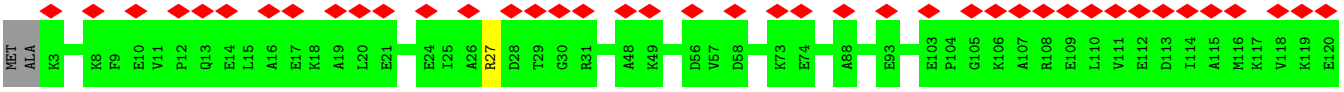



• Molecule 34: 50S ribosomal protein L7Ae

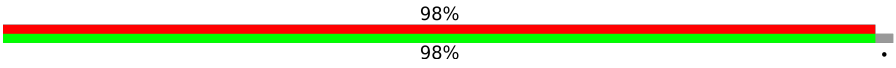
Chain BH:

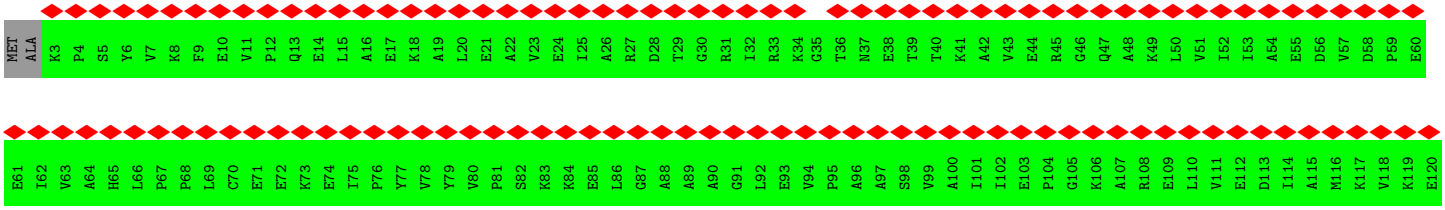



• Molecule 34: 50S ribosomal protein L7Ae

Chain BI:

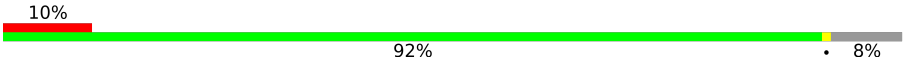


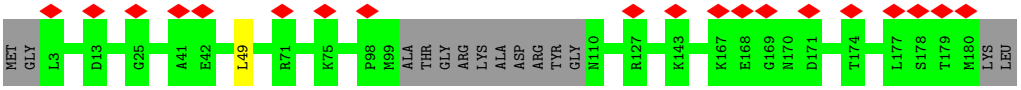





• Molecule 35: 50S ribosomal protein L10e

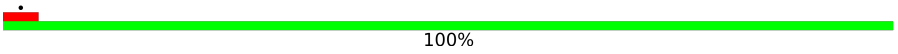
Chain BJ:

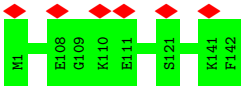



• Molecule 36: 50S ribosomal protein L13

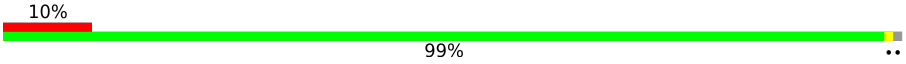
Chain BK:

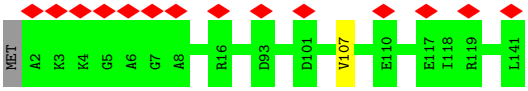



• Molecule 37: 50S ribosomal protein L14

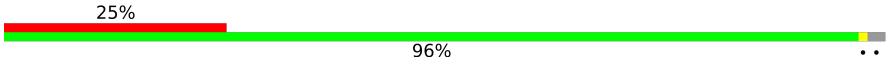
Chain BL:

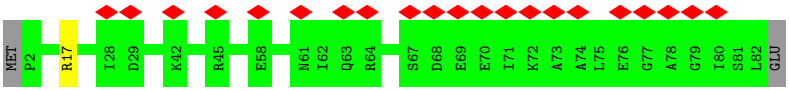



• Molecule 38: 50S ribosomal protein L14e

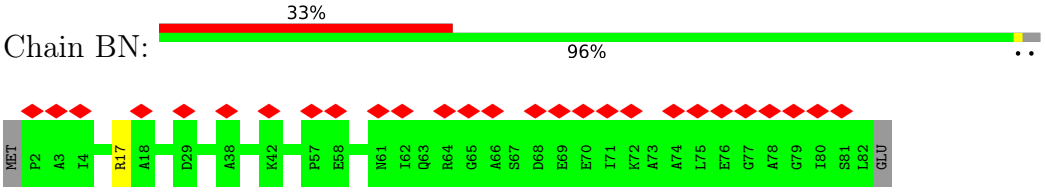
Chain BM:



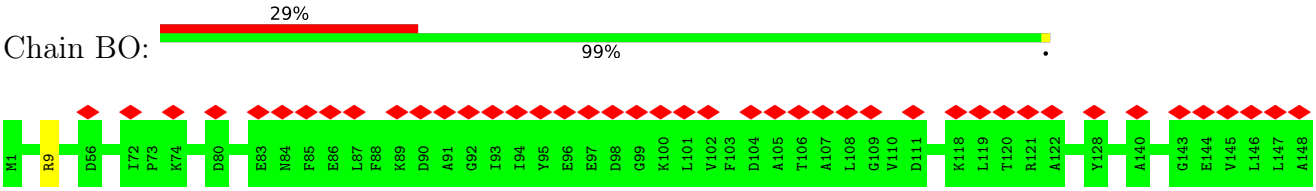

• Molecule 38: 50S ribosomal protein L14e

Chain BN:



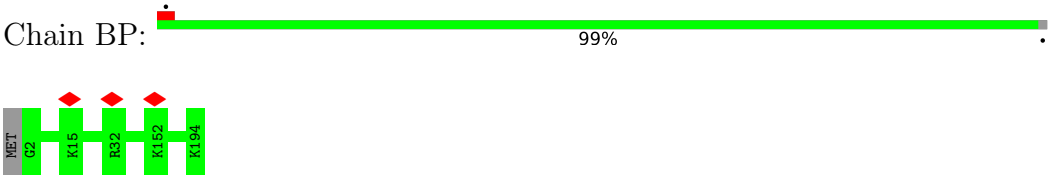

• Molecule 39: 50S ribosomal protein L15

Chain BO:



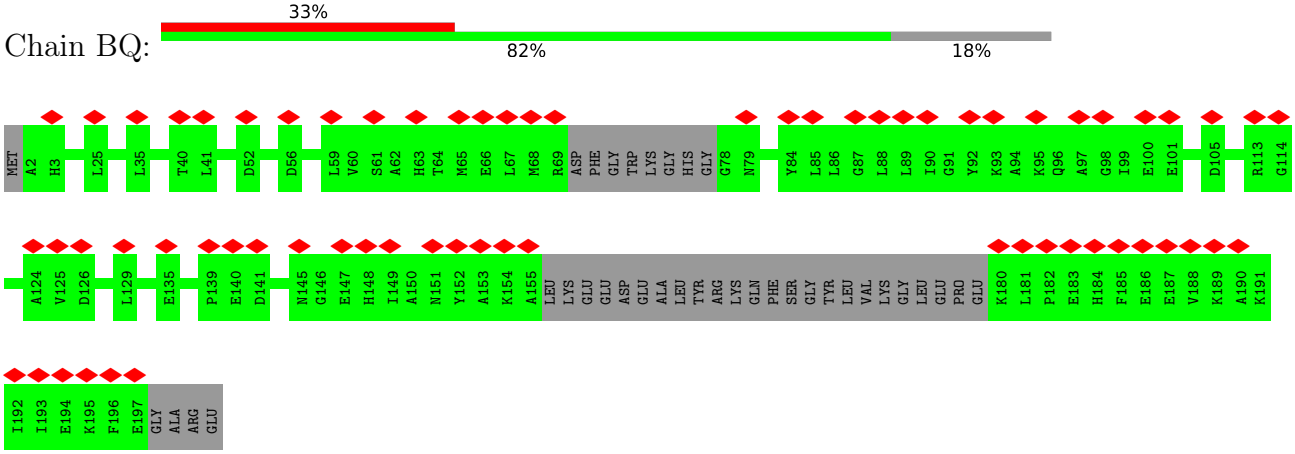

• Molecule 40: 50S ribosomal protein L15e

Chain BP:



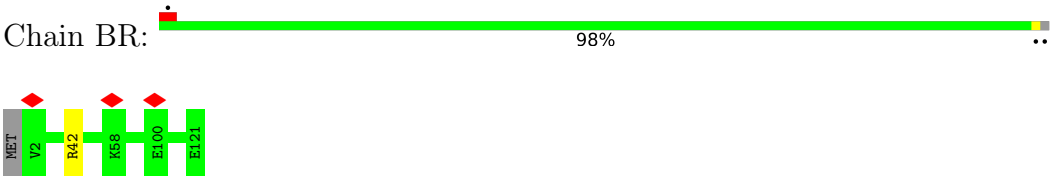

• Molecule 41: 50S ribosomal protein L18

Chain BQ:



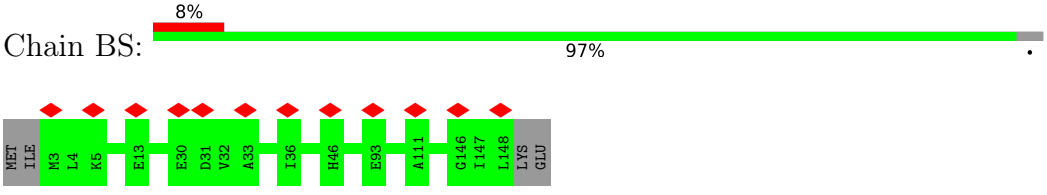

• Molecule 42: 50S ribosomal protein L18e

Chain BR:



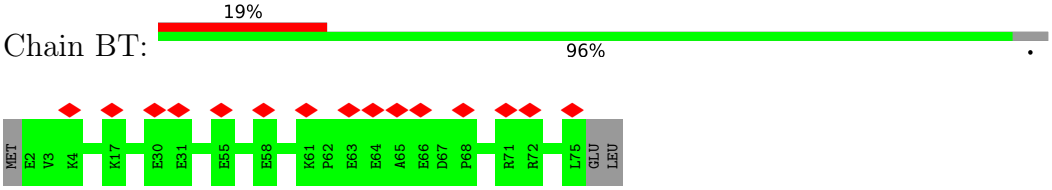

• Molecule 43: 50S ribosomal protein L19e

Chain BS:



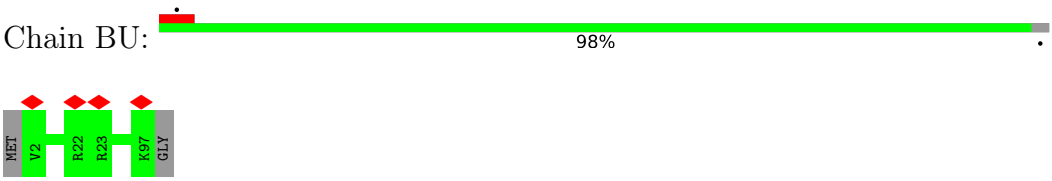
• Molecule 44: 50S ribosomal protein L18Ae

Chain BT:



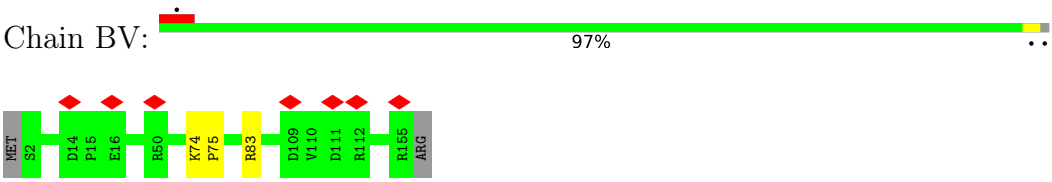

• Molecule 45: 50S ribosomal protein L21e

Chain BU:



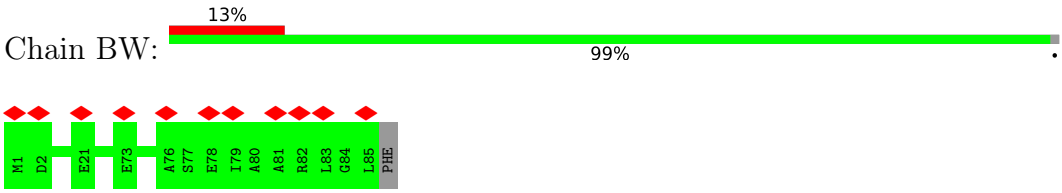

• Molecule 46: 50S ribosomal protein L22

Chain BV:



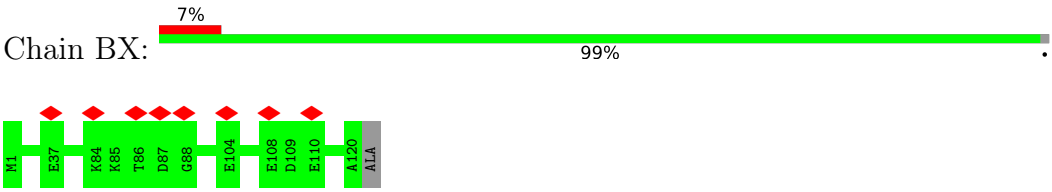

• Molecule 47: 50S ribosomal protein L23

Chain BW:



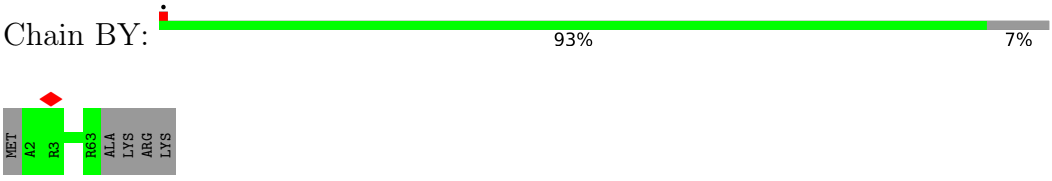

• Molecule 48: 50S ribosomal protein L24

Chain BX:



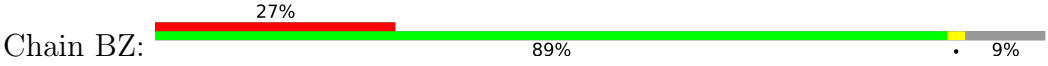

• Molecule 49: 50S ribosomal protein L24e

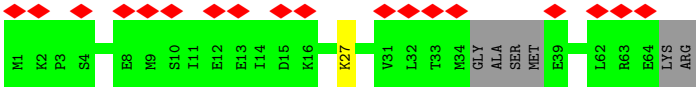
Chain BY:




• Molecule 50: 50S ribosomal protein L29

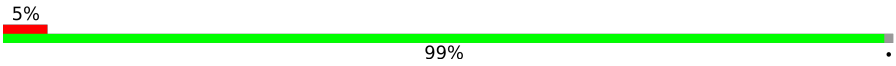
Chain BZ:

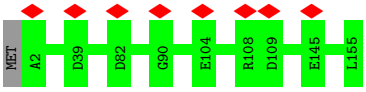





• Molecule 51: 50S ribosomal protein L30

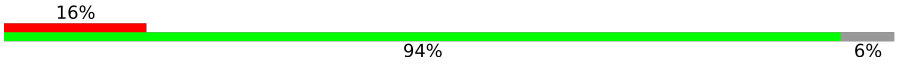
Chain Ba:

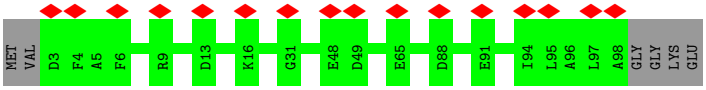



• Molecule 52: 50S ribosomal protein L30e

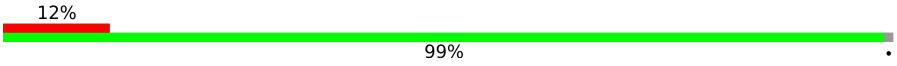
Chain Bb:

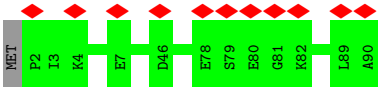



• Molecule 53: 50S ribosomal protein L31e

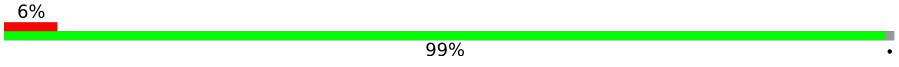
Chain Bc:

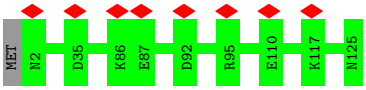



• Molecule 54: 50S ribosomal protein L32e

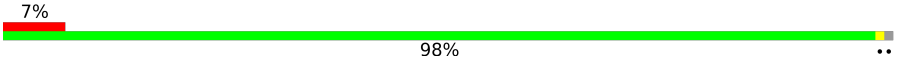
Chain Bd:

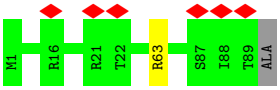



• Molecule 55: 50S ribosomal protein L34e

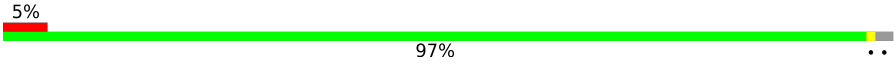
Chain Be:

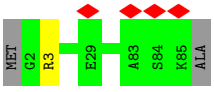



• Molecule 56: 50S ribosomal protein L37Ae

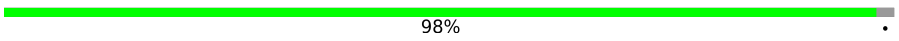
Chain Bg:




• Molecule 57: 50S ribosomal protein L37e

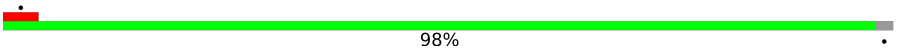
Chain Bh:

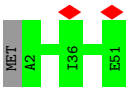




• Molecule 58: 50S ribosomal protein L39e

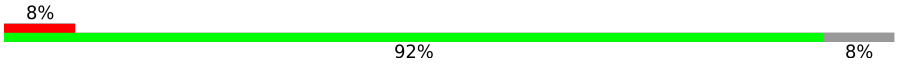
Chain Bi:

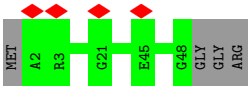



• Molecule 59: 50S ribosomal protein L40e

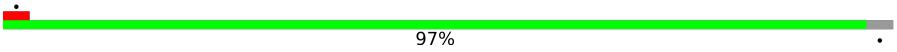
Chain Bj:




• Molecule 60: LSU ribosomal protein L41E

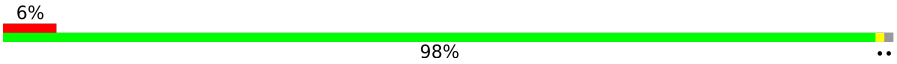
Chain Bk:

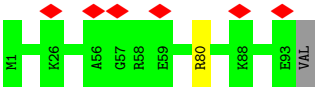




• Molecule 61: 50S ribosomal protein L44e

Chain Bl:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 53737 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 34 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | 29000 | Depositor |
| Image detector | FEI FALCON III (4k x 4k) | Depositor |
| Maximum map value | 0.441 | Depositor |
| Minimum map value | -0.245 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.011 | Depositor |
| Recommended contour level | 0.05 | Depositor |
| Map size (Å) | 408.0, 408.0, 408.0 | wwPDB |
| Map dimensions | 480, 480, 480 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.85, 0.85, 0.85 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, A2M, OMG, OMC, LV2, OMU, 5MC, B8T, ZN, 6MZ, MA6, 4AC, LHH, 2MG, 4SU

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 | Aa | 1.19 | 25/33361 (0.1%) | 1.15 | 100/52003 (0.2%) |
| 2 | Ab | 0.39 | 0/1611 | 0.47 | 0/2179 |
| 3 | Ac | 0.33 | 0/1546 | 0.50 | 0/2075 |
| 4 | Ad | 0.38 | 0/1578 | 0.51 | 0/2119 |
| 5 | Ae | 0.40 | 0/1477 | 0.52 | 0/1980 |
| 6 | Af | 0.45 | 0/1991 | 0.49 | 0/2688 |
| 7 | Ag | 0.30 | 0/1779 | 0.47 | 0/2396 |
| 8 | Ah | 0.36 | 0/968 | 0.51 | 0/1300 |
| 9 | Ai | 0.37 | 0/1748 | 0.48 | 0/2347 |
| 10 | Aj | 0.43 | 0/1039 | 0.51 | 0/1397 |
| 11 | Ak | 0.42 | 0/991 | 0.53 | 0/1322 |
| 12 | Al | 0.34 | 0/1068 | 0.53 | 0/1430 |
| 13 | Am | 0.31 | 0/810 | 0.49 | 0/1087 |
| 14 | An | 0.61 | 2/968 (0.2%) | 0.58 | 1/1304 (0.1%) |
| 15 | Ao | 0.44 | 0/1139 | 0.50 | 0/1518 |
| 16 | Ap | 0.36 | 0/1113 | 0.49 | 0/1500 |
| 17 | Aq | 0.39 | 0/1241 | 0.47 | 0/1667 |
| 18 | Ar | 0.35 | 0/457 | 0.48 | 0/602 |
| 19 | As | 0.29 | 0/899 | 0.47 | 0/1214 |
| 20 | At | 0.30 | 0/545 | 0.48 | 0/725 |
| 21 | Au | 0.37 | 0/970 | 0.49 | 0/1295 |
| 22 | Av | 0.40 | 0/1249 | 0.48 | 0/1687 |
| 23 | Aw | 0.41 | 0/790 | 0.50 | 0/1063 |
| 24 | Ax | 0.26 | 0/469 | 0.49 | 0/633 |
| 25 | Ay | 0.37 | 0/501 | 0.52 | 0/672 |
| 26 | Az | 0.28 | 0/440 | 0.44 | 0/599 |
| 27 | BA | 1.58 | 139/66981 (0.2%) | 1.39 | 489/104453 (0.5%) |
| 28 | BB | 1.06 | 0/2993 | 1.17 | 14/4668 (0.3%) |
| 29 | BC | 0.69 | 0/1860 | 0.66 | 0/2511 |
| 30 | BD | 0.65 | 0/2815 | 0.62 | 0/3795 |
| 31 | BE | 0.63 | 0/2066 | 0.61 | 0/2785 |
| 32 | BF | 0.48 | 0/1330 | 0.60 | 0/1778 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 33 | BG | 0.56 | 0/1490 | 0.57 | 0/2006 |
| 34 | BH | 0.46 | 0/941 | 0.53 | 0/1272 |
| 34 | BI | 0.33 | 0/941 | 0.50 | 0/1272 |
| 35 | BJ | 0.61 | 0/1407 | 0.63 | 1/1891 (0.1%) |
| 36 | BK | 0.67 | 0/1165 | 0.68 | 0/1558 |
| 37 | BL | 0.65 | 1/1067 (0.1%) | 0.62 | 0/1435 |
| 38 | BM | 0.50 | 0/614 | 0.58 | 0/824 |
| 38 | BN | 0.47 | 0/614 | 0.56 | 0/824 |
| 39 | BO | 0.55 | 0/1187 | 0.62 | 0/1583 |
| 40 | BP | 0.73 | 0/1621 | 0.61 | 0/2163 |
| 41 | BQ | 0.47 | 0/1342 | 0.54 | 0/1804 |
| 42 | BR | 0.58 | 0/971 | 0.59 | 0/1301 |
| 43 | BS | 0.59 | 0/1216 | 0.59 | 0/1607 |
| 44 | BT | 0.58 | 0/636 | 0.57 | 0/852 |
| 45 | BU | 0.62 | 0/806 | 0.58 | 0/1080 |
| 46 | BV | 0.73 | 2/1259 (0.2%) | 0.65 | 1/1688 (0.1%) |
| 47 | BW | 0.56 | 0/690 | 0.56 | 0/925 |
| 48 | BX | 0.58 | 0/1007 | 0.59 | 0/1344 |
| 49 | BY | 0.63 | 0/538 | 0.54 | 0/716 |
| 50 | BZ | 0.47 | 0/506 | 0.57 | 0/668 |
| 51 | Ba | 0.61 | 0/1259 | 0.63 | 0/1680 |
| 52 | Bb | 0.47 | 0/742 | 0.53 | 0/1001 |
| 53 | Bc | 0.60 | 0/736 | 0.53 | 0/990 |
| 54 | Bd | 0.66 | 0/1044 | 0.60 | 0/1394 |
| 55 | Be | 0.60 | 0/746 | 0.66 | 0/997 |
| 56 | Bg | 0.63 | 0/640 | 0.65 | 0/855 |
| 57 | Bh | 0.77 | 0/524 | 0.66 | 0/692 |
| 58 | Bi | 0.69 | 0/441 | 0.60 | 0/588 |
| 59 | Bj | 0.55 | 0/381 | 0.55 | 0/505 |
| 60 | Bk | 0.54 | 0/351 | 0.67 | 0/454 |
| 61 | Bl | 0.61 | 0/796 | 0.61 | 0/1056 |
| All | All | 1.19 | 169/166471 (0.1%) | 1.11 | 606/245817 (0.2%) |

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 |
|---|---|---|---|
| 14 | An | 0 | 1 |

All (169) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 46 | BV | 75 | PRO | N-CA | 13.70 | 1.70 | 1.47 |
| 14 | An | 125 | PRO | N-CA | 13.65 | 1.70 | 1.47 |
| 1 | Aa | 1463 | G | N1-C2 | -6.60 | 1.32 | 1.37 |
| 1 | Aa | 763 | G | N1-C2 | -6.49 | 1.32 | 1.37 |
| 1 | Aa | 1445 | C | C4-C5 | -6.41 | 1.37 | 1.43 |
| 1 | Aa | 849 | C | N1-C6 | -6.37 | 1.33 | 1.37 |
| 27 | BA | 1806 | C | N1-C6 | -6.30 | 1.33 | 1.37 |
| 27 | BA | 1446 | G | C6-N1 | -6.28 | 1.35 | 1.39 |
| 27 | BA | 1961 | C | C4-C5 | -6.20 | 1.38 | 1.43 |
| 27 | BA | 915 | C | C5-C6 | -6.14 | 1.29 | 1.34 |
| 27 | BA | 2178 | C | C4-C5 | -6.09 | 1.38 | 1.43 |
| 27 | BA | 1958 | C | C4-C5 | -6.06 | 1.38 | 1.43 |
| 27 | BA | 1918 | C | N1-C6 | -6.00 | 1.33 | 1.37 |
| 1 | Aa | 1445 | C | N1-C6 | -5.99 | 1.33 | 1.37 |
| 27 | BA | 2136 | C | C4-C5 | -5.98 | 1.38 | 1.43 |
| 1 | Aa | 887 | C | O3'-P | -5.97 | 1.53 | 1.61 |
| 14 | An | 124 | ILE | C-N | 5.97 | 1.45 | 1.34 |
| 46 | BV | 74 | LYS | C-N | 5.96 | 1.45 | 1.34 |
| 1 | Aa | 1463 | G | C8-N7 | -5.96 | 1.27 | 1.30 |
| 27 | BA | 232 | A | N9-C4 | -5.88 | 1.34 | 1.37 |
| 1 | Aa | 1474 | G | C6-N1 | -5.84 | 1.35 | 1.39 |
| 27 | BA | 2185 | C | C4-C5 | -5.81 | 1.38 | 1.43 |
| 27 | BA | 2874 | C | N1-C6 | -5.80 | 1.33 | 1.37 |
| 27 | BA | 1757 | C | C4-C5 | -5.80 | 1.38 | 1.43 |
| 1 | Aa | 1445 | C | C5-C6 | -5.79 | 1.29 | 1.34 |
| 27 | BA | 1114 | C | C4-C5 | -5.77 | 1.38 | 1.43 |
| 27 | BA | 1050 | C | N1-C6 | -5.74 | 1.33 | 1.37 |
| 1 | Aa | 1458 | C | C5-C6 | -5.72 | 1.29 | 1.34 |
| 27 | BA | 2643 | C | N1-C6 | -5.68 | 1.33 | 1.37 |
| 27 | BA | 2820 | G | C6-N1 | -5.68 | 1.35 | 1.39 |
| 27 | BA | 689 | C | C4-C5 | -5.68 | 1.38 | 1.43 |
| 27 | BA | 2061 | G | N1-C2 | -5.66 | 1.33 | 1.37 |
| 1 | Aa | 1466 | G | C6-N1 | -5.65 | 1.35 | 1.39 |
| 1 | Aa | 1432 | A | N9-C4 | -5.64 | 1.34 | 1.37 |
| 1 | Aa | 706 | G | C6-N1 | -5.63 | 1.35 | 1.39 |
| 1 | Aa | 1471 | U | C4-C5 | -5.61 | 1.38 | 1.43 |
| 27 | BA | 1805 | C | C4-C5 | -5.59 | 1.38 | 1.43 |
| 27 | BA | 946 | G | C6-N1 | -5.59 | 1.35 | 1.39 |
| 27 | BA | 2621 | C | C5-C6 | -5.58 | 1.29 | 1.34 |
| 27 | BA | 1379 | G | C6-N1 | -5.56 | 1.35 | 1.39 |
| 27 | BA | 900 | C | C4-C5 | -5.55 | 1.38 | 1.43 |
| 27 | BA | 954 | C | C4-C5 | -5.54 | 1.38 | 1.43 |
| 27 | BA | 2062 | G | N9-C4 | -5.53 | 1.33 | 1.38 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 893 | C | C4-C5 | -5.52 | 1.38 | 1.43 |
| 37 | BL | 107 | VAL | C-N | -5.52 | 1.21 | 1.34 |
| 27 | BA | 994 | C | C4-C5 | -5.52 | 1.38 | 1.43 |
| 27 | BA | 691 | G | C6-N1 | -5.52 | 1.35 | 1.39 |
| 27 | BA | 2060 | C | N1-C6 | -5.52 | 1.33 | 1.37 |
| 27 | BA | 1784 | C | C4-C5 | -5.51 | 1.38 | 1.43 |
| 27 | BA | 2340 | G | C6-N1 | -5.50 | 1.35 | 1.39 |
| 1 | Aa | 761 | A | N9-C4 | -5.47 | 1.34 | 1.37 |
| 27 | BA | 2111 | G | C6-N1 | -5.47 | 1.35 | 1.39 |
| 27 | BA | 1445 | G | C6-N1 | -5.47 | 1.35 | 1.39 |
| 27 | BA | 2746 | G | N1-C2 | -5.46 | 1.33 | 1.37 |
| 27 | BA | 2012 | A | C6-N6 | -5.45 | 1.29 | 1.33 |
| 27 | BA | 2061 | G | C6-N1 | -5.45 | 1.35 | 1.39 |
| 27 | BA | 241 | G | N1-C2 | -5.44 | 1.33 | 1.37 |
| 27 | BA | 1336 | C | N1-C6 | -5.44 | 1.33 | 1.37 |
| 27 | BA | 941 | C | C5-C6 | -5.44 | 1.29 | 1.34 |
| 27 | BA | 1771 | C | C5-C6 | -5.44 | 1.29 | 1.34 |
| 27 | BA | 1818 | C | C5-C6 | -5.44 | 1.29 | 1.34 |
| 27 | BA | 1806 | C | C4-C5 | -5.43 | 1.38 | 1.43 |
| 27 | BA | 2132 | C | C4-C5 | -5.42 | 1.38 | 1.43 |
| 27 | BA | 46 | C | C5-C6 | -5.42 | 1.30 | 1.34 |
| 1 | Aa | 1466 | G | N1-C2 | -5.41 | 1.33 | 1.37 |
| 27 | BA | 1091 | C | C5-C6 | -5.41 | 1.30 | 1.34 |
| 27 | BA | 807 | G | C6-N1 | -5.39 | 1.35 | 1.39 |
| 27 | BA | 181 | A | N7-C5 | -5.38 | 1.36 | 1.39 |
| 27 | BA | 1805 | C | C5-C6 | -5.38 | 1.30 | 1.34 |
| 27 | BA | 1366 | C | C4-C5 | -5.38 | 1.38 | 1.43 |
| 27 | BA | 1115 | C | C5-C6 | -5.37 | 1.30 | 1.34 |
| 27 | BA | 1938 | A | N7-C5 | -5.35 | 1.36 | 1.39 |
| 27 | BA | 2621 | C | N1-C6 | -5.34 | 1.33 | 1.37 |
| 27 | BA | 484 | C | C4-C5 | -5.34 | 1.38 | 1.43 |
| 27 | BA | 1960 | C | C5-C6 | -5.34 | 1.30 | 1.34 |
| 27 | BA | 784 | C | C4-C5 | -5.33 | 1.38 | 1.43 |
| 27 | BA | 1442 | C | C5-C6 | -5.33 | 1.30 | 1.34 |
| 1 | Aa | 1458 | C | N1-C6 | -5.32 | 1.33 | 1.37 |
| 27 | BA | 2866 | A | N9-C4 | -5.32 | 1.34 | 1.37 |
| 27 | BA | 661 | G | N1-C2 | -5.30 | 1.33 | 1.37 |
| 1 | Aa | 1473 | C | C4-C5 | -5.29 | 1.38 | 1.43 |
| 27 | BA | 1466 | C | C4-C5 | -5.29 | 1.38 | 1.43 |
| 27 | BA | 1775 | G | C6-N1 | -5.28 | 1.35 | 1.39 |
| 27 | BA | 2813 | C | N1-C6 | -5.28 | 1.33 | 1.37 |
| 27 | BA | 711 | C | C4-C5 | -5.28 | 1.38 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 889 | G | C6-N1 | -5.28 | 1.35 | 1.39 |
| 27 | BA | 915 | C | C4-C5 | -5.27 | 1.38 | 1.43 |
| 27 | BA | 954 | C | C5-C6 | -5.25 | 1.30 | 1.34 |
| 27 | BA | 177 | G | C6-N1 | -5.25 | 1.35 | 1.39 |
| 27 | BA | 2788 | C | N1-C6 | -5.25 | 1.33 | 1.37 |
| 27 | BA | 2087 | C | C4-C5 | -5.25 | 1.38 | 1.43 |
| 27 | BA | 466 | C | C5-C6 | -5.24 | 1.30 | 1.34 |
| 27 | BA | 2621 | C | C4-C5 | -5.24 | 1.38 | 1.43 |
| 27 | BA | 897 | G | C6-N1 | -5.24 | 1.35 | 1.39 |
| 27 | BA | 1374 | C | N1-C6 | -5.23 | 1.34 | 1.37 |
| 27 | BA | 1960 | C | C4-C5 | -5.23 | 1.38 | 1.43 |
| 27 | BA | 859 | G | C6-N1 | -5.23 | 1.35 | 1.39 |
| 27 | BA | 1920 | G | C6-N1 | -5.22 | 1.35 | 1.39 |
| 27 | BA | 1404 | G | C6-N1 | -5.22 | 1.35 | 1.39 |
| 27 | BA | 1277 | C | C5-C6 | -5.21 | 1.30 | 1.34 |
| 27 | BA | 2179 | A | C6-N6 | -5.21 | 1.29 | 1.33 |
| 27 | BA | 961 | A | C6-N6 | -5.21 | 1.29 | 1.33 |
| 27 | BA | 2949 | A | C6-N6 | -5.21 | 1.29 | 1.33 |
| 1 | Aa | 1341 | C | N1-C6 | -5.20 | 1.34 | 1.37 |
| 27 | BA | 1918 | C | C5-C6 | -5.20 | 1.30 | 1.34 |
| 27 | BA | 919 | C | C4-C5 | -5.19 | 1.38 | 1.43 |
| 27 | BA | 2107 | C | N1-C6 | -5.19 | 1.34 | 1.37 |
| 27 | BA | 2161 | G | N1-C2 | -5.19 | 1.33 | 1.37 |
| 27 | BA | 348 | A | C6-N6 | -5.18 | 1.29 | 1.33 |
| 27 | BA | 676 | G | C6-N1 | -5.18 | 1.35 | 1.39 |
| 1 | Aa | 1460 | G | C2-N2 | -5.18 | 1.29 | 1.34 |
| 27 | BA | 1916 | C | N3-C4 | -5.17 | 1.30 | 1.33 |
| 27 | BA | 810 | G | C6-N1 | -5.17 | 1.35 | 1.39 |
| 27 | BA | 182 | A | N7-C5 | -5.17 | 1.36 | 1.39 |
| 27 | BA | 1433 | C | C4-C5 | -5.16 | 1.38 | 1.43 |
| 1 | Aa | 850 | A | N7-C5 | -5.16 | 1.36 | 1.39 |
| 27 | BA | 2185 | C | C5-C6 | -5.15 | 1.30 | 1.34 |
| 27 | BA | 796 | A | N9-C4 | -5.15 | 1.34 | 1.37 |
| 27 | BA | 2350 | C | C5-C6 | -5.15 | 1.30 | 1.34 |
| 27 | BA | 1961 | C | C5-C6 | -5.14 | 1.30 | 1.34 |
| 27 | BA | 2831 | C | N1-C6 | -5.14 | 1.34 | 1.37 |
| 27 | BA | 1365 | C | C4-C5 | -5.13 | 1.38 | 1.43 |
| 27 | BA | 711 | C | N1-C6 | -5.13 | 1.34 | 1.37 |
| 27 | BA | 1913 | A | N9-C4 | -5.12 | 1.34 | 1.37 |
| 27 | BA | 1832 | C | C4-C5 | -5.12 | 1.38 | 1.43 |
| 1 | Aa | 1359 | C | N1-C6 | -5.12 | 1.34 | 1.37 |
| 27 | BA | 1520 | G | C8-N7 | -5.11 | 1.27 | 1.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 673 | A | C6-N6 | -5.11 | 1.29 | 1.33 |
| 27 | BA | 672 | C | N3-C4 | -5.10 | 1.30 | 1.33 |
| 27 | BA | 1933 | C | N1-C6 | -5.10 | 1.34 | 1.37 |
| 27 | BA | 676 | G | C8-N7 | -5.09 | 1.27 | 1.30 |
| 27 | BA | 1783 | C | N1-C6 | -5.09 | 1.34 | 1.37 |
| 27 | BA | 926 | G | C6-N1 | -5.09 | 1.35 | 1.39 |
| 27 | BA | 941 | C | C4-C5 | -5.09 | 1.38 | 1.43 |
| 27 | BA | 2683 | C | C4-C5 | -5.09 | 1.38 | 1.43 |
| 27 | BA | 1788 | G | C6-N1 | -5.08 | 1.35 | 1.39 |
| 27 | BA | 681 | C | C5-C6 | -5.08 | 1.30 | 1.34 |
| 27 | BA | 2342 | C | C5-C6 | -5.08 | 1.30 | 1.34 |
| 27 | BA | 798 | C | C4-N4 | -5.08 | 1.29 | 1.33 |
| 27 | BA | 920 | G | C8-N7 | -5.07 | 1.27 | 1.30 |
| 27 | BA | 1784 | C | N3-C4 | -5.07 | 1.30 | 1.33 |
| 27 | BA | 174 | C | N1-C6 | -5.07 | 1.34 | 1.37 |
| 1 | Aa | 763 | G | N9-C4 | -5.07 | 1.33 | 1.38 |
| 27 | BA | 2061 | G | C2-N2 | -5.06 | 1.29 | 1.34 |
| 27 | BA | 1401 | G | N9-C4 | -5.05 | 1.33 | 1.38 |
| 27 | BA | 2062 | G | C2-N2 | -5.05 | 1.29 | 1.34 |
| 27 | BA | 2704 | A | C6-N6 | -5.05 | 1.29 | 1.33 |
| 27 | BA | 2361 | C | C4-C5 | -5.04 | 1.39 | 1.43 |
| 1 | Aa | 763 | G | C6-N1 | -5.04 | 1.36 | 1.39 |
| 27 | BA | 2103 | C | C4-C5 | -5.04 | 1.39 | 1.43 |
| 27 | BA | 2549 | G | N1-C2 | -5.03 | 1.33 | 1.37 |
| 27 | BA | 2149 | C | C5-C6 | -5.03 | 1.30 | 1.34 |
| 27 | BA | 123 | C | C4-C5 | -5.02 | 1.39 | 1.43 |
| 1 | Aa | 280 | G | C6-N1 | -5.02 | 1.36 | 1.39 |
| 27 | BA | 914 | C | N1-C6 | -5.02 | 1.34 | 1.37 |
| 27 | BA | 2073 | A | C5-C6 | -5.02 | 1.36 | 1.41 |
| 27 | BA | 656 | G | C8-N7 | -5.02 | 1.27 | 1.30 |
| 27 | BA | 1041 | C | C4-C5 | -5.02 | 1.39 | 1.43 |
| 27 | BA | 1082 | C | N1-C6 | -5.02 | 1.34 | 1.37 |
| 27 | BA | 466 | C | N1-C6 | -5.01 | 1.34 | 1.37 |
| 27 | BA | 908 | G | C8-N7 | -5.01 | 1.27 | 1.30 |
| 27 | BA | 195 | A | N9-C4 | -5.01 | 1.34 | 1.37 |
| 27 | BA | 1114 | C | C5-C6 | -5.01 | 1.30 | 1.34 |
| 27 | BA | 2061 | G | N7-C5 | -5.01 | 1.36 | 1.39 |
| 27 | BA | 2822 | G | N1-C2 | -5.01 | 1.33 | 1.37 |
| 27 | BA | 2091 | A | C6-N6 | -5.01 | 1.29 | 1.33 |
| 27 | BA | 688 | G | C8-N7 | -5.00 | 1.27 | 1.30 |
| 27 | BA | 666 | A | C6-N6 | -5.00 | 1.29 | 1.33 |
| 27 | BA | 1762 | C | N1-C6 | -5.00 | 1.34 | 1.37 |

All (606) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 28 | BB | 31 | C | N1-C2-O2 | 9.66 | 124.69 | 118.90 |
| 27 | BA | 2136 | C | C2-N1-C1' | 8.97 | 128.67 | 118.80 |
| 27 | BA | 2187 | U | N3-C4-O4 | 8.57 | 125.40 | 119.40 |
| 1 | Aa | 1369 | G | N1-C2-N2 | -8.51 | 108.54 | 116.20 |
| 27 | BA | 1450 | C | C2-N1-C1' | 8.49 | 128.14 | 118.80 |
| 27 | BA | 3029 | C | N3-C2-O2 | -8.48 | 115.96 | 121.90 |
| 27 | BA | 994 | C | C5-C4-N4 | -8.41 | 114.31 | 120.20 |
| 27 | BA | 2312 | C | C2-N1-C1' | 8.38 | 128.02 | 118.80 |
| 27 | BA | 549 | G | O4'-C1'-N9 | 8.32 | 114.86 | 108.20 |
| 27 | BA | 1433 | C | C2-N1-C1' | 8.21 | 127.83 | 118.80 |
| 27 | BA | 1433 | C | N1-C2-O2 | 8.13 | 123.78 | 118.90 |
| 1 | Aa | 1445 | C | C2-N1-C1' | 8.09 | 127.69 | 118.80 |
| 14 | An | 125 | PRO | CA-N-CD | -8.02 | 100.27 | 111.50 |
| 1 | Aa | 1445 | C | N1-C2-O2 | 7.98 | 123.69 | 118.90 |
| 27 | BA | 2140 | C | C5-C4-N4 | -7.92 | 114.66 | 120.20 |
| 27 | BA | 547 | C | N1-C2-O2 | 7.91 | 123.65 | 118.90 |
| 1 | Aa | 1463 | G | N3-C2-N2 | 7.86 | 125.40 | 119.90 |
| 27 | BA | 216 | C | N3-C4-C5 | 7.81 | 125.02 | 121.90 |
| 27 | BA | 527 | G | OP1-P-OP2 | 7.79 | 131.29 | 119.60 |
| 27 | BA | 2062 | G | C2-N3-C4 | -7.77 | 108.01 | 111.90 |
| 28 | BB | 31 | C | N3-C2-O2 | -7.77 | 116.46 | 121.90 |
| 27 | BA | 1916 | C | C2-N1-C1' | 7.76 | 127.33 | 118.80 |
| 27 | BA | 35 | G | C2-N3-C4 | -7.66 | 108.07 | 111.90 |
| 46 | BV | 75 | PRO | CA-N-CD | -7.62 | 100.83 | 111.50 |
| 27 | BA | 2136 | C | C6-N1-C1' | -7.53 | 111.76 | 120.80 |
| 27 | BA | 661 | G | N1-C2-N2 | -7.53 | 109.43 | 116.20 |
| 1 | Aa | 281 | C | C2-N1-C1' | 7.47 | 127.02 | 118.80 |
| 27 | BA | 776 | C | C2-N1-C1' | 7.46 | 127.01 | 118.80 |
| 27 | BA | 2826 | C | C2-N1-C1' | 7.46 | 127.00 | 118.80 |
| 1 | Aa | 1445 | C | C5-C4-N4 | -7.40 | 115.02 | 120.20 |
| 1 | Aa | 888 | A | O5'-P-OP2 | 7.39 | 119.57 | 110.70 |
| 27 | BA | 1958 | C | C2-N1-C1' | 7.39 | 126.93 | 118.80 |
| 1 | Aa | 700 | C | C2-N1-C1' | 7.37 | 126.91 | 118.80 |
| 27 | BA | 1119 | C | C2-N1-C1' | 7.33 | 126.86 | 118.80 |
| 27 | BA | 2007 | C | N1-C2-O2 | 7.31 | 123.29 | 118.90 |
| 27 | BA | 2683 | C | C2-N1-C1' | 7.31 | 126.84 | 118.80 |
| 27 | BA | 1958 | C | N1-C2-O2 | 7.30 | 123.28 | 118.90 |
| 27 | BA | 504 | G | N7-C8-N9 | 7.30 | 116.75 | 113.10 |
| 27 | BA | 1918 | C | C5-C4-N4 | -7.29 | 115.10 | 120.20 |
| 1 | Aa | 340 | C | C5-C4-N4 | -7.28 | 115.10 | 120.20 |
| 27 | BA | 1958 | C | C5-C4-N4 | -7.21 | 115.15 | 120.20 |
| 27 | BA | 1961 | C | N1-C2-O2 | 7.20 | 123.22 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 2699 | G | N3-C4-N9 | -7.17 | 121.70 | 126.00 |
| 27 | BA | 2683 | C | N1-C2-O2 | 7.13 | 123.18 | 118.90 |
| 27 | BA | 2177 | C | N1-C2-O2 | 7.13 | 123.18 | 118.90 |
| 27 | BA | 547 | C | C2-N1-C1' | 7.09 | 126.60 | 118.80 |
| 27 | BA | 1358 | G | N3-C4-N9 | -7.06 | 121.76 | 126.00 |
| 27 | BA | 676 | G | C2-N3-C4 | -7.06 | 108.37 | 111.90 |
| 27 | BA | 776 | C | N1-C2-O2 | 7.05 | 123.13 | 118.90 |
| 27 | BA | 661 | G | C2-N3-C4 | -7.04 | 108.38 | 111.90 |
| 27 | BA | 2826 | C | N1-C2-O2 | 7.02 | 123.11 | 118.90 |
| 27 | BA | 2149 | C | C2-N1-C1' | 7.02 | 126.52 | 118.80 |
| 27 | BA | 2187 | U | C5-C4-O4 | -7.01 | 121.69 | 125.90 |
| 27 | BA | 2061 | G | C2-N3-C4 | -7.00 | 108.40 | 111.90 |
| 27 | BA | 2562 | C | N3-C4-C5 | 6.90 | 124.66 | 121.90 |
| 27 | BA | 2190 | C | N1-C2-O2 | 6.88 | 123.03 | 118.90 |
| 27 | BA | 2877 | G | C2-N3-C4 | -6.87 | 108.47 | 111.90 |
| 27 | BA | 1928 | C | C5-C4-N4 | -6.83 | 115.42 | 120.20 |
| 27 | BA | 2043 | G | O4'-C1'-N9 | 6.83 | 113.66 | 108.20 |
| 27 | BA | 767 | G | C6-C5-N7 | -6.79 | 126.33 | 130.40 |
| 1 | Aa | 1431 | G | C2-N3-C4 | -6.76 | 108.52 | 111.90 |
| 27 | BA | 66 | C | N1-C2-O2 | 6.73 | 122.94 | 118.90 |
| 1 | Aa | 1006 | C | C2'-C3'-O3' | 6.73 | 124.47 | 113.70 |
| 27 | BA | 1271 | C | C2-N1-C1' | 6.72 | 126.19 | 118.80 |
| 1 | Aa | 1445 | C | C6-N1-C1' | -6.71 | 112.75 | 120.80 |
| 27 | BA | 1449 | U | C2-N1-C1' | 6.71 | 125.75 | 117.70 |
| 28 | BB | 31 | C | C2-N1-C1' | 6.68 | 126.15 | 118.80 |
| 27 | BA | 277 | C | C2-N1-C1' | 6.67 | 126.13 | 118.80 |
| 1 | Aa | 1473 | C | C5-C4-N4 | -6.66 | 115.54 | 120.20 |
| 1 | Aa | 1347 | C | N1-C2-O2 | 6.65 | 122.89 | 118.90 |
| 27 | BA | 2177 | C | C2-N1-C1' | 6.61 | 126.07 | 118.80 |
| 1 | Aa | 1369 | G | N3-C2-N2 | 6.59 | 124.52 | 119.90 |
| 27 | BA | 654 | C | N1-C2-O2 | 6.59 | 122.86 | 118.90 |
| 1 | Aa | 1464 | G | C5-C6-O6 | -6.59 | 124.64 | 128.60 |
| 27 | BA | 1450 | C | N1-C2-O2 | 6.58 | 122.85 | 118.90 |
| 27 | BA | 2185 | C | N1-C2-O2 | 6.58 | 122.84 | 118.90 |
| 1 | Aa | 1069 | U | C5-C4-O4 | -6.55 | 121.97 | 125.90 |
| 27 | BA | 807 | G | C2-N3-C4 | -6.54 | 108.63 | 111.90 |
| 27 | BA | 2136 | C | N1-C2-O2 | 6.54 | 122.82 | 118.90 |
| 27 | BA | 2129 | C | C5-C4-N4 | -6.53 | 115.63 | 120.20 |
| 1 | Aa | 1242 | C | C2-N1-C1' | 6.51 | 125.97 | 118.80 |
| 35 | BJ | 49 | LEU | CB-CG-CD2 | 6.51 | 122.07 | 111.00 |
| 27 | BA | 1269 | G | C8-N9-C4 | -6.51 | 103.80 | 106.40 |
| 27 | BA | 76 | U | C5-C4-O4 | -6.50 | 122.00 | 125.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 1237 | C | N1-C2-O2 | 6.49 | 122.80 | 118.90 |
| 27 | BA | 915 | C | N1-C2-O2 | 6.48 | 122.79 | 118.90 |
| 27 | BA | 1777 | G | C2-N3-C4 | -6.48 | 108.66 | 111.90 |
| 27 | BA | 2119 | C | N1-C2-O2 | 6.48 | 122.79 | 118.90 |
| 27 | BA | 1767 | G | P-O3'-C3' | 6.48 | 127.47 | 119.70 |
| 27 | BA | 2136 | C | C5-C4-N4 | -6.47 | 115.67 | 120.20 |
| 27 | BA | 1918 | C | N3-C4-N4 | 6.46 | 122.52 | 118.00 |
| 27 | BA | 2149 | C | N1-C2-O2 | 6.45 | 122.77 | 118.90 |
| 27 | BA | 136 | C | N3-C4-C5 | 6.45 | 124.48 | 121.90 |
| 1 | Aa | 1464 | G | N1-C6-O6 | 6.45 | 123.77 | 119.90 |
| 27 | BA | 508 | G | C2-N3-C4 | -6.44 | 108.68 | 111.90 |
| 1 | Aa | 297 | C | N1-C2-O2 | 6.44 | 122.76 | 118.90 |
| 27 | BA | 767 | G | N3-C4-N9 | 6.40 | 129.84 | 126.00 |
| 27 | BA | 2297 | C | N1-C2-O2 | 6.40 | 122.74 | 118.90 |
| 27 | BA | 2791 | G | C8-N9-C4 | -6.39 | 103.84 | 106.40 |
| 27 | BA | 955 | C | N3-C4-C5 | 6.36 | 124.44 | 121.90 |
| 27 | BA | 689 | C | N1-C2-O2 | 6.35 | 122.71 | 118.90 |
| 27 | BA | 973 | G | C2-N3-C4 | -6.33 | 108.74 | 111.90 |
| 27 | BA | 804 | C | N1-C2-O2 | 6.32 | 122.69 | 118.90 |
| 1 | Aa | 183 | C | N1-C2-O2 | 6.32 | 122.69 | 118.90 |
| 27 | BA | 2007 | C | C2-N1-C1' | 6.29 | 125.72 | 118.80 |
| 27 | BA | 842 | C | C5-C4-N4 | -6.28 | 115.81 | 120.20 |
| 27 | BA | 2695 | C | N1-C2-O2 | 6.28 | 122.67 | 118.90 |
| 27 | BA | 2822 | G | N1-C2-N2 | -6.27 | 110.56 | 116.20 |
| 27 | BA | 994 | C | N3-C4-N4 | 6.27 | 122.39 | 118.00 |
| 27 | BA | 1048 | C | C5-C4-N4 | -6.26 | 115.81 | 120.20 |
| 27 | BA | 76 | U | N3-C4-O4 | 6.26 | 123.78 | 119.40 |
| 27 | BA | 2822 | G | C2-N3-C4 | -6.25 | 108.78 | 111.90 |
| 27 | BA | 1536 | C | C2-N1-C1' | 6.24 | 125.67 | 118.80 |
| 27 | BA | 1433 | C | C6-N1-C1' | -6.24 | 113.32 | 120.80 |
| 1 | Aa | 481 | C | C2-N1-C1' | 6.23 | 125.65 | 118.80 |
| 1 | Aa | 297 | C | C2-N1-C1' | 6.23 | 125.65 | 118.80 |
| 1 | Aa | 1069 | U | N3-C4-O4 | 6.23 | 123.76 | 119.40 |
| 27 | BA | 1903 | U | N3-C4-O4 | 6.22 | 123.76 | 119.40 |
| 27 | BA | 2664 | C | C2-N1-C1' | 6.22 | 125.64 | 118.80 |
| 27 | BA | 1116 | A | N1-C6-N6 | 6.22 | 122.33 | 118.60 |
| 27 | BA | 2367 | C | C6-N1-C2 | -6.22 | 117.81 | 120.30 |
| 27 | BA | 1401 | G | N3-C4-N9 | -6.21 | 122.27 | 126.00 |
| 27 | BA | 1041 | C | C2-N1-C1' | 6.21 | 125.63 | 118.80 |
| 27 | BA | 1266 | C | C5-C4-N4 | -6.21 | 115.86 | 120.20 |
| 27 | BA | 851 | G | C8-N9-C4 | -6.20 | 103.92 | 106.40 |
| 27 | BA | 918 | U | C2-N1-C1' | 6.18 | 125.11 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 954 | C | N3-C4-C5 | 6.17 | 124.37 | 121.90 |
| 27 | BA | 2350 | C | N3-C4-C5 | 6.16 | 124.36 | 121.90 |
| 1 | Aa | 644 | C | N1-C2-O2 | 6.15 | 122.59 | 118.90 |
| 1 | Aa | 520 | G | P-O3'-C3' | 6.15 | 127.08 | 119.70 |
| 1 | Aa | 884 | C | C2-N1-C1' | 6.14 | 125.56 | 118.80 |
| 27 | BA | 2118 | G | C2-N3-C4 | -6.14 | 108.83 | 111.90 |
| 27 | BA | 889 | G | C2-N3-C4 | -6.12 | 108.84 | 111.90 |
| 27 | BA | 2297 | C | N3-C2-O2 | -6.12 | 117.61 | 121.90 |
| 27 | BA | 2819 | C | N1-C2-O2 | 6.11 | 122.57 | 118.90 |
| 1 | Aa | 1242 | C | N1-C2-O2 | 6.11 | 122.56 | 118.90 |
| 27 | BA | 689 | C | C2-N1-C1' | 6.11 | 125.52 | 118.80 |
| 27 | BA | 1365 | C | C2-N1-C1' | 6.10 | 125.51 | 118.80 |
| 27 | BA | 1960 | C | N1-C2-O2 | 6.10 | 122.56 | 118.90 |
| 27 | BA | 1365 | C | N1-C2-O2 | 6.10 | 122.56 | 118.90 |
| 27 | BA | 1958 | C | C6-N1-C1' | -6.10 | 113.48 | 120.80 |
| 27 | BA | 1916 | C | N1-C2-O2 | 6.10 | 122.56 | 118.90 |
| 27 | BA | 2312 | C | N1-C2-O2 | 6.10 | 122.56 | 118.90 |
| 1 | Aa | 281 | C | N1-C2-O2 | 6.10 | 122.56 | 118.90 |
| 1 | Aa | 515 | C | C2-N1-C1' | 6.09 | 125.50 | 118.80 |
| 27 | BA | 806 | G | C8-N9-C4 | -6.09 | 103.97 | 106.40 |
| 27 | BA | 661 | G | N3-C2-N2 | 6.08 | 124.16 | 119.90 |
| 27 | BA | 1450 | C | C6-N1-C1' | -6.08 | 113.50 | 120.80 |
| 27 | BA | 1463 | C | C5-C4-N4 | -6.07 | 115.95 | 120.20 |
| 1 | Aa | 1030 | C | C2-N1-C1' | 6.07 | 125.48 | 118.80 |
| 1 | Aa | 515 | C | N1-C2-O2 | 6.07 | 122.54 | 118.90 |
| 27 | BA | 2107 | C | C2-N1-C1' | 6.06 | 125.46 | 118.80 |
| 27 | BA | 1114 | C | C5-C4-N4 | -6.04 | 115.97 | 120.20 |
| 27 | BA | 876 | G | O4'-C1'-N9 | 6.04 | 113.03 | 108.20 |
| 27 | BA | 953 | C | C5-C4-N4 | -6.04 | 115.97 | 120.20 |
| 27 | BA | 1277 | C | C2-N1-C1' | 6.03 | 125.43 | 118.80 |
| 27 | BA | 2190 | C | C2-N1-C1' | 6.02 | 125.42 | 118.80 |
| 27 | BA | 2826 | C | C6-N1-C1' | -6.02 | 113.58 | 120.80 |
| 27 | BA | 2140 | C | N3-C4-C5 | 6.01 | 124.31 | 121.90 |
| 27 | BA | 2991 | C | C2-N1-C1' | 6.01 | 125.41 | 118.80 |
| 27 | BA | 1237 | C | N3-C2-O2 | -6.01 | 117.70 | 121.90 |
| 27 | BA | 1924 | C | C5-C4-N4 | -5.99 | 116.01 | 120.20 |
| 27 | BA | 1502 | C | C5-C4-N4 | -5.98 | 116.02 | 120.20 |
| 27 | BA | 2854 | C | C5-C4-N4 | -5.97 | 116.02 | 120.20 |
| 27 | BA | 915 | C | C2-N1-C1' | 5.96 | 125.36 | 118.80 |
| 27 | BA | 956 | C | C2-N1-C1' | 5.96 | 125.36 | 118.80 |
| 27 | BA | 1805 | C | C5-C4-N4 | -5.96 | 116.03 | 120.20 |
| 1 | Aa | 1463 | G | C4-C5-N7 | 5.96 | 113.19 | 110.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 2837 | C | N1-C2-O2 | 5.95 | 122.47 | 118.90 |
| 27 | BA | 1284 | C | C2-N1-C1' | 5.94 | 125.33 | 118.80 |
| 27 | BA | 1769 | C | C2-N1-C1' | 5.93 | 125.33 | 118.80 |
| 27 | BA | 2313 | C | C5-C4-N4 | -5.93 | 116.05 | 120.20 |
| 27 | BA | 809 | C | C2-N1-C1' | 5.93 | 125.32 | 118.80 |
| 27 | BA | 309 | C | C2-N1-C1' | 5.93 | 125.32 | 118.80 |
| 27 | BA | 491 | G | C2-N3-C4 | -5.93 | 108.94 | 111.90 |
| 27 | BA | 1916 | C | C6-N1-C2 | -5.93 | 117.93 | 120.30 |
| 28 | BB | 50 | G | N3-C2-N2 | 5.93 | 124.05 | 119.90 |
| 27 | BA | 893 | C | C5-C4-N4 | -5.92 | 116.05 | 120.20 |
| 27 | BA | 277 | C | N1-C2-O2 | 5.92 | 122.45 | 118.90 |
| 27 | BA | 2740 | C | C2-N1-C1' | 5.92 | 125.31 | 118.80 |
| 1 | Aa | 700 | C | C6-N1-C1' | -5.92 | 113.70 | 120.80 |
| 27 | BA | 955 | C | C5-C4-N4 | -5.91 | 116.06 | 120.20 |
| 27 | BA | 189 | C | C2-N1-C1' | 5.91 | 125.30 | 118.80 |
| 27 | BA | 1184 | C | N3-C2-O2 | -5.91 | 117.77 | 121.90 |
| 27 | BA | 1756 | C | C2-N1-C1' | 5.89 | 125.28 | 118.80 |
| 27 | BA | 946 | G | C2-N3-C4 | -5.89 | 108.95 | 111.90 |
| 27 | BA | 1706 | G | N7-C8-N9 | 5.88 | 116.04 | 113.10 |
| 27 | BA | 1933 | C | N3-C4-C5 | 5.88 | 124.25 | 121.90 |
| 27 | BA | 464 | C | C5-C4-N4 | -5.88 | 116.08 | 120.20 |
| 27 | BA | 1496 | C | N1-C2-O2 | 5.88 | 122.43 | 118.90 |
| 27 | BA | 185 | G | C8-N9-C4 | -5.88 | 104.05 | 106.40 |
| 27 | BA | 1370 | G | C2-N3-C4 | -5.88 | 108.96 | 111.90 |
| 27 | BA | 122 | C | C2-N1-C1' | 5.87 | 125.26 | 118.80 |
| 27 | BA | 2185 | C | C5-C4-N4 | -5.87 | 116.09 | 120.20 |
| 27 | BA | 804 | C | C2-N1-C1' | 5.87 | 125.26 | 118.80 |
| 27 | BA | 2185 | C | C2-N1-C1' | 5.87 | 125.26 | 118.80 |
| 27 | BA | 26 | C | C2-N1-C1' | 5.86 | 125.25 | 118.80 |
| 27 | BA | 1655 | C | C2-N1-C1' | 5.85 | 125.24 | 118.80 |
| 27 | BA | 2723 | C | N1-C2-O2 | 5.84 | 122.41 | 118.90 |
| 27 | BA | 2685 | G | C8-N9-C4 | -5.84 | 104.06 | 106.40 |
| 27 | BA | 2603 | C | C5-C4-N4 | -5.84 | 116.11 | 120.20 |
| 27 | BA | 956 | C | C6-N1-C1' | -5.84 | 113.79 | 120.80 |
| 27 | BA | 2477 | C | N1-C2-O2 | 5.82 | 122.39 | 118.90 |
| 27 | BA | 2513 | C | C2-N1-C1' | 5.82 | 125.20 | 118.80 |
| 27 | BA | 2534 | A | C8-N9-C4 | -5.81 | 103.48 | 105.80 |
| 1 | Aa | 1369 | G | C6-C5-N7 | -5.81 | 126.92 | 130.40 |
| 1 | Aa | 1394 | C | C2-N1-C1' | 5.80 | 125.18 | 118.80 |
| 27 | BA | 2125 | G | C2-N3-C4 | -5.80 | 109.00 | 111.90 |
| 27 | BA | 1956 | G | C2-N3-C4 | -5.80 | 109.00 | 111.90 |
| 27 | BA | 50 | G | C4-N9-C1' | 5.80 | 134.04 | 126.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | Aa | 850 | A | N7-C8-N9 | 5.79 | 116.69 | 113.80 |
| 27 | BA | 2312 | C | C6-N1-C1' | -5.78 | 113.86 | 120.80 |
| 27 | BA | 2339 | G | C2-N3-C4 | -5.78 | 109.01 | 111.90 |
| 27 | BA | 1404 | G | C2-N3-C4 | -5.76 | 109.02 | 111.90 |
| 1 | Aa | 1325 | G | N1-C2-N2 | -5.76 | 111.01 | 116.20 |
| 27 | BA | 1435 | G | C2-N3-C4 | -5.76 | 109.02 | 111.90 |
| 27 | BA | 2837 | C | C2-N1-C1' | 5.76 | 125.13 | 118.80 |
| 27 | BA | 1358 | G | N9-C4-C5 | 5.76 | 107.70 | 105.40 |
| 27 | BA | 1278 | C | C2-N1-C1' | 5.75 | 125.13 | 118.80 |
| 1 | Aa | 763 | G | C2-N3-C4 | -5.74 | 109.03 | 111.90 |
| 27 | BA | 2873 | C | C2-N1-C1' | 5.74 | 125.12 | 118.80 |
| 27 | BA | 650 | C | C5-C4-N4 | -5.74 | 116.18 | 120.20 |
| 27 | BA | 1401 | G | N3-C4-C5 | 5.74 | 131.47 | 128.60 |
| 27 | BA | 484 | C | N1-C2-O2 | 5.74 | 122.34 | 118.90 |
| 27 | BA | 1536 | C | N1-C2-O2 | 5.73 | 122.34 | 118.90 |
| 27 | BA | 2177 | C | C6-N1-C1' | -5.72 | 113.93 | 120.80 |
| 27 | BA | 207 | A | C8-N9-C4 | -5.72 | 103.51 | 105.80 |
| 27 | BA | 918 | U | N1-C2-O2 | 5.72 | 126.80 | 122.80 |
| 27 | BA | 520 | G | O4'-C1'-N9 | 5.71 | 112.77 | 108.20 |
| 27 | BA | 922 | G | N7-C8-N9 | 5.71 | 115.96 | 113.10 |
| 27 | BA | 1520 | G | C2-N3-C4 | -5.71 | 109.05 | 111.90 |
| 27 | BA | 515 | G | C2-N3-C4 | -5.71 | 109.05 | 111.90 |
| 28 | BB | 121 | G | C4-N9-C1' | 5.70 | 133.91 | 126.50 |
| 28 | BB | 121 | G | N3-C4-N9 | 5.70 | 129.42 | 126.00 |
| 27 | BA | 1271 | C | C6-N1-C1' | -5.68 | 113.98 | 120.80 |
| 27 | BA | 1323 | G | C2-N3-C4 | -5.68 | 109.06 | 111.90 |
| 27 | BA | 2181 | G | C8-N9-C4 | -5.68 | 104.13 | 106.40 |
| 27 | BA | 906 | G | C8-N9-C4 | -5.68 | 104.13 | 106.40 |
| 1 | Aa | 691 | C | N1-C2-O2 | 5.68 | 122.31 | 118.90 |
| 27 | BA | 1286 | G | N7-C8-N9 | 5.67 | 115.94 | 113.10 |
| 27 | BA | 2445 | C | C2-N1-C1' | 5.67 | 125.04 | 118.80 |
| 27 | BA | 962 | U | C5-C4-O4 | -5.67 | 122.50 | 125.90 |
| 27 | BA | 2507 | G | C8-N9-C1' | 5.67 | 134.37 | 127.00 |
| 27 | BA | 2699 | G | N3-C4-C5 | 5.67 | 131.43 | 128.60 |
| 27 | BA | 1360 | G | N7-C8-N9 | 5.66 | 115.93 | 113.10 |
| 27 | BA | 1100 | G | C2-N3-C4 | -5.66 | 109.07 | 111.90 |
| 28 | BB | 121 | G | C6-C5-N7 | -5.66 | 127.00 | 130.40 |
| 27 | BA | 180 | G | N7-C8-N9 | 5.66 | 115.93 | 113.10 |
| 27 | BA | 2473 | C | N1-C2-O2 | 5.66 | 122.30 | 118.90 |
| 27 | BA | 2163 | G | C2-N3-C4 | -5.65 | 109.07 | 111.90 |
| 27 | BA | 1804 | C | N1-C2-O2 | 5.65 | 122.29 | 118.90 |
| 1 | Aa | 1473 | C | N1-C2-O2 | 5.64 | 122.29 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 741 | C | N3-C4-C5 | 5.64 | 124.16 | 121.90 |
| 27 | BA | 2438 | A | O4'-C1'-N9 | 5.64 | 112.72 | 108.20 |
| 27 | BA | 2342 | C | C2-N1-C1' | 5.64 | 125.00 | 118.80 |
| 27 | BA | 2500 | C | C5-C4-N4 | -5.64 | 116.25 | 120.20 |
| 27 | BA | 591 | C | C5-C4-N4 | -5.64 | 116.25 | 120.20 |
| 27 | BA | 66 | C | C2-N1-C1' | 5.63 | 125.00 | 118.80 |
| 27 | BA | 427 | G | C8-N9-C4 | -5.63 | 104.15 | 106.40 |
| 27 | BA | 893 | C | N1-C2-O2 | 5.63 | 122.28 | 118.90 |
| 27 | BA | 1656 | C | C2-N1-C1' | 5.63 | 125.00 | 118.80 |
| 28 | BB | 60 | C | C2-N1-C1' | 5.63 | 125.00 | 118.80 |
| 27 | BA | 1116 | A | C5-C6-N6 | -5.63 | 119.20 | 123.70 |
| 27 | BA | 2496 | C | C5-C4-N4 | -5.63 | 116.26 | 120.20 |
| 27 | BA | 2879 | A | N7-C8-N9 | 5.63 | 116.61 | 113.80 |
| 1 | Aa | 81 | C | N1-C2-O2 | 5.62 | 122.27 | 118.90 |
| 27 | BA | 1086 | G | C2-N3-C4 | -5.62 | 109.09 | 111.90 |
| 27 | BA | 2119 | C | C2-N1-C1' | 5.62 | 124.98 | 118.80 |
| 27 | BA | 1830 | G | N7-C8-N9 | 5.62 | 115.91 | 113.10 |
| 27 | BA | 1469 | C | C2-N1-C1' | 5.61 | 124.97 | 118.80 |
| 1 | Aa | 316 | C | C2-N1-C1' | 5.61 | 124.97 | 118.80 |
| 27 | BA | 378 | U | P-O3'-C3' | 5.60 | 126.42 | 119.70 |
| 27 | BA | 2135 | C | C5-C4-N4 | -5.60 | 116.28 | 120.20 |
| 1 | Aa | 281 | C | C6-N1-C1' | -5.60 | 114.08 | 120.80 |
| 27 | BA | 504 | G | C5-N7-C8 | -5.60 | 101.50 | 104.30 |
| 27 | BA | 903 | G | N3-C4-N9 | -5.60 | 122.64 | 126.00 |
| 27 | BA | 1809 | C | N1-C2-O2 | 5.60 | 122.26 | 118.90 |
| 27 | BA | 1931 | G | N7-C8-N9 | 5.60 | 115.90 | 113.10 |
| 1 | Aa | 763 | G | C5-C6-O6 | 5.59 | 131.96 | 128.60 |
| 1 | Aa | 1451 | A | O4'-C1'-N9 | 5.59 | 112.67 | 108.20 |
| 1 | Aa | 1463 | G | N1-C2-N2 | -5.59 | 111.17 | 116.20 |
| 27 | BA | 1414 | C | C2-N1-C1' | 5.58 | 124.94 | 118.80 |
| 27 | BA | 177 | G | C8-N9-C4 | -5.58 | 104.17 | 106.40 |
| 27 | BA | 2695 | C | C2-N1-C1' | 5.58 | 124.94 | 118.80 |
| 27 | BA | 128 | U | N3-C4-O4 | 5.57 | 123.30 | 119.40 |
| 27 | BA | 473 | C | N3-C4-C5 | 5.57 | 124.13 | 121.90 |
| 27 | BA | 2417 | C | N3-C4-N4 | 5.57 | 121.90 | 118.00 |
| 27 | BA | 1447 | G | C2-N3-C4 | -5.56 | 109.12 | 111.90 |
| 27 | BA | 2312 | C | C6-N1-C2 | -5.56 | 118.08 | 120.30 |
| 27 | BA | 2363 | C | C2-N1-C1' | 5.56 | 124.92 | 118.80 |
| 27 | BA | 1837 | A | C5-N7-C8 | -5.56 | 101.12 | 103.90 |
| 1 | Aa | 1466 | G | N1-C2-N2 | -5.55 | 111.20 | 116.20 |
| 27 | BA | 915 | C | N3-C4-C5 | 5.55 | 124.12 | 121.90 |
| 27 | BA | 185 | G | N7-C8-N9 | 5.55 | 115.87 | 113.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 2344 | G | C8-N9-C4 | -5.55 | 104.18 | 106.40 |
| 27 | BA | 2007 | C | N3-C2-O2 | -5.54 | 118.02 | 121.90 |
| 1 | Aa | 1295 | C | C2-N1-C1' | 5.54 | 124.90 | 118.80 |
| 1 | Aa | 515 | C | C6-N1-C1' | -5.54 | 114.15 | 120.80 |
| 27 | BA | 451 | C | C2-N1-C1' | 5.54 | 124.90 | 118.80 |
| 27 | BA | 1254 | C | N1-C2-O2 | 5.54 | 122.22 | 118.90 |
| 27 | BA | 2533 | C | C2-N1-C1' | 5.54 | 124.90 | 118.80 |
| 27 | BA | 2820 | G | C2-N3-C4 | -5.54 | 109.13 | 111.90 |
| 27 | BA | 1325 | A | N7-C8-N9 | 5.54 | 116.57 | 113.80 |
| 27 | BA | 1433 | C | C5-C4-N4 | -5.54 | 116.32 | 120.20 |
| 27 | BA | 2290 | C | N3-C2-O2 | -5.54 | 118.02 | 121.90 |
| 27 | BA | 1100 | G | N7-C8-N9 | 5.53 | 115.86 | 113.10 |
| 27 | BA | 2599 | C | N1-C2-O2 | 5.53 | 122.22 | 118.90 |
| 27 | BA | 2290 | C | N1-C2-O2 | 5.53 | 122.22 | 118.90 |
| 27 | BA | 1768 | C | O4'-C1'-N1 | 5.53 | 112.62 | 108.20 |
| 27 | BA | 566 | G | C2-N3-C4 | -5.52 | 109.14 | 111.90 |
| 27 | BA | 1358 | G | C8-N9-C1' | 5.51 | 134.16 | 127.00 |
| 1 | Aa | 1450 | C | N3-C4-C5 | 5.50 | 124.10 | 121.90 |
| 27 | BA | 2599 | C | C2-N1-C1' | 5.50 | 124.85 | 118.80 |
| 27 | BA | 2874 | C | C2-N1-C1' | 5.50 | 124.85 | 118.80 |
| 27 | BA | 1903 | U | C5-C4-O4 | -5.50 | 122.60 | 125.90 |
| 1 | Aa | 1341 | C | N1-C2-O2 | 5.50 | 122.20 | 118.90 |
| 27 | BA | 200 | C | C2-N1-C1' | 5.49 | 124.84 | 118.80 |
| 27 | BA | 2694 | C | C5-C4-N4 | -5.49 | 116.36 | 120.20 |
| 27 | BA | 547 | C | N3-C2-O2 | -5.48 | 118.06 | 121.90 |
| 1 | Aa | 1345 | C | C2-N1-C1' | 5.48 | 124.83 | 118.80 |
| 28 | BB | 34 | G | N3-C4-N9 | 5.47 | 129.28 | 126.00 |
| 27 | BA | 1082 | C | N1-C2-O2 | 5.47 | 122.18 | 118.90 |
| 27 | BA | 2678 | G | N7-C8-N9 | 5.47 | 115.84 | 113.10 |
| 1 | Aa | 520 | G | O4'-C1'-N9 | -5.47 | 103.82 | 108.20 |
| 27 | BA | 2339 | G | N1-C2-N2 | -5.46 | 111.28 | 116.20 |
| 27 | BA | 2342 | C | N1-C2-O2 | 5.46 | 122.18 | 118.90 |
| 27 | BA | 2723 | C | N3-C2-O2 | -5.45 | 118.08 | 121.90 |
| 1 | Aa | 264 | C | N1-C2-O2 | 5.45 | 122.17 | 118.90 |
| 27 | BA | 1875 | C | N1-C2-O2 | 5.44 | 122.17 | 118.90 |
| 1 | Aa | 589 | C | N1-C2-O2 | 5.44 | 122.16 | 118.90 |
| 1 | Aa | 343 | C | C2-N1-C1' | 5.44 | 124.78 | 118.80 |
| 27 | BA | 1119 | C | C6-N1-C1' | -5.44 | 114.28 | 120.80 |
| 27 | BA | 547 | C | C5-C4-N4 | -5.44 | 116.39 | 120.20 |
| 1 | Aa | 763 | G | N3-C4-N9 | -5.43 | 122.74 | 126.00 |
| 27 | BA | 1706 | G | N1-C2-N2 | -5.43 | 111.31 | 116.20 |
| 27 | BA | 1114 | C | C2-N1-C1' | 5.43 | 124.77 | 118.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 1637 | G | C2-N3-C4 | -5.43 | 109.18 | 111.90 |
| 27 | BA | 1469 | C | N1-C2-O2 | 5.43 | 122.16 | 118.90 |
| 27 | BA | 2120 | C | C2-N1-C1' | 5.43 | 124.77 | 118.80 |
| 27 | BA | 1117 | G | C2-N3-C4 | -5.43 | 109.19 | 111.90 |
| 27 | BA | 181 | A | N7-C8-N9 | 5.42 | 116.51 | 113.80 |
| 27 | BA | 1269 | G | N7-C8-N9 | 5.42 | 115.81 | 113.10 |
| 27 | BA | 1534 | U | C2-N1-C1' | 5.42 | 124.20 | 117.70 |
| 27 | BA | 167 | G | C8-N9-C4 | -5.42 | 104.23 | 106.40 |
| 27 | BA | 352 | C | N3-C4-C5 | 5.42 | 124.07 | 121.90 |
| 27 | BA | 2711 | G | C2-N3-C4 | -5.42 | 109.19 | 111.90 |
| 27 | BA | 807 | G | N7-C8-N9 | 5.42 | 115.81 | 113.10 |
| 1 | Aa | 1463 | G | N9-C4-C5 | -5.41 | 103.23 | 105.40 |
| 27 | BA | 439 | G | N1-C2-N2 | -5.41 | 111.33 | 116.20 |
| 27 | BA | 2125 | G | N1-C2-N2 | -5.41 | 111.33 | 116.20 |
| 27 | BA | 719 | C | C2-N1-C1' | 5.41 | 124.75 | 118.80 |
| 27 | BA | 1948 | C | C5-C4-N4 | -5.41 | 116.42 | 120.20 |
| 1 | Aa | 489 | C | C2-N1-C1' | 5.40 | 124.74 | 118.80 |
| 27 | BA | 1927 | G | N3-C4-N9 | -5.40 | 122.76 | 126.00 |
| 27 | BA | 504 | G | C2-N3-C4 | -5.40 | 109.20 | 111.90 |
| 27 | BA | 1504 | C | N1-C2-O2 | 5.40 | 122.14 | 118.90 |
| 27 | BA | 953 | C | N3-C4-C5 | 5.40 | 124.06 | 121.90 |
| 1 | Aa | 94 | C | P-O3'-C3' | 5.39 | 126.17 | 119.70 |
| 1 | Aa | 1457 | G | C8-N9-C4 | -5.39 | 104.24 | 106.40 |
| 27 | BA | 784 | C | C5-C4-N4 | -5.39 | 116.43 | 120.20 |
| 27 | BA | 547 | C | C6-N1-C1' | -5.39 | 114.34 | 120.80 |
| 27 | BA | 933 | G | C8-N9-C4 | -5.38 | 104.25 | 106.40 |
| 27 | BA | 2129 | C | C2-N1-C1' | 5.38 | 124.72 | 118.80 |
| 1 | Aa | 644 | C | N3-C2-O2 | -5.38 | 118.13 | 121.90 |
| 27 | BA | 154 | C | C2-N1-C1' | 5.38 | 124.72 | 118.80 |
| 27 | BA | 2378 | C | N1-C2-O2 | 5.38 | 122.13 | 118.90 |
| 27 | BA | 1102 | G | N3-C4-N9 | -5.38 | 122.77 | 126.00 |
| 27 | BA | 1391 | C | C2-N1-C1' | 5.38 | 124.71 | 118.80 |
| 27 | BA | 309 | C | C6-N1-C1' | -5.37 | 114.35 | 120.80 |
| 27 | BA | 784 | C | N3-C4-C5 | 5.37 | 124.05 | 121.90 |
| 27 | BA | 1806 | C | C2-N1-C1' | 5.37 | 124.71 | 118.80 |
| 27 | BA | 2819 | C | C2-N1-C1' | 5.37 | 124.70 | 118.80 |
| 27 | BA | 1056 | C | N1-C2-O2 | 5.37 | 122.12 | 118.90 |
| 27 | BA | 1145 | C | N1-C2-O2 | 5.37 | 122.12 | 118.90 |
| 1 | Aa | 324 | C | N1-C2-O2 | 5.36 | 122.12 | 118.90 |
| 1 | Aa | 873 | G | N7-C8-N9 | 5.36 | 115.78 | 113.10 |
| 1 | Aa | 1369 | G | C4-N9-C1' | 5.36 | 133.46 | 126.50 |
| 27 | BA | 441 | A | C8-N9-C4 | -5.36 | 103.66 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 1514 | G | C2-N3-C4 | -5.35 | 109.22 | 111.90 |
| 27 | BA | 1053 | U | C5-C4-O4 | -5.35 | 122.69 | 125.90 |
| 27 | BA | 1958 | C | N3-C4-N4 | 5.35 | 121.75 | 118.00 |
| 27 | BA | 1033 | C | C2-N1-C1' | 5.35 | 124.68 | 118.80 |
| 27 | BA | 1113 | C | C5-C4-N4 | -5.34 | 116.46 | 120.20 |
| 27 | BA | 915 | C | C5-C4-N4 | -5.34 | 116.46 | 120.20 |
| 27 | BA | 79 | G | C8-N9-C4 | -5.34 | 104.27 | 106.40 |
| 27 | BA | 1809 | C | C2-N1-C1' | 5.34 | 124.67 | 118.80 |
| 27 | BA | 2683 | C | C6-N1-C1' | -5.34 | 114.40 | 120.80 |
| 27 | BA | 2621 | C | C5-C4-N4 | -5.33 | 116.47 | 120.20 |
| 1 | Aa | 887 | C | P-O3'-C3' | 5.33 | 126.10 | 119.70 |
| 27 | BA | 857 | C | C2-N1-C1' | 5.33 | 124.67 | 118.80 |
| 27 | BA | 245 | G | N1-C2-N2 | -5.33 | 111.40 | 116.20 |
| 1 | Aa | 1347 | C | C2-N1-C1' | 5.33 | 124.66 | 118.80 |
| 27 | BA | 776 | C | N3-C2-O2 | -5.33 | 118.17 | 121.90 |
| 27 | BA | 906 | G | N7-C8-N9 | 5.33 | 115.76 | 113.10 |
| 27 | BA | 380 | G | C2-N3-C4 | -5.32 | 109.24 | 111.90 |
| 27 | BA | 2664 | C | N1-C2-O2 | 5.32 | 122.09 | 118.90 |
| 1 | Aa | 1460 | G | C8-N9-C4 | -5.31 | 104.28 | 106.40 |
| 27 | BA | 1058 | C | N1-C2-O2 | 5.31 | 122.09 | 118.90 |
| 1 | Aa | 850 | A | C5-N7-C8 | -5.30 | 101.25 | 103.90 |
| 27 | BA | 2760 | G | O4'-C1'-N9 | 5.30 | 112.44 | 108.20 |
| 1 | Aa | 1345 | C | N1-C2-O2 | 5.30 | 122.08 | 118.90 |
| 27 | BA | 2694 | C | N3-C4-C5 | 5.30 | 124.02 | 121.90 |
| 27 | BA | 1917 | A | N7-C8-N9 | 5.30 | 116.45 | 113.80 |
| 27 | BA | 2109 | C | C5-C4-N4 | -5.29 | 116.49 | 120.20 |
| 27 | BA | 2822 | G | N7-C8-N9 | 5.29 | 115.75 | 113.10 |
| 27 | BA | 1254 | C | C2-N1-C1' | 5.29 | 124.62 | 118.80 |
| 27 | BA | 1099 | C | C2-N1-C1' | 5.29 | 124.61 | 118.80 |
| 27 | BA | 2668 | A | N7-C8-N9 | 5.29 | 116.44 | 113.80 |
| 27 | BA | 2113 | C | N3-C4-C5 | 5.28 | 124.01 | 121.90 |
| 27 | BA | 199 | C | C2-N1-C1' | 5.28 | 124.61 | 118.80 |
| 27 | BA | 186 | A | C8-N9-C4 | -5.28 | 103.69 | 105.80 |
| 27 | BA | 1041 | C | C5-C4-N4 | -5.28 | 116.50 | 120.20 |
| 27 | BA | 2132 | C | C2-N1-C1' | 5.28 | 124.61 | 118.80 |
| 27 | BA | 1045 | G | C2-N3-C4 | -5.28 | 109.26 | 111.90 |
| 27 | BA | 1325 | A | C8-N9-C4 | -5.28 | 103.69 | 105.80 |
| 1 | Aa | 1056 | C | C2-N1-C1' | 5.27 | 124.60 | 118.80 |
| 27 | BA | 176 | C | C2-N1-C1' | 5.27 | 124.60 | 118.80 |
| 27 | BA | 2685 | G | P-O3'-C3' | 5.27 | 126.03 | 119.70 |
| 27 | BA | 714 | G | C2-N3-C4 | -5.27 | 109.27 | 111.90 |
| 27 | BA | 806 | G | N7-C8-N9 | 5.27 | 115.73 | 113.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 1323 | G | N7-C8-N9 | 5.26 | 115.73 | 113.10 |
| 27 | BA | 186 | A | N7-C8-N9 | 5.26 | 116.43 | 113.80 |
| 27 | BA | 904 | G | C2-N3-C4 | -5.26 | 109.27 | 111.90 |
| 27 | BA | 1485 | C | C5-C4-N4 | -5.26 | 116.52 | 120.20 |
| 27 | BA | 1938 | A | N7-C8-N9 | 5.26 | 116.43 | 113.80 |
| 27 | BA | 2588 | C | C2-N1-C1' | 5.26 | 124.58 | 118.80 |
| 27 | BA | 1612 | C | N1-C2-O2 | 5.26 | 122.05 | 118.90 |
| 27 | BA | 2161 | G | P-O3'-C3' | 5.25 | 126.00 | 119.70 |
| 27 | BA | 2664 | C | C6-N1-C1' | -5.25 | 114.50 | 120.80 |
| 27 | BA | 809 | C | N1-C2-O2 | 5.25 | 122.05 | 118.90 |
| 27 | BA | 1931 | G | C8-N9-C4 | -5.25 | 104.30 | 106.40 |
| 27 | BA | 210 | A | N7-C8-N9 | 5.25 | 116.42 | 113.80 |
| 27 | BA | 654 | C | C2-N1-C1' | 5.25 | 124.57 | 118.80 |
| 27 | BA | 50 | G | C8-N9-C1' | -5.24 | 120.18 | 127.00 |
| 27 | BA | 1371 | G | C2-N3-C4 | -5.24 | 109.28 | 111.90 |
| 27 | BA | 2254 | C | N3-C2-O2 | -5.24 | 118.23 | 121.90 |
| 27 | BA | 1271 | C | N1-C2-O2 | 5.24 | 122.04 | 118.90 |
| 27 | BA | 2148 | C | C2-N1-C1' | 5.24 | 124.56 | 118.80 |
| 1 | Aa | 316 | C | P-O3'-C3' | 5.23 | 125.98 | 119.70 |
| 1 | Aa | 517 | A | N1-C6-N6 | -5.23 | 115.46 | 118.60 |
| 27 | BA | 1102 | G | C2-N3-C4 | -5.23 | 109.28 | 111.90 |
| 27 | BA | 2087 | C | N1-C2-O2 | 5.23 | 122.04 | 118.90 |
| 27 | BA | 2589 | C | N1-C2-O2 | 5.23 | 122.04 | 118.90 |
| 27 | BA | 2501 | C | C5-C4-N4 | -5.23 | 116.54 | 120.20 |
| 27 | BA | 2138 | G | N7-C8-N9 | 5.22 | 115.71 | 113.10 |
| 27 | BA | 2625 | C | C2-N1-C1' | 5.22 | 124.55 | 118.80 |
| 27 | BA | 1401 | G | C2-N3-C4 | -5.22 | 109.29 | 111.90 |
| 27 | BA | 954 | C | C5-C4-N4 | -5.22 | 116.55 | 120.20 |
| 27 | BA | 1277 | C | C6-N1-C1' | -5.22 | 114.54 | 120.80 |
| 27 | BA | 2788 | C | N3-C4-C5 | 5.21 | 123.99 | 121.90 |
| 27 | BA | 425 | C | N3-C4-C5 | 5.21 | 123.98 | 121.90 |
| 27 | BA | 797 | C | C5-C4-N4 | -5.21 | 116.55 | 120.20 |
| 27 | BA | 1114 | C | N1-C2-O2 | 5.21 | 122.03 | 118.90 |
| 27 | BA | 719 | C | N1-C2-O2 | 5.21 | 122.02 | 118.90 |
| 27 | BA | 2440 | G | C4-N9-C1' | 5.21 | 133.27 | 126.50 |
| 27 | BA | 2873 | C | N1-C2-O2 | 5.21 | 122.02 | 118.90 |
| 27 | BA | 2701 | G | N7-C8-N9 | 5.21 | 115.70 | 113.10 |
| 27 | BA | 46 | C | C2-N1-C1' | 5.20 | 124.52 | 118.80 |
| 27 | BA | 425 | C | C5-C4-N4 | -5.20 | 116.56 | 120.20 |
| 27 | BA | 876 | G | C8-N9-C1' | 5.20 | 133.76 | 127.00 |
| 27 | BA | 2161 | G | C8-N9-C4 | -5.20 | 104.32 | 106.40 |
| 27 | BA | 1255 | C | C2-N1-C1' | 5.20 | 124.52 | 118.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 28 | BB | 121 | G | C8-N9-C1' | -5.20 | 120.24 | 127.00 |
| 1 | Aa | 260 | C | C2-N1-C1' | 5.20 | 124.52 | 118.80 |
| 27 | BA | 277 | C | C6-N1-C1' | -5.20 | 114.56 | 120.80 |
| 27 | BA | 856 | C | N1-C2-O2 | 5.19 | 122.02 | 118.90 |
| 27 | BA | 908 | G | C2-N3-C4 | -5.19 | 109.30 | 111.90 |
| 27 | BA | 955 | C | C2-N3-C4 | -5.19 | 117.31 | 119.90 |
| 27 | BA | 1937 | A | N7-C8-N9 | 5.19 | 116.39 | 113.80 |
| 27 | BA | 729 | C | C2-N1-C1' | 5.19 | 124.51 | 118.80 |
| 27 | BA | 1784 | C | N1-C2-O2 | 5.19 | 122.01 | 118.90 |
| 27 | BA | 2686 | G | C4-N9-C1' | 5.19 | 133.24 | 126.50 |
| 1 | Aa | 1325 | G | N3-C2-N2 | 5.18 | 123.53 | 119.90 |
| 27 | BA | 836 | C | C2-N1-C1' | 5.18 | 124.50 | 118.80 |
| 27 | BA | 2431 | A | N7-C8-N9 | 5.18 | 116.39 | 113.80 |
| 1 | Aa | 1347 | C | N3-C2-O2 | -5.18 | 118.27 | 121.90 |
| 27 | BA | 241 | G | C2-N3-C4 | -5.18 | 109.31 | 111.90 |
| 27 | BA | 205 | G | C5-C6-O6 | 5.18 | 131.71 | 128.60 |
| 27 | BA | 1132 | C | C2-N1-C1' | 5.18 | 124.50 | 118.80 |
| 27 | BA | 1268 | G | C8-N9-C4 | -5.18 | 104.33 | 106.40 |
| 27 | BA | 2668 | A | C8-N9-C4 | -5.18 | 103.73 | 105.80 |
| 27 | BA | 1058 | C | C2-N1-C1' | 5.18 | 124.49 | 118.80 |
| 27 | BA | 1916 | C | C6-N1-C1' | -5.18 | 114.59 | 120.80 |
| 1 | Aa | 863 | A | P-O3'-C3' | 5.17 | 125.90 | 119.70 |
| 27 | BA | 1073 | G | C2-N3-C4 | -5.17 | 109.32 | 111.90 |
| 27 | BA | 1082 | C | C2-N1-C1' | 5.17 | 124.48 | 118.80 |
| 27 | BA | 199 | C | N1-C2-O2 | 5.17 | 122.00 | 118.90 |
| 27 | BA | 2678 | G | C8-N9-C4 | -5.17 | 104.33 | 106.40 |
| 27 | BA | 689 | C | C5-C4-N4 | -5.16 | 116.59 | 120.20 |
| 27 | BA | 1767 | G | N7-C8-N9 | 5.16 | 115.68 | 113.10 |
| 27 | BA | 1915 | A | N7-C8-N9 | 5.16 | 116.38 | 113.80 |
| 27 | BA | 228 | C | N1-C2-O2 | 5.16 | 121.99 | 118.90 |
| 27 | BA | 2683 | C | N3-C2-O2 | -5.16 | 118.29 | 121.90 |
| 28 | BB | 31 | C | C6-N1-C2 | -5.16 | 118.24 | 120.30 |
| 27 | BA | 1938 | A | C8-N9-C4 | -5.15 | 103.74 | 105.80 |
| 1 | Aa | 840 | G | C2-N3-C4 | -5.15 | 109.33 | 111.90 |
| 27 | BA | 523 | C | N1-C2-O2 | 5.15 | 121.99 | 118.90 |
| 27 | BA | 1366 | C | C2-N1-C1' | 5.15 | 124.47 | 118.80 |
| 27 | BA | 2699 | G | C2-N3-C4 | -5.15 | 109.33 | 111.90 |
| 27 | BA | 696 | G | C2-N3-C4 | -5.15 | 109.33 | 111.90 |
| 27 | BA | 497 | G | N3-C4-N9 | -5.15 | 122.91 | 126.00 |
| 27 | BA | 1450 | C | C6-N1-C2 | -5.15 | 118.24 | 120.30 |
| 1 | Aa | 1072 | C | C2-N1-C1' | 5.14 | 124.46 | 118.80 |
| 27 | BA | 506 | G | C2-N3-C4 | -5.14 | 109.33 | 111.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 28 | BB | 51 | G | N1-C2-N2 | -5.14 | 111.57 | 116.20 |
| 1 | Aa | 1162 | C | N1-C2-O2 | 5.14 | 121.98 | 118.90 |
| 27 | BA | 940 | C | C2-N1-C1' | 5.14 | 124.45 | 118.80 |
| 27 | BA | 2477 | C | C5-C4-N4 | -5.14 | 116.60 | 120.20 |
| 1 | Aa | 1015 | C | N3-C4-C5 | 5.14 | 123.95 | 121.90 |
| 27 | BA | 41 | C | N3-C4-C5 | 5.14 | 123.95 | 121.90 |
| 1 | Aa | 316 | C | N1-C2-O2 | 5.14 | 121.98 | 118.90 |
| 1 | Aa | 1161 | C | N1-C2-O2 | 5.14 | 121.98 | 118.90 |
| 27 | BA | 654 | C | N3-C2-O2 | -5.14 | 118.31 | 121.90 |
| 27 | BA | 1783 | C | N1-C2-O2 | 5.13 | 121.98 | 118.90 |
| 27 | BA | 1751 | G | C2-N3-C4 | -5.13 | 109.34 | 111.90 |
| 27 | BA | 2344 | G | N7-C8-N9 | 5.13 | 115.67 | 113.10 |
| 27 | BA | 1835 | G | N1-C2-N2 | -5.13 | 111.59 | 116.20 |
| 27 | BA | 962 | U | N3-C4-O4 | 5.12 | 122.99 | 119.40 |
| 1 | Aa | 1372 | C | C2-N1-C1' | 5.12 | 124.44 | 118.80 |
| 27 | BA | 465 | C | N3-C4-C5 | 5.12 | 123.95 | 121.90 |
| 27 | BA | 877 | C | C5-C4-N4 | -5.12 | 116.62 | 120.20 |
| 27 | BA | 2954 | C | N3-C4-C5 | 5.12 | 123.95 | 121.90 |
| 27 | BA | 2468 | C | C2-N1-C1' | 5.12 | 124.43 | 118.80 |
| 27 | BA | 1392 | C | C5-C4-N4 | -5.12 | 116.62 | 120.20 |
| 1 | Aa | 154 | C | C2-N1-C1' | 5.11 | 124.42 | 118.80 |
| 1 | Aa | 1392 | G | C8-N9-C4 | -5.11 | 104.36 | 106.40 |
| 27 | BA | 2995 | C | C2-N1-C1' | 5.11 | 124.42 | 118.80 |
| 27 | BA | 208 | A | N7-C8-N9 | 5.11 | 116.35 | 113.80 |
| 27 | BA | 772 | A | C5-C6-N6 | -5.11 | 119.61 | 123.70 |
| 27 | BA | 2081 | G | C2-N3-C4 | -5.11 | 109.35 | 111.90 |
| 27 | BA | 776 | C | C6-N1-C1' | -5.11 | 114.67 | 120.80 |
| 27 | BA | 53 | C | C2-N1-C1' | 5.10 | 124.41 | 118.80 |
| 1 | Aa | 691 | C | C2-N1-C1' | 5.10 | 124.41 | 118.80 |
| 1 | Aa | 1445 | C | N3-C2-O2 | -5.10 | 118.33 | 121.90 |
| 27 | BA | 123 | C | C5-C4-N4 | -5.10 | 116.63 | 120.20 |
| 27 | BA | 1445 | G | C2-N3-C4 | -5.10 | 109.35 | 111.90 |
| 27 | BA | 1765 | G | C8-N9-C4 | -5.10 | 104.36 | 106.40 |
| 27 | BA | 1916 | C | C5-C6-N1 | 5.10 | 123.55 | 121.00 |
| 27 | BA | 2874 | C | N1-C2-O2 | 5.10 | 121.96 | 118.90 |
| 27 | BA | 830 | G | O4'-C1'-N9 | 5.09 | 112.28 | 108.20 |
| 27 | BA | 1450 | C | C5-C6-N1 | 5.09 | 123.55 | 121.00 |
| 27 | BA | 2138 | G | C8-N9-C4 | -5.09 | 104.36 | 106.40 |
| 1 | Aa | 105 | C | C2-N1-C1' | 5.09 | 124.40 | 118.80 |
| 27 | BA | 125 | G | C2-N3-C4 | -5.09 | 109.35 | 111.90 |
| 27 | BA | 1092 | C | N1-C2-O2 | 5.09 | 121.95 | 118.90 |
| 1 | Aa | 260 | C | N1-C2-O2 | 5.09 | 121.95 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 1352 | C | C5-C4-N4 | -5.09 | 116.64 | 120.20 |
| 27 | BA | 180 | G | C2-N3-C4 | -5.09 | 109.36 | 111.90 |
| 27 | BA | 956 | C | N1-C2-O2 | 5.08 | 121.95 | 118.90 |
| 27 | BA | 2141 | G | C2-N3-C4 | -5.08 | 109.36 | 111.90 |
| 27 | BA | 30 | C | N1-C2-O2 | 5.08 | 121.95 | 118.90 |
| 27 | BA | 1154 | A | C8-N9-C4 | -5.08 | 103.77 | 105.80 |
| 27 | BA | 2763 | C | C2-N1-C1' | 5.08 | 124.39 | 118.80 |
| 27 | BA | 1744 | C | C2-N1-C1' | 5.08 | 124.39 | 118.80 |
| 27 | BA | 2190 | C | C6-N1-C1' | -5.08 | 114.71 | 120.80 |
| 27 | BA | 1960 | C | C2-N1-C1' | 5.08 | 124.38 | 118.80 |
| 27 | BA | 2113 | C | C5-C4-N4 | -5.07 | 116.65 | 120.20 |
| 27 | BA | 2361 | C | C5-C4-N4 | -5.07 | 116.65 | 120.20 |
| 27 | BA | 852 | G | C2-N3-C4 | -5.07 | 109.37 | 111.90 |
| 27 | BA | 2254 | C | C6-N1-C2 | -5.07 | 118.27 | 120.30 |
| 27 | BA | 3029 | C | N1-C2-O2 | 5.07 | 121.94 | 118.90 |
| 27 | BA | 1579 | G | C2-N3-C4 | -5.06 | 109.37 | 111.90 |
| 27 | BA | 1360 | G | C8-N9-C4 | -5.06 | 104.38 | 106.40 |
| 27 | BA | 3029 | C | C6-N1-C2 | -5.06 | 118.28 | 120.30 |
| 28 | BB | 50 | G | N1-C2-N2 | -5.06 | 111.65 | 116.20 |
| 27 | BA | 1037 | C | N3-C4-C5 | 5.05 | 123.92 | 121.90 |
| 27 | BA | 1536 | C | C6-N1-C1' | -5.05 | 114.73 | 120.80 |
| 27 | BA | 61 | A | N7-C8-N9 | 5.05 | 116.32 | 113.80 |
| 27 | BA | 1257 | G | N1-C2-N2 | -5.05 | 111.66 | 116.20 |
| 1 | Aa | 1431 | G | N1-C2-N2 | -5.05 | 111.66 | 116.20 |
| 27 | BA | 1449 | U | C6-N1-C1' | -5.05 | 114.13 | 121.20 |
| 27 | BA | 1789 | G | N3-C2-N2 | -5.05 | 116.37 | 119.90 |
| 27 | BA | 2062 | G | N1-C2-N3 | 5.05 | 126.93 | 123.90 |
| 27 | BA | 2120 | C | C6-N1-C1' | -5.05 | 114.74 | 120.80 |
| 1 | Aa | 1369 | G | N1-C2-N3 | 5.05 | 126.93 | 123.90 |
| 27 | BA | 2312 | C | N3-C4-N4 | 5.05 | 121.53 | 118.00 |
| 1 | Aa | 255 | C | C2-N1-C1' | 5.04 | 124.34 | 118.80 |
| 27 | BA | 1257 | G | C2-N3-C4 | -5.04 | 109.38 | 111.90 |
| 27 | BA | 1504 | C | C2-N1-C1' | 5.04 | 124.35 | 118.80 |
| 27 | BA | 2507 | G | C4-N9-C1' | -5.04 | 119.94 | 126.50 |
| 27 | BA | 1115 | C | C2-N1-C1' | 5.04 | 124.34 | 118.80 |
| 1 | Aa | 1453 | G | N3-C4-N9 | -5.04 | 122.98 | 126.00 |
| 27 | BA | 174 | C | C2-N1-C1' | 5.04 | 124.34 | 118.80 |
| 27 | BA | 245 | G | N3-C2-N2 | 5.03 | 123.42 | 119.90 |
| 1 | Aa | 729 | C | C2-N1-C1' | 5.03 | 124.33 | 118.80 |
| 27 | BA | 681 | C | C5-C4-N4 | -5.02 | 116.69 | 120.20 |
| 27 | BA | 1133 | C | C2-N1-C1' | 5.02 | 124.33 | 118.80 |
| 1 | Aa | 81 | C | N3-C2-O2 | -5.02 | 118.39 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | Aa | 1345 | C | C6-N1-C1' | -5.02 | 114.78 | 120.80 |
| 27 | BA | 2043 | G | N3-C4-N9 | -5.02 | 122.99 | 126.00 |
| 27 | BA | 767 | G | N3-C4-C5 | -5.02 | 126.09 | 128.60 |
| 27 | BA | 2361 | C | N1-C2-O2 | 5.02 | 121.91 | 118.90 |
| 27 | BA | 946 | G | N1-C2-N2 | -5.02 | 111.69 | 116.20 |
| 28 | BB | 121 | G | C4-C5-N7 | 5.02 | 112.81 | 110.80 |
| 1 | Aa | 1410 | C | N1-C2-O2 | 5.02 | 121.91 | 118.90 |
| 27 | BA | 776 | C | C6-N1-C2 | -5.01 | 118.30 | 120.30 |
| 27 | BA | 2139 | G | C8-N9-C4 | -5.01 | 104.40 | 106.40 |
| 27 | BA | 856 | C | C2-N1-C1' | 5.01 | 124.31 | 118.80 |
| 27 | BA | 2078 | C | C5-C4-N4 | -5.01 | 116.69 | 120.20 |
| 27 | BA | 1832 | C | C5-C4-N4 | -5.00 | 116.70 | 120.20 |
| 27 | BA | 2546 | C | N1-C2-O2 | 5.00 | 121.90 | 118.90 |
| 27 | BA | 2696 | G | N7-C8-N9 | 5.00 | 115.60 | 113.10 |
| 1 | Aa | 316 | C | N3-C2-O2 | -5.00 | 118.40 | 121.90 |
| 27 | BA | 2087 | C | C2-N1-C1' | 5.00 | 124.30 | 118.80 |
| 27 | BA | 2150 | U | C5-C6-N1 | 5.00 | 125.20 | 122.70 |
| 27 | BA | 2087 | C | C5-C4-N4 | -5.00 | 116.70 | 120.20 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 14 | An | 126 | HIS | 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 PDB entries followed by that with respect to all EM entries.

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 | Ab | 194/201 (96%) | 181 (93%) | 13 (7%) | 0 | 100 | 100 |
| 3 | Ac | 193/209 (92%) | 181 (94%) | 12 (6%) | 0 | 100 | 100 |
| 4 | Ad | 188/200 (94%) | 172 (92%) | 16 (8%) | 0 | 100 | 100 |
| 5 | Ae | 172/180 (96%) | 162 (94%) | 10 (6%) | 0 | 100 | 100 |
| 6 | Af | 239/243 (98%) | 222 (93%) | 17 (7%) | 0 | 100 | 100 |
| 7 | Ag | 221/235 (94%) | 207 (94%) | 14 (6%) | 0 | 100 | 100 |
| 8 | Ah | 121/125 (97%) | 109 (90%) | 12 (10%) | 0 | 100 | 100 |
| 9 | Ai | 212/215 (99%) | 200 (94%) | 12 (6%) | 0 | 100 | 100 |
| 10 | Aj | 127/130 (98%) | 115 (91%) | 12 (9%) | 0 | 100 | 100 |
| 11 | Ak | 123/130 (95%) | 114 (93%) | 9 (7%) | 0 | 100 | 100 |
| 12 | Al | 131/135 (97%) | 123 (94%) | 8 (6%) | 0 | 100 | 100 |
| 13 | Am | 98/102 (96%) | 90 (92%) | 8 (8%) | 0 | 100 | 100 |
| 14 | An | 125/140 (89%) | 120 (96%) | 5 (4%) | 0 | 100 | 100 |
| 15 | Ao | 141/147 (96%) | 137 (97%) | 4 (3%) | 0 | 100 | 100 |
| 16 | Ap | 133/149 (89%) | 114 (86%) | 19 (14%) | 0 | 100 | 100 |
| 17 | Aq | 147/151 (97%) | 141 (96%) | 6 (4%) | 0 | 100 | 100 |
| 18 | Ar | 52/56 (93%) | 47 (90%) | 5 (10%) | 0 | 100 | 100 |
| 19 | As | 106/114 (93%) | 100 (94%) | 6 (6%) | 0 | 100 | 100 |
| 20 | At | 62/67 (92%) | 60 (97%) | 2 (3%) | 0 | 100 | 100 |
| 21 | Au | 114/133 (86%) | 108 (95%) | 6 (5%) | 0 | 100 | 100 |
| 22 | Av | 147/150 (98%) | 134 (91%) | 13 (9%) | 0 | 100 | 100 |
| 23 | Aw | 93/98 (95%) | 89 (96%) | 4 (4%) | 0 | 100 | 100 |
| 24 | Ax | 59/65 (91%) | 57 (97%) | 2 (3%) | 0 | 100 | 100 |
| 25 | Ay | 62/70 (89%) | 55 (89%) | 7 (11%) | 0 | 100 | 100 |
| 26 | Az | 53/62 (86%) | 47 (89%) | 6 (11%) | 0 | 100 | 100 |
| 29 | BC | 235/239 (98%) | 209 (89%) | 26 (11%) | 0 | 100 | 100 |
| 30 | BD | 342/346 (99%) | 311 (91%) | 31 (9%) | 0 | 100 | 100 |
| 31 | BE | 253/255 (99%) | 232 (92%) | 21 (8%) | 0 | 100 | 100 |
| 32 | BF | 165/183 (90%) | 136 (82%) | 29 (18%) | 0 | 100 | 100 |
| 33 | BG | 181/184 (98%) | 168 (93%) | 13 (7%) | 0 | 100 | 100 |
| 34 | BH | 119/123 (97%) | 111 (93%) | 8 (7%) | 0 | 100 | 100 |
| 34 | BI | 119/123 (97%) | 106 (89%) | 13 (11%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 35 | BJ | 164/182 (90%) | 149 (91%) | 15 (9%) | 0 | 100 | 100 |
| 36 | BK | 140/142 (99%) | 132 (94%) | 8 (6%) | 0 | 100 | 100 |
| 37 | BL | 138/141 (98%) | 128 (93%) | 10 (7%) | 0 | 100 | 100 |
| 38 | BM | 79/83 (95%) | 72 (91%) | 7 (9%) | 0 | 100 | 100 |
| 38 | BN | 79/83 (95%) | 69 (87%) | 10 (13%) | 0 | 100 | 100 |
| 39 | BO | 146/148 (99%) | 129 (88%) | 17 (12%) | 0 | 100 | 100 |
| 40 | BP | 191/194 (98%) | 178 (93%) | 13 (7%) | 0 | 100 | 100 |
| 41 | BQ | 158/201 (79%) | 144 (91%) | 14 (9%) | 0 | 100 | 100 |
| 42 | BR | 118/121 (98%) | 106 (90%) | 12 (10%) | 0 | 100 | 100 |
| 43 | BS | 144/150 (96%) | 128 (89%) | 16 (11%) | 0 | 100 | 100 |
| 44 | BT | 72/77 (94%) | 68 (94%) | 4 (6%) | 0 | 100 | 100 |
| 45 | BU | 94/98 (96%) | 88 (94%) | 6 (6%) | 0 | 100 | 100 |
| 46 | BV | 152/156 (97%) | 143 (94%) | 9 (6%) | 0 | 100 | 100 |
| 47 | BW | 83/86 (96%) | 71 (86%) | 12 (14%) | 0 | 100 | 100 |
| 48 | BX | 118/121 (98%) | 111 (94%) | 7 (6%) | 0 | 100 | 100 |
| 49 | BY | 60/67 (90%) | 59 (98%) | 1 (2%) | 0 | 100 | 100 |
| 50 | BZ | 56/66 (85%) | 54 (96%) | 2 (4%) | 0 | 100 | 100 |
| 51 | Ba | 152/155 (98%) | 142 (93%) | 10 (7%) | 0 | 100 | 100 |
| 52 | Bb | 94/102 (92%) | 86 (92%) | 8 (8%) | 0 | 100 | 100 |
| 53 | Bc | 87/90 (97%) | 84 (97%) | 3 (3%) | 0 | 100 | 100 |
| 54 | Bd | 122/125 (98%) | 113 (93%) | 9 (7%) | 0 | 100 | 100 |
| 55 | Be | 87/90 (97%) | 77 (88%) | 10 (12%) | 0 | 100 | 100 |
| 56 | Bg | 82/86 (95%) | 78 (95%) | 4 (5%) | 0 | 100 | 100 |
| 57 | Bh | 60/63 (95%) | 58 (97%) | 2 (3%) | 0 | 100 | 100 |
| 58 | Bi | 48/51 (94%) | 43 (90%) | 5 (10%) | 0 | 100 | 100 |
| 59 | Bj | 45/51 (88%) | 39 (87%) | 6 (13%) | 0 | 100 | 100 |
| 60 | Bk | 34/37 (92%) | 33 (97%) | 1 (3%) | 0 | 100 | 100 |
| 61 | Bl | 91/94 (97%) | 88 (97%) | 3 (3%) | 0 | 100 | 100 |
| All | All | 7621/8020 (95%) | 7028 (92%) | 593 (8%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 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 PDB entries followed by that with respect to all EM entries.

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 | Ab | 170/175 (97%) | 170 (100%) | 0 | 100 | 100 |
| 3 | Ac | 154/168 (92%) | 154 (100%) | 0 | 100 | 100 |
| 4 | Ad | 162/169 (96%) | 162 (100%) | 0 | 100 | 100 |
| 5 | Ae | 153/156 (98%) | 153 (100%) | 0 | 100 | 100 |
| 6 | Af | 210/212 (99%) | 210 (100%) | 0 | 100 | 100 |
| 7 | Ag | 185/197 (94%) | 185 (100%) | 0 | 100 | 100 |
| 8 | Ah | 104/105 (99%) | 104 (100%) | 0 | 100 | 100 |
| 9 | Ai | 183/184 (100%) | 183 (100%) | 0 | 100 | 100 |
| 10 | Aj | 106/107 (99%) | 106 (100%) | 0 | 100 | 100 |
| 11 | Ak | 101/105 (96%) | 101 (100%) | 0 | 100 | 100 |
| 12 | Al | 110/112 (98%) | 110 (100%) | 0 | 100 | 100 |
| 13 | Am | 89/91 (98%) | 89 (100%) | 0 | 100 | 100 |
| 14 | An | 94/108 (87%) | 94 (100%) | 0 | 100 | 100 |
| 15 | Ao | 117/120 (98%) | 117 (100%) | 0 | 100 | 100 |
| 16 | Ap | 111/123 (90%) | 111 (100%) | 0 | 100 | 100 |
| 17 | Aq | 129/131 (98%) | 128 (99%) | 1 (1%) | 81 | 92 |
| 18 | Ar | 45/46 (98%) | 45 (100%) | 0 | 100 | 100 |
| 19 | As | 96/101 (95%) | 96 (100%) | 0 | 100 | 100 |
| 20 | At | 58/61 (95%) | 58 (100%) | 0 | 100 | 100 |
| 21 | Au | 104/117 (89%) | 103 (99%) | 1 (1%) | 76 | 90 |
| 22 | Av | 125/126 (99%) | 125 (100%) | 0 | 100 | 100 |
| 23 | Aw | 85/88 (97%) | 85 (100%) | 0 | 100 | 100 |
| 24 | Ax | 53/56 (95%) | 53 (100%) | 0 | 100 | 100 |
| 25 | Ay | 53/59 (90%) | 53 (100%) | 0 | 100 | 100 |
| 26 | Az | 49/55 (89%) | 49 (100%) | 0 | 100 | 100 |
| 29 | BC | 185/187 (99%) | 185 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 30 | BD | 288/289 (100%) | 288 (100%) | 0 | 100 | 100 |
| 31 | BE | 212/212 (100%) | 212 (100%) | 0 | 100 | 100 |
| 32 | BF | 130/155 (84%) | 128 (98%) | 2 (2%) | 65 | 85 |
| 33 | BG | 158/159 (99%) | 157 (99%) | 1 (1%) | 86 | 94 |
| 34 | BH | 99/100 (99%) | 98 (99%) | 1 (1%) | 76 | 90 |
| 34 | BI | 99/100 (99%) | 99 (100%) | 0 | 100 | 100 |
| 35 | BJ | 144/153 (94%) | 144 (100%) | 0 | 100 | 100 |
| 36 | BK | 120/120 (100%) | 120 (100%) | 0 | 100 | 100 |
| 37 | BL | 104/105 (99%) | 104 (100%) | 0 | 100 | 100 |
| 38 | BM | 63/65 (97%) | 62 (98%) | 1 (2%) | 62 | 84 |
| 38 | BN | 63/65 (97%) | 62 (98%) | 1 (2%) | 62 | 84 |
| 39 | BO | 116/116 (100%) | 115 (99%) | 1 (1%) | 78 | 91 |
| 40 | BP | 161/162 (99%) | 161 (100%) | 0 | 100 | 100 |
| 41 | BQ | 138/167 (83%) | 138 (100%) | 0 | 100 | 100 |
| 42 | BR | 101/102 (99%) | 100 (99%) | 1 (1%) | 76 | 90 |
| 43 | BS | 120/124 (97%) | 120 (100%) | 0 | 100 | 100 |
| 44 | BT | 69/72 (96%) | 69 (100%) | 0 | 100 | 100 |
| 45 | BU | 84/85 (99%) | 84 (100%) | 0 | 100 | 100 |
| 46 | BV | 129/131 (98%) | 128 (99%) | 1 (1%) | 81 | 92 |
| 47 | BW | 75/76 (99%) | 75 (100%) | 0 | 100 | 100 |
| 48 | BX | 109/109 (100%) | 109 (100%) | 0 | 100 | 100 |
| 49 | BY | 54/58 (93%) | 54 (100%) | 0 | 100 | 100 |
| 50 | BZ | 57/61 (93%) | 56 (98%) | 1 (2%) | 59 | 82 |
| 51 | Ba | 132/133 (99%) | 132 (100%) | 0 | 100 | 100 |
| 52 | Bb | 76/80 (95%) | 76 (100%) | 0 | 100 | 100 |
| 53 | Bc | 75/76 (99%) | 75 (100%) | 0 | 100 | 100 |
| 54 | Bd | 106/107 (99%) | 106 (100%) | 0 | 100 | 100 |
| 55 | Be | 80/80 (100%) | 79 (99%) | 1 (1%) | 69 | 87 |
| 56 | Bg | 62/63 (98%) | 61 (98%) | 1 (2%) | 62 | 84 |
| 57 | Bh | 50/51 (98%) | 50 (100%) | 0 | 100 | 100 |
| 58 | Bi | 45/46 (98%) | 45 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 59 | Bj | 36/38 (95%) | 36 (100%) | 0 | 100 100 |
| 60 | Bk | 34/35 (97%) | 34 (100%) | 0 | 100 100 |
| 61 | Bl | 83/84 (99%) | 82 (99%) | 1 (1%) | 71 88 |
| All | All | 6503/6738 (96%) | 6488 (100%) | 15 (0%) | 93 98 |

All (15) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 17 | Aq | 9 | ARG |
| 21 | Au | 38 | LYS |
| 32 | BF | 152 | ARG |
| 32 | BF | 177 | LYS |
| 33 | BG | 59 | PHE |
| 34 | BH | 27 | ARG |
| 38 | BM | 17 | ARG |
| 38 | BN | 17 | ARG |
| 39 | BO | 9 | ARG |
| 42 | BR | 42 | ARG |
| 46 | BV | 83 | ARG |
| 50 | BZ | 27 | LYS |
| 55 | Be | 63 | ARG |
| 56 | Bg | 3 | ARG |
| 61 | Bl | 80 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | Ab | 104 | GLN |
| 13 | Am | 25 | GLN |
| 18 | Ar | 7 | ASN |
| 19 | As | 29 | HIS |
| 30 | BD | 237 | ASN |
| 30 | BD | 255 | GLN |
| 32 | BF | 161 | HIS |
| 38 | BN | 63 | GLN |
| 39 | BO | 25 | HIS |
| 39 | BO | 45 | GLN |
| 42 | BR | 77 | HIS |
| 43 | BS | 143 | GLN |
| 51 | Ba | 33 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 53 | Bc | 16 | ASN |

### 5.3.3 RNA

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | Aa | 1428/1498 (95%) | 274 (19%) | 0 |
| 27 | BA | 2876/3037 (94%) | 668 (23%) | 46 (1%) |
| 28 | BB | 124/126 (98%) | 26 (20%) | 2 (1%) |
| All | All | 4428/4661 (95%) | 968 (21%) | 48 (1%) |

All (968) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Aa | 4 | C |
| 1 | Aa | 17 | C |
| 1 | Aa | 33 | U |
| 1 | Aa | 45 | U |
| 1 | Aa | 47 | A |
| 1 | Aa | 52 | OMU |
| 1 | Aa | 54 | C |
| 1 | Aa | 55 | G |
| 1 | Aa | 57 | G |
| 1 | Aa | 60 | A |
| 1 | Aa | 66 | C |
| 1 | Aa | 77 | C |
| 1 | Aa | 94 | C |
| 1 | Aa | 95 | A |
| 1 | Aa | 100 | C |
| 1 | Aa | 109 | A |
| 1 | Aa | 111 | C |
| 1 | Aa | 126 | G |
| 1 | Aa | 143 | C |
| 1 | Aa | 169 | G |
| 1 | Aa | 179 | G |
| 1 | Aa | 180 | G |
| 1 | Aa | 188 | G |
| 1 | Aa | 192 | A |
| 1 | Aa | 194 | A |
| 1 | Aa | 195 | G |
| 1 | Aa | 214 | G |
| 1 | Aa | 219 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Aa | 232 | U |
| 1 | Aa | 233 | U |
| 1 | Aa | 235 | G |
| 1 | Aa | 236 | G |
| 1 | Aa | 239 | G |
| 1 | Aa | 254 | G |
| 1 | Aa | 255 | C |
| 1 | Aa | 268 | A |
| 1 | Aa | 270 | A |
| 1 | Aa | 277 | C |
| 1 | Aa | 289 | G |
| 1 | Aa | 294 | A |
| 1 | Aa | 316 | C |
| 1 | Aa | 317 | A |
| 1 | Aa | 333 | C |
| 1 | Aa | 335 | G |
| 1 | Aa | 340 | C |
| 1 | Aa | 341 | A |
| 1 | Aa | 342 | G |
| 1 | Aa | 344 | A |
| 1 | Aa | 350 | G |
| 1 | Aa | 355 | C |
| 1 | Aa | 360 | C |
| 1 | Aa | 372 | C |
| 1 | Aa | 382 | OMG |
| 1 | Aa | 385 | A |
| 1 | Aa | 394 | G |
| 1 | Aa | 415 | U |
| 1 | Aa | 428 | A |
| 1 | Aa | 431 | G |
| 1 | Aa | 440 | A |
| 1 | Aa | 441 | U |
| 1 | Aa | 442 | A |
| 1 | Aa | 443 | A |
| 1 | Aa | 446 | OMG |
| 1 | Aa | 453 | A |
| 1 | Aa | 454 | A |
| 1 | Aa | 456 | G |
| 1 | Aa | 457 | 5MC |
| 1 | Aa | 463 | G |
| 1 | Aa | 464 | 5MC |
| 1 | Aa | 466 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Aa | 469 | G |
| 1 | Aa | 472 | G |
| 1 | Aa | 477 | A |
| 1 | Aa | 478 | A |
| 1 | Aa | 492 | A |
| 1 | Aa | 506 | U |
| 1 | Aa | 508 | A |
| 1 | Aa | 509 | U |
| 1 | Aa | 511 | G |
| 1 | Aa | 517 | A |
| 1 | Aa | 518 | A |
| 1 | Aa | 521 | C |
| 1 | Aa | 522 | G |
| 1 | Aa | 524 | C |
| 1 | Aa | 541 | A |
| 1 | Aa | 547 | U |
| 1 | Aa | 575 | G |
| 1 | Aa | 578 | U |
| 1 | Aa | 579 | G |
| 1 | Aa | 599 | U |
| 1 | Aa | 611 | A |
| 1 | Aa | 621 | U |
| 1 | Aa | 633 | A |
| 1 | Aa | 634 | G |
| 1 | Aa | 661 | A |
| 1 | Aa | 668 | G |
| 1 | Aa | 669 | U |
| 1 | Aa | 677 | G |
| 1 | Aa | 694 | G |
| 1 | Aa | 695 | U |
| 1 | Aa | 701 | G |
| 1 | Aa | 704 | G |
| 1 | Aa | 708 | G |
| 1 | Aa | 719 | G |
| 1 | Aa | 723 | A |
| 1 | Aa | 727 | A |
| 1 | Aa | 738 | A |
| 1 | Aa | 739 | U |
| 1 | Aa | 740 | A |
| 1 | Aa | 748 | A |
| 1 | Aa | 759 | U |
| 1 | Aa | 763 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Aa | 774 | A |
| 1 | Aa | 790 | U |
| 1 | Aa | 793 | A |
| 1 | Aa | 815 | A |
| 1 | Aa | 822 | A |
| 1 | Aa | 840 | G |
| 1 | Aa | 864 | A |
| 1 | Aa | 869 | A |
| 1 | Aa | 872 | G |
| 1 | Aa | 876 | OMG |
| 1 | Aa | 877 | G |
| 1 | Aa | 879 | G |
| 1 | Aa | 884 | C |
| 1 | Aa | 885 | U |
| 1 | Aa | 886 | A |
| 1 | Aa | 888 | A |
| 1 | Aa | 892 | OMG |
| 1 | Aa | 896 | G |
| 1 | Aa | 901 | U |
| 1 | Aa | 906 | U |
| 1 | Aa | 911 | U |
| 1 | Aa | 914 | G |
| 1 | Aa | 917 | 5MU |
| 1 | Aa | 920 | A |
| 1 | Aa | 922 | G |
| 1 | Aa | 925 | G |
| 1 | Aa | 926 | G |
| 1 | Aa | 927 | G |
| 1 | Aa | 928 | A |
| 1 | Aa | 941 | G |
| 1 | Aa | 943 | G |
| 1 | Aa | 959 | C |
| 1 | Aa | 960 | C |
| 1 | Aa | 961 | A |
| 1 | Aa | 962 | G |
| 1 | Aa | 969 | G |
| 1 | Aa | 972 | C |
| 1 | Aa | 975 | G |
| 1 | Aa | 979 | G |
| 1 | Aa | 987 | G |
| 1 | Aa | 989 | G |
| 1 | Aa | 993 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Aa | 1008 | G |
| 1 | Aa | 1009 | U |
| 1 | Aa | 1010 | C |
| 1 | Aa | 1038 | G |
| 1 | Aa | 1039 | U |
| 1 | Aa | 1044 | U |
| 1 | Aa | 1045 | A |
| 1 | Aa | 1046 | A |
| 1 | Aa | 1069 | U |
| 1 | Aa | 1076 | U |
| 1 | Aa | 1077 | C |
| 1 | Aa | 1078 | C |
| 1 | Aa | 1079 | U |
| 1 | Aa | 1084 | G |
| 1 | Aa | 1085 | C |
| 1 | Aa | 1086 | U |
| 1 | Aa | 1088 | G |
| 1 | Aa | 1091 | A |
| 1 | Aa | 1092 | G |
| 1 | Aa | 1098 | A |
| 1 | Aa | 1111 | C |
| 1 | Aa | 1115 | G |
| 1 | Aa | 1116 | G |
| 1 | Aa | 1119 | A |
| 1 | Aa | 1120 | U |
| 1 | Aa | 1123 | G |
| 1 | Aa | 1131 | A |
| 1 | Aa | 1132 | A |
| 1 | Aa | 1133 | G |
| 1 | Aa | 1135 | A |
| 1 | Aa | 1136 | G |
| 1 | Aa | 1146 | G |
| 1 | Aa | 1148 | A |
| 1 | Aa | 1149 | G |
| 1 | Aa | 1152 | C |
| 1 | Aa | 1154 | G |
| 1 | Aa | 1157 | U |
| 1 | Aa | 1158 | G |
| 1 | Aa | 1163 | G |
| 1 | Aa | 1164 | A |
| 1 | Aa | 1168 | C |
| 1 | Aa | 1169 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Aa | 1170 | C |
| 1 | Aa | 1171 | C |
| 1 | Aa | 1172 | G |
| 1 | Aa | 1176 | U |
| 1 | Aa | 1179 | A |
| 1 | Aa | 1180 | C |
| 1 | Aa | 1181 | G |
| 1 | Aa | 1187 | U |
| 1 | Aa | 1190 | A |
| 1 | Aa | 1191 | A |
| 1 | Aa | 1193 | G |
| 1 | Aa | 1200 | A |
| 1 | Aa | 1208 | A |
| 1 | Aa | 1209 | U |
| 1 | Aa | 1212 | G |
| 1 | Aa | 1218 | G |
| 1 | Aa | 1221 | A |
| 1 | Aa | 1222 | G |
| 1 | Aa | 1224 | G |
| 1 | Aa | 1225 | G |
| 1 | Aa | 1230 | G |
| 1 | Aa | 1232 | A |
| 1 | Aa | 1246 | C |
| 1 | Aa | 1250 | C |
| 1 | Aa | 1251 | A |
| 1 | Aa | 1252 | G |
| 1 | Aa | 1258 | A |
| 1 | Aa | 1260 | C |
| 1 | Aa | 1272 | C |
| 1 | Aa | 1275 | OMG |
| 1 | Aa | 1276 | 5MC |
| 1 | Aa | 1279 | G |
| 1 | Aa | 1284 | A |
| 1 | Aa | 1286 | G |
| 1 | Aa | 1288 | U |
| 1 | Aa | 1292 | A |
| 1 | Aa | 1297 | U |
| 1 | Aa | 1298 | A |
| 1 | Aa | 1299 | G |
| 1 | Aa | 1305 | G |
| 1 | Aa | 1312 | A |
| 1 | Aa | 1316 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Aa | 1322 | G |
| 1 | Aa | 1325 | G |
| 1 | Aa | 1328 | U |
| 1 | Aa | 1331 | G |
| 1 | Aa | 1334 | C |
| 1 | Aa | 1337 | G |
| 1 | Aa | 1349 | C |
| 1 | Aa | 1350 | A |
| 1 | Aa | 1352 | 5MC |
| 1 | Aa | 1353 | G |
| 1 | Aa | 1354 | OMC |
| 1 | Aa | 1358 | OMU |
| 1 | Aa | 1359 | C |
| 1 | Aa | 1371 | G |
| 1 | Aa | 1392 | G |
| 1 | Aa | 1398 | C |
| 1 | Aa | 1400 | U |
| 1 | Aa | 1402 | G |
| 1 | Aa | 1403 | G |
| 1 | Aa | 1407 | G |
| 1 | Aa | 1431 | G |
| 1 | Aa | 1433 | G |
| 1 | Aa | 1436 | G |
| 1 | Aa | 1441 | A |
| 1 | Aa | 1442 | A |
| 1 | Aa | 1446 | G |
| 1 | Aa | 1447 | U |
| 1 | Aa | 1451 | A |
| 1 | Aa | 1452 | A |
| 1 | Aa | 1453 | G |
| 1 | Aa | 1455 | U |
| 1 | Aa | 1466 | G |
| 1 | Aa | 1475 | G |
| 1 | Aa | 1477 | U |
| 1 | Aa | 1478 | 5MC |
| 1 | Aa | 1479 | G |
| 27 | BA | 12 | C |
| 27 | BA | 15 | U |
| 27 | BA | 16 | G |
| 27 | BA | 18 | C |
| 27 | BA | 19 | A |
| 27 | BA | 21 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | BA | 34 | OMU |
| 27 | BA | 43 | C |
| 27 | BA | 49 | G |
| 27 | BA | 55 | C |
| 27 | BA | 73 | A |
| 27 | BA | 80 | A |
| 27 | BA | 83 | A |
| 27 | BA | 84 | G |
| 27 | BA | 94 | G |
| 27 | BA | 100 | G |
| 27 | BA | 108 | U |
| 27 | BA | 109 | C |
| 27 | BA | 110 | G |
| 27 | BA | 113 | C |
| 27 | BA | 127 | A |
| 27 | BA | 128 | U |
| 27 | BA | 129 | G |
| 27 | BA | 132 | A |
| 27 | BA | 133 | C |
| 27 | BA | 135 | U |
| 27 | BA | 139 | G |
| 27 | BA | 144 | U |
| 27 | BA | 148 | G |
| 27 | BA | 149 | C |
| 27 | BA | 150 | C |
| 27 | BA | 153 | A |
| 27 | BA | 159 | A |
| 27 | BA | 160 | G |
| 27 | BA | 161 | U |
| 27 | BA | 162 | C |
| 27 | BA | 172 | A |
| 27 | BA | 187 | A |
| 27 | BA | 190 | A |
| 27 | BA | 206 | G |
| 27 | BA | 207 | A |
| 27 | BA | 208 | A |
| 27 | BA | 213 | A |
| 27 | BA | 215 | OMG |
| 27 | BA | 217 | A |
| 27 | BA | 218 | A |
| 27 | BA | 219 | A |
| 27 | BA | 220 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | BA | 221 | G |
| 27 | BA | 224 | A |
| 27 | BA | 239 | G |
| 27 | BA | 241 | G |
| 27 | BA | 247 | A |
| 27 | BA | 251 | G |
| 27 | BA | 257 | G |
| 27 | BA | 269 | C |
| 27 | BA | 281 | A |
| 27 | BA | 283 | G |
| 27 | BA | 285 | U |
| 27 | BA | 294 | G |
| 27 | BA | 295 | U |
| 27 | BA | 301 | U |
| 27 | BA | 302 | G |
| 27 | BA | 303 | U |
| 27 | BA | 304 | A |
| 27 | BA | 310 | C |
| 27 | BA | 311 | G |
| 27 | BA | 312 | C |
| 27 | BA | 314 | G |
| 27 | BA | 315 | A |
| 27 | BA | 316 | G |
| 27 | BA | 317 | G |
| 27 | BA | 318 | A |
| 27 | BA | 323 | U |
| 27 | BA | 324 | G |
| 27 | BA | 328 | G |
| 27 | BA | 340 | U |
| 27 | BA | 341 | C |
| 27 | BA | 350 | C |
| 27 | BA | 353 | OMG |
| 27 | BA | 360 | G |
| 27 | BA | 363 | A |
| 27 | BA | 368 | G |
| 27 | BA | 369 | A |
| 27 | BA | 370 | A |
| 27 | BA | 377 | G |
| 27 | BA | 379 | A |
| 27 | BA | 382 | C |
| 27 | BA | 384 | U |
| 27 | BA | 385 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | BA | 386 | A |
| 27 | BA | 393 | G |
| 27 | BA | 398 | C |
| 27 | BA | 399 | C |
| 27 | BA | 401 | G |
| 27 | BA | 404 | G |
| 27 | BA | 405 | U |
| 27 | BA | 408 | C |
| 27 | BA | 414 | G |
| 27 | BA | 419 | OMG |
| 27 | BA | 429 | U |
| 27 | BA | 430 | A |
| 27 | BA | 432 | C |
| 27 | BA | 440 | A |
| 27 | BA | 444 | U |
| 27 | BA | 445 | G |
| 27 | BA | 451 | C |
| 27 | BA | 460 | C |
| 27 | BA | 461 | C |
| 27 | BA | 472 | A |
| 27 | BA | 475 | U |
| 27 | BA | 476 | C |
| 27 | BA | 480 | A |
| 27 | BA | 482 | A |
| 27 | BA | 488 | A2M |
| 27 | BA | 490 | C |
| 27 | BA | 496 | A |
| 27 | BA | 505 | A2M |
| 27 | BA | 506 | G |
| 27 | BA | 514 | U |
| 27 | BA | 520 | G |
| 27 | BA | 531 | G |
| 27 | BA | 540 | A |
| 27 | BA | 542 | A |
| 27 | BA | 543 | G |
| 27 | BA | 545 | G |
| 27 | BA | 546 | C |
| 27 | BA | 547 | C |
| 27 | BA | 551 | A |
| 27 | BA | 567 | G |
| 27 | BA | 568 | A |
| 27 | BA | 569 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | BA | 570 | G |
| 27 | BA | 581 | A |
| 27 | BA | 584 | G |
| 27 | BA | 602 | G |
| 27 | BA | 609 | C |
| 27 | BA | 610 | G |
| 27 | BA | 612 | G |
| 27 | BA | 613 | C |
| 27 | BA | 615 | A |
| 27 | BA | 616 | C |
| 27 | BA | 622 | A |
| 27 | BA | 623 | G |
| 27 | BA | 629 | G |
| 27 | BA | 634 | G |
| 27 | BA | 635 | G |
| 27 | BA | 636 | U |
| 27 | BA | 654 | C |
| 27 | BA | 658 | C |
| 27 | BA | 662 | G |
| 27 | BA | 666 | A |
| 27 | BA | 677 | A |
| 27 | BA | 683 | C |
| 27 | BA | 688 | G |
| 27 | BA | 694 | A |
| 27 | BA | 701 | G |
| 27 | BA | 707 | C |
| 27 | BA | 708 | A |
| 27 | BA | 715 | A |
| 27 | BA | 716 | A |
| 27 | BA | 717 | G |
| 27 | BA | 733 | C |
| 27 | BA | 734 | A |
| 27 | BA | 735 | G |
| 27 | BA | 736 | G |
| 27 | BA | 740 | G |
| 27 | BA | 747 | G |
| 27 | BA | 753 | G |
| 27 | BA | 754 | OMC |
| 27 | BA | 755 | G |
| 27 | BA | 757 | G |
| 27 | BA | 774 | C |
| 27 | BA | 801 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | BA | 802 | A |
| 27 | BA | 812 | U |
| 27 | BA | 827 | G |
| 27 | BA | 832 | A |
| 27 | BA | 835 | C |
| 27 | BA | 842 | C |
| 27 | BA | 844 | G |
| 27 | BA | 848 | G |
| 27 | BA | 849 | A2M |
| 27 | BA | 852 | G |
| 27 | BA | 856 | C |
| 27 | BA | 860 | C |
| 27 | BA | 867 | U |
| 27 | BA | 870 | U |
| 27 | BA | 875 | 5MU |
| 27 | BA | 891 | G |
| 27 | BA | 892 | A |
| 27 | BA | 893 | C |
| 27 | BA | 896 | C |
| 27 | BA | 903 | G |
| 27 | BA | 904 | G |
| 27 | BA | 910 | A |
| 27 | BA | 912 | OMG |
| 27 | BA | 913 | G |
| 27 | BA | 919 | C |
| 27 | BA | 920 | G |
| 27 | BA | 933 | G |
| 27 | BA | 940 | C |
| 27 | BA | 943 | G |
| 27 | BA | 945 | C |
| 27 | BA | 950 | U |
| 27 | BA | 951 | A |
| 27 | BA | 955 | C |
| 27 | BA | 956 | C |
| 27 | BA | 966 | C |
| 27 | BA | 969 | G |
| 27 | BA | 974 | A |
| 27 | BA | 988 | G |
| 27 | BA | 994 | C |
| 27 | BA | 995 | A |
| 27 | BA | 999 | A |
| 27 | BA | 1001 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | BA | 1003 | G |
| 27 | BA | 1005 | G |
| 27 | BA | 1009 | U |
| 27 | BA | 1010 | A |
| 27 | BA | 1012 | G |
| 27 | BA | 1014 | G |
| 27 | BA | 1016 | C |
| 27 | BA | 1017 | G |
| 27 | BA | 1018 | A |
| 27 | BA | 1019 | A |
| 27 | BA | 1021 | G |
| 27 | BA | 1022 | C |
| 27 | BA | 1023 | C |
| 27 | BA | 1024 | U |
| 27 | BA | 1026 | C |
| 27 | BA | 1027 | G |
| 27 | BA | 1031 | C |
| 27 | BA | 1039 | A |
| 27 | BA | 1041 | C |
| 27 | BA | 1048 | C |
| 27 | BA | 1055 | C |
| 27 | BA | 1056 | C |
| 27 | BA | 1058 | C |
| 27 | BA | 1062 | A |
| 27 | BA | 1063 | G |
| 27 | BA | 1069 | C |
| 27 | BA | 1076 | G |
| 27 | BA | 1077 | G |
| 27 | BA | 1079 | G |
| 27 | BA | 1089 | A |
| 27 | BA | 1090 | G |
| 27 | BA | 1102 | G |
| 27 | BA | 1103 | A |
| 27 | BA | 1111 | A |
| 27 | BA | 1116 | A |
| 27 | BA | 1117 | G |
| 27 | BA | 1118 | A |
| 27 | BA | 1119 | C |
| 27 | BA | 1125 | U |
| 27 | BA | 1129 | G |
| 27 | BA | 1130 | G |
| 27 | BA | 1136 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | BA | 1139 | U |
| 27 | BA | 1140 | G |
| 27 | BA | 1149 | G |
| 27 | BA | 1151 | G |
| 27 | BA | 1156 | U |
| 27 | BA | 1157 | C |
| 27 | BA | 1158 | C |
| 27 | BA | 1159 | A |
| 27 | BA | 1165 | U |
| 27 | BA | 1167 | U |
| 27 | BA | 1175 | C |
| 27 | BA | 1177 | U |
| 27 | BA | 1179 | G |
| 27 | BA | 1180 | A |
| 27 | BA | 1183 | G |
| 27 | BA | 1184 | C |
| 27 | BA | 1185 | G |
| 27 | BA | 1243 | A |
| 27 | BA | 1244 | G |
| 27 | BA | 1247 | C |
| 27 | BA | 1248 | A |
| 27 | BA | 1249 | G |
| 27 | BA | 1250 | G |
| 27 | BA | 1251 | G |
| 27 | BA | 1260 | A |
| 27 | BA | 1264 | G |
| 27 | BA | 1265 | A2M |
| 27 | BA | 1266 | C |
| 27 | BA | 1270 | G |
| 27 | BA | 1307 | A |
| 27 | BA | 1310 | G |
| 27 | BA | 1313 | C |
| 27 | BA | 1318 | A |
| 27 | BA | 1320 | C |
| 27 | BA | 1321 | G |
| 27 | BA | 1322 | G |
| 27 | BA | 1323 | G |
| 27 | BA | 1336 | C |
| 27 | BA | 1347 | G |
| 27 | BA | 1361 | A |
| 27 | BA | 1362 | G |
| 27 | BA | 1371 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | BA | 1372 | A |
| 27 | BA | 1373 | C |
| 27 | BA | 1379 | G |
| 27 | BA | 1385 | G |
| 27 | BA | 1388 | G |
| 27 | BA | 1391 | C |
| 27 | BA | 1409 | A |
| 27 | BA | 1410 | U |
| 27 | BA | 1436 | U |
| 27 | BA | 1437 | A |
| 27 | BA | 1438 | G |
| 27 | BA | 1457 | A |
| 27 | BA | 1461 | U |
| 27 | BA | 1477 | U |
| 27 | BA | 1479 | G |
| 27 | BA | 1480 | OMU |
| 27 | BA | 1485 | C |
| 27 | BA | 1487 | U |
| 27 | BA | 1490 | C |
| 27 | BA | 1517 | A2M |
| 27 | BA | 1521 | A |
| 27 | BA | 1525 | OMG |
| 27 | BA | 1533 | A |
| 27 | BA | 1547 | G |
| 27 | BA | 1548 | 5MU |
| 27 | BA | 1551 | OMU |
| 27 | BA | 1556 | G |
| 27 | BA | 1560 | C |
| 27 | BA | 1563 | C |
| 27 | BA | 1565 | C |
| 27 | BA | 1568 | G |
| 27 | BA | 1571 | C |
| 27 | BA | 1581 | C |
| 27 | BA | 1594 | G |
| 27 | BA | 1606 | A |
| 27 | BA | 1617 | U |
| 27 | BA | 1624 | A |
| 27 | BA | 1626 | A |
| 27 | BA | 1635 | G |
| 27 | BA | 1636 | A |
| 27 | BA | 1637 | G |
| 27 | BA | 1639 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | BA | 1640 | C |
| 27 | BA | 1646 | U |
| 27 | BA | 1647 | G |
| 27 | BA | 1650 | G |
| 27 | BA | 1652 | G |
| 27 | BA | 1657 | G |
| 27 | BA | 1660 | U |
| 27 | BA | 1662 | A |
| 27 | BA | 1664 | A |
| 27 | BA | 1671 | A |
| 27 | BA | 1672 | U |
| 27 | BA | 1673 | G |
| 27 | BA | 1674 | G |
| 27 | BA | 1675 | C |
| 27 | BA | 1681 | G |
| 27 | BA | 1682 | U |
| 27 | BA | 1683 | A |
| 27 | BA | 1685 | G |
| 27 | BA | 1692 | U |
| 27 | BA | 1693 | C |
| 27 | BA | 1699 | A |
| 27 | BA | 1704 | U |
| 27 | BA | 1706 | G |
| 27 | BA | 1715 | A |
| 27 | BA | 1716 | A |
| 27 | BA | 1734 | U |
| 27 | BA | 1742 | G |
| 27 | BA | 1743 | A |
| 27 | BA | 1752 | A |
| 27 | BA | 1754 | A |
| 27 | BA | 1755 | A |
| 27 | BA | 1761 | A |
| 27 | BA | 1762 | C |
| 27 | BA | 1763 | U |
| 27 | BA | 1764 | G |
| 27 | BA | 1767 | G |
| 27 | BA | 1768 | C |
| 27 | BA | 1769 | C |
| 27 | BA | 1771 | C |
| 27 | BA | 1773 | G |
| 27 | BA | 1785 | U |
| 27 | BA | 1792 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | BA | 1793 | G |
| 27 | BA | 1794 | U |
| 27 | BA | 1795 | C |
| 27 | BA | 1799 | OMG |
| 27 | BA | 1800 | G |
| 27 | BA | 1801 | A |
| 27 | BA | 1822 | G |
| 27 | BA | 1824 | A |
| 27 | BA | 1827 | U |
| 27 | BA | 1842 | C |
| 27 | BA | 1848 | A |
| 27 | BA | 1849 | A |
| 27 | BA | 1853 | G |
| 27 | BA | 1855 | G |
| 27 | BA | 1859 | G |
| 27 | BA | 1861 | G |
| 27 | BA | 1884 | G |
| 27 | BA | 1891 | G |
| 27 | BA | 1892 | OMG |
| 27 | BA | 1897 | C |
| 27 | BA | 1901 | A |
| 27 | BA | 1904 | G |
| 27 | BA | 1908 | A |
| 27 | BA | 1909 | G |
| 27 | BA | 1914 | A |
| 27 | BA | 1928 | C |
| 27 | BA | 1929 | U |
| 27 | BA | 1930 | A |
| 27 | BA | 1933 | C |
| 27 | BA | 1945 | G |
| 27 | BA | 1946 | U |
| 27 | BA | 1956 | G |
| 27 | BA | 1957 | A |
| 27 | BA | 1991 | A |
| 27 | BA | 2002 | A |
| 27 | BA | 2014 | A |
| 27 | BA | 2018 | OMC |
| 27 | BA | 2019 | OMG |
| 27 | BA | 2026 | A |
| 27 | BA | 2027 | C |
| 27 | BA | 2029 | A |
| 27 | BA | 2033 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | BA | 2036 | U |
| 27 | BA | 2038 | U |
| 27 | BA | 2042 | G |
| 27 | BA | 2043 | G |
| 27 | BA | 2048 | G |
| 27 | BA | 2049 | A |
| 27 | BA | 2051 | A |
| 27 | BA | 2053 | U |
| 27 | BA | 2054 | C |
| 27 | BA | 2055 | 5MC |
| 27 | BA | 2067 | A |
| 27 | BA | 2068 | U |
| 27 | BA | 2073 | A |
| 27 | BA | 2074 | C |
| 27 | BA | 2076 | U |
| 27 | BA | 2077 | G |
| 27 | BA | 2078 | C |
| 27 | BA | 2080 | U |
| 27 | BA | 2083 | A |
| 27 | BA | 2084 | U |
| 27 | BA | 2085 | G |
| 27 | BA | 2088 | G |
| 27 | BA | 2099 | C |
| 27 | BA | 2104 | U |
| 27 | BA | 2105 | G |
| 27 | BA | 2106 | U |
| 27 | BA | 2119 | C |
| 27 | BA | 2125 | G |
| 27 | BA | 2135 | C |
| 27 | BA | 2139 | G |
| 27 | BA | 2143 | A |
| 27 | BA | 2144 | U |
| 27 | BA | 2145 | A |
| 27 | BA | 2148 | C |
| 27 | BA | 2152 | OMG |
| 27 | BA | 2153 | G |
| 27 | BA | 2155 | C |
| 27 | BA | 2162 | U |
| 27 | BA | 2164 | G |
| 27 | BA | 2167 | A |
| 27 | BA | 2173 | G |
| 27 | BA | 2174 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | BA | 2175 | C |
| 27 | BA | 2181 | G |
| 27 | BA | 2182 | G |
| 27 | BA | 2194 | A |
| 27 | BA | 2214 | C |
| 27 | BA | 2216 | G |
| 27 | BA | 2217 | G |
| 27 | BA | 2218 | G |
| 27 | BA | 2219 | G |
| 27 | BA | 2220 | G |
| 27 | BA | 2221 | U |
| 27 | BA | 2222 | G |
| 27 | BA | 2223 | C |
| 27 | BA | 2224 | G |
| 27 | BA | 2226 | A |
| 27 | BA | 2227 | G |
| 27 | BA | 2228 | C |
| 27 | BA | 2229 | G |
| 27 | BA | 2230 | U |
| 27 | BA | 2238 | A |
| 27 | BA | 2240 | G |
| 27 | BA | 2241 | C |
| 27 | BA | 2243 | U |
| 27 | BA | 2244 | C |
| 27 | BA | 2245 | G |
| 27 | BA | 2247 | A |
| 27 | BA | 2248 | G |
| 27 | BA | 2249 | C |
| 27 | BA | 2250 | C |
| 27 | BA | 2257 | C |
| 27 | BA | 2258 | C |
| 27 | BA | 2260 | G |
| 27 | BA | 2261 | G |
| 27 | BA | 2265 | G |
| 27 | BA | 2269 | G |
| 27 | BA | 2270 | A |
| 27 | BA | 2271 | G |
| 27 | BA | 2275 | C |
| 27 | BA | 2279 | U |
| 27 | BA | 2281 | A |
| 27 | BA | 2282 | G |
| 27 | BA | 2283 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | BA | 2284 | C |
| 27 | BA | 2291 | C |
| 27 | BA | 2292 | A |
| 27 | BA | 2293 | C |
| 27 | BA | 2303 | U |
| 27 | BA | 2318 | G |
| 27 | BA | 2321 | G |
| 27 | BA | 2327 | A |
| 27 | BA | 2328 | C |
| 27 | BA | 2337 | G |
| 27 | BA | 2340 | G |
| 27 | BA | 2353 | OMG |
| 27 | BA | 2358 | G |
| 27 | BA | 2360 | A |
| 27 | BA | 2369 | A |
| 27 | BA | 2379 | OMG |
| 27 | BA | 2382 | G |
| 27 | BA | 2385 | G |
| 27 | BA | 2386 | C |
| 27 | BA | 2389 | OMU |
| 27 | BA | 2390 | A |
| 27 | BA | 2391 | A |
| 27 | BA | 2392 | G |
| 27 | BA | 2403 | G |
| 27 | BA | 2406 | G |
| 27 | BA | 2409 | C |
| 27 | BA | 2423 | A |
| 27 | BA | 2425 | A |
| 27 | BA | 2428 | G |
| 27 | BA | 2443 | G |
| 27 | BA | 2445 | C |
| 27 | BA | 2448 | G |
| 27 | BA | 2453 | G |
| 27 | BA | 2460 | A |
| 27 | BA | 2464 | G |
| 27 | BA | 2465 | A |
| 27 | BA | 2482 | A |
| 27 | BA | 2483 | A |
| 27 | BA | 2489 | G |
| 27 | BA | 2491 | C |
| 27 | BA | 2497 | G |
| 27 | BA | 2498 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | BA | 2510 | U |
| 27 | BA | 2520 | G |
| 27 | BA | 2530 | U |
| 27 | BA | 2531 | G |
| 27 | BA | 2534 | A |
| 27 | BA | 2535 | G |
| 27 | BA | 2536 | A |
| 27 | BA | 2539 | A |
| 27 | BA | 2545 | OMC |
| 27 | BA | 2550 | OMG |
| 27 | BA | 2552 | A |
| 27 | BA | 2563 | G |
| 27 | BA | 2568 | OMG |
| 27 | BA | 2572 | G |
| 27 | BA | 2573 | A |
| 27 | BA | 2578 | C |
| 27 | BA | 2579 | C |
| 27 | BA | 2580 | A |
| 27 | BA | 2581 | 4SU |
| 27 | BA | 2582 | A |
| 27 | BA | 2585 | G |
| 27 | BA | 2589 | C |
| 27 | BA | 2595 | OMC |
| 27 | BA | 2596 | U |
| 27 | BA | 2598 | G |
| 27 | BA | 2606 | G |
| 27 | BA | 2609 | G |
| 27 | BA | 2610 | OMU |
| 27 | BA | 2622 | A |
| 27 | BA | 2632 | U |
| 27 | BA | 2633 | G |
| 27 | BA | 2638 | A |
| 27 | BA | 2642 | G |
| 27 | BA | 2646 | A |
| 27 | BA | 2660 | C |
| 27 | BA | 2669 | A |
| 27 | BA | 2670 | A |
| 27 | BA | 2671 | G |
| 27 | BA | 2676 | A |
| 27 | BA | 2677 | C |
| 27 | BA | 2682 | G |
| 27 | BA | 2685 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | BA | 2686 | G |
| 27 | BA | 2703 | G |
| 27 | BA | 2706 | A |
| 27 | BA | 2707 | G |
| 27 | BA | 2713 | A |
| 27 | BA | 2717 | U |
| 27 | BA | 2718 | A |
| 27 | BA | 2719 | U |
| 27 | BA | 2733 | U |
| 27 | BA | 2734 | G |
| 27 | BA | 2735 | G |
| 27 | BA | 2737 | C |
| 27 | BA | 2738 | G |
| 27 | BA | 2741 | U |
| 27 | BA | 2742 | G |
| 27 | BA | 2748 | A |
| 27 | BA | 2749 | A |
| 27 | BA | 2750 | G |
| 27 | BA | 2752 | C |
| 27 | BA | 2754 | C |
| 27 | BA | 2767 | A |
| 27 | BA | 2768 | G |
| 27 | BA | 2775 | G |
| 27 | BA | 2776 | G |
| 27 | BA | 2777 | A |
| 27 | BA | 2778 | G |
| 27 | BA | 2787 | U |
| 27 | BA | 2794 | U |
| 27 | BA | 2810 | G |
| 27 | BA | 2814 | A |
| 27 | BA | 2815 | U |
| 27 | BA | 2816 | A |
| 27 | BA | 2817 | G |
| 27 | BA | 2822 | G |
| 27 | BA | 2827 | U |
| 27 | BA | 2835 | A |
| 27 | BA | 2836 | G |
| 27 | BA | 2837 | C |
| 27 | BA | 2839 | G |
| 27 | BA | 2850 | A |
| 27 | BA | 2853 | G |
| 27 | BA | 2861 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | BA | 2862 | G |
| 27 | BA | 2867 | A |
| 27 | BA | 2868 | G |
| 27 | BA | 2878 | A |
| 27 | BA | 2879 | A |
| 27 | BA | 2883 | A |
| 27 | BA | 2884 | G |
| 27 | BA | 2937 | G |
| 27 | BA | 2945 | G |
| 27 | BA | 2946 | A |
| 27 | BA | 2952 | A |
| 27 | BA | 2959 | U |
| 27 | BA | 2960 | G |
| 27 | BA | 2961 | A |
| 27 | BA | 2971 | G |
| 27 | BA | 2976 | A |
| 27 | BA | 2982 | G |
| 27 | BA | 2985 | G |
| 27 | BA | 2990 | A |
| 27 | BA | 2995 | C |
| 27 | BA | 3001 | C |
| 27 | BA | 3007 | G |
| 27 | BA | 3008 | C |
| 27 | BA | 3014 | C |
| 27 | BA | 3020 | G |
| 27 | BA | 3024 | G |
| 27 | BA | 3027 | U |
| 27 | BA | 3030 | U |
| 27 | BA | 3031 | A |
| 27 | BA | 3032 | C |
| 27 | BA | 3034 | G |
| 27 | BA | 3036 | G |
| 28 | BB | 4 | A |
| 28 | BB | 5 | C |
| 28 | BB | 12 | C |
| 28 | BB | 25 | C |
| 28 | BB | 26 | C |
| 28 | BB | 32 | C |
| 28 | BB | 34 | G |
| 28 | BB | 35 | U |
| 28 | BB | 36 | C |
| 28 | BB | 39 | G |

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*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 28 | BB | 41 | U |
| 28 | BB | 42 | U |
| 28 | BB | 43 | C |
| 28 | BB | 44 | G |
| 28 | BB | 47 | C |
| 28 | BB | 49 | C |
| 28 | BB | 53 | A |
| 28 | BB | 57 | A |
| 28 | BB | 79 | G |
| 28 | BB | 89 | C |
| 28 | BB | 94 | A |
| 28 | BB | 95 | G |
| 28 | BB | 101 | G |
| 28 | BB | 115 | G |
| 28 | BB | 116 | C |
| 28 | BB | 124 | C |

All (48) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | BA | 108 | U |
| 27 | BA | 128 | U |
| 27 | BA | 134 | C |
| 27 | BA | 147 | U |
| 27 | BA | 187 | A |
| 27 | BA | 268 | A |
| 27 | BA | 378 | U |
| 27 | BA | 392 | C |
| 27 | BA | 404 | G |
| 27 | BA | 471 | U |
| 27 | BA | 687 | A |
| 27 | BA | 912 | OMG |
| 27 | BA | 973 | G |
| 27 | BA | 987 | G |
| 27 | BA | 1002 | G |
| 27 | BA | 1178 | A |
| 27 | BA | 1182 | A |
| 27 | BA | 1360 | G |
| 27 | BA | 1436 | U |
| 27 | BA | 1520 | G |
| 27 | BA | 1636 | A |
| 27 | BA | 1671 | A |

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*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | BA | 1673 | G |
| 27 | BA | 1691 | U |
| 27 | BA | 1741 | C |
| 27 | BA | 1753 | G |
| 27 | BA | 1767 | G |
| 27 | BA | 1799 | OMG |
| 27 | BA | 1928 | C |
| 27 | BA | 2053 | U |
| 27 | BA | 2154 | A |
| 27 | BA | 2161 | G |
| 27 | BA | 2173 | G |
| 27 | BA | 2216 | G |
| 27 | BA | 2239 | G |
| 27 | BA | 2268 | G |
| 27 | BA | 2282 | G |
| 27 | BA | 2482 | A |
| 27 | BA | 2496 | C |
| 27 | BA | 2534 | A |
| 27 | BA | 2545 | OMC |
| 27 | BA | 2571 | OMC |
| 27 | BA | 2685 | G |
| 27 | BA | 2836 | G |
| 27 | BA | 2945 | G |
| 27 | BA | 3026 | G |
| 28 | BB | 3 | U |
| 28 | BB | 56 | U |

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

229 non-standard protein/DNA/RNA residues are modelled in this entry.

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 | $\#\|Z\| > 2$ |
| 27 | OMG | BA | 2010 | 27 | 18,26,27 | 2.13 | 6 (33%) | 19,38,41 | 1.40 | 3 (15%) |
| 27 | 4AC | BA | 3023 | 27 | 21,24,25 | 3.17 | 9 (42%) | 29,34,37 | 1.33 | 7 (24%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 1 | OMU | Aa | 1358 | 1 | 19,22,23 | 2.52 | 7 (36%) | 26,31,34 | 2.31 | 8 (30%) |
| 1 | 4AC | Aa | 525 | 1 | 21,24,25 | 3.00 | 10 (47%) | 29,34,37 | 1.88 | 6 (20%) |
| 1 | B8T | Aa | 1141 | 1 | 19,22,23 | 0.81 | 0 | 26,31,34 | 0.76 | 0 |
| 1 | OMG | Aa | 532 | 1 | 18,26,27 | 2.14 | 7 (38%) | 19,38,41 | 1.37 | 3 (15%) |
| 27 | OMC | BA | 561 | 27 | 19,22,23 | 2.59 | 7 (36%) | 26,31,34 | 0.94 | 1 (3%) |
| 27 | OMG | BA | 63 | 27 | 18,26,27 | 2.13 | 5 (27%) | 19,38,41 | 1.74 | 5 (26%) |
| 27 | 4AC | BA | 2797 | 27 | 21,24,25 | 2.96 | 10 (47%) | 29,34,37 | 1.17 | 3 (10%) |
| 1 | 4AC | Aa | 847 | 1 | 21,24,25 | 3.09 | 10 (47%) | 29,34,37 | 1.19 | 3 (10%) |
| 27 | OMG | BA | 723 | 27 | 18,26,27 | 2.18 | 8 (44%) | 19,38,41 | 1.82 | 4 (21%) |
| 1 | OMU | Aa | 8 | 1 | 19,22,23 | 2.73 | 7 (36%) | 26,31,34 | 1.85 | 8 (30%) |
| 27 | OMG | BA | 2152 | 27 | 18,26,27 | 2.01 | 5 (27%) | 19,38,41 | 1.53 | 4 (21%) |
| 27 | OMG | BA | 2379 | 27 | 18,26,27 | 2.14 | 5 (27%) | 19,38,41 | 1.82 | 4 (21%) |
| 27 | OMC | BA | 2124 | 27 | 19,22,23 | 2.58 | 7 (36%) | 26,31,34 | 1.08 | 3 (11%) |
| 27 | OMG | BA | 2728 | 27 | 18,26,27 | 2.20 | 6 (33%) | 19,38,41 | 1.58 | 4 (21%) |
| 27 | OMU | BA | 619 | 27 | 19,22,23 | 2.81 | 7 (36%) | 26,31,34 | 1.79 | 6 (23%) |
| 27 | OMG | BA | 674 | 27 | 18,26,27 | 1.85 | 6 (33%) | 19,38,41 | 1.69 | 7 (36%) |
| 27 | OMG | BA | 1558 | 27 | 18,26,27 | 2.13 | 7 (38%) | 19,38,41 | 1.54 | 6 (31%) |
| 27 | 4AC | BA | 2997 | 27 | 21,24,25 | 3.17 | 9 (42%) | 29,34,37 | 1.22 | 3 (10%) |
| 27 | A2M | BA | 212 | 27 | 18,25,26 | 0.89 | 1 (5%) | 18,36,39 | 1.44 | 3 (16%) |
| 27 | OMU | BA | 1319 | 27 | 19,22,23 | 2.75 | 7 (36%) | 26,31,34 | 1.70 | 5 (19%) |
| 1 | 4AC | Aa | 730 | 1 | 21,24,25 | 3.06 | 10 (47%) | 29,34,37 | 1.68 | 5 (17%) |
| 1 | 4AC | Aa | 1459 | 1 | 21,24,25 | 2.56 | 7 (33%) | 29,34,37 | 1.66 | 8 (27%) |
| 27 | 4AC | BA | 799 | 27 | 21,24,25 | 2.98 | 10 (47%) | 29,34,37 | 1.33 | 3 (10%) |
| 1 | OMG | Aa | 852 | 1 | 18,26,27 | 2.09 | 5 (27%) | 19,38,41 | 1.32 | 3 (15%) |
| 1 | OMU | Aa | 304 | 1 | 19,22,23 | 2.87 | 7 (36%) | 26,31,34 | 1.71 | 4 (15%) |
| 27 | 4AC | BA | 1427 | 27 | 21,24,25 | 2.99 | 9 (42%) | 29,34,37 | 1.27 | 4 (13%) |
| 27 | 4AC | BA | 244 | 27 | 21,24,25 | 2.99 | 10 (47%) | 29,34,37 | 1.21 | 4 (13%) |
| 27 | OMC | BA | 2545 | 27 | 19,22,23 | 2.58 | 7 (36%) | 26,31,34 | 1.29 | 2 (7%) |
| 27 | 4SU | BA | 2581 | 27 | 18,21,22 | 4.00 | 8 (44%) | 26,30,33 | 2.26 | 5 (19%) |
| 1 | 4AC | Aa | 1007 | 1 | 21,24,25 | 1.07 | 1 (4%) | 29,34,37 | 1.16 | 4 (13%) |
| 27 | OMC | BA | 1790 | 27 | 19,22,23 | 2.51 | 7 (36%) | 26,31,34 | 1.12 | 1 (3%) |
| 27 | 5MU | BA | 1548 | 27 | 19,22,23 | 4.67 | 7 (36%) | 28,32,35 | 3.64 | 10 (35%) |
| 1 | 5MC | Aa | 1352 | 1 | 18,22,23 | 3.42 | 7 (38%) | 26,32,35 | 1.15 | 3 (11%) |
| 27 | 5MC | BA | 2605 | 27 | 18,22,23 | 3.26 | 7 (38%) | 26,32,35 | 0.90 | 1 (3%) |
| 27 | OMG | BA | 1953 | 27 | 18,26,27 | 2.21 | 7 (38%) | 19,38,41 | 1.73 | 4 (21%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 27 | OMC | BA | 1750 | 27 | 19,22,23 | 2.54 | 7 (36%) | 26,31,34 | 1.22 | 5 (19%) |
| 1 | OMU | Aa | 240 | 1 | 19,22,23 | 2.88 | 7 (36%) | 26,31,34 | 1.76 | 4 (15%) |
| 27 | 4AC | BA | 2832 | 27 | 21,24,25 | 3.03 | 10 (47%) | 29,34,37 | 1.29 | 4 (13%) |
| 27 | OMU | BA | 768 | 27 | 19,22,23 | 2.74 | 7 (36%) | 26,31,34 | 1.74 | 4 (15%) |
| 27 | OMG | BA | 2521 | 27 | 18,26,27 | 2.18 | 7 (38%) | 19,38,41 | 1.55 | 3 (15%) |
| 1 | 5MC | Aa | 457 | 1 | 18,22,23 | 4.90 | 15 (83%) | 26,32,35 | 1.12 | 1 (3%) |
| 27 | OMG | BA | 2527 | 27 | 18,26,27 | 2.10 | 6 (33%) | 19,38,41 | 1.38 | 3 (15%) |
| 27 | 4AC | BA | 2121 | 27 | 21,24,25 | 2.90 | 10 (47%) | 29,34,37 | 1.33 | 4 (13%) |
| 1 | 4AC | Aa | 818 | 1 | 21,24,25 | 3.11 | 10 (47%) | 29,34,37 | 1.57 | 5 (17%) |
| 1 | OMG | Aa | 498 | 1 | 18,26,27 | 2.23 | 7 (38%) | 19,38,41 | 1.37 | 3 (15%) |
| 27 | 4AC | BA | 1396 | 27 | 21,24,25 | 3.07 | 10 (47%) | 29,34,37 | 1.45 | 6 (20%) |
| 27 | 4AC | BA | 201 | 27 | 21,24,25 | 2.89 | 10 (47%) | 29,34,37 | 1.65 | 6 (20%) |
| 27 | 5MC | BA | 2863 | 27 | 18,22,23 | 3.13 | 7 (38%) | 26,32,35 | 1.23 | 4 (15%) |
| 27 | 4AC | BA | 925 | 27 | 21,24,25 | 1.06 | 1 (4%) | 29,34,37 | 1.55 | 6 (20%) |
| 27 | OMG | BA | 2745 | 27 | 18,26,27 | 2.16 | 6 (33%) | 19,38,41 | 1.75 | 4 (21%) |
| 27 | A2M | BA | 872 | 27 | 18,25,26 | 4.15 | 9 (50%) | 18,36,39 | 3.01 | 4 (22%) |
| 27 | 4AC | BA | 1431 | 27 | 21,24,25 | 3.15 | 10 (47%) | 29,34,37 | 1.41 | 6 (20%) |
| 27 | OMG | BA | 2528 | 27 | 18,26,27 | 2.31 | 6 (33%) | 19,38,41 | 1.97 | 5 (26%) |
| 27 | 5MU | BA | 875 | 27 | 19,22,23 | 4.58 | 7 (36%) | 28,32,35 | 3.71 | 11 (39%) |
| 27 | OMU | BA | 1340 | 27 | 19,22,23 | 2.65 | 7 (36%) | 26,31,34 | 1.71 | 5 (19%) |
| 1 | 5MC | Aa | 1004 | 1 | 18,22,23 | 3.24 | 7 (38%) | 26,32,35 | 1.14 | 2 (7%) |
| 27 | OMG | BA | 365 | 27 | 18,26,27 | 2.04 | 7 (38%) | 19,38,41 | 1.44 | 3 (15%) |
| 27 | OMC | BA | 718 | 27 | 19,22,23 | 2.65 | 7 (36%) | 26,31,34 | 1.30 | 4 (15%) |
| 27 | 5MU | BA | 1085 | 27 | 19,22,23 | 4.18 | 7 (36%) | 28,32,35 | 4.37 | 11 (39%) |
| 27 | 5MU | BA | 2688 | 27 | 19,22,23 | 4.44 | 7 (36%) | 28,32,35 | 3.70 | 11 (39%) |
| 27 | OMG | BA | 552 | 27 | 18,26,27 | 2.18 | 7 (38%) | 19,38,41 | 1.56 | 5 (26%) |
| 27 | A2M | BA | 756 | 27 | 18,25,26 | 4.21 | 8 (44%) | 18,36,39 | 2.86 | 4 (22%) |
| 27 | OMG | BA | 2168 | 27 | 18,26,27 | 2.19 | 7 (38%) | 19,38,41 | 1.54 | 6 (31%) |
| 1 | OMC | Aa | 535 | 1 | 19,22,23 | 2.71 | 7 (36%) | 26,31,34 | 0.93 | 0 |
| 1 | OMU | Aa | 52 | 1 | 19,22,23 | 2.82 | 7 (36%) | 26,31,34 | 1.62 | 4 (15%) |
| 27 | 4AC | BA | 56 | 27 | 21,24,25 | 3.10 | 9 (42%) | 29,34,37 | 1.35 | 5 (17%) |
| 1 | MA6 | Aa | 1467 | 1 | 18,26,27 | 1.41 | 3 (16%) | 19,38,41 | 3.11 | 2 (10%) |
| 27 | 4AC | BA | 858 | 27 | 21,24,25 | 2.97 | 10 (47%) | 29,34,37 | 1.65 | 2 (6%) |
| 27 | 4AC | BA | 433 | 27 | 21,24,25 | 3.00 | 9 (42%) | 29,34,37 | 1.23 | 3 (10%) |
| 1 | OMG | Aa | 994 | 1 | 18,26,27 | 2.43 | 8 (44%) | 19,38,41 | 1.45 | 4 (21%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 27 | 5MC | BA | 2055 | 27 | 18,22,23 | 3.24 | 7 (38%) | 26,32,35 | 1.11 | 1 (3%) |
| 27 | OMG | BA | 1940 | 27 | 18,26,27 | 2.05 | 6 (33%) | 19,38,41 | 1.26 | 3 (15%) |
| 27 | B8T | BA | 357 | 27 | 19,22,23 | 0.79 | 0 | 26,31,34 | 0.85 | 1 (3%) |
| 27 | A2M | BA | 825 | 27 | 18,25,26 | 4.12 | 9 (50%) | 18,36,39 | 2.85 | 3 (16%) |
| 27 | 4AC | BA | 376 | 27 | 21,24,25 | 3.01 | 9 (42%) | 29,34,37 | 1.32 | 5 (17%) |
| 1 | 2MG | Aa | 670 | 1 | 18,26,27 | 2.27 | 7 (38%) | 16,38,41 | 1.24 | 2 (12%) |
| 27 | OMU | BA | 1480 | 27 | 19,22,23 | 2.72 | 7 (36%) | 26,31,34 | 1.59 | 4 (15%) |
| 1 | 4AC | Aa | 682 | 1 | 21,24,25 | 3.23 | 9 (42%) | 29,34,37 | 1.47 | 5 (17%) |
| 27 | OMG | BA | 575 | 27 | 18,26,27 | 2.15 | 7 (38%) | 19,38,41 | 1.42 | 4 (21%) |
| 27 | 4AC | BA | 778 | 27 | 21,24,25 | 3.14 | 10 (47%) | 29,34,37 | 1.04 | 2 (6%) |
| 27 | OMG | BA | 2019 | 27 | 18,26,27 | 2.41 | 8 (44%) | 19,38,41 | 1.70 | 4 (21%) |
| 1 | 5MC | Aa | 942 | 1 | 18,22,23 | 3.37 | 7 (38%) | 26,32,35 | 1.04 | 2 (7%) |
| 27 | A2M | BA | 1400 | 27 | 18,25,26 | 4.07 | 10 (55%) | 18,36,39 | 2.89 | 4 (22%) |
| 27 | 4AC | BA | 1434 | 27 | 21,24,25 | 2.91 | 10 (47%) | 29,34,37 | 1.70 | 6 (20%) |
| 27 | 4AC | BA | 2159 | 27 | 21,24,25 | 2.98 | 10 (47%) | 29,34,37 | 1.32 | 5 (17%) |
| 27 | OMG | BA | 2568 | 27 | 18,26,27 | 1.01 | 1 (5%) | 19,38,41 | 1.06 | 2 (10%) |
| 27 | 4AC | BA | 418 | 27 | 21,24,25 | 3.20 | 10 (47%) | 29,34,37 | 1.17 | 4 (13%) |
| 27 | OMG | BA | 1799 | 27 | 18,26,27 | 2.33 | 8 (44%) | 19,38,41 | 1.64 | 5 (26%) |
| 1 | 4AC | Aa | 41 | 1 | 21,24,25 | 3.26 | 9 (42%) | 29,34,37 | 1.68 | 5 (17%) |
| 27 | 4AC | BA | 730 | 27 | 21,24,25 | 3.16 | 10 (47%) | 29,34,37 | 1.37 | 5 (17%) |
| 27 | OMC | BA | 2018 | 27 | 19,22,23 | 2.36 | 7 (36%) | 26,31,34 | 1.07 | 3 (11%) |
| 27 | OMG | BA | 1106 | 27 | 18,26,27 | 2.11 | 7 (38%) | 19,38,41 | 1.42 | 3 (15%) |
| 1 | OMG | Aa | 446 | 1 | 18,26,27 | 2.20 | 7 (38%) | 19,38,41 | 1.40 | 4 (21%) |
| 1 | OMG | Aa | 1275 | 1 | 18,26,27 | 1.04 | 1 (5%) | 19,38,41 | 1.08 | 2 (10%) |
| 27 | 4AC | BA | 1955 | 27 | 21,24,25 | 2.89 | 10 (47%) | 29,34,37 | 1.16 | 4 (13%) |
| 1 | LHH | Aa | 1020 | 1 | 22,25,26 | 2.56 | 5 (22%) | 29,35,38 | 1.85 | 8 (27%) |
| 27 | 5MU | BA | 537 | 27 | 19,22,23 | 4.44 | 7 (36%) | 28,32,35 | 3.88 | 10 (35%) |
| 27 | OMG | BA | 800 | 27 | 18,26,27 | 1.97 | 6 (33%) | 19,38,41 | 1.25 | 4 (21%) |
| 27 | 4AC | BA | 1470 | 27 | 21,24,25 | 3.05 | 9 (42%) | 29,34,37 | 1.55 | 6 (20%) |
| 27 | OMG | BA | 2550 | 27 | 18,26,27 | 2.09 | 6 (33%) | 19,38,41 | 2.06 | 6 (31%) |
| 27 | 5MU | BA | 298 | 27 | 19,22,23 | 4.46 | 7 (36%) | 28,32,35 | 3.72 | 10 (35%) |
| 1 | 4AC | Aa | 697 | 1 | 21,24,25 | 3.24 | 9 (42%) | 29,34,37 | 1.64 | 6 (20%) |
| 27 | 4AC | BA | 3009 | 27 | 21,24,25 | 3.09 | 10 (47%) | 29,34,37 | 1.22 | 3 (10%) |
| 27 | OMU | BA | 1969 | 27 | 19,22,23 | 2.75 | 7 (36%) | 26,31,34 | 1.73 | 5 (19%) |
| 27 | OMG | BA | 1525 | 27 | 18,26,27 | 2.23 | 7 (38%) | 19,38,41 | 1.64 | 4 (21%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 1 | 6MZ | Aa | 1449 | 1 | 18,25,26 | 0.77 | 0 | 16,36,39 | 1.94 | 3 (18%) |
| 27 | 4AC | BA | 1337 | 27 | 21,24,25 | 3.01 | 10 (47%) | 29,34,37 | 1.18 | 3 (10%) |
| 27 | A2M | BA | 488 | 27 | 18,25,26 | 4.06 | 8 (44%) | 18,36,39 | 2.96 | 4 (22%) |
| 27 | OMG | BA | 2657 | 27 | 18,26,27 | 2.18 | 7 (38%) | 19,38,41 | 1.49 | 3 (15%) |
| 1 | OMG | Aa | 138 | 1 | 18,26,27 | 2.27 | 7 (38%) | 19,38,41 | 1.40 | 3 (15%) |
| 1 | LHH | Aa | 229 | 1 | 22,25,26 | 2.50 | 5 (22%) | 29,35,38 | 1.70 | 6 (20%) |
| 1 | 5MC | Aa | 672 | 1 | 18,22,23 | 3.12 | 7 (38%) | 26,32,35 | 1.20 | 2 (7%) |
| 1 | 4AC | Aa | 1217 | 1 | 21,24,25 | 3.44 | 9 (42%) | 29,34,37 | 1.59 | 6 (20%) |
| 27 | LHH | BA | 617 | 27 | 22,25,26 | 2.53 | 5 (22%) | 29,35,38 | 1.66 | 6 (20%) |
| 27 | 5MC | BA | 2070 | 27 | 18,22,23 | 0.95 | 2 (11%) | 26,32,35 | 1.20 | 3 (11%) |
| 1 | OMG | Aa | 771 | 1 | 18,26,27 | 2.24 | 7 (38%) | 19,38,41 | 1.37 | 4 (21%) |
| 27 | OMG | BA | 912 | 27 | 18,26,27 | 2.21 | 7 (38%) | 19,38,41 | 2.02 | 4 (21%) |
| 27 | OMU | BA | 2542 | 27 | 19,22,23 | 2.70 | 7 (36%) | 26,31,34 | 1.75 | 5 (19%) |
| 27 | A2M | BA | 932 | 27 | 18,25,26 | 4.18 | 8 (44%) | 18,36,39 | 2.67 | 4 (22%) |
| 1 | 4AC | Aa | 136 | 1 | 21,24,25 | 3.33 | 9 (42%) | 29,34,37 | 1.72 | 5 (17%) |
| 27 | 4AC | BA | 1810 | 27 | 21,24,25 | 3.05 | 10 (47%) | 29,34,37 | 1.44 | 5 (17%) |
| 1 | OMG | Aa | 659 | 1 | 18,26,27 | 2.19 | 8 (44%) | 19,38,41 | 1.35 | 4 (21%) |
| 27 | A2M | BA | 505 | 27 | 18,25,26 | 4.08 | 8 (44%) | 18,36,39 | 3.44 | 6 (33%) |
| 1 | 5MC | Aa | 1476 | 1 | 18,22,23 | 4.81 | 15 (83%) | 26,32,35 | 1.20 | 2 (7%) |
| 27 | OMU | BA | 1551 | 27 | 19,22,23 | 2.93 | 7 (36%) | 26,31,34 | 1.77 | 5 (19%) |
| 27 | OMC | BA | 2571 | 27 | 19,22,23 | 2.66 | 7 (36%) | 26,31,34 | 1.28 | 4 (15%) |
| 27 | 4AC | BA | 805 | 27 | 21,24,25 | 2.86 | 10 (47%) | 29,34,37 | 1.40 | 7 (24%) |
| 1 | 4AC | Aa | 5 | 1 | 21,24,25 | 3.13 | 10 (47%) | 29,34,37 | 1.64 | 5 (17%) |
| 27 | OMU | BA | 34 | 27 | 19,22,23 | 2.62 | 7 (36%) | 26,31,34 | 1.63 | 4 (15%) |
| 27 | A2M | BA | 1265 | 27 | 18,25,26 | 4.19 | 6 (33%) | 18,36,39 | 3.27 | 4 (22%) |
| 27 | A2M | BA | 2702 | 27 | 18,25,26 | 4.02 | 9 (50%) | 18,36,39 | 2.59 | 4 (22%) |
| 1 | OMC | Aa | 1361 | 1,27 | 19,22,23 | 2.56 | 7 (36%) | 26,31,34 | 0.82 | 0 |
| 1 | B8T | Aa | 1262 | 1 | 19,22,23 | 0.78 | 0 | 26,31,34 | 0.93 | 1 (3%) |
| 1 | OMC | Aa | 825 | 1 | 19,22,23 | 2.62 | 7 (36%) | 26,31,34 | 0.86 | 0 |
| 1 | OMC | Aa | 752 | 1 | 19,22,23 | 2.69 | 7 (36%) | 26,31,34 | 0.98 | 1 (3%) |
| 27 | A2M | BA | 879 | 27 | 18,25,26 | 4.12 | 7 (38%) | 18,36,39 | 2.95 | 4 (22%) |
| 27 | OMG | BA | 1398 | 27 | 18,26,27 | 2.09 | 5 (27%) | 19,38,41 | 1.37 | 3 (15%) |
| 27 | OMG | BA | 2353 | 27 | 18,26,27 | 2.06 | 6 (33%) | 19,38,41 | 1.46 | 4 (21%) |
| 1 | OMG | Aa | 1026 | 1 | 18,26,27 | 2.25 | 7 (38%) | 19,38,41 | 1.35 | 4 (21%) |
| 27 | 4AC | BA | 2780 | 27 | 21,24,25 | 3.13 | 9 (42%) | 29,34,37 | 1.67 | 7 (24%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 27 | 5MC | BA | 2035 | 27 | 18,22,23 | 4.78 | 15 (83%) | 26,32,35 | 1.19 | 2 (7%) |
| 27 | 5MU | BA | 572 | 27 | 19,22,23 | 4.45 | 7 (36%) | 28,32,35 | 3.73 | 12 (42%) |
| 1 | 5MU | Aa | 917 | 1 | 19,22,23 | 1.39 | 4 (21%) | 28,32,35 | 2.22 | 6 (21%) |
| 27 | OMC | BA | 754 | 27 | 19,22,23 | 2.71 | 7 (36%) | 26,31,34 | 0.99 | 0 |
| 27 | OMG | BA | 419 | 27 | 18,26,27 | 2.17 | 5 (27%) | 19,38,41 | 3.64 | 6 (31%) |
| 1 | MA6 | Aa | 1468 | 1 | 18,26,27 | 1.33 | 1 (5%) | 19,38,41 | 3.30 | 2 (10%) |
| 27 | 4AC | BA | 501 | 27 | 21,24,25 | 3.05 | 9 (42%) | 29,34,37 | 1.32 | 3 (10%) |
| 27 | 5MU | BA | 1905 | 27 | 19,22,23 | 4.46 | 7 (36%) | 28,32,35 | 3.81 | 11 (39%) |
| 1 | 5MC | Aa | 464 | 1 | 18,22,23 | 3.34 | 7 (38%) | 26,32,35 | 1.22 | 2 (7%) |
| 27 | 4AC | BA | 1375 | 27 | 21,24,25 | 3.10 | 10 (47%) | 29,34,37 | 1.32 | 4 (13%) |
| 27 | 5MU | BA | 2384 | 27 | 19,22,23 | 4.63 | 7 (36%) | 28,32,35 | 3.73 | 12 (42%) |
| 1 | 4AC | Aa | 458 | 1 | 21,24,25 | 1.02 | 1 (4%) | 29,34,37 | 1.19 | 3 (10%) |
| 1 | LV2 | Aa | 918 | 1 | 20,23,24 | 0.94 | 0 | 26,33,36 | 0.81 | 0 |
| 27 | 4AC | BA | 124 | 27 | 21,24,25 | 2.91 | 10 (47%) | 29,34,37 | 1.21 | 3 (10%) |
| 27 | OMG | BA | 353 | 27 | 18,26,27 | 2.44 | 8 (44%) | 19,38,41 | 1.90 | 5 (26%) |
| 27 | OMG | BA | 833 | 27 | 18,26,27 | 2.27 | 8 (44%) | 19,38,41 | 1.71 | 4 (21%) |
| 27 | 4AC | BA | 1899 | 27 | 21,24,25 | 2.96 | 10 (47%) | 29,34,37 | 1.26 | 4 (13%) |
| 1 | 4AC | Aa | 827 | 1 | 21,24,25 | 3.18 | 9 (42%) | 29,34,37 | 1.24 | 4 (13%) |
| 27 | OMU | BA | 657 | 27 | 19,22,23 | 2.56 | 6 (31%) | 26,31,34 | 1.65 | 6 (23%) |
| 1 | 4AC | Aa | 501 | 1 | 21,24,25 | 3.24 | 9 (42%) | 29,34,37 | 1.51 | 5 (17%) |
| 27 | OMU | BA | 453 | 27 | 19,22,23 | 2.72 | 7 (36%) | 26,31,34 | 1.82 | 5 (19%) |
| 27 | OMG | BA | 215 | 27 | 18,26,27 | 2.27 | 7 (38%) | 19,38,41 | 1.91 | 4 (21%) |
| 1 | 4AC | Aa | 358 | 1 | 21,24,25 | 3.25 | 9 (42%) | 29,34,37 | 1.60 | 5 (17%) |
| 1 | A2M | Aa | 352 | 1 | 18,25,26 | 0.94 | 1 (5%) | 18,36,39 | 1.29 | 2 (11%) |
| 1 | OMG | Aa | 1025 | 1 | 18,26,27 | 2.17 | 7 (38%) | 19,38,41 | 1.41 | 3 (15%) |
| 27 | OMU | BA | 2389 | 27 | 19,22,23 | 1.29 | 3 (15%) | 26,31,34 | 1.84 | 6 (23%) |
| 1 | OMG | Aa | 320 | 1 | 18,26,27 | 2.25 | 7 (38%) | 19,38,41 | 1.42 | 3 (15%) |
| 27 | 4AC | BA | 2590 | 27 | 21,24,25 | 3.04 | 10 (47%) | 29,34,37 | 1.20 | 5 (17%) |
| 27 | OMG | BA | 64 | 27 | 18,26,27 | 2.01 | 6 (33%) | 19,38,41 | 1.37 | 3 (15%) |
| 27 | 4AC | BA | 1934 | 27 | 21,24,25 | 2.98 | 9 (42%) | 29,34,37 | 1.31 | 4 (13%) |
| 27 | OMG | BA | 290 | 27 | 18,26,27 | 2.21 | 8 (44%) | 19,38,41 | 1.64 | 4 (21%) |
| 1 | 4AC | Aa | 373 | 1 | 21,24,25 | 3.15 | 9 (42%) | 29,34,37 | 1.45 | 6 (20%) |
| 27 | OMU | BA | 2656 | 27 | 19,22,23 | 2.65 | 7 (36%) | 26,31,34 | 1.67 | 4 (15%) |
| 1 | OMG | Aa | 892 | 1 | 18,26,27 | 2.18 | 7 (38%) | 19,38,41 | 1.35 | 3 (15%) |
| 1 | 5MC | Aa | 1478 | 1 | 18,22,23 | 3.03 | 7 (38%) | 26,32,35 | 1.48 | 6 (23%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 1 | OMC | Aa | 190 | 1 | 19,22,23 | 2.74 | 7 (36%) | 26,31,34 | 0.89 | 0 |
| 1 | 4AC | Aa | 569 | 1 | 21,24,25 | 3.15 | 9 (42%) | 29,34,37 | 1.40 | 5 (17%) |
| 27 | OMG | BA | 2324 | 27 | 18,26,27 | 2.19 | 7 (38%) | 19,38,41 | 1.43 | 3 (15%) |
| 27 | LHH | BA | 2457 | 27 | 22,25,26 | 2.52 | 5 (22%) | 29,35,38 | 2.16 | 7 (24%) |
| 1 | OMC | Aa | 296 | 1 | 19,22,23 | 2.62 | 7 (36%) | 26,31,34 | 0.96 | 1 (3%) |
| 27 | A2M | BA | 849 | 27 | 18,25,26 | 4.04 | 8 (44%) | 18,36,39 | 3.29 | 6 (33%) |
| 27 | OMC | BA | 2595 | 27 | 19,22,23 | 2.57 | 7 (36%) | 26,31,34 | 1.27 | 3 (11%) |
| 27 | OMC | BA | 1820 | 27 | 19,22,23 | 2.58 | 7 (36%) | 26,31,34 | 1.29 | 5 (19%) |
| 27 | 4AC | BA | 2838 | 27 | 21,24,25 | 3.16 | 9 (42%) | 29,34,37 | 1.30 | 4 (13%) |
| 27 | OMU | BA | 2610 | 27 | 19,22,23 | 3.04 | 8 (42%) | 26,31,34 | 1.83 | 4 (15%) |
| 1 | OMG | Aa | 913 | 1 | 18,26,27 | 2.40 | 8 (44%) | 19,38,41 | 2.05 | 6 (31%) |
| 27 | 5MC | BA | 944 | 27 | 18,22,23 | 2.92 | 7 (38%) | 26,32,35 | 1.31 | 3 (11%) |
| 27 | OMG | BA | 1892 | 27 | 18,26,27 | 2.12 | 7 (38%) | 19,38,41 | 1.37 | 3 (15%) |
| 27 | 4SU | BA | 2553 | 27 | 18,21,22 | 3.87 | 8 (44%) | 26,30,33 | 1.94 | 5 (19%) |
| 27 | 4AC | BA | 713 | 27 | 21,24,25 | 3.04 | 9 (42%) | 29,34,37 | 1.17 | 2 (6%) |
| 27 | 4AC | BA | 335 | 27 | 21,24,25 | 3.13 | 9 (42%) | 29,34,37 | 1.14 | 3 (10%) |
| 27 | A2M | BA | 1517 | 27 | 18,25,26 | 3.93 | 7 (38%) | 18,36,39 | 2.89 | 3 (16%) |
| 27 | OMU | BA | 1776 | 27 | 19,22,23 | 2.71 | 7 (36%) | 26,31,34 | 1.79 | 6 (23%) |
| 27 | 4AC | BA | 1305 | 27 | 21,24,25 | 3.31 | 10 (47%) | 29,34,37 | 1.55 | 6 (20%) |
| 27 | 5MC | BA | 1696 | 27 | 18,22,23 | 3.02 | 7 (38%) | 26,32,35 | 1.07 | 2 (7%) |
| 27 | LHH | BA | 526 | 27 | 22,25,26 | 2.41 | 5 (22%) | 29,35,38 | 1.77 | 7 (24%) |
| 27 | OMG | BA | 763 | 27 | 18,26,27 | 2.15 | 7 (38%) | 19,38,41 | 1.47 | 4 (21%) |
| 27 | OMG | BA | 2016 | 27 | 18,26,27 | 2.23 | 6 (33%) | 19,38,41 | 1.59 | 4 (21%) |
| 27 | 4AC | BA | 27 | 27 | 21,24,25 | 3.17 | 10 (47%) | 29,34,37 | 1.35 | 5 (17%) |
| 1 | OMG | Aa | 450 | 1 | 18,26,27 | 2.16 | 7 (38%) | 19,38,41 | 1.30 | 3 (15%) |
| 27 | OMC | BA | 2047 | 27 | 19,22,23 | 2.56 | 7 (36%) | 26,31,34 | 1.06 | 1 (3%) |
| 27 | LHH | BA | 2955 | 27 | 22,25,26 | 2.39 | 5 (22%) | 29,35,38 | 2.00 | 6 (20%) |
| 1 | OMC | Aa | 1354 | 1 | 19,22,23 | 2.75 | 7 (36%) | 26,31,34 | 1.03 | 2 (7%) |
| 27 | 4AC | BA | 1357 | 27 | 21,24,25 | 3.02 | 10 (47%) | 29,34,37 | 1.38 | 6 (20%) |
| 1 | OMG | Aa | 1265 | 1 | 18,26,27 | 2.27 | 8 (44%) | 19,38,41 | 1.42 | 3 (15%) |
| 1 | 4AC | Aa | 605 | 1 | 21,24,25 | 3.30 | 9 (42%) | 29,34,37 | 1.91 | 7 (24%) |
| 1 | OMG | Aa | 1107 | 1 | 18,26,27 | 2.30 | 8 (44%) | 19,38,41 | 1.43 | 4 (21%) |
| 27 | 5MC | BA | 2075 | 27 | 18,22,23 | 2.86 | 7 (38%) | 26,32,35 | 1.02 | 1 (3%) |
| 1 | B8T | Aa | 1051 | 1 | 19,22,23 | 0.80 | 0 | 26,31,34 | 0.89 | 1 (3%) |
| 27 | 4AC | BA | 2992 | 27 | 21,24,25 | 3.32 | 10 (47%) | 29,34,37 | 1.39 | 5 (17%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 1 | OMG | Aa | 246 | 1 | 18,26,27 | 2.14 | 7 (38%) | 19,38,41 | 1.36 | 3 (15%) |
| 27 | OMG | BA | 2672 | 27 | 18,26,27 | 2.14 | 6 (33%) | 19,38,41 | 1.74 | 4 (21%) |
| 1 | OMG | Aa | 876 | 1 | 18,26,27 | 2.30 | 8 (44%) | 19,38,41 | 1.37 | 4 (21%) |
| 27 | OMC | BA | 869 | 27 | 19,22,23 | 2.60 | 7 (36%) | 26,31,34 | 1.06 | 2 (7%) |
| 27 | 5MC | BA | 1965 | 27 | 18,22,23 | 2.86 | 7 (38%) | 26,32,35 | 1.15 | 2 (7%) |
| 1 | 5MC | Aa | 1276 | 1 | 18,22,23 | 4.83 | 16 (88%) | 26,32,35 | 1.16 | 2 (7%) |
| 27 | 4AC | BA | 1543 | 27 | 21,24,25 | 3.12 | 9 (42%) | 29,34,37 | 1.21 | 4 (13%) |
| 1 | 5MC | Aa | 854 | 1 | 18,22,23 | 2.93 | 7 (38%) | 26,32,35 | 1.46 | 5 (19%) |
| 1 | OMG | Aa | 382 | 1 | 18,26,27 | 2.18 | 7 (38%) | 19,38,41 | 1.44 | 3 (15%) |
| 27 | OMC | BA | 2630 | 27 | 19,22,23 | 2.48 | 7 (36%) | 26,31,34 | 1.10 | 2 (7%) |
| 27 | 4AC | BA | 1641 | 27 | 21,24,25 | 3.13 | 9 (42%) | 29,34,37 | 1.25 | 5 (17%) |
| 1 | OMG | Aa | 636 | 1 | 18,26,27 | 2.31 | 7 (38%) | 19,38,41 | 1.32 | 3 (15%) |
| 1 | OMG | Aa | 381 | 1 | 18,26,27 | 2.22 | 8 (44%) | 19,38,41 | 1.44 | 4 (21%) |
| 27 | OMC | BA | 250 | 27 | 19,22,23 | 2.66 | 7 (36%) | 26,31,34 | 1.42 | 5 (19%) |
| 1 | 4AC | Aa | 298 | 1 | 21,24,25 | 3.17 | 9 (42%) | 29,34,37 | 1.61 | 5 (17%) |
| 1 | OMG | Aa | 1434 | 1 | 18,26,27 | 2.16 | 7 (38%) | 19,38,41 | 1.47 | 3 (15%) |
| 1 | OMU | Aa | 479 | 1 | 19,22,23 | 2.97 | 8 (42%) | 26,31,34 | 1.69 | 5 (19%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 27 | OMG | BA | 2010 | 27 | - | 0/5/27/28 | 0/3/3/3 |
| 27 | 4AC | BA | 3023 | 27 | - | 2/11/29/30 | 0/2/2/2 |
| 1 | OMU | Aa | 1358 | 1 | - | 3/9/27/28 | 0/2/2/2 |
| 1 | 4AC | Aa | 525 | 1 | - | 5/11/29/30 | 0/2/2/2 |
| 1 | B8T | Aa | 1141 | 1 | - | 0/7/27/28 | 0/2/2/2 |
| 1 | OMG | Aa | 532 | 1 | - | 2/5/27/28 | 0/3/3/3 |
| 27 | OMC | BA | 561 | 27 | - | 0/9/27/28 | 0/2/2/2 |
| 27 | OMG | BA | 63 | 27 | - | 0/5/27/28 | 0/3/3/3 |
| 27 | 4AC | BA | 2797 | 27 | - | 0/11/29/30 | 0/2/2/2 |
| 1 | 4AC | Aa | 847 | 1 | - | 0/11/29/30 | 0/2/2/2 |
| 27 | OMG | BA | 723 | 27 | - | 1/5/27/28 | 0/3/3/3 |
| 1 | OMU | Aa | 8 | 1 | - | 3/9/27/28 | 0/2/2/2 |
| 27 | OMG | BA | 2152 | 27 | - | 2/5/27/28 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 27 | OMG | BA | 2379 | 27 | - | 3/5/27/28 | 0/3/3/3 |
| 27 | OMC | BA | 2124 | 27 | - | 0/9/27/28 | 0/2/2/2 |
| 27 | OMG | BA | 2728 | 27 | - | 0/5/27/28 | 0/3/3/3 |
| 27 | OMU | BA | 619 | 27 | - | 1/9/27/28 | 0/2/2/2 |
| 27 | OMG | BA | 674 | 27 | - | 0/5/27/28 | 0/3/3/3 |
| 27 | OMG | BA | 1558 | 27 | - | 0/5/27/28 | 0/3/3/3 |
| 27 | 4AC | BA | 2997 | 27 | - | 0/11/29/30 | 0/2/2/2 |
| 27 | A2M | BA | 212 | 27 | - | 1/5/27/28 | 0/3/3/3 |
| 27 | OMU | BA | 1319 | 27 | - | 0/9/27/28 | 0/2/2/2 |
| 1 | 4AC | Aa | 730 | 1 | - | 2/11/29/30 | 0/2/2/2 |
| 1 | 4AC | Aa | 1459 | 1 | - | 0/11/29/30 | 0/2/2/2 |
| 27 | 4AC | BA | 799 | 27 | - | 0/11/29/30 | 0/2/2/2 |
| 1 | OMG | Aa | 852 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | OMU | Aa | 304 | 1 | - | 1/9/27/28 | 0/2/2/2 |
| 27 | 4AC | BA | 1427 | 27 | - | 0/11/29/30 | 0/2/2/2 |
| 27 | 4AC | BA | 244 | 27 | - | 1/11/29/30 | 0/2/2/2 |
| 27 | OMC | BA | 2545 | 27 | - | 1/9/27/28 | 0/2/2/2 |
| 27 | 4SU | BA | 2581 | 27 | - | 2/7/25/26 | 0/2/2/2 |
| 1 | 4AC | Aa | 1007 | 1 | - | 2/11/29/30 | 0/2/2/2 |
| 27 | OMC | BA | 1790 | 27 | - | 2/9/27/28 | 0/2/2/2 |
| 27 | 5MU | BA | 1548 | 27 | - | 2/7/25/26 | 0/2/2/2 |
| 1 | 5MC | Aa | 1352 | 1 | - | 2/7/25/26 | 0/2/2/2 |
| 27 | 5MC | BA | 2605 | 27 | - | 0/7/25/26 | 0/2/2/2 |
| 27 | OMG | BA | 1953 | 27 | - | 2/5/27/28 | 0/3/3/3 |
| 27 | OMC | BA | 1750 | 27 | - | 0/9/27/28 | 0/2/2/2 |
| 1 | OMU | Aa | 240 | 1 | - | 0/9/27/28 | 0/2/2/2 |
| 27 | 4AC | BA | 2832 | 27 | - | 1/11/29/30 | 0/2/2/2 |
| 27 | OMU | BA | 768 | 27 | - | 0/9/27/28 | 0/2/2/2 |
| 27 | OMG | BA | 2521 | 27 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | 5MC | Aa | 457 | 1 | - | 2/7/25/26 | 0/2/2/2 |
| 27 | OMG | BA | 2527 | 27 | - | 2/5/27/28 | 0/3/3/3 |
| 27 | 4AC | BA | 2121 | 27 | - | 0/11/29/30 | 0/2/2/2 |
| 1 | 4AC | Aa | 818 | 1 | - | 2/11/29/30 | 0/2/2/2 |
| 1 | OMG | Aa | 498 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 27 | 4AC | BA | 1396 | 27 | - | 2/11/29/30 | 0/2/2/2 |
| 27 | 4AC | BA | 201 | 27 | - | 2/11/29/30 | 0/2/2/2 |
| 27 | 5MC | BA | 2863 | 27 | - | 0/7/25/26 | 0/2/2/2 |
| 27 | 4AC | BA | 925 | 27 | - | 2/11/29/30 | 0/2/2/2 |
| 27 | OMG | BA | 2745 | 27 | - | 0/5/27/28 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 27 | A2M | BA | 872 | 27 | - | 0/5/27/28 | 0/3/3/3 |
| 27 | 4AC | BA | 1431 | 27 | - | 0/11/29/30 | 0/2/2/2 |
| 27 | OMG | BA | 2528 | 27 | - | 0/5/27/28 | 0/3/3/3 |
| 27 | 5MU | BA | 875 | 27 | - | 2/7/25/26 | 0/2/2/2 |
| 27 | OMU | BA | 1340 | 27 | - | 0/9/27/28 | 0/2/2/2 |
| 1 | 5MC | Aa | 1004 | 1 | - | 2/7/25/26 | 0/2/2/2 |
| 27 | OMG | BA | 365 | 27 | - | 1/5/27/28 | 0/3/3/3 |
| 27 | OMC | BA | 718 | 27 | - | 0/9/27/28 | 0/2/2/2 |
| 27 | 5MU | BA | 1085 | 27 | - | 0/7/25/26 | 0/2/2/2 |
| 27 | 5MU | BA | 2688 | 27 | - | 0/7/25/26 | 0/2/2/2 |
| 27 | OMG | BA | 552 | 27 | - | 0/5/27/28 | 0/3/3/3 |
| 27 | A2M | BA | 756 | 27 | - | 0/5/27/28 | 0/3/3/3 |
| 27 | OMG | BA | 2168 | 27 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | OMC | Aa | 535 | 1 | - | 0/9/27/28 | 0/2/2/2 |
| 1 | OMU | Aa | 52 | 1 | - | 2/9/27/28 | 0/2/2/2 |
| 27 | 4AC | BA | 56 | 27 | - | 0/11/29/30 | 0/2/2/2 |
| 1 | MA6 | Aa | 1467 | 1 | - | 0/7/29/30 | 0/3/3/3 |
| 27 | 4AC | BA | 858 | 27 | - | 2/11/29/30 | 0/2/2/2 |
| 27 | 4AC | BA | 433 | 27 | - | 0/11/29/30 | 0/2/2/2 |
| 1 | OMG | Aa | 994 | 1 | - | 1/5/27/28 | 0/3/3/3 |
| 27 | 5MC | BA | 2055 | 27 | - | 2/7/25/26 | 0/2/2/2 |
| 27 | OMG | BA | 1940 | 27 | - | 2/5/27/28 | 0/3/3/3 |
| 27 | B8T | BA | 357 | 27 | - | 0/7/27/28 | 0/2/2/2 |
| 27 | A2M | BA | 825 | 27 | - | 0/5/27/28 | 0/3/3/3 |
| 27 | 4AC | BA | 376 | 27 | - | 0/11/29/30 | 0/2/2/2 |
| 1 | 2MG | Aa | 670 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 27 | OMU | BA | 1480 | 27 | - | 2/9/27/28 | 0/2/2/2 |
| 1 | 4AC | Aa | 682 | 1 | - | 0/11/29/30 | 0/2/2/2 |
| 27 | OMG | BA | 575 | 27 | - | 2/5/27/28 | 0/3/3/3 |
| 27 | 4AC | BA | 778 | 27 | - | 0/11/29/30 | 0/2/2/2 |
| 27 | OMG | BA | 2019 | 27 | - | 2/5/27/28 | 0/3/3/3 |
| 1 | 5MC | Aa | 942 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 27 | A2M | BA | 1400 | 27 | - | 1/5/27/28 | 0/3/3/3 |
| 27 | 4AC | BA | 1434 | 27 | - | 2/11/29/30 | 0/2/2/2 |
| 27 | 4AC | BA | 2159 | 27 | - | 0/11/29/30 | 0/2/2/2 |
| 27 | OMG | BA | 2568 | 27 | - | 3/5/27/28 | 0/3/3/3 |
| 27 | 4AC | BA | 418 | 27 | - | 0/11/29/30 | 0/2/2/2 |
| 27 | OMG | BA | 1799 | 27 | - | 3/5/27/28 | 0/3/3/3 |
| 1 | 4AC | Aa | 41 | 1 | - | 2/11/29/30 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 27 | 4AC | BA | 730 | 27 | - | 0/11/29/30 | 0/2/2/2 |
| 27 | OMC | BA | 2018 | 27 | - | 2/9/27/28 | 0/2/2/2 |
| 27 | OMG | BA | 1106 | 27 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | OMG | Aa | 446 | 1 | - | 2/5/27/28 | 0/3/3/3 |
| 1 | OMG | Aa | 1275 | 1 | - | 1/5/27/28 | 0/3/3/3 |
| 27 | 4AC | BA | 1955 | 27 | - | 2/11/29/30 | 0/2/2/2 |
| 1 | LHH | Aa | 1020 | 1 | - | 4/13/31/32 | 0/2/2/2 |
| 27 | 5MU | BA | 537 | 27 | - | 0/7/25/26 | 0/2/2/2 |
| 27 | OMG | BA | 800 | 27 | - | 0/5/27/28 | 0/3/3/3 |
| 27 | 4AC | BA | 1470 | 27 | - | 0/11/29/30 | 0/2/2/2 |
| 27 | OMG | BA | 2550 | 27 | - | 2/5/27/28 | 0/3/3/3 |
| 27 | 5MU | BA | 298 | 27 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 4AC | Aa | 697 | 1 | - | 4/11/29/30 | 0/2/2/2 |
| 27 | 4AC | BA | 3009 | 27 | - | 2/11/29/30 | 0/2/2/2 |
| 27 | OMU | BA | 1969 | 27 | - | 0/9/27/28 | 0/2/2/2 |
| 27 | OMG | BA | 1525 | 27 | - | 2/5/27/28 | 0/3/3/3 |
| 1 | 6MZ | Aa | 1449 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 27 | 4AC | BA | 1337 | 27 | - | 2/11/29/30 | 0/2/2/2 |
| 27 | A2M | BA | 488 | 27 | - | 3/5/27/28 | 0/3/3/3 |
| 27 | OMG | BA | 2657 | 27 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | OMG | Aa | 138 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | LHH | Aa | 229 | 1 | - | 3/13/31/32 | 0/2/2/2 |
| 1 | 5MC | Aa | 672 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 4AC | Aa | 1217 | 1 | - | 4/11/29/30 | 0/2/2/2 |
| 27 | LHH | BA | 617 | 27 | - | 5/13/31/32 | 0/2/2/2 |
| 27 | 5MC | BA | 2070 | 27 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMG | Aa | 771 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 27 | OMG | BA | 912 | 27 | - | 0/5/27/28 | 0/3/3/3 |
| 27 | OMU | BA | 2542 | 27 | - | 0/9/27/28 | 0/2/2/2 |
| 27 | A2M | BA | 932 | 27 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | 4AC | Aa | 136 | 1 | - | 2/11/29/30 | 0/2/2/2 |
| 27 | 4AC | BA | 1810 | 27 | - | 2/11/29/30 | 0/2/2/2 |
| 1 | OMG | Aa | 659 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 27 | A2M | BA | 505 | 27 | - | 2/5/27/28 | 0/3/3/3 |
| 1 | 5MC | Aa | 1476 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 27 | OMU | BA | 1551 | 27 | - | 3/9/27/28 | 0/2/2/2 |
| 27 | OMC | BA | 2571 | 27 | - | 2/9/27/28 | 0/2/2/2 |
| 27 | 4AC | BA | 805 | 27 | - | 0/11/29/30 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 1 | 4AC | Aa | 5 | 1 | - | 4/11/29/30 | 0/2/2/2 |
| 27 | OMU | BA | 34 | 27 | - | 1/9/27/28 | 0/2/2/2 |
| 27 | A2M | BA | 1265 | 27 | - | 2/5/27/28 | 0/3/3/3 |
| 27 | A2M | BA | 2702 | 27 | - | 1/5/27/28 | 0/3/3/3 |
| 1 | OMC | Aa | 1361 | 1,27 | - | 0/9/27/28 | 0/2/2/2 |
| 1 | B8T | Aa | 1262 | 1 | - | 0/7/27/28 | 0/2/2/2 |
| 1 | OMC | Aa | 825 | 1 | - | 0/9/27/28 | 0/2/2/2 |
| 1 | OMC | Aa | 752 | 1 | - | 0/9/27/28 | 0/2/2/2 |
| 27 | A2M | BA | 879 | 27 | - | 0/5/27/28 | 0/3/3/3 |
| 27 | OMG | BA | 1398 | 27 | - | 0/5/27/28 | 0/3/3/3 |
| 27 | OMG | BA | 2353 | 27 | - | 2/5/27/28 | 0/3/3/3 |
| 1 | OMG | Aa | 1026 | 1 | - | 1/5/27/28 | 0/3/3/3 |
| 27 | 4AC | BA | 2780 | 27 | - | 0/11/29/30 | 0/2/2/2 |
| 27 | 5MC | BA | 2035 | 27 | - | 0/7/25/26 | 0/2/2/2 |
| 27 | 5MU | BA | 572 | 27 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MU | Aa | 917 | 1 | - | 2/7/25/26 | 0/2/2/2 |
| 27 | OMC | BA | 754 | 27 | - | 2/9/27/28 | 0/2/2/2 |
| 27 | OMG | BA | 419 | 27 | - | 2/5/27/28 | 0/3/3/3 |
| 1 | MA6 | Aa | 1468 | 1 | - | 2/7/29/30 | 0/3/3/3 |
| 27 | 4AC | BA | 501 | 27 | - | 0/11/29/30 | 0/2/2/2 |
| 27 | 5MU | BA | 1905 | 27 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MC | Aa | 464 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 27 | 4AC | BA | 1375 | 27 | - | 2/11/29/30 | 0/2/2/2 |
| 27 | 5MU | BA | 2384 | 27 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 4AC | Aa | 458 | 1 | - | 6/11/29/30 | 0/2/2/2 |
| 1 | LV2 | Aa | 918 | 1 | - | 0/9/29/30 | 0/2/2/2 |
| 27 | 4AC | BA | 124 | 27 | - | 0/11/29/30 | 0/2/2/2 |
| 27 | OMG | BA | 353 | 27 | - | 2/5/27/28 | 0/3/3/3 |
| 27 | OMG | BA | 833 | 27 | - | 0/5/27/28 | 0/3/3/3 |
| 27 | 4AC | BA | 1899 | 27 | - | 0/11/29/30 | 0/2/2/2 |
| 1 | 4AC | Aa | 827 | 1 | - | 0/11/29/30 | 0/2/2/2 |
| 27 | OMU | BA | 657 | 27 | - | 1/9/27/28 | 0/2/2/2 |
| 1 | 4AC | Aa | 501 | 1 | - | 0/11/29/30 | 0/2/2/2 |
| 27 | OMU | BA | 453 | 27 | - | 2/9/27/28 | 0/2/2/2 |
| 27 | OMG | BA | 215 | 27 | - | 2/5/27/28 | 0/3/3/3 |
| 1 | 4AC | Aa | 358 | 1 | - | 2/11/29/30 | 0/2/2/2 |
| 1 | A2M | Aa | 352 | 1 | - | 1/5/27/28 | 0/3/3/3 |
| 1 | OMG | Aa | 1025 | 1 | - | 1/5/27/28 | 0/3/3/3 |
| 27 | OMU | BA | 2389 | 27 | - | 2/9/27/28 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 1 | OMG | Aa | 320 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 27 | 4AC | BA | 2590 | 27 | - | 0/11/29/30 | 0/2/2/2 |
| 27 | OMG | BA | 64 | 27 | - | 2/5/27/28 | 0/3/3/3 |
| 27 | 4AC | BA | 1934 | 27 | - | 0/11/29/30 | 0/2/2/2 |
| 27 | OMG | BA | 290 | 27 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | 4AC | Aa | 373 | 1 | - | 0/11/29/30 | 0/2/2/2 |
| 27 | OMU | BA | 2656 | 27 | - | 0/9/27/28 | 0/2/2/2 |
| 1 | OMG | Aa | 892 | 1 | - | 3/5/27/28 | 0/3/3/3 |
| 1 | 5MC | Aa | 1478 | 1 | - | 3/7/25/26 | 0/2/2/2 |
| 1 | OMC | Aa | 190 | 1 | - | 2/9/27/28 | 0/2/2/2 |
| 1 | 4AC | Aa | 569 | 1 | - | 0/11/29/30 | 0/2/2/2 |
| 27 | OMG | BA | 2324 | 27 | - | 0/5/27/28 | 0/3/3/3 |
| 27 | LHH | BA | 2457 | 27 | - | 4/13/31/32 | 0/2/2/2 |
| 1 | OMC | Aa | 296 | 1 | - | 0/9/27/28 | 0/2/2/2 |
| 27 | A2M | BA | 849 | 27 | - | 2/5/27/28 | 0/3/3/3 |
| 27 | OMC | BA | 2595 | 27 | - | 2/9/27/28 | 0/2/2/2 |
| 27 | OMC | BA | 1820 | 27 | - | 0/9/27/28 | 0/2/2/2 |
| 27 | 4AC | BA | 2838 | 27 | - | 2/11/29/30 | 0/2/2/2 |
| 27 | OMU | BA | 2610 | 27 | - | 3/9/27/28 | 0/2/2/2 |
| 1 | OMG | Aa | 913 | 1 | - | 2/5/27/28 | 0/3/3/3 |
| 27 | 5MC | BA | 944 | 27 | - | 0/7/25/26 | 0/2/2/2 |
| 27 | OMG | BA | 1892 | 27 | - | 1/5/27/28 | 0/3/3/3 |
| 27 | 4SU | BA | 2553 | 27 | - | 0/7/25/26 | 0/2/2/2 |
| 27 | 4AC | BA | 713 | 27 | - | 0/11/29/30 | 0/2/2/2 |
| 27 | 4AC | BA | 335 | 27 | - | 0/11/29/30 | 0/2/2/2 |
| 27 | A2M | BA | 1517 | 27 | - | 1/5/27/28 | 0/3/3/3 |
| 27 | OMU | BA | 1776 | 27 | - | 0/9/27/28 | 0/2/2/2 |
| 27 | 4AC | BA | 1305 | 27 | - | 2/11/29/30 | 0/2/2/2 |
| 27 | 5MC | BA | 1696 | 27 | - | 0/7/25/26 | 0/2/2/2 |
| 27 | LHH | BA | 526 | 27 | - | 1/13/31/32 | 0/2/2/2 |
| 27 | OMG | BA | 763 | 27 | - | 0/5/27/28 | 0/3/3/3 |
| 27 | OMG | BA | 2016 | 27 | - | 0/5/27/28 | 0/3/3/3 |
| 27 | 4AC | BA | 27 | 27 | - | 2/11/29/30 | 0/2/2/2 |
| 1 | OMG | Aa | 450 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 27 | OMC | BA | 2047 | 27 | - | 0/9/27/28 | 0/2/2/2 |
| 27 | LHH | BA | 2955 | 27 | - | 3/13/31/32 | 0/2/2/2 |
| 1 | OMC | Aa | 1354 | 1 | - | 2/9/27/28 | 0/2/2/2 |
| 27 | 4AC | BA | 1357 | 27 | - | 0/11/29/30 | 0/2/2/2 |
| 1 | OMG | Aa | 1265 | 1 | - | 0/5/27/28 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 1 | 4AC | Aa | 605 | 1 | - | 1/11/29/30 | 0/2/2/2 |
| 1 | OMG | Aa | 1107 | 1 | - | 3/5/27/28 | 0/3/3/3 |
| 27 | 5MC | BA | 2075 | 27 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | B8T | Aa | 1051 | 1 | - | 0/7/27/28 | 0/2/2/2 |
| 27 | 4AC | BA | 2992 | 27 | - | 3/11/29/30 | 0/2/2/2 |
| 1 | OMG | Aa | 246 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 27 | OMG | BA | 2672 | 27 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | OMG | Aa | 876 | 1 | - | 2/5/27/28 | 0/3/3/3 |
| 27 | OMC | BA | 869 | 27 | - | 2/9/27/28 | 0/2/2/2 |
| 27 | 5MC | BA | 1965 | 27 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MC | Aa | 1276 | 1 | - | 2/7/25/26 | 0/2/2/2 |
| 27 | 4AC | BA | 1543 | 27 | - | 3/11/29/30 | 0/2/2/2 |
| 1 | 5MC | Aa | 854 | 1 | - | 1/7/25/26 | 0/2/2/2 |
| 1 | OMG | Aa | 382 | 1 | - | 2/5/27/28 | 0/3/3/3 |
| 27 | OMC | BA | 2630 | 27 | - | 0/9/27/28 | 0/2/2/2 |
| 27 | 4AC | BA | 1641 | 27 | - | 2/11/29/30 | 0/2/2/2 |
| 1 | OMG | Aa | 636 | 1 | - | 2/5/27/28 | 0/3/3/3 |
| 1 | OMG | Aa | 381 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 27 | OMC | BA | 250 | 27 | - | 0/9/27/28 | 0/2/2/2 |
| 1 | 4AC | Aa | 298 | 1 | - | 0/11/29/30 | 0/2/2/2 |
| 1 | OMG | Aa | 1434 | 1 | - | 1/5/27/28 | 0/3/3/3 |
| 1 | OMU | Aa | 479 | 1 | - | 1/9/27/28 | 0/2/2/2 |

All (1672) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 1265 | A2M | O4'-C1' | 14.99 | 1.62 | 1.41 |
| 27 | BA | 756 | A2M | O4'-C1' | 14.76 | 1.61 | 1.41 |
| 27 | BA | 932 | A2M | O4'-C1' | 14.62 | 1.61 | 1.41 |
| 27 | BA | 872 | A2M | O4'-C1' | 14.38 | 1.61 | 1.41 |
| 27 | BA | 879 | A2M | O4'-C1' | 14.34 | 1.61 | 1.41 |
| 27 | BA | 849 | A2M | O4'-C1' | 14.21 | 1.60 | 1.41 |
| 27 | BA | 825 | A2M | O4'-C1' | 14.09 | 1.60 | 1.41 |
| 27 | BA | 505 | A2M | O4'-C1' | 13.96 | 1.60 | 1.41 |
| 27 | BA | 488 | A2M | O4'-C1' | 13.84 | 1.60 | 1.41 |
| 27 | BA | 2702 | A2M | O4'-C1' | 13.72 | 1.60 | 1.41 |
| 27 | BA | 1400 | A2M | O4'-C1' | 13.59 | 1.60 | 1.41 |
| 27 | BA | 1517 | A2M | O4'-C1' | 13.45 | 1.59 | 1.41 |
| 1 | Aa | 1476 | 5MC | C2'-C3' | -10.81 | 1.23 | 1.53 |
| 1 | Aa | 1276 | 5MC | C2'-C3' | -10.79 | 1.23 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 1548 | 5MU | C2-N1 | 10.67 | 1.55 | 1.38 |
| 27 | BA | 298 | 5MU | C2-N1 | 10.58 | 1.55 | 1.38 |
| 27 | BA | 1548 | 5MU | C6-N1 | 10.54 | 1.56 | 1.38 |
| 27 | BA | 875 | 5MU | C2-N1 | 10.51 | 1.55 | 1.38 |
| 1 | Aa | 457 | 5MC | C2'-C3' | -10.49 | 1.24 | 1.53 |
| 27 | BA | 2035 | 5MC | C2'-C3' | -10.37 | 1.24 | 1.53 |
| 27 | BA | 537 | 5MU | C2-N1 | 10.31 | 1.55 | 1.38 |
| 27 | BA | 572 | 5MU | C2-N1 | 10.22 | 1.54 | 1.38 |
| 27 | BA | 2688 | 5MU | C2-N1 | 10.20 | 1.54 | 1.38 |
| 27 | BA | 1085 | 5MU | C2-N1 | 10.18 | 1.54 | 1.38 |
| 27 | BA | 1905 | 5MU | C2-N1 | 10.11 | 1.54 | 1.38 |
| 27 | BA | 2384 | 5MU | C2-N1 | 10.10 | 1.54 | 1.38 |
| 27 | BA | 875 | 5MU | C6-N1 | 10.05 | 1.55 | 1.38 |
| 27 | BA | 2384 | 5MU | C6-N1 | 9.92 | 1.55 | 1.38 |
| 27 | BA | 2384 | 5MU | C4-C5 | 9.52 | 1.60 | 1.44 |
| 27 | BA | 298 | 5MU | C6-N1 | 9.42 | 1.54 | 1.38 |
| 27 | BA | 572 | 5MU | C6-N1 | 9.39 | 1.54 | 1.38 |
| 27 | BA | 1905 | 5MU | C6-N1 | 9.37 | 1.54 | 1.38 |
| 27 | BA | 2688 | 5MU | C6-N1 | 9.25 | 1.53 | 1.38 |
| 27 | BA | 537 | 5MU | C6-N1 | 9.25 | 1.53 | 1.38 |
| 1 | Aa | 457 | 5MC | C6-C5 | 9.12 | 1.49 | 1.34 |
| 27 | BA | 1548 | 5MU | C4-C5 | 9.00 | 1.59 | 1.44 |
| 27 | BA | 2035 | 5MC | C6-C5 | 8.90 | 1.49 | 1.34 |
| 1 | Aa | 1276 | 5MC | C6-C5 | 8.80 | 1.49 | 1.34 |
| 1 | Aa | 1020 | LHH | O2-C2 | 8.79 | 1.40 | 1.23 |
| 27 | BA | 537 | 5MU | C4-C5 | 8.77 | 1.59 | 1.44 |
| 27 | BA | 2688 | 5MU | C4-C5 | 8.74 | 1.59 | 1.44 |
| 1 | Aa | 1476 | 5MC | C6-C5 | 8.63 | 1.48 | 1.34 |
| 27 | BA | 1905 | 5MU | C4-C5 | 8.58 | 1.59 | 1.44 |
| 27 | BA | 572 | 5MU | C4-C5 | 8.57 | 1.59 | 1.44 |
| 1 | Aa | 1352 | 5MC | C6-C5 | 8.55 | 1.48 | 1.34 |
| 27 | BA | 526 | LHH | O2-C2 | 8.54 | 1.39 | 1.23 |
| 27 | BA | 617 | LHH | O2-C2 | 8.53 | 1.39 | 1.23 |
| 27 | BA | 2581 | 4SU | C4-N3 | 8.53 | 1.46 | 1.37 |
| 27 | BA | 2955 | LHH | O2-C2 | 8.53 | 1.39 | 1.23 |
| 1 | Aa | 229 | LHH | O2-C2 | 8.53 | 1.39 | 1.23 |
| 27 | BA | 875 | 5MU | C4-C5 | 8.52 | 1.58 | 1.44 |
| 27 | BA | 2457 | LHH | O2-C2 | 8.48 | 1.39 | 1.23 |
| 1 | Aa | 942 | 5MC | C6-C5 | 8.46 | 1.48 | 1.34 |
| 27 | BA | 2055 | 5MC | C6-C5 | 8.43 | 1.48 | 1.34 |
| 27 | BA | 298 | 5MU | C4-C5 | 8.39 | 1.58 | 1.44 |
| 27 | BA | 2605 | 5MC | C6-C5 | 8.28 | 1.48 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 2581 | 4SU | C2-N1 | 8.27 | 1.51 | 1.38 |
| 27 | BA | 875 | 5MU | C4-N3 | -8.26 | 1.23 | 1.38 |
| 27 | BA | 2553 | 4SU | C2-N1 | 8.25 | 1.51 | 1.38 |
| 1 | Aa | 464 | 5MC | C6-C5 | 8.22 | 1.48 | 1.34 |
| 27 | BA | 1085 | 5MU | C6-N1 | 8.13 | 1.51 | 1.38 |
| 27 | BA | 2688 | 5MU | C4-N3 | -8.08 | 1.23 | 1.38 |
| 27 | BA | 1905 | 5MU | C4-N3 | -8.07 | 1.23 | 1.38 |
| 27 | BA | 2384 | 5MU | C4-N3 | -8.01 | 1.24 | 1.38 |
| 27 | BA | 572 | 5MU | C4-N3 | -8.00 | 1.24 | 1.38 |
| 27 | BA | 537 | 5MU | C4-N3 | -7.93 | 1.24 | 1.38 |
| 27 | BA | 1085 | 5MU | C4-C5 | 7.89 | 1.57 | 1.44 |
| 1 | Aa | 672 | 5MC | C6-C5 | 7.81 | 1.47 | 1.34 |
| 27 | BA | 1085 | 5MU | C4-N3 | -7.80 | 1.24 | 1.38 |
| 27 | BA | 298 | 5MU | C4-N3 | -7.80 | 1.24 | 1.38 |
| 1 | Aa | 1004 | 5MC | C6-C5 | 7.74 | 1.47 | 1.34 |
| 1 | Aa | 1217 | 4AC | C4-N3 | 7.57 | 1.46 | 1.32 |
| 27 | BA | 2863 | 5MC | C6-C5 | 7.55 | 1.47 | 1.34 |
| 27 | BA | 2553 | 4SU | C4-N3 | 7.48 | 1.45 | 1.37 |
| 27 | BA | 1548 | 5MU | C4-N3 | -7.48 | 1.25 | 1.38 |
| 1 | Aa | 1478 | 5MC | C6-C5 | 7.46 | 1.46 | 1.34 |
| 27 | BA | 2610 | OMU | C2-N1 | 7.39 | 1.50 | 1.38 |
| 27 | BA | 1400 | A2M | O4'-C4' | -7.31 | 1.28 | 1.45 |
| 27 | BA | 2992 | 4AC | C4-N3 | 7.22 | 1.45 | 1.32 |
| 27 | BA | 1696 | 5MC | C6-C5 | 7.17 | 1.46 | 1.34 |
| 27 | BA | 1305 | 4AC | C4-N3 | 7.13 | 1.45 | 1.32 |
| 27 | BA | 1551 | OMU | C2-N1 | 7.11 | 1.49 | 1.38 |
| 1 | Aa | 358 | 4AC | C4-N3 | 7.11 | 1.45 | 1.32 |
| 1 | Aa | 605 | 4AC | C4-N3 | 7.07 | 1.45 | 1.32 |
| 1 | Aa | 697 | 4AC | C4-N3 | 7.07 | 1.45 | 1.32 |
| 1 | Aa | 682 | 4AC | C4-N3 | 7.07 | 1.45 | 1.32 |
| 27 | BA | 2702 | A2M | O4'-C4' | -7.06 | 1.29 | 1.45 |
| 1 | Aa | 136 | 4AC | C4-N3 | 7.06 | 1.45 | 1.32 |
| 1 | Aa | 501 | 4AC | C4-N3 | 7.05 | 1.45 | 1.32 |
| 27 | BA | 505 | A2M | O4'-C4' | -7.04 | 1.29 | 1.45 |
| 27 | BA | 825 | A2M | O4'-C4' | -7.04 | 1.29 | 1.45 |
| 27 | BA | 1431 | 4AC | C4-N3 | 7.03 | 1.45 | 1.32 |
| 1 | Aa | 479 | OMU | C2-N3 | 6.98 | 1.50 | 1.38 |
| 27 | BA | 2997 | 4AC | C4-N3 | 6.96 | 1.44 | 1.32 |
| 27 | BA | 418 | 4AC | C4-N3 | 6.94 | 1.44 | 1.32 |
| 1 | Aa | 298 | 4AC | C4-N3 | 6.94 | 1.44 | 1.32 |
| 27 | BA | 730 | 4AC | C4-N3 | 6.93 | 1.44 | 1.32 |
| 27 | BA | 2838 | 4AC | C4-N3 | 6.92 | 1.44 | 1.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Aa | 479 | OMU | C2-N1 | 6.92 | 1.49 | 1.38 |
| 27 | BA | 3023 | 4AC | C4-N3 | 6.92 | 1.44 | 1.32 |
| 1 | Aa | 41 | 4AC | C4-N3 | 6.90 | 1.44 | 1.32 |
| 27 | BA | 778 | 4AC | C4-N3 | 6.88 | 1.44 | 1.32 |
| 27 | BA | 488 | A2M | O4'-C4' | -6.88 | 1.29 | 1.45 |
| 1 | Aa | 847 | 4AC | C4-N3 | 6.86 | 1.44 | 1.32 |
| 27 | BA | 27 | 4AC | C4-N3 | 6.84 | 1.44 | 1.32 |
| 27 | BA | 1337 | 4AC | C4-N3 | 6.84 | 1.44 | 1.32 |
| 1 | Aa | 818 | 4AC | C4-N3 | 6.84 | 1.44 | 1.32 |
| 27 | BA | 872 | A2M | O4'-C4' | -6.83 | 1.29 | 1.45 |
| 27 | BA | 1934 | 4AC | C4-N3 | 6.83 | 1.44 | 1.32 |
| 27 | BA | 1375 | 4AC | C4-N3 | 6.81 | 1.44 | 1.32 |
| 1 | Aa | 373 | 4AC | C4-N3 | 6.80 | 1.44 | 1.32 |
| 27 | BA | 56 | 4AC | C4-N3 | 6.80 | 1.44 | 1.32 |
| 27 | BA | 433 | 4AC | C4-N3 | 6.80 | 1.44 | 1.32 |
| 27 | BA | 858 | 4AC | C4-N3 | 6.80 | 1.44 | 1.32 |
| 27 | BA | 1517 | A2M | O4'-C4' | -6.79 | 1.29 | 1.45 |
| 27 | BA | 944 | 5MC | C6-C5 | 6.79 | 1.45 | 1.34 |
| 27 | BA | 1810 | 4AC | C4-N3 | 6.79 | 1.44 | 1.32 |
| 1 | Aa | 240 | OMU | C2-N1 | 6.79 | 1.49 | 1.38 |
| 1 | Aa | 5 | 4AC | C4-N3 | 6.78 | 1.44 | 1.32 |
| 1 | Aa | 827 | 4AC | C4-N3 | 6.77 | 1.44 | 1.32 |
| 27 | BA | 2075 | 5MC | C6-C5 | 6.77 | 1.45 | 1.34 |
| 27 | BA | 1396 | 4AC | C4-N3 | 6.75 | 1.44 | 1.32 |
| 27 | BA | 2159 | 4AC | C4-N3 | 6.74 | 1.44 | 1.32 |
| 27 | BA | 2832 | 4AC | C4-N3 | 6.74 | 1.44 | 1.32 |
| 1 | Aa | 569 | 4AC | C4-N3 | 6.73 | 1.44 | 1.32 |
| 27 | BA | 932 | A2M | O4'-C4' | -6.73 | 1.30 | 1.45 |
| 27 | BA | 1543 | 4AC | C4-N3 | 6.72 | 1.44 | 1.32 |
| 27 | BA | 376 | 4AC | C4-N3 | 6.72 | 1.44 | 1.32 |
| 27 | BA | 1357 | 4AC | C4-N3 | 6.72 | 1.44 | 1.32 |
| 27 | BA | 3009 | 4AC | C4-N3 | 6.71 | 1.44 | 1.32 |
| 27 | BA | 2780 | 4AC | C4-N3 | 6.71 | 1.44 | 1.32 |
| 27 | BA | 335 | 4AC | C4-N3 | 6.69 | 1.44 | 1.32 |
| 27 | BA | 501 | 4AC | C4-N3 | 6.69 | 1.44 | 1.32 |
| 1 | Aa | 854 | 5MC | C6-C5 | 6.69 | 1.45 | 1.34 |
| 1 | Aa | 304 | OMU | C2-N1 | 6.68 | 1.49 | 1.38 |
| 27 | BA | 2610 | OMU | C2-N3 | 6.67 | 1.49 | 1.38 |
| 27 | BA | 1899 | 4AC | C4-N3 | 6.67 | 1.44 | 1.32 |
| 27 | BA | 1641 | 4AC | C4-N3 | 6.66 | 1.44 | 1.32 |
| 27 | BA | 244 | 4AC | C4-N3 | 6.66 | 1.44 | 1.32 |
| 27 | BA | 756 | A2M | O4'-C4' | -6.64 | 1.30 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 619 | OMU | C2-N1 | 6.63 | 1.49 | 1.38 |
| 1 | Aa | 730 | 4AC | C4-N3 | 6.61 | 1.44 | 1.32 |
| 1 | Aa | 52 | OMU | C2-N1 | 6.60 | 1.49 | 1.38 |
| 27 | BA | 799 | 4AC | C4-N3 | 6.58 | 1.44 | 1.32 |
| 27 | BA | 1470 | 4AC | C4-N3 | 6.55 | 1.44 | 1.32 |
| 27 | BA | 879 | A2M | O4'-C4' | -6.54 | 1.30 | 1.45 |
| 27 | BA | 1965 | 5MC | C6-C5 | 6.54 | 1.45 | 1.34 |
| 27 | BA | 2581 | 4SU | C2-N3 | 6.48 | 1.49 | 1.38 |
| 1 | Aa | 1352 | 5MC | C4-N3 | 6.48 | 1.45 | 1.34 |
| 27 | BA | 2590 | 4AC | C4-N3 | 6.48 | 1.44 | 1.32 |
| 27 | BA | 1265 | A2M | O4'-C4' | -6.48 | 1.30 | 1.45 |
| 27 | BA | 849 | A2M | O4'-C4' | -6.48 | 1.30 | 1.45 |
| 1 | Aa | 304 | OMU | C2-N3 | 6.45 | 1.49 | 1.38 |
| 27 | BA | 1969 | OMU | C2-N1 | 6.45 | 1.48 | 1.38 |
| 1 | Aa | 525 | 4AC | C4-N3 | 6.45 | 1.44 | 1.32 |
| 27 | BA | 1427 | 4AC | C4-N3 | 6.43 | 1.44 | 1.32 |
| 27 | BA | 1776 | OMU | C2-N1 | 6.43 | 1.48 | 1.38 |
| 27 | BA | 768 | OMU | C2-N1 | 6.42 | 1.48 | 1.38 |
| 27 | BA | 2121 | 4AC | C4-N3 | 6.40 | 1.43 | 1.32 |
| 27 | BA | 1319 | OMU | C2-N1 | 6.40 | 1.48 | 1.38 |
| 1 | Aa | 240 | OMU | C2-N3 | 6.39 | 1.49 | 1.38 |
| 27 | BA | 2797 | 4AC | C4-N3 | 6.39 | 1.43 | 1.32 |
| 1 | Aa | 457 | 5MC | C4-N3 | 6.38 | 1.44 | 1.34 |
| 27 | BA | 713 | 4AC | C4-N3 | 6.38 | 1.43 | 1.32 |
| 27 | BA | 1319 | OMU | C2-N3 | 6.36 | 1.49 | 1.38 |
| 1 | Aa | 8 | OMU | C2-N1 | 6.35 | 1.48 | 1.38 |
| 27 | BA | 1955 | 4AC | C4-N3 | 6.31 | 1.43 | 1.32 |
| 27 | BA | 1551 | OMU | C2-N3 | 6.29 | 1.49 | 1.38 |
| 1 | Aa | 1004 | 5MC | C4-N3 | 6.29 | 1.44 | 1.34 |
| 27 | BA | 2553 | 4SU | C2-N3 | 6.29 | 1.49 | 1.38 |
| 1 | Aa | 1476 | 5MC | C4-N3 | 6.27 | 1.44 | 1.34 |
| 1 | Aa | 41 | 4AC | C6-C5 | 6.25 | 1.49 | 1.35 |
| 27 | BA | 619 | OMU | C2-N3 | 6.25 | 1.49 | 1.38 |
| 27 | BA | 453 | OMU | C2-N1 | 6.25 | 1.48 | 1.38 |
| 1 | Aa | 1276 | 5MC | C4-N3 | 6.24 | 1.44 | 1.34 |
| 1 | Aa | 52 | OMU | C2-N3 | 6.24 | 1.49 | 1.38 |
| 27 | BA | 1434 | 4AC | C4-N3 | 6.23 | 1.43 | 1.32 |
| 1 | Aa | 942 | 5MC | C4-N3 | 6.22 | 1.44 | 1.34 |
| 1 | Aa | 136 | 4AC | C6-C5 | 6.22 | 1.49 | 1.35 |
| 27 | BA | 805 | 4AC | C4-N3 | 6.22 | 1.43 | 1.32 |
| 27 | BA | 201 | 4AC | C4-N3 | 6.22 | 1.43 | 1.32 |
| 1 | Aa | 847 | 4AC | C6-C5 | 6.21 | 1.49 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 2992 | 4AC | C6-C5 | 6.21 | 1.49 | 1.35 |
| 27 | BA | 2605 | 5MC | C4-N3 | 6.21 | 1.44 | 1.34 |
| 1 | Aa | 464 | 5MC | C4-N3 | 6.20 | 1.44 | 1.34 |
| 1 | Aa | 358 | 4AC | C6-C5 | 6.19 | 1.49 | 1.35 |
| 27 | BA | 2542 | OMU | C2-N1 | 6.15 | 1.48 | 1.38 |
| 27 | BA | 2035 | 5MC | C4-N3 | 6.15 | 1.44 | 1.34 |
| 27 | BA | 657 | OMU | C2-N1 | 6.14 | 1.48 | 1.38 |
| 27 | BA | 1480 | OMU | C2-N1 | 6.13 | 1.48 | 1.38 |
| 27 | BA | 1305 | 4AC | C6-C5 | 6.12 | 1.49 | 1.35 |
| 1 | Aa | 1217 | 4AC | C6-C5 | 6.09 | 1.49 | 1.35 |
| 27 | BA | 768 | OMU | C2-N3 | 6.09 | 1.48 | 1.38 |
| 1 | Aa | 818 | 4AC | C6-C5 | 6.09 | 1.49 | 1.35 |
| 27 | BA | 1340 | OMU | C2-N1 | 6.09 | 1.48 | 1.38 |
| 27 | BA | 2863 | 5MC | C4-N3 | 6.08 | 1.44 | 1.34 |
| 1 | Aa | 1354 | OMC | C2-N3 | 6.06 | 1.48 | 1.36 |
| 27 | BA | 2997 | 4AC | C6-C5 | 6.06 | 1.49 | 1.35 |
| 1 | Aa | 5 | 4AC | C6-C5 | 6.06 | 1.49 | 1.35 |
| 27 | BA | 1969 | OMU | C2-N3 | 6.05 | 1.48 | 1.38 |
| 1 | Aa | 457 | 5MC | C2-N3 | 6.04 | 1.48 | 1.36 |
| 27 | BA | 3009 | 4AC | C6-C5 | 6.04 | 1.49 | 1.35 |
| 27 | BA | 869 | OMC | C2-N3 | 6.04 | 1.48 | 1.36 |
| 27 | BA | 418 | 4AC | C6-C5 | 6.00 | 1.49 | 1.35 |
| 1 | Aa | 535 | OMC | C2-N3 | 5.98 | 1.48 | 1.36 |
| 27 | BA | 124 | 4AC | C4-N3 | 5.97 | 1.43 | 1.32 |
| 27 | BA | 2542 | OMU | C2-N3 | 5.96 | 1.48 | 1.38 |
| 1 | Aa | 464 | 5MC | C2-N3 | 5.96 | 1.48 | 1.36 |
| 1 | Aa | 1352 | 5MC | C2-N3 | 5.96 | 1.48 | 1.36 |
| 1 | Aa | 8 | OMU | C2-N3 | 5.94 | 1.48 | 1.38 |
| 27 | BA | 2656 | OMU | C2-N3 | 5.94 | 1.48 | 1.38 |
| 1 | Aa | 827 | 4AC | C6-C5 | 5.93 | 1.48 | 1.35 |
| 27 | BA | 2581 | 4SU | C5-C4 | 5.93 | 1.50 | 1.42 |
| 27 | BA | 1696 | 5MC | C4-N3 | 5.93 | 1.44 | 1.34 |
| 27 | BA | 2553 | 4SU | C6-C5 | 5.92 | 1.48 | 1.35 |
| 27 | BA | 453 | OMU | C2-N3 | 5.92 | 1.48 | 1.38 |
| 1 | Aa | 501 | 4AC | C6-C5 | 5.92 | 1.48 | 1.35 |
| 1 | Aa | 697 | 4AC | C6-C5 | 5.91 | 1.48 | 1.35 |
| 1 | Aa | 682 | 4AC | C6-C5 | 5.90 | 1.48 | 1.35 |
| 27 | BA | 2035 | 5MC | C2-N3 | 5.90 | 1.48 | 1.36 |
| 1 | Aa | 373 | 4AC | C6-C5 | 5.90 | 1.48 | 1.35 |
| 1 | Aa | 569 | 4AC | C6-C5 | 5.89 | 1.48 | 1.35 |
| 27 | BA | 1480 | OMU | C2-N3 | 5.89 | 1.48 | 1.38 |
| 27 | BA | 56 | 4AC | C6-C5 | 5.88 | 1.48 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Aa | 942 | 5MC | C2-N3 | 5.88 | 1.48 | 1.36 |
| 1 | Aa | 605 | 4AC | C7-N4 | 5.87 | 1.48 | 1.37 |
| 1 | Aa | 1476 | 5MC | C2-N3 | 5.86 | 1.48 | 1.36 |
| 27 | BA | 2581 | 4SU | C6-C5 | 5.85 | 1.48 | 1.35 |
| 27 | BA | 2656 | OMU | C2-N1 | 5.84 | 1.47 | 1.38 |
| 1 | Aa | 1276 | 5MC | C2-N3 | 5.84 | 1.48 | 1.36 |
| 1 | Aa | 752 | OMC | C2-N3 | 5.83 | 1.48 | 1.36 |
| 27 | BA | 1641 | 4AC | C6-C5 | 5.82 | 1.48 | 1.35 |
| 1 | Aa | 854 | 5MC | C4-N3 | 5.81 | 1.44 | 1.34 |
| 1 | Aa | 730 | 4AC | C6-C5 | 5.81 | 1.48 | 1.35 |
| 27 | BA | 1820 | OMC | C2-N3 | 5.80 | 1.48 | 1.36 |
| 27 | BA | 730 | 4AC | C6-C5 | 5.80 | 1.48 | 1.35 |
| 1 | Aa | 1459 | 4AC | C4-N3 | 5.79 | 1.42 | 1.32 |
| 1 | Aa | 190 | OMC | C2-N3 | 5.79 | 1.48 | 1.36 |
| 27 | BA | 1375 | 4AC | C6-C5 | 5.78 | 1.48 | 1.35 |
| 27 | BA | 2055 | 5MC | C4-N3 | 5.77 | 1.43 | 1.34 |
| 27 | BA | 353 | OMG | C2-N3 | 5.77 | 1.47 | 1.33 |
| 27 | BA | 754 | OMC | C2-N3 | 5.77 | 1.48 | 1.36 |
| 1 | Aa | 1004 | 5MC | C2-N3 | 5.76 | 1.48 | 1.36 |
| 27 | BA | 501 | 4AC | C6-C5 | 5.75 | 1.48 | 1.35 |
| 27 | BA | 3023 | 4AC | C6-C5 | 5.74 | 1.48 | 1.35 |
| 1 | Aa | 672 | 5MC | C4-N3 | 5.74 | 1.43 | 1.34 |
| 1 | Aa | 605 | 4AC | C6-C5 | 5.74 | 1.48 | 1.35 |
| 27 | BA | 250 | OMC | C2-N3 | 5.73 | 1.48 | 1.36 |
| 27 | BA | 1396 | 4AC | C7-N4 | 5.72 | 1.47 | 1.37 |
| 1 | Aa | 136 | 4AC | C7-N4 | 5.72 | 1.47 | 1.37 |
| 1 | Aa | 298 | 4AC | C7-N4 | 5.71 | 1.47 | 1.37 |
| 27 | BA | 335 | 4AC | C6-C5 | 5.71 | 1.48 | 1.35 |
| 27 | BA | 2590 | 4AC | C6-C5 | 5.71 | 1.48 | 1.35 |
| 27 | BA | 1340 | OMU | C2-N3 | 5.70 | 1.48 | 1.38 |
| 27 | BA | 713 | 4AC | C6-C5 | 5.70 | 1.48 | 1.35 |
| 27 | BA | 2528 | OMG | C2-N3 | 5.69 | 1.47 | 1.33 |
| 27 | BA | 1776 | OMU | C2-N3 | 5.69 | 1.48 | 1.38 |
| 27 | BA | 34 | OMU | C2-N1 | 5.69 | 1.47 | 1.38 |
| 27 | BA | 1431 | 4AC | C7-N4 | 5.68 | 1.47 | 1.37 |
| 27 | BA | 2553 | 4SU | C5-C4 | 5.68 | 1.49 | 1.42 |
| 27 | BA | 718 | OMC | C2-N3 | 5.67 | 1.47 | 1.36 |
| 1 | Aa | 697 | 4AC | C7-N4 | 5.66 | 1.47 | 1.37 |
| 1 | Aa | 825 | OMC | C2-N3 | 5.65 | 1.47 | 1.36 |
| 1 | Aa | 1361 | OMC | C2-N3 | 5.65 | 1.47 | 1.36 |
| 27 | BA | 27 | 4AC | C6-C5 | 5.64 | 1.48 | 1.35 |
| 27 | BA | 778 | 4AC | C6-C5 | 5.64 | 1.48 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 858 | 4AC | C6-C5 | 5.64 | 1.48 | 1.35 |
| 27 | BA | 2832 | 4AC | C6-C5 | 5.64 | 1.48 | 1.35 |
| 27 | BA | 1470 | 4AC | C6-C5 | 5.63 | 1.48 | 1.35 |
| 27 | BA | 2838 | 4AC | C6-C5 | 5.61 | 1.48 | 1.35 |
| 27 | BA | 1305 | 4AC | C7-N4 | 5.61 | 1.47 | 1.37 |
| 27 | BA | 1750 | OMC | C2-N3 | 5.60 | 1.47 | 1.36 |
| 1 | Aa | 41 | 4AC | C7-N4 | 5.59 | 1.47 | 1.37 |
| 27 | BA | 1543 | 4AC | C6-C5 | 5.59 | 1.48 | 1.35 |
| 27 | BA | 2075 | 5MC | C4-N3 | 5.59 | 1.43 | 1.34 |
| 27 | BA | 2610 | OMU | C6-C5 | 5.58 | 1.48 | 1.35 |
| 27 | BA | 2780 | 4AC | C7-N4 | 5.58 | 1.47 | 1.37 |
| 1 | Aa | 358 | 4AC | C7-N4 | 5.58 | 1.47 | 1.37 |
| 1 | Aa | 525 | 4AC | C6-C5 | 5.57 | 1.48 | 1.35 |
| 1 | Aa | 1217 | 4AC | C7-N4 | 5.57 | 1.47 | 1.37 |
| 1 | Aa | 854 | 5MC | C2-N3 | 5.56 | 1.47 | 1.36 |
| 27 | BA | 1337 | 4AC | C6-C5 | 5.56 | 1.48 | 1.35 |
| 27 | BA | 418 | 4AC | C7-N4 | 5.55 | 1.47 | 1.37 |
| 27 | BA | 657 | OMU | C2-N3 | 5.54 | 1.47 | 1.38 |
| 1 | Aa | 298 | 4AC | C6-C5 | 5.54 | 1.47 | 1.35 |
| 27 | BA | 2838 | 4AC | C7-N4 | 5.54 | 1.47 | 1.37 |
| 27 | BA | 1548 | 5MU | C6-C5 | 5.53 | 1.43 | 1.34 |
| 27 | BA | 2780 | 4AC | C6-C5 | 5.53 | 1.47 | 1.35 |
| 27 | BA | 34 | OMU | C2-N3 | 5.53 | 1.47 | 1.38 |
| 1 | Aa | 569 | 4AC | C7-N4 | 5.52 | 1.47 | 1.37 |
| 27 | BA | 1543 | 4AC | C7-N4 | 5.51 | 1.47 | 1.37 |
| 1 | Aa | 994 | OMG | C2-N3 | 5.50 | 1.46 | 1.33 |
| 1 | Aa | 1358 | OMU | C2-N1 | 5.50 | 1.47 | 1.38 |
| 1 | Aa | 827 | 4AC | C7-N4 | 5.48 | 1.47 | 1.37 |
| 27 | BA | 1427 | 4AC | C6-C5 | 5.48 | 1.47 | 1.35 |
| 1 | Aa | 913 | OMG | C2-N3 | 5.48 | 1.46 | 1.33 |
| 27 | BA | 3023 | 4AC | C7-N4 | 5.47 | 1.47 | 1.37 |
| 27 | BA | 2384 | 5MU | C6-C5 | 5.47 | 1.43 | 1.34 |
| 27 | BA | 27 | 4AC | C7-N4 | 5.47 | 1.47 | 1.37 |
| 1 | Aa | 296 | OMC | C2-N3 | 5.46 | 1.47 | 1.36 |
| 27 | BA | 1357 | 4AC | C6-C5 | 5.46 | 1.47 | 1.35 |
| 27 | BA | 2992 | 4AC | C7-N4 | 5.46 | 1.47 | 1.37 |
| 27 | BA | 561 | OMC | C2-N3 | 5.46 | 1.47 | 1.36 |
| 1 | Aa | 190 | OMC | C6-C5 | 5.46 | 1.47 | 1.35 |
| 1 | Aa | 636 | OMG | C2-N3 | 5.44 | 1.46 | 1.33 |
| 1 | Aa | 501 | 4AC | C7-N4 | 5.43 | 1.47 | 1.37 |
| 27 | BA | 2545 | OMC | C2-N3 | 5.43 | 1.47 | 1.36 |
| 27 | BA | 1551 | OMU | C6-C5 | 5.43 | 1.47 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 201 | 4AC | C6-C5 | 5.41 | 1.47 | 1.35 |
| 1 | Aa | 672 | 5MC | C2-N3 | 5.41 | 1.47 | 1.36 |
| 27 | BA | 2124 | OMC | C2-N3 | 5.41 | 1.47 | 1.36 |
| 1 | Aa | 682 | 4AC | C7-N4 | 5.40 | 1.47 | 1.37 |
| 27 | BA | 2630 | OMC | C2-N3 | 5.40 | 1.47 | 1.36 |
| 27 | BA | 2797 | 4AC | C6-C5 | 5.40 | 1.47 | 1.35 |
| 27 | BA | 2457 | LHH | C7-N4 | 5.39 | 1.47 | 1.37 |
| 27 | BA | 2159 | 4AC | C6-C5 | 5.38 | 1.47 | 1.35 |
| 27 | BA | 376 | 4AC | C6-C5 | 5.37 | 1.47 | 1.35 |
| 27 | BA | 805 | 4AC | C7-N4 | 5.37 | 1.47 | 1.37 |
| 27 | BA | 1434 | 4AC | C6-C5 | 5.36 | 1.47 | 1.35 |
| 27 | BA | 2019 | OMG | C2-N3 | 5.35 | 1.46 | 1.33 |
| 27 | BA | 2055 | 5MC | C2-N3 | 5.35 | 1.47 | 1.36 |
| 27 | BA | 2571 | OMC | C2-N3 | 5.34 | 1.47 | 1.36 |
| 1 | Aa | 752 | OMC | C6-C5 | 5.34 | 1.47 | 1.35 |
| 1 | Aa | 1217 | 4AC | C2-N3 | 5.34 | 1.47 | 1.36 |
| 27 | BA | 244 | 4AC | C6-C5 | 5.34 | 1.47 | 1.35 |
| 27 | BA | 1790 | OMC | C2-N3 | 5.31 | 1.47 | 1.36 |
| 27 | BA | 2863 | 5MC | C2-N3 | 5.31 | 1.47 | 1.36 |
| 1 | Aa | 1478 | 5MC | C4-N3 | 5.30 | 1.43 | 1.34 |
| 1 | Aa | 876 | OMG | C2-N3 | 5.30 | 1.46 | 1.33 |
| 27 | BA | 1955 | 4AC | C6-C5 | 5.30 | 1.47 | 1.35 |
| 27 | BA | 1375 | 4AC | C7-N4 | 5.30 | 1.47 | 1.37 |
| 27 | BA | 2595 | OMC | C2-N3 | 5.29 | 1.47 | 1.36 |
| 1 | Aa | 1361 | OMC | C6-C5 | 5.29 | 1.47 | 1.35 |
| 27 | BA | 1810 | 4AC | C6-C5 | 5.29 | 1.47 | 1.35 |
| 1 | Aa | 1358 | OMU | C2-N3 | 5.29 | 1.47 | 1.38 |
| 27 | BA | 730 | 4AC | C7-N4 | 5.29 | 1.47 | 1.37 |
| 1 | Aa | 240 | OMU | C6-C5 | 5.28 | 1.47 | 1.35 |
| 1 | Aa | 535 | OMC | C6-C5 | 5.28 | 1.47 | 1.35 |
| 1 | Aa | 373 | 4AC | C7-N4 | 5.27 | 1.47 | 1.37 |
| 27 | BA | 124 | 4AC | C7-N4 | 5.27 | 1.46 | 1.37 |
| 27 | BA | 1810 | 4AC | C7-N4 | 5.26 | 1.46 | 1.37 |
| 1 | Aa | 296 | OMC | C6-C5 | 5.26 | 1.47 | 1.35 |
| 1 | Aa | 1478 | 5MC | C2-N3 | 5.26 | 1.47 | 1.36 |
| 27 | BA | 215 | OMG | C2-N3 | 5.26 | 1.46 | 1.33 |
| 27 | BA | 124 | 4AC | C6-C5 | 5.26 | 1.47 | 1.35 |
| 27 | BA | 335 | 4AC | C7-N4 | 5.26 | 1.46 | 1.37 |
| 27 | BA | 799 | 4AC | C6-C5 | 5.25 | 1.47 | 1.35 |
| 27 | BA | 1396 | 4AC | C6-C5 | 5.25 | 1.47 | 1.35 |
| 27 | BA | 2121 | 4AC | C6-C5 | 5.23 | 1.47 | 1.35 |
| 27 | BA | 1431 | 4AC | C6-C5 | 5.22 | 1.47 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 2571 | OMC | C6-C5 | 5.22 | 1.47 | 1.35 |
| 27 | BA | 1899 | 4AC | C6-C5 | 5.22 | 1.47 | 1.35 |
| 1 | Aa | 818 | 4AC | C7-N4 | 5.21 | 1.46 | 1.37 |
| 27 | BA | 778 | 4AC | C7-N4 | 5.21 | 1.46 | 1.37 |
| 27 | BA | 1965 | 5MC | C4-N3 | 5.20 | 1.42 | 1.34 |
| 27 | BA | 799 | 4AC | C7-N4 | 5.20 | 1.46 | 1.37 |
| 27 | BA | 1899 | 4AC | C7-N4 | 5.19 | 1.46 | 1.37 |
| 27 | BA | 2018 | OMC | C2-N3 | 5.19 | 1.46 | 1.36 |
| 1 | Aa | 479 | OMU | C6-C5 | 5.18 | 1.47 | 1.35 |
| 27 | BA | 1696 | 5MC | C2-N3 | 5.18 | 1.46 | 1.36 |
| 1 | Aa | 1217 | 4AC | C4-N4 | 5.18 | 1.47 | 1.39 |
| 27 | BA | 433 | 4AC | C7-N4 | 5.18 | 1.46 | 1.37 |
| 27 | BA | 1470 | 4AC | C7-N4 | 5.17 | 1.46 | 1.37 |
| 27 | BA | 2159 | 4AC | C7-N4 | 5.17 | 1.46 | 1.37 |
| 27 | BA | 2075 | 5MC | C2-N3 | 5.17 | 1.46 | 1.36 |
| 1 | Aa | 1107 | OMG | C2-N3 | 5.17 | 1.45 | 1.33 |
| 27 | BA | 944 | 5MC | C2-N3 | 5.16 | 1.46 | 1.36 |
| 1 | Aa | 320 | OMG | C2-N3 | 5.16 | 1.45 | 1.33 |
| 1 | Aa | 304 | OMU | C6-C5 | 5.16 | 1.47 | 1.35 |
| 1 | Aa | 138 | OMG | C2-N3 | 5.16 | 1.45 | 1.33 |
| 27 | BA | 201 | 4AC | C7-N4 | 5.15 | 1.46 | 1.37 |
| 27 | BA | 3009 | 4AC | C7-N4 | 5.14 | 1.46 | 1.37 |
| 27 | BA | 244 | 4AC | C7-N4 | 5.14 | 1.46 | 1.37 |
| 27 | BA | 2521 | OMG | C2-N3 | 5.14 | 1.45 | 1.33 |
| 27 | BA | 2047 | OMC | C6-C5 | 5.13 | 1.47 | 1.35 |
| 27 | BA | 2797 | 4AC | C7-N4 | 5.13 | 1.46 | 1.37 |
| 1 | Aa | 825 | OMC | C6-C5 | 5.13 | 1.47 | 1.35 |
| 27 | BA | 713 | 4AC | C7-N4 | 5.12 | 1.46 | 1.37 |
| 27 | BA | 1641 | 4AC | C7-N4 | 5.11 | 1.46 | 1.37 |
| 1 | Aa | 1354 | OMC | C6-C5 | 5.11 | 1.46 | 1.35 |
| 1 | Aa | 52 | OMU | C6-C5 | 5.10 | 1.46 | 1.35 |
| 27 | BA | 944 | 5MC | C4-N3 | 5.10 | 1.42 | 1.34 |
| 27 | BA | 1357 | 4AC | C7-N4 | 5.10 | 1.46 | 1.37 |
| 1 | Aa | 1265 | OMG | C2-N3 | 5.08 | 1.45 | 1.33 |
| 1 | Aa | 8 | OMU | C6-C5 | 5.08 | 1.46 | 1.35 |
| 27 | BA | 1427 | 4AC | C7-N4 | 5.07 | 1.46 | 1.37 |
| 27 | BA | 1434 | 4AC | C7-N4 | 5.07 | 1.46 | 1.37 |
| 27 | BA | 2016 | OMG | C2-N3 | 5.07 | 1.45 | 1.33 |
| 1 | Aa | 771 | OMG | C2-N3 | 5.06 | 1.45 | 1.33 |
| 27 | BA | 2605 | 5MC | C2-N3 | 5.06 | 1.46 | 1.36 |
| 27 | BA | 2832 | 4AC | C7-N4 | 5.05 | 1.46 | 1.37 |
| 27 | BA | 754 | OMC | C6-C5 | 5.05 | 1.46 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 2590 | 4AC | C7-N4 | 5.05 | 1.46 | 1.37 |
| 1 | Aa | 730 | 4AC | C7-N4 | 5.04 | 1.46 | 1.37 |
| 27 | BA | 619 | OMU | C6-C5 | 5.04 | 1.46 | 1.35 |
| 1 | Aa | 1026 | OMG | C2-N3 | 5.04 | 1.45 | 1.33 |
| 27 | BA | 2047 | OMC | C2-N3 | 5.04 | 1.46 | 1.36 |
| 27 | BA | 63 | OMG | C2-N3 | 5.02 | 1.45 | 1.33 |
| 1 | Aa | 605 | 4AC | C2-N3 | 5.02 | 1.46 | 1.36 |
| 27 | BA | 2997 | 4AC | C7-N4 | 5.02 | 1.46 | 1.37 |
| 27 | BA | 250 | OMC | C6-C5 | 5.01 | 1.46 | 1.35 |
| 27 | BA | 2780 | 4AC | C2-N1 | 5.00 | 1.50 | 1.40 |
| 27 | BA | 1953 | OMG | C2-N3 | 5.00 | 1.45 | 1.33 |
| 27 | BA | 376 | 4AC | C7-N4 | 4.99 | 1.46 | 1.37 |
| 27 | BA | 2545 | OMC | C6-C5 | 4.99 | 1.46 | 1.35 |
| 1 | Aa | 5 | 4AC | C7-N4 | 4.99 | 1.46 | 1.37 |
| 27 | BA | 1934 | 4AC | C6-C5 | 4.99 | 1.46 | 1.35 |
| 27 | BA | 2992 | 4AC | C2-N3 | 4.97 | 1.46 | 1.36 |
| 27 | BA | 912 | OMG | C2-N3 | 4.97 | 1.45 | 1.33 |
| 1 | Aa | 498 | OMG | C2-N3 | 4.97 | 1.45 | 1.33 |
| 27 | BA | 501 | 4AC | C7-N4 | 4.97 | 1.46 | 1.37 |
| 27 | BA | 1934 | 4AC | C7-N4 | 4.97 | 1.46 | 1.37 |
| 27 | BA | 833 | OMG | C2-N3 | 4.97 | 1.45 | 1.33 |
| 27 | BA | 1305 | 4AC | C2-N3 | 4.96 | 1.46 | 1.36 |
| 1 | Aa | 670 | 2MG | C2-N2 | 4.96 | 1.44 | 1.33 |
| 27 | BA | 433 | 4AC | C6-C5 | 4.94 | 1.46 | 1.35 |
| 27 | BA | 2780 | 4AC | C2-N3 | 4.93 | 1.46 | 1.36 |
| 27 | BA | 3023 | 4AC | C2-N3 | 4.92 | 1.46 | 1.36 |
| 27 | BA | 754 | OMC | C4-N3 | 4.92 | 1.44 | 1.34 |
| 1 | Aa | 41 | 4AC | C2-N1 | 4.92 | 1.50 | 1.40 |
| 1 | Aa | 381 | OMG | C2-N3 | 4.92 | 1.45 | 1.33 |
| 27 | BA | 1480 | OMU | C6-C5 | 4.91 | 1.46 | 1.35 |
| 27 | BA | 353 | OMG | C4-N3 | 4.91 | 1.49 | 1.37 |
| 27 | BA | 561 | OMC | C6-C5 | 4.91 | 1.46 | 1.35 |
| 27 | BA | 526 | LHH | C7-N4 | 4.91 | 1.46 | 1.37 |
| 27 | BA | 2657 | OMG | C2-N3 | 4.90 | 1.45 | 1.33 |
| 1 | Aa | 136 | 4AC | C2-N3 | 4.90 | 1.46 | 1.36 |
| 27 | BA | 1892 | OMG | C2-N3 | 4.90 | 1.45 | 1.33 |
| 27 | BA | 1543 | 4AC | C2-N3 | 4.89 | 1.46 | 1.36 |
| 27 | BA | 730 | 4AC | C2-N1 | 4.89 | 1.50 | 1.40 |
| 27 | BA | 2992 | 4AC | C2-N1 | 4.89 | 1.50 | 1.40 |
| 1 | Aa | 525 | 4AC | C7-N4 | 4.89 | 1.46 | 1.37 |
| 1 | Aa | 373 | 4AC | C2-N3 | 4.89 | 1.46 | 1.36 |
| 1 | Aa | 682 | 4AC | C2-N3 | 4.89 | 1.46 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 2838 | 4AC | C2-N3 | 4.89 | 1.46 | 1.36 |
| 1 | Aa | 1020 | LHH | C7-N4 | 4.89 | 1.46 | 1.37 |
| 27 | BA | 2595 | OMC | C6-C5 | 4.89 | 1.46 | 1.35 |
| 1 | Aa | 136 | 4AC | C2-N1 | 4.89 | 1.50 | 1.40 |
| 1 | Aa | 382 | OMG | C2-N3 | 4.88 | 1.45 | 1.33 |
| 27 | BA | 1969 | OMU | C6-C5 | 4.88 | 1.46 | 1.35 |
| 1 | Aa | 446 | OMG | C2-N3 | 4.88 | 1.45 | 1.33 |
| 1 | Aa | 450 | OMG | C2-N3 | 4.88 | 1.45 | 1.33 |
| 27 | BA | 718 | OMC | C4-N3 | 4.87 | 1.44 | 1.34 |
| 27 | BA | 2728 | OMG | C2-N3 | 4.87 | 1.45 | 1.33 |
| 1 | Aa | 298 | 4AC | C2-N3 | 4.87 | 1.46 | 1.36 |
| 1 | Aa | 1217 | 4AC | C2-N1 | 4.87 | 1.50 | 1.40 |
| 27 | BA | 1965 | 5MC | C2-N3 | 4.86 | 1.46 | 1.36 |
| 27 | BA | 1750 | OMC | C6-C5 | 4.86 | 1.46 | 1.35 |
| 27 | BA | 778 | 4AC | C2-N1 | 4.86 | 1.50 | 1.40 |
| 1 | Aa | 659 | OMG | C2-N3 | 4.86 | 1.45 | 1.33 |
| 27 | BA | 1337 | 4AC | C7-N4 | 4.85 | 1.46 | 1.37 |
| 27 | BA | 1641 | 4AC | C2-N1 | 4.85 | 1.50 | 1.40 |
| 27 | BA | 56 | 4AC | C7-N4 | 4.85 | 1.46 | 1.37 |
| 27 | BA | 1810 | 4AC | C2-N3 | 4.85 | 1.46 | 1.36 |
| 1 | Aa | 827 | 4AC | C2-N3 | 4.85 | 1.46 | 1.36 |
| 27 | BA | 2324 | OMG | C2-N3 | 4.84 | 1.45 | 1.33 |
| 27 | BA | 453 | OMU | C6-C5 | 4.84 | 1.46 | 1.35 |
| 27 | BA | 2019 | OMG | C4-N3 | 4.84 | 1.49 | 1.37 |
| 27 | BA | 2124 | OMC | C6-C5 | 4.84 | 1.46 | 1.35 |
| 27 | BA | 2997 | 4AC | C2-N3 | 4.84 | 1.46 | 1.36 |
| 1 | Aa | 246 | OMG | C2-N3 | 4.83 | 1.44 | 1.33 |
| 27 | BA | 2838 | 4AC | C2-N1 | 4.83 | 1.50 | 1.40 |
| 27 | BA | 718 | OMC | C6-C5 | 4.83 | 1.46 | 1.35 |
| 1 | Aa | 358 | 4AC | C2-N3 | 4.82 | 1.46 | 1.36 |
| 1 | Aa | 373 | 4AC | C2-N1 | 4.82 | 1.50 | 1.40 |
| 27 | BA | 376 | 4AC | C2-N3 | 4.82 | 1.46 | 1.36 |
| 27 | BA | 335 | 4AC | C2-N1 | 4.82 | 1.50 | 1.40 |
| 1 | Aa | 1025 | OMG | C2-N3 | 4.81 | 1.44 | 1.33 |
| 27 | BA | 1799 | OMG | C2-N3 | 4.81 | 1.44 | 1.33 |
| 27 | BA | 250 | OMC | C4-N3 | 4.81 | 1.44 | 1.34 |
| 27 | BA | 2672 | OMG | C2-N3 | 4.80 | 1.44 | 1.33 |
| 27 | BA | 1955 | 4AC | C7-N4 | 4.80 | 1.46 | 1.37 |
| 27 | BA | 2379 | OMG | C2-N3 | 4.79 | 1.44 | 1.33 |
| 27 | BA | 290 | OMG | C2-N3 | 4.79 | 1.44 | 1.33 |
| 27 | BA | 869 | OMC | C4-N3 | 4.79 | 1.44 | 1.34 |
| 1 | Aa | 605 | 4AC | C2-N1 | 4.78 | 1.50 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 56 | 4AC | C2-N3 | 4.78 | 1.46 | 1.36 |
| 1 | Aa | 682 | 4AC | C2-N1 | 4.78 | 1.50 | 1.40 |
| 27 | BA | 2353 | OMG | C2-N3 | 4.78 | 1.44 | 1.33 |
| 1 | Aa | 1354 | OMC | C4-N3 | 4.78 | 1.44 | 1.34 |
| 27 | BA | 27 | 4AC | C2-N3 | 4.78 | 1.46 | 1.36 |
| 27 | BA | 2528 | OMG | C4-N3 | 4.77 | 1.48 | 1.37 |
| 1 | Aa | 994 | OMG | C4-N3 | 4.77 | 1.48 | 1.37 |
| 27 | BA | 1398 | OMG | C2-N3 | 4.77 | 1.44 | 1.33 |
| 27 | BA | 805 | 4AC | C6-C5 | 4.76 | 1.46 | 1.35 |
| 27 | BA | 869 | OMC | C6-C5 | 4.75 | 1.46 | 1.35 |
| 27 | BA | 1799 | OMG | C6-N1 | 4.75 | 1.44 | 1.37 |
| 1 | Aa | 501 | 4AC | C2-N1 | 4.75 | 1.50 | 1.40 |
| 27 | BA | 617 | LHH | C7-N4 | 4.74 | 1.46 | 1.37 |
| 27 | BA | 298 | 5MU | C6-C5 | 4.74 | 1.42 | 1.34 |
| 1 | Aa | 569 | 4AC | C2-N3 | 4.74 | 1.46 | 1.36 |
| 27 | BA | 572 | 5MU | C6-C5 | 4.74 | 1.42 | 1.34 |
| 1 | Aa | 892 | OMG | C2-N3 | 4.74 | 1.44 | 1.33 |
| 27 | BA | 2688 | 5MU | C6-C5 | 4.73 | 1.42 | 1.34 |
| 1 | Aa | 1434 | OMG | C2-N3 | 4.73 | 1.44 | 1.33 |
| 27 | BA | 34 | OMU | C6-C5 | 4.73 | 1.46 | 1.35 |
| 27 | BA | 27 | 4AC | C2-N1 | 4.73 | 1.50 | 1.40 |
| 1 | Aa | 697 | 4AC | C2-N1 | 4.72 | 1.50 | 1.40 |
| 27 | BA | 1525 | OMG | C2-N3 | 4.72 | 1.44 | 1.33 |
| 27 | BA | 1790 | OMC | C6-C5 | 4.72 | 1.46 | 1.35 |
| 1 | Aa | 229 | LHH | C7-N4 | 4.72 | 1.45 | 1.37 |
| 27 | BA | 2010 | OMG | C2-N3 | 4.71 | 1.44 | 1.33 |
| 1 | Aa | 697 | 4AC | C2-N3 | 4.71 | 1.45 | 1.36 |
| 27 | BA | 1106 | OMG | C2-N3 | 4.70 | 1.44 | 1.33 |
| 1 | Aa | 605 | 4AC | C4-N4 | 4.70 | 1.46 | 1.39 |
| 27 | BA | 418 | 4AC | C2-N3 | 4.70 | 1.45 | 1.36 |
| 27 | BA | 433 | 4AC | C2-N3 | 4.70 | 1.45 | 1.36 |
| 1 | Aa | 501 | 4AC | C2-N3 | 4.69 | 1.45 | 1.36 |
| 27 | BA | 1396 | 4AC | C2-N3 | 4.69 | 1.45 | 1.36 |
| 1 | Aa | 913 | OMG | C4-N3 | 4.68 | 1.48 | 1.37 |
| 27 | BA | 2550 | OMG | C2-N3 | 4.68 | 1.44 | 1.33 |
| 1 | Aa | 535 | OMC | C4-N3 | 4.68 | 1.43 | 1.34 |
| 27 | BA | 2527 | OMG | C2-N3 | 4.68 | 1.44 | 1.33 |
| 1 | Aa | 670 | 2MG | C4-N3 | 4.68 | 1.48 | 1.37 |
| 27 | BA | 713 | 4AC | C2-N3 | 4.67 | 1.45 | 1.36 |
| 1 | Aa | 525 | 4AC | C2-N1 | 4.67 | 1.50 | 1.40 |
| 27 | BA | 1431 | 4AC | C2-N1 | 4.67 | 1.50 | 1.40 |
| 1 | Aa | 5 | 4AC | C2-N3 | 4.67 | 1.45 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Aa | 1459 | 4AC | C6-C5 | 4.66 | 1.45 | 1.35 |
| 1 | Aa | 847 | 4AC | C7-N4 | 4.66 | 1.45 | 1.37 |
| 1 | Aa | 752 | OMC | C4-N3 | 4.66 | 1.43 | 1.34 |
| 27 | BA | 1305 | 4AC | C4-N4 | 4.66 | 1.46 | 1.39 |
| 27 | BA | 433 | 4AC | C2-N1 | 4.65 | 1.50 | 1.40 |
| 27 | BA | 2745 | OMG | C2-N3 | 4.65 | 1.44 | 1.33 |
| 1 | Aa | 525 | 4AC | C2-N3 | 4.65 | 1.45 | 1.36 |
| 27 | BA | 1776 | OMU | C6-C5 | 4.65 | 1.45 | 1.35 |
| 27 | BA | 1431 | 4AC | C2-N3 | 4.65 | 1.45 | 1.36 |
| 27 | BA | 1810 | 4AC | C2-N1 | 4.64 | 1.50 | 1.40 |
| 27 | BA | 723 | OMG | C2-N3 | 4.64 | 1.44 | 1.33 |
| 1 | Aa | 852 | OMG | C2-N3 | 4.64 | 1.44 | 1.33 |
| 27 | BA | 1375 | 4AC | C2-N3 | 4.63 | 1.45 | 1.36 |
| 27 | BA | 1470 | 4AC | C2-N1 | 4.63 | 1.50 | 1.40 |
| 1 | Aa | 532 | OMG | C2-N3 | 4.63 | 1.44 | 1.33 |
| 27 | BA | 2553 | 4SU | C4-S4 | -4.62 | 1.59 | 1.68 |
| 27 | BA | 2630 | OMC | C6-C5 | 4.62 | 1.45 | 1.35 |
| 27 | BA | 335 | 4AC | C2-N3 | 4.62 | 1.45 | 1.36 |
| 27 | BA | 1934 | 4AC | C2-N3 | 4.62 | 1.45 | 1.36 |
| 27 | BA | 768 | OMU | C6-C5 | 4.62 | 1.45 | 1.35 |
| 27 | BA | 418 | 4AC | C2-N1 | 4.61 | 1.50 | 1.40 |
| 1 | Aa | 1217 | 4AC | CM7-C7 | 4.61 | 1.60 | 1.50 |
| 27 | BA | 3009 | 4AC | C2-N1 | 4.61 | 1.50 | 1.40 |
| 1 | Aa | 298 | 4AC | C2-N1 | 4.61 | 1.50 | 1.40 |
| 27 | BA | 2595 | OMC | C2-N1 | 4.61 | 1.50 | 1.40 |
| 27 | BA | 858 | 4AC | C2-N3 | 4.61 | 1.45 | 1.36 |
| 27 | BA | 537 | 5MU | C6-C5 | 4.60 | 1.42 | 1.34 |
| 1 | Aa | 190 | OMC | C4-N3 | 4.60 | 1.43 | 1.34 |
| 27 | BA | 376 | 4AC | C2-N1 | 4.60 | 1.50 | 1.40 |
| 1 | Aa | 457 | 5MC | C6-N1 | 4.60 | 1.45 | 1.38 |
| 1 | Aa | 358 | 4AC | C2-N1 | 4.60 | 1.50 | 1.40 |
| 27 | BA | 2997 | 4AC | C2-N1 | 4.59 | 1.50 | 1.40 |
| 27 | BA | 2121 | 4AC | C7-N4 | 4.59 | 1.45 | 1.37 |
| 27 | BA | 1340 | OMU | C6-C5 | 4.59 | 1.45 | 1.35 |
| 27 | BA | 875 | 5MU | C6-C5 | 4.59 | 1.42 | 1.34 |
| 27 | BA | 1396 | 4AC | C2-N1 | 4.59 | 1.49 | 1.40 |
| 27 | BA | 1319 | OMU | C6-C5 | 4.59 | 1.45 | 1.35 |
| 27 | BA | 799 | 4AC | C2-N3 | 4.59 | 1.45 | 1.36 |
| 1 | Aa | 818 | 4AC | C2-N3 | 4.58 | 1.45 | 1.36 |
| 1 | Aa | 457 | 5MC | O4'-C1' | -4.58 | 1.31 | 1.42 |
| 27 | BA | 244 | 4AC | C2-N3 | 4.58 | 1.45 | 1.36 |
| 1 | Aa | 41 | 4AC | C2-N3 | 4.57 | 1.45 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 778 | 4AC | C2-N3 | 4.57 | 1.45 | 1.36 |
| 27 | BA | 3009 | 4AC | C2-N3 | 4.57 | 1.45 | 1.36 |
| 27 | BA | 1357 | 4AC | C2-N1 | 4.57 | 1.49 | 1.40 |
| 27 | BA | 1820 | OMC | C4-N3 | 4.56 | 1.43 | 1.34 |
| 27 | BA | 3023 | 4AC | C2-N1 | 4.56 | 1.49 | 1.40 |
| 27 | BA | 552 | OMG | C2-N3 | 4.56 | 1.44 | 1.33 |
| 27 | BA | 1337 | 4AC | C2-N3 | 4.56 | 1.45 | 1.36 |
| 1 | Aa | 136 | 4AC | C4-N4 | 4.56 | 1.46 | 1.39 |
| 1 | Aa | 818 | 4AC | C2-N1 | 4.55 | 1.49 | 1.40 |
| 1 | Aa | 697 | 4AC | C4-N4 | 4.55 | 1.46 | 1.39 |
| 1 | Aa | 825 | OMC | C4-N3 | 4.55 | 1.43 | 1.34 |
| 27 | BA | 730 | 4AC | C2-N3 | 4.55 | 1.45 | 1.36 |
| 27 | BA | 713 | 4AC | C2-N1 | 4.55 | 1.49 | 1.40 |
| 1 | Aa | 5 | 4AC | C2-N1 | 4.55 | 1.49 | 1.40 |
| 27 | BA | 1427 | 4AC | C2-N1 | 4.55 | 1.49 | 1.40 |
| 27 | BA | 1470 | 4AC | C2-N3 | 4.54 | 1.45 | 1.36 |
| 1 | Aa | 1107 | OMG | C4-N3 | 4.54 | 1.48 | 1.37 |
| 27 | BA | 2016 | OMG | C4-N3 | 4.54 | 1.48 | 1.37 |
| 1 | Aa | 636 | OMG | C4-N3 | 4.53 | 1.48 | 1.37 |
| 27 | BA | 2832 | 4AC | C2-N3 | 4.53 | 1.45 | 1.36 |
| 1 | Aa | 847 | 4AC | C2-N1 | 4.53 | 1.49 | 1.40 |
| 1 | Aa | 569 | 4AC | C2-N1 | 4.52 | 1.49 | 1.40 |
| 27 | BA | 2992 | 4AC | C4-N4 | 4.52 | 1.46 | 1.39 |
| 1 | Aa | 847 | 4AC | C2-N3 | 4.52 | 1.45 | 1.36 |
| 27 | BA | 1934 | 4AC | C2-N1 | 4.51 | 1.49 | 1.40 |
| 27 | BA | 1525 | OMG | C4-N3 | 4.51 | 1.48 | 1.37 |
| 27 | BA | 63 | OMG | C4-N3 | 4.51 | 1.48 | 1.37 |
| 27 | BA | 2955 | LHH | C7-N4 | 4.51 | 1.45 | 1.37 |
| 27 | BA | 501 | 4AC | C2-N3 | 4.51 | 1.45 | 1.36 |
| 1 | Aa | 1476 | 5MC | O4'-C1' | -4.50 | 1.31 | 1.42 |
| 27 | BA | 1790 | OMC | C4-N3 | 4.50 | 1.43 | 1.34 |
| 27 | BA | 1899 | 4AC | C2-N1 | 4.50 | 1.49 | 1.40 |
| 1 | Aa | 876 | OMG | C4-N3 | 4.50 | 1.48 | 1.37 |
| 27 | BA | 365 | OMG | C2-N3 | 4.50 | 1.44 | 1.33 |
| 27 | BA | 2571 | OMC | C4-N3 | 4.49 | 1.43 | 1.34 |
| 27 | BA | 1641 | 4AC | C2-N3 | 4.48 | 1.45 | 1.36 |
| 27 | BA | 1899 | 4AC | C2-N3 | 4.48 | 1.45 | 1.36 |
| 27 | BA | 1305 | 4AC | C2-N1 | 4.48 | 1.49 | 1.40 |
| 1 | Aa | 730 | 4AC | C2-N3 | 4.48 | 1.45 | 1.36 |
| 27 | BA | 2035 | 5MC | O4'-C1' | -4.47 | 1.31 | 1.42 |
| 1 | Aa | 138 | OMG | C4-N3 | 4.47 | 1.48 | 1.37 |
| 1 | Aa | 1276 | 5MC | O4'-C1' | -4.47 | 1.31 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 2159 | 4AC | C2-N3 | 4.47 | 1.45 | 1.36 |
| 27 | BA | 56 | 4AC | C2-N1 | 4.46 | 1.49 | 1.40 |
| 27 | BA | 2542 | OMU | C6-C5 | 4.46 | 1.45 | 1.35 |
| 27 | BA | 1905 | 5MU | C6-C5 | 4.46 | 1.41 | 1.34 |
| 27 | BA | 244 | 4AC | C2-N1 | 4.45 | 1.49 | 1.40 |
| 27 | BA | 501 | 4AC | C2-N1 | 4.45 | 1.49 | 1.40 |
| 27 | BA | 1940 | OMG | C2-N3 | 4.45 | 1.44 | 1.33 |
| 27 | BA | 2521 | OMG | C4-N3 | 4.44 | 1.48 | 1.37 |
| 1 | Aa | 827 | 4AC | C2-N1 | 4.43 | 1.49 | 1.40 |
| 1 | Aa | 1276 | 5MC | C6-N1 | 4.43 | 1.45 | 1.38 |
| 1 | Aa | 1358 | OMU | C6-C5 | 4.43 | 1.45 | 1.35 |
| 27 | BA | 2656 | OMU | C6-C5 | 4.43 | 1.45 | 1.35 |
| 1 | Aa | 320 | OMG | C4-N3 | 4.43 | 1.48 | 1.37 |
| 1 | Aa | 1361 | OMC | C4-N3 | 4.43 | 1.43 | 1.34 |
| 1 | Aa | 1265 | OMG | C4-N3 | 4.43 | 1.48 | 1.37 |
| 27 | BA | 1427 | 4AC | C2-N3 | 4.42 | 1.45 | 1.36 |
| 27 | BA | 2168 | OMG | C2-N3 | 4.42 | 1.43 | 1.33 |
| 27 | BA | 2124 | OMC | C4-N3 | 4.42 | 1.43 | 1.34 |
| 27 | BA | 1375 | 4AC | C2-N1 | 4.42 | 1.49 | 1.40 |
| 27 | BA | 1357 | 4AC | C2-N3 | 4.41 | 1.45 | 1.36 |
| 1 | Aa | 190 | OMC | C4-N4 | 4.41 | 1.44 | 1.33 |
| 1 | Aa | 682 | 4AC | C4-N4 | 4.41 | 1.46 | 1.39 |
| 1 | Aa | 730 | 4AC | C4-N4 | 4.41 | 1.46 | 1.39 |
| 1 | Aa | 1026 | OMG | C4-N3 | 4.41 | 1.48 | 1.37 |
| 1 | Aa | 1476 | 5MC | C6-N1 | 4.40 | 1.45 | 1.38 |
| 27 | BA | 2590 | 4AC | C2-N1 | 4.39 | 1.49 | 1.40 |
| 27 | BA | 561 | OMC | C4-N3 | 4.39 | 1.43 | 1.34 |
| 1 | Aa | 771 | OMG | C4-N3 | 4.39 | 1.48 | 1.37 |
| 27 | BA | 250 | OMC | C4-N4 | 4.39 | 1.44 | 1.33 |
| 27 | BA | 124 | 4AC | C2-N3 | 4.38 | 1.45 | 1.36 |
| 27 | BA | 2581 | 4SU | C4-S4 | -4.38 | 1.60 | 1.68 |
| 27 | BA | 2571 | OMC | C4-N4 | 4.38 | 1.44 | 1.33 |
| 27 | BA | 1543 | 4AC | C2-N1 | 4.38 | 1.49 | 1.40 |
| 27 | BA | 763 | OMG | C2-N3 | 4.37 | 1.43 | 1.33 |
| 27 | BA | 2797 | 4AC | C2-N1 | 4.37 | 1.49 | 1.40 |
| 27 | BA | 2121 | 4AC | C2-N1 | 4.37 | 1.49 | 1.40 |
| 27 | BA | 1434 | 4AC | C2-N3 | 4.37 | 1.45 | 1.36 |
| 27 | BA | 858 | 4AC | C2-N1 | 4.36 | 1.49 | 1.40 |
| 27 | BA | 2832 | 4AC | C2-N1 | 4.36 | 1.49 | 1.40 |
| 27 | BA | 2018 | OMC | C6-C5 | 4.35 | 1.45 | 1.35 |
| 27 | BA | 1750 | OMC | C4-N3 | 4.35 | 1.43 | 1.34 |
| 27 | BA | 718 | OMC | C2-N1 | 4.35 | 1.49 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 2152 | OMG | C2-N3 | 4.34 | 1.43 | 1.33 |
| 1 | Aa | 296 | OMC | C4-N3 | 4.34 | 1.43 | 1.34 |
| 1 | Aa | 41 | 4AC | C4-N4 | 4.33 | 1.46 | 1.39 |
| 27 | BA | 575 | OMG | C2-N3 | 4.33 | 1.43 | 1.33 |
| 1 | Aa | 1354 | OMC | C4-N4 | 4.33 | 1.44 | 1.33 |
| 27 | BA | 1953 | OMG | C4-N3 | 4.33 | 1.47 | 1.37 |
| 27 | BA | 419 | OMG | O6-C6 | -4.33 | 1.14 | 1.23 |
| 1 | Aa | 381 | OMG | C4-N3 | 4.33 | 1.47 | 1.37 |
| 27 | BA | 2035 | 5MC | C6-N1 | 4.32 | 1.45 | 1.38 |
| 27 | BA | 944 | 5MC | C6-N1 | 4.32 | 1.45 | 1.38 |
| 27 | BA | 657 | OMU | C6-C5 | 4.32 | 1.45 | 1.35 |
| 1 | Aa | 1354 | OMC | C2-N1 | 4.31 | 1.49 | 1.40 |
| 27 | BA | 723 | OMG | C4-N3 | 4.31 | 1.47 | 1.37 |
| 27 | BA | 2121 | 4AC | C2-N3 | 4.31 | 1.45 | 1.36 |
| 27 | BA | 805 | 4AC | C2-N3 | 4.31 | 1.45 | 1.36 |
| 27 | BA | 2324 | OMG | C4-N3 | 4.30 | 1.47 | 1.37 |
| 27 | BA | 2595 | OMC | C4-N3 | 4.30 | 1.43 | 1.34 |
| 27 | BA | 2545 | OMC | C4-N3 | 4.30 | 1.43 | 1.34 |
| 27 | BA | 858 | 4AC | C7-N4 | 4.30 | 1.45 | 1.37 |
| 27 | BA | 2672 | OMG | C4-N3 | 4.30 | 1.47 | 1.37 |
| 27 | BA | 2630 | OMC | C4-N3 | 4.30 | 1.43 | 1.34 |
| 27 | BA | 1820 | OMC | C6-C5 | 4.29 | 1.45 | 1.35 |
| 27 | BA | 1337 | 4AC | C2-N1 | 4.29 | 1.49 | 1.40 |
| 1 | Aa | 501 | 4AC | CM7-C7 | 4.29 | 1.59 | 1.50 |
| 1 | Aa | 498 | OMG | C4-N3 | 4.29 | 1.47 | 1.37 |
| 1 | Aa | 535 | OMC | C4-N4 | 4.28 | 1.44 | 1.33 |
| 1 | Aa | 659 | OMG | C4-N3 | 4.26 | 1.47 | 1.37 |
| 1 | Aa | 892 | OMG | C4-N3 | 4.26 | 1.47 | 1.37 |
| 27 | BA | 800 | OMG | C2-N3 | 4.26 | 1.43 | 1.33 |
| 27 | BA | 833 | OMG | C4-N3 | 4.26 | 1.47 | 1.37 |
| 27 | BA | 763 | OMG | C4-N3 | 4.25 | 1.47 | 1.37 |
| 27 | BA | 2379 | OMG | C4-N3 | 4.25 | 1.47 | 1.37 |
| 27 | BA | 799 | 4AC | C2-N1 | 4.25 | 1.49 | 1.40 |
| 1 | Aa | 1276 | 5MC | C4-N4 | 4.25 | 1.45 | 1.34 |
| 1 | Aa | 5 | 4AC | C4-N4 | 4.25 | 1.45 | 1.39 |
| 27 | BA | 1375 | 4AC | CM7-C7 | 4.25 | 1.59 | 1.50 |
| 27 | BA | 2124 | OMC | C2-N1 | 4.24 | 1.49 | 1.40 |
| 27 | BA | 2797 | 4AC | CM7-C7 | 4.24 | 1.59 | 1.50 |
| 27 | BA | 124 | 4AC | C2-N1 | 4.24 | 1.49 | 1.40 |
| 27 | BA | 2590 | 4AC | C2-N3 | 4.24 | 1.44 | 1.36 |
| 1 | Aa | 852 | OMG | C4-N3 | 4.23 | 1.47 | 1.37 |
| 1 | Aa | 457 | 5MC | C4-N4 | 4.22 | 1.45 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 2159 | 4AC | C2-N1 | 4.22 | 1.49 | 1.40 |
| 1 | Aa | 1459 | 4AC | C2-N1 | 4.22 | 1.49 | 1.40 |
| 27 | BA | 2035 | 5MC | C2-N1 | 4.22 | 1.49 | 1.40 |
| 27 | BA | 201 | 4AC | C2-N3 | 4.21 | 1.44 | 1.36 |
| 27 | BA | 1955 | 4AC | C2-N3 | 4.21 | 1.44 | 1.36 |
| 1 | Aa | 1476 | 5MC | C4-N4 | 4.21 | 1.45 | 1.34 |
| 1 | Aa | 457 | 5MC | C2-N1 | 4.21 | 1.49 | 1.40 |
| 27 | BA | 1398 | OMG | C4-N3 | 4.20 | 1.47 | 1.37 |
| 27 | BA | 805 | 4AC | C2-N1 | 4.20 | 1.49 | 1.40 |
| 1 | Aa | 501 | 4AC | C4-N4 | 4.19 | 1.45 | 1.39 |
| 27 | BA | 1434 | 4AC | C2-N1 | 4.19 | 1.49 | 1.40 |
| 1 | Aa | 1352 | 5MC | C2-N1 | 4.19 | 1.49 | 1.40 |
| 27 | BA | 2571 | OMC | C2-N1 | 4.19 | 1.49 | 1.40 |
| 27 | BA | 250 | OMC | C2-N1 | 4.19 | 1.49 | 1.40 |
| 1 | Aa | 457 | 5MC | C2'-C1' | 4.19 | 1.66 | 1.53 |
| 1 | Aa | 450 | OMG | C4-N3 | 4.18 | 1.47 | 1.37 |
| 1 | Aa | 827 | 4AC | CM7-C7 | 4.18 | 1.59 | 1.50 |
| 27 | BA | 2010 | OMG | C4-N3 | 4.18 | 1.47 | 1.37 |
| 27 | BA | 2657 | OMG | C4-N3 | 4.18 | 1.47 | 1.37 |
| 1 | Aa | 446 | OMG | C4-N3 | 4.17 | 1.47 | 1.37 |
| 1 | Aa | 358 | 4AC | C4-N4 | 4.17 | 1.45 | 1.39 |
| 27 | BA | 1305 | 4AC | CM7-C7 | 4.17 | 1.59 | 1.50 |
| 27 | BA | 2047 | OMC | C4-N3 | 4.16 | 1.42 | 1.34 |
| 27 | BA | 335 | 4AC | CM7-C7 | 4.16 | 1.59 | 1.50 |
| 1 | Aa | 752 | OMC | C2-N1 | 4.15 | 1.49 | 1.40 |
| 1 | Aa | 730 | 4AC | C2-N1 | 4.15 | 1.49 | 1.40 |
| 27 | BA | 1955 | 4AC | CM7-C7 | 4.15 | 1.59 | 1.50 |
| 1 | Aa | 1020 | LHH | C4-N4 | 4.15 | 1.45 | 1.39 |
| 27 | BA | 2728 | OMG | C4-N3 | 4.14 | 1.47 | 1.37 |
| 27 | BA | 552 | OMG | C4-N3 | 4.14 | 1.47 | 1.37 |
| 1 | Aa | 190 | OMC | C2-N1 | 4.13 | 1.48 | 1.40 |
| 27 | BA | 2527 | OMG | C4-N3 | 4.13 | 1.47 | 1.37 |
| 27 | BA | 2550 | OMG | C4-N3 | 4.13 | 1.47 | 1.37 |
| 1 | Aa | 818 | 4AC | C4-N4 | 4.13 | 1.45 | 1.39 |
| 27 | BA | 1427 | 4AC | CM7-C7 | 4.13 | 1.59 | 1.50 |
| 27 | BA | 1558 | OMG | C2-N3 | 4.13 | 1.43 | 1.33 |
| 1 | Aa | 296 | OMC | C2-N1 | 4.12 | 1.48 | 1.40 |
| 1 | Aa | 605 | 4AC | CM7-C7 | 4.12 | 1.59 | 1.50 |
| 1 | Aa | 1478 | 5MC | C2-N1 | 4.12 | 1.48 | 1.40 |
| 1 | Aa | 1025 | OMG | C4-N3 | 4.12 | 1.47 | 1.37 |
| 27 | BA | 418 | 4AC | CM7-C7 | 4.12 | 1.59 | 1.50 |
| 1 | Aa | 464 | 5MC | C2-N1 | 4.11 | 1.48 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 1810 | 4AC | CM7-C7 | 4.11 | 1.59 | 1.50 |
| 1 | Aa | 382 | OMG | C4-N3 | 4.11 | 1.47 | 1.37 |
| 27 | BA | 2047 | OMC | C4-N4 | 4.11 | 1.43 | 1.33 |
| 27 | BA | 290 | OMG | C4-N3 | 4.11 | 1.47 | 1.37 |
| 27 | BA | 2797 | 4AC | C2-N3 | 4.11 | 1.44 | 1.36 |
| 1 | Aa | 825 | OMC | C4-N4 | 4.10 | 1.43 | 1.33 |
| 1 | Aa | 942 | 5MC | C4-N4 | 4.10 | 1.44 | 1.34 |
| 1 | Aa | 752 | OMC | C4-N4 | 4.10 | 1.43 | 1.33 |
| 27 | BA | 2605 | 5MC | C2-N1 | 4.10 | 1.48 | 1.40 |
| 27 | BA | 2035 | 5MC | C4-N4 | 4.09 | 1.44 | 1.34 |
| 27 | BA | 1940 | OMG | C4-N3 | 4.09 | 1.47 | 1.37 |
| 27 | BA | 2832 | 4AC | CM7-C7 | 4.09 | 1.59 | 1.50 |
| 1 | Aa | 246 | OMG | C4-N3 | 4.09 | 1.47 | 1.37 |
| 27 | BA | 2838 | 4AC | CM7-C7 | 4.09 | 1.59 | 1.50 |
| 27 | BA | 2590 | 4AC | CM7-C7 | 4.09 | 1.59 | 1.50 |
| 1 | Aa | 942 | 5MC | C6-N1 | 4.09 | 1.45 | 1.38 |
| 27 | BA | 730 | 4AC | CM7-C7 | 4.08 | 1.59 | 1.50 |
| 27 | BA | 1641 | 4AC | CM7-C7 | 4.08 | 1.59 | 1.50 |
| 27 | BA | 1892 | OMG | C4-N3 | 4.08 | 1.47 | 1.37 |
| 27 | BA | 799 | 4AC | CM7-C7 | 4.08 | 1.59 | 1.50 |
| 27 | BA | 64 | OMG | C2-N3 | 4.07 | 1.43 | 1.33 |
| 1 | Aa | 136 | 4AC | CM7-C7 | 4.07 | 1.59 | 1.50 |
| 27 | BA | 501 | 4AC | C4-N4 | 4.07 | 1.45 | 1.39 |
| 27 | BA | 778 | 4AC | CM7-C7 | 4.07 | 1.59 | 1.50 |
| 27 | BA | 754 | OMC | C2-N1 | 4.07 | 1.48 | 1.40 |
| 27 | BA | 27 | 4AC | CM7-C7 | 4.07 | 1.59 | 1.50 |
| 27 | BA | 1820 | OMC | C2-N1 | 4.06 | 1.48 | 1.40 |
| 27 | BA | 2997 | 4AC | CM7-C7 | 4.06 | 1.59 | 1.50 |
| 27 | BA | 419 | OMG | C2-N3 | 4.05 | 1.43 | 1.33 |
| 27 | BA | 2047 | OMC | C2-N1 | 4.05 | 1.48 | 1.40 |
| 27 | BA | 2152 | OMG | C4-N3 | 4.05 | 1.47 | 1.37 |
| 1 | Aa | 296 | OMC | C4-N4 | 4.05 | 1.43 | 1.33 |
| 27 | BA | 27 | 4AC | C4-N4 | 4.04 | 1.45 | 1.39 |
| 1 | Aa | 827 | 4AC | C4-N4 | 4.04 | 1.45 | 1.39 |
| 1 | Aa | 1459 | 4AC | C7-N4 | 4.04 | 1.44 | 1.37 |
| 27 | BA | 2035 | 5MC | C2'-C1' | 4.04 | 1.66 | 1.53 |
| 1 | Aa | 1434 | OMG | C4-N3 | 4.04 | 1.47 | 1.37 |
| 27 | BA | 2168 | OMG | C4-N3 | 4.03 | 1.47 | 1.37 |
| 27 | BA | 617 | LHH | C4-N4 | 4.03 | 1.45 | 1.39 |
| 27 | BA | 1543 | 4AC | CM7-C7 | 4.03 | 1.58 | 1.50 |
| 1 | Aa | 479 | OMU | C4-N3 | 4.03 | 1.45 | 1.38 |
| 1 | Aa | 1276 | 5MC | C2'-C1' | 4.03 | 1.66 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 2353 | OMG | C4-N3 | 4.03 | 1.47 | 1.37 |
| 1 | Aa | 1459 | 4AC | C2-N3 | 4.03 | 1.44 | 1.36 |
| 27 | BA | 912 | OMG | C4-N3 | 4.02 | 1.47 | 1.37 |
| 27 | BA | 713 | 4AC | CM7-C7 | 4.02 | 1.58 | 1.50 |
| 27 | BA | 1558 | OMG | C4-N3 | 4.02 | 1.47 | 1.37 |
| 27 | BA | 1820 | OMC | C4-N4 | 4.02 | 1.43 | 1.33 |
| 1 | Aa | 457 | 5MC | C5'-C4' | -4.02 | 1.39 | 1.51 |
| 27 | BA | 201 | 4AC | C2-N1 | 4.02 | 1.48 | 1.40 |
| 27 | BA | 2055 | 5MC | C6-N1 | 4.02 | 1.44 | 1.38 |
| 27 | BA | 3023 | 4AC | CM7-C7 | 4.01 | 1.58 | 1.50 |
| 1 | Aa | 464 | 5MC | C6-N1 | 4.01 | 1.44 | 1.38 |
| 27 | BA | 561 | OMC | C4-N4 | 4.01 | 1.43 | 1.33 |
| 1 | Aa | 569 | 4AC | C4-N4 | 4.01 | 1.45 | 1.39 |
| 27 | BA | 778 | 4AC | C4-N4 | 4.00 | 1.45 | 1.39 |
| 1 | Aa | 1004 | 5MC | C4-N4 | 4.00 | 1.44 | 1.34 |
| 27 | BA | 1431 | 4AC | CM7-C7 | 4.00 | 1.58 | 1.50 |
| 27 | BA | 1431 | 4AC | C4-N4 | 4.00 | 1.45 | 1.39 |
| 1 | Aa | 1352 | 5MC | C4-N4 | 4.00 | 1.44 | 1.34 |
| 27 | BA | 1396 | 4AC | CM7-C7 | 4.00 | 1.58 | 1.50 |
| 27 | BA | 2992 | 4AC | CM7-C7 | 3.99 | 1.58 | 1.50 |
| 1 | Aa | 535 | OMC | C2-N1 | 3.99 | 1.48 | 1.40 |
| 27 | BA | 718 | OMC | C4-N4 | 3.99 | 1.43 | 1.33 |
| 1 | Aa | 373 | 4AC | C4-N4 | 3.99 | 1.45 | 1.39 |
| 27 | BA | 215 | OMG | C4-N3 | 3.98 | 1.47 | 1.37 |
| 1 | Aa | 1276 | 5MC | C2-N1 | 3.98 | 1.48 | 1.40 |
| 27 | BA | 1337 | 4AC | CM7-C7 | 3.98 | 1.58 | 1.50 |
| 27 | BA | 433 | 4AC | CM7-C7 | 3.97 | 1.58 | 1.50 |
| 1 | Aa | 1276 | 5MC | C5'-C4' | -3.96 | 1.39 | 1.51 |
| 1 | Aa | 1352 | 5MC | C6-N1 | 3.96 | 1.44 | 1.38 |
| 27 | BA | 1955 | 4AC | C2-N1 | 3.96 | 1.48 | 1.40 |
| 27 | BA | 3009 | 4AC | CM7-C7 | 3.95 | 1.58 | 1.50 |
| 1 | Aa | 994 | OMG | C2-N2 | 3.95 | 1.43 | 1.34 |
| 27 | BA | 869 | OMC | C2-N1 | 3.95 | 1.48 | 1.40 |
| 27 | BA | 2630 | OMC | C2-N1 | 3.95 | 1.48 | 1.40 |
| 27 | BA | 2121 | 4AC | CM7-C7 | 3.94 | 1.58 | 1.50 |
| 27 | BA | 858 | 4AC | CM7-C7 | 3.94 | 1.58 | 1.50 |
| 27 | BA | 1750 | OMC | C2-N1 | 3.94 | 1.48 | 1.40 |
| 27 | BA | 56 | 4AC | CM7-C7 | 3.93 | 1.58 | 1.50 |
| 27 | BA | 2605 | 5MC | C6-N1 | 3.93 | 1.44 | 1.38 |
| 27 | BA | 754 | OMC | C4-N4 | 3.93 | 1.43 | 1.33 |
| 27 | BA | 1790 | OMC | C2-N1 | 3.93 | 1.48 | 1.40 |
| 1 | Aa | 229 | LHH | C4-N4 | 3.92 | 1.45 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 1934 | 4AC | CM7-C7 | 3.92 | 1.58 | 1.50 |
| 27 | BA | 2745 | OMG | C4-N3 | 3.92 | 1.46 | 1.37 |
| 1 | Aa | 532 | OMG | C4-N3 | 3.91 | 1.46 | 1.37 |
| 27 | BA | 805 | 4AC | CM7-C7 | 3.91 | 1.58 | 1.50 |
| 27 | BA | 1357 | 4AC | CM7-C7 | 3.91 | 1.58 | 1.50 |
| 1 | Aa | 1004 | 5MC | C2-N1 | 3.91 | 1.48 | 1.40 |
| 27 | BA | 2545 | OMC | C4-N4 | 3.90 | 1.43 | 1.33 |
| 1 | Aa | 1476 | 5MC | C5'-C4' | -3.90 | 1.39 | 1.51 |
| 27 | BA | 575 | OMG | C4-N3 | 3.90 | 1.46 | 1.37 |
| 1 | Aa | 682 | 4AC | CM7-C7 | 3.89 | 1.58 | 1.50 |
| 27 | BA | 2780 | 4AC | CM7-C7 | 3.89 | 1.58 | 1.50 |
| 1 | Aa | 298 | 4AC | C4-N4 | 3.89 | 1.45 | 1.39 |
| 27 | BA | 730 | 4AC | C4-N4 | 3.89 | 1.45 | 1.39 |
| 27 | BA | 561 | OMC | C2-N1 | 3.88 | 1.48 | 1.40 |
| 27 | BA | 1106 | OMG | C4-N3 | 3.88 | 1.46 | 1.37 |
| 27 | BA | 1470 | 4AC | CM7-C7 | 3.88 | 1.58 | 1.50 |
| 1 | Aa | 825 | OMC | C2-N1 | 3.88 | 1.48 | 1.40 |
| 27 | BA | 3023 | 4AC | C4-N4 | 3.87 | 1.45 | 1.39 |
| 1 | Aa | 304 | OMU | C4-N3 | 3.87 | 1.45 | 1.38 |
| 27 | BA | 419 | OMG | C2-N1 | 3.86 | 1.47 | 1.37 |
| 1 | Aa | 942 | 5MC | C2-N1 | 3.86 | 1.48 | 1.40 |
| 27 | BA | 419 | OMG | C4-N3 | 3.86 | 1.46 | 1.37 |
| 27 | BA | 944 | 5MC | C2-N1 | 3.86 | 1.48 | 1.40 |
| 27 | BA | 56 | 4AC | C4-N4 | 3.86 | 1.45 | 1.39 |
| 27 | BA | 124 | 4AC | CM7-C7 | 3.86 | 1.58 | 1.50 |
| 27 | BA | 418 | 4AC | C4-N4 | 3.86 | 1.45 | 1.39 |
| 1 | Aa | 1476 | 5MC | C2'-C1' | 3.86 | 1.65 | 1.53 |
| 27 | BA | 1750 | OMC | C4-N4 | 3.86 | 1.43 | 1.33 |
| 27 | BA | 2018 | OMC | C4-N3 | 3.85 | 1.42 | 1.34 |
| 27 | BA | 2997 | 4AC | C4-N4 | 3.85 | 1.45 | 1.39 |
| 1 | Aa | 464 | 5MC | C4-N4 | 3.85 | 1.44 | 1.34 |
| 27 | BA | 768 | OMU | C4-N3 | 3.84 | 1.45 | 1.38 |
| 27 | BA | 453 | OMU | C4-N3 | 3.83 | 1.45 | 1.38 |
| 27 | BA | 1905 | 5MU | O4-C4 | -3.83 | 1.16 | 1.23 |
| 27 | BA | 2863 | 5MC | C2-N1 | 3.83 | 1.48 | 1.40 |
| 1 | Aa | 41 | 4AC | CM7-C7 | 3.82 | 1.58 | 1.50 |
| 27 | BA | 1319 | OMU | C4-N3 | 3.82 | 1.45 | 1.38 |
| 1 | Aa | 569 | 4AC | CM7-C7 | 3.81 | 1.58 | 1.50 |
| 27 | BA | 201 | 4AC | CM7-C7 | 3.81 | 1.58 | 1.50 |
| 1 | Aa | 847 | 4AC | CM7-C7 | 3.81 | 1.58 | 1.50 |
| 27 | BA | 1790 | OMC | C4-N4 | 3.81 | 1.42 | 1.33 |
| 27 | BA | 2055 | 5MC | C2-N1 | 3.81 | 1.48 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Aa | 240 | OMU | C4-N3 | 3.81 | 1.45 | 1.38 |
| 1 | Aa | 298 | 4AC | CM7-C7 | 3.80 | 1.58 | 1.50 |
| 1 | Aa | 1476 | 5MC | C2-N1 | 3.80 | 1.48 | 1.40 |
| 1 | Aa | 672 | 5MC | C2-N1 | 3.79 | 1.48 | 1.40 |
| 27 | BA | 2590 | 4AC | C4-N4 | 3.79 | 1.45 | 1.39 |
| 27 | BA | 1551 | OMU | C4-N3 | 3.79 | 1.45 | 1.38 |
| 27 | BA | 800 | OMG | C4-N3 | 3.79 | 1.46 | 1.37 |
| 27 | BA | 1641 | 4AC | C4-N4 | 3.79 | 1.45 | 1.39 |
| 27 | BA | 2035 | 5MC | C5'-C4' | -3.79 | 1.39 | 1.51 |
| 1 | Aa | 525 | 4AC | CM7-C7 | 3.79 | 1.58 | 1.50 |
| 27 | BA | 2124 | OMC | C4-N4 | 3.78 | 1.42 | 1.33 |
| 1 | Aa | 1004 | 5MC | C6-N1 | 3.78 | 1.44 | 1.38 |
| 27 | BA | 244 | 4AC | CM7-C7 | 3.78 | 1.58 | 1.50 |
| 27 | BA | 1799 | OMG | C2-N2 | 3.77 | 1.43 | 1.34 |
| 1 | Aa | 670 | 2MG | C2-N1 | 3.77 | 1.42 | 1.36 |
| 27 | BA | 763 | OMG | C6-N1 | 3.76 | 1.43 | 1.37 |
| 27 | BA | 1558 | OMG | C6-N1 | 3.75 | 1.43 | 1.37 |
| 27 | BA | 1899 | 4AC | CM7-C7 | 3.75 | 1.58 | 1.50 |
| 27 | BA | 2595 | OMC | C4-N4 | 3.75 | 1.42 | 1.33 |
| 27 | BA | 1965 | 5MC | C2-N1 | 3.74 | 1.48 | 1.40 |
| 27 | BA | 619 | OMU | C4-N3 | 3.74 | 1.45 | 1.38 |
| 27 | BA | 376 | 4AC | CM7-C7 | 3.74 | 1.58 | 1.50 |
| 27 | BA | 575 | OMG | C6-N1 | 3.74 | 1.43 | 1.37 |
| 27 | BA | 365 | OMG | C4-N3 | 3.72 | 1.46 | 1.37 |
| 1 | Aa | 373 | 4AC | CM7-C7 | 3.72 | 1.58 | 1.50 |
| 27 | BA | 2542 | OMU | C4-N3 | 3.71 | 1.45 | 1.38 |
| 1 | Aa | 52 | OMU | C4-N3 | 3.71 | 1.45 | 1.38 |
| 27 | BA | 713 | 4AC | C4-N4 | 3.71 | 1.45 | 1.39 |
| 1 | Aa | 1361 | OMC | C2-N1 | 3.70 | 1.48 | 1.40 |
| 27 | BA | 1776 | OMU | O4-C4 | -3.70 | 1.17 | 1.24 |
| 27 | BA | 2159 | 4AC | CM7-C7 | 3.70 | 1.58 | 1.50 |
| 27 | BA | 2610 | OMU | C4-N3 | 3.70 | 1.45 | 1.38 |
| 27 | BA | 2457 | LHH | C4-N4 | 3.69 | 1.45 | 1.39 |
| 27 | BA | 1470 | 4AC | C4-N4 | 3.69 | 1.45 | 1.39 |
| 1 | Aa | 847 | 4AC | C4-N4 | 3.68 | 1.45 | 1.39 |
| 1 | Aa | 358 | 4AC | CM7-C7 | 3.68 | 1.58 | 1.50 |
| 1 | Aa | 854 | 5MC | C4-N4 | 3.68 | 1.43 | 1.34 |
| 27 | BA | 353 | OMG | C2-N2 | 3.68 | 1.42 | 1.34 |
| 27 | BA | 552 | OMG | C6-N1 | 3.67 | 1.43 | 1.37 |
| 1 | Aa | 1026 | OMG | C2-N2 | 3.66 | 1.42 | 1.34 |
| 1 | Aa | 1467 | MA6 | C5-C4 | -3.66 | 1.31 | 1.40 |
| 27 | BA | 2863 | 5MC | C4-N4 | 3.66 | 1.43 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 501 | 4AC | CM7-C7 | 3.66 | 1.58 | 1.50 |
| 27 | BA | 335 | 4AC | C4-N4 | 3.66 | 1.45 | 1.39 |
| 27 | BA | 2055 | 5MC | C4-N4 | 3.65 | 1.43 | 1.34 |
| 27 | BA | 1543 | 4AC | C4-N4 | 3.64 | 1.45 | 1.39 |
| 1 | Aa | 697 | 4AC | CM7-C7 | 3.64 | 1.58 | 1.50 |
| 27 | BA | 2838 | 4AC | C4-N4 | 3.64 | 1.45 | 1.39 |
| 27 | BA | 2780 | 4AC | C4-N4 | 3.64 | 1.45 | 1.39 |
| 27 | BA | 1799 | OMG | C4-N3 | 3.64 | 1.46 | 1.37 |
| 27 | BA | 617 | LHH | C2-N3 | 3.62 | 1.43 | 1.36 |
| 27 | BA | 1434 | 4AC | CM7-C7 | 3.60 | 1.58 | 1.50 |
| 27 | BA | 34 | OMU | O4-C4 | -3.59 | 1.17 | 1.24 |
| 1 | Aa | 457 | 5MC | O3'-C3' | 3.58 | 1.51 | 1.43 |
| 27 | BA | 674 | OMG | C2-N3 | 3.58 | 1.41 | 1.33 |
| 27 | BA | 1696 | 5MC | C2-N1 | 3.58 | 1.47 | 1.40 |
| 27 | BA | 1340 | OMU | O4-C4 | -3.57 | 1.17 | 1.24 |
| 27 | BA | 64 | OMG | C4-N3 | 3.57 | 1.46 | 1.37 |
| 27 | BA | 419 | OMG | C2-N2 | 3.56 | 1.42 | 1.34 |
| 1 | Aa | 1020 | LHH | C2-N3 | 3.56 | 1.43 | 1.36 |
| 27 | BA | 2018 | OMC | C2-N1 | 3.55 | 1.47 | 1.40 |
| 27 | BA | 1400 | A2M | C5-C4 | -3.54 | 1.31 | 1.40 |
| 27 | BA | 572 | 5MU | O4-C4 | -3.54 | 1.16 | 1.23 |
| 1 | Aa | 913 | OMG | C2-N2 | 3.54 | 1.42 | 1.34 |
| 1 | Aa | 1358 | OMU | O4-C4 | -3.53 | 1.17 | 1.24 |
| 27 | BA | 875 | 5MU | O4-C4 | -3.53 | 1.16 | 1.23 |
| 27 | BA | 215 | OMG | O6-C6 | -3.53 | 1.16 | 1.23 |
| 27 | BA | 1969 | OMU | O4-C4 | -3.53 | 1.17 | 1.24 |
| 1 | Aa | 1361 | OMC | C4-N4 | 3.52 | 1.42 | 1.33 |
| 1 | Aa | 5 | 4AC | CM7-C7 | 3.52 | 1.57 | 1.50 |
| 27 | BA | 2168 | OMG | C2-N2 | 3.52 | 1.42 | 1.34 |
| 27 | BA | 657 | OMU | O4-C4 | -3.52 | 1.17 | 1.24 |
| 27 | BA | 1696 | 5MC | C4-N4 | 3.52 | 1.43 | 1.34 |
| 27 | BA | 2545 | OMC | C2-N1 | 3.51 | 1.47 | 1.40 |
| 27 | BA | 2019 | OMG | C2-N2 | 3.51 | 1.42 | 1.34 |
| 27 | BA | 1965 | 5MC | C4-N4 | 3.50 | 1.43 | 1.34 |
| 27 | BA | 674 | OMG | C4-N3 | 3.49 | 1.45 | 1.37 |
| 27 | BA | 2863 | 5MC | C6-N1 | 3.49 | 1.44 | 1.38 |
| 27 | BA | 1480 | OMU | C4-N3 | 3.49 | 1.44 | 1.38 |
| 1 | Aa | 854 | 5MC | C2-N1 | 3.49 | 1.47 | 1.40 |
| 1 | Aa | 229 | LHH | C2-N3 | 3.49 | 1.43 | 1.36 |
| 27 | BA | 2745 | OMG | O6-C6 | -3.49 | 1.16 | 1.23 |
| 1 | Aa | 672 | 5MC | C4-N4 | 3.49 | 1.43 | 1.34 |
| 27 | BA | 244 | 4AC | C4-N4 | 3.48 | 1.44 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 1434 | 4AC | C4-N4 | 3.48 | 1.44 | 1.39 |
| 27 | BA | 2035 | 5MC | O3'-C3' | 3.47 | 1.51 | 1.43 |
| 27 | BA | 505 | A2M | C5-C4 | -3.47 | 1.31 | 1.40 |
| 1 | Aa | 672 | 5MC | C6-N1 | 3.47 | 1.44 | 1.38 |
| 1 | Aa | 1265 | OMG | C2-N2 | 3.47 | 1.42 | 1.34 |
| 27 | BA | 2550 | OMG | O6-C6 | -3.47 | 1.16 | 1.23 |
| 27 | BA | 2656 | OMU | C4-N3 | 3.46 | 1.44 | 1.38 |
| 1 | Aa | 876 | OMG | C2-N2 | 3.46 | 1.42 | 1.34 |
| 27 | BA | 2728 | OMG | C2-N2 | 3.46 | 1.42 | 1.34 |
| 27 | BA | 1357 | 4AC | C4-N4 | 3.45 | 1.44 | 1.39 |
| 27 | BA | 1965 | 5MC | O2-C2 | -3.44 | 1.17 | 1.23 |
| 27 | BA | 2545 | OMC | O2-C2 | -3.44 | 1.17 | 1.23 |
| 27 | BA | 215 | OMG | C2-N2 | 3.44 | 1.42 | 1.34 |
| 27 | BA | 912 | OMG | O6-C6 | -3.44 | 1.16 | 1.23 |
| 1 | Aa | 1478 | 5MC | C4-N4 | 3.44 | 1.43 | 1.34 |
| 1 | Aa | 381 | OMG | C2-N2 | 3.44 | 1.42 | 1.34 |
| 27 | BA | 912 | OMG | C5-C4 | -3.44 | 1.34 | 1.43 |
| 27 | BA | 2018 | OMC | O2-C2 | -3.43 | 1.17 | 1.23 |
| 1 | Aa | 636 | OMG | C2-N2 | 3.43 | 1.42 | 1.34 |
| 1 | Aa | 138 | OMG | C2-N2 | 3.43 | 1.42 | 1.34 |
| 1 | Aa | 1476 | 5MC | O2-C2 | -3.43 | 1.17 | 1.23 |
| 1 | Aa | 771 | OMG | C2-N2 | 3.43 | 1.42 | 1.34 |
| 27 | BA | 1480 | OMU | O4-C4 | -3.42 | 1.17 | 1.24 |
| 27 | BA | 2605 | 5MC | C4-N4 | 3.42 | 1.43 | 1.34 |
| 1 | Aa | 1478 | 5MC | C6-N1 | 3.42 | 1.43 | 1.38 |
| 27 | BA | 2542 | OMU | O4-C4 | -3.41 | 1.17 | 1.24 |
| 27 | BA | 1696 | 5MC | C6-N1 | 3.41 | 1.43 | 1.38 |
| 27 | BA | 1340 | OMU | C4-N3 | 3.41 | 1.44 | 1.38 |
| 1 | Aa | 136 | 4AC | C5-C4 | 3.41 | 1.48 | 1.40 |
| 27 | BA | 1305 | 4AC | C5-C4 | 3.40 | 1.48 | 1.40 |
| 27 | BA | 2018 | OMC | C4-N4 | 3.40 | 1.41 | 1.33 |
| 27 | BA | 2152 | OMG | C5-C4 | -3.40 | 1.34 | 1.43 |
| 27 | BA | 1085 | 5MU | O2-C2 | -3.40 | 1.16 | 1.23 |
| 27 | BA | 833 | OMG | C2-N2 | 3.39 | 1.42 | 1.34 |
| 27 | BA | 869 | OMC | C4-N4 | 3.39 | 1.41 | 1.33 |
| 27 | BA | 1969 | OMU | C4-N3 | 3.39 | 1.44 | 1.38 |
| 27 | BA | 2379 | OMG | O6-C6 | -3.39 | 1.16 | 1.23 |
| 27 | BA | 2457 | LHH | C2-N3 | 3.39 | 1.43 | 1.36 |
| 27 | BA | 3009 | 4AC | C4-N4 | 3.38 | 1.44 | 1.39 |
| 27 | BA | 2075 | 5MC | C2-N1 | 3.38 | 1.47 | 1.40 |
| 1 | Aa | 659 | OMG | C2-N2 | 3.38 | 1.42 | 1.34 |
| 27 | BA | 1085 | 5MU | O4-C4 | -3.37 | 1.17 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 1965 | 5MC | C6-N1 | 3.37 | 1.43 | 1.38 |
| 27 | BA | 754 | OMC | O2-C2 | -3.37 | 1.17 | 1.23 |
| 27 | BA | 298 | 5MU | O4-C4 | -3.37 | 1.17 | 1.23 |
| 1 | Aa | 498 | OMG | C2-N2 | 3.37 | 1.42 | 1.34 |
| 27 | BA | 2550 | OMG | C5-C4 | -3.36 | 1.34 | 1.43 |
| 27 | BA | 1337 | 4AC | C4-N4 | 3.35 | 1.44 | 1.39 |
| 27 | BA | 526 | LHH | C2-N3 | 3.35 | 1.43 | 1.36 |
| 27 | BA | 453 | OMU | O4-C4 | -3.35 | 1.18 | 1.24 |
| 1 | Aa | 1107 | OMG | C2-N2 | 3.35 | 1.42 | 1.34 |
| 1 | Aa | 8 | OMU | O4-C4 | -3.35 | 1.18 | 1.24 |
| 27 | BA | 825 | A2M | C5-C4 | -3.35 | 1.32 | 1.40 |
| 27 | BA | 2630 | OMC | O2-C2 | -3.35 | 1.17 | 1.23 |
| 1 | Aa | 1358 | OMU | C4-N3 | 3.34 | 1.44 | 1.38 |
| 27 | BA | 537 | 5MU | O4-C4 | -3.34 | 1.17 | 1.23 |
| 27 | BA | 2672 | OMG | O6-C6 | -3.34 | 1.16 | 1.23 |
| 27 | BA | 2832 | 4AC | C4-N4 | 3.34 | 1.44 | 1.39 |
| 1 | Aa | 1476 | 5MC | O3'-C3' | 3.34 | 1.50 | 1.43 |
| 27 | BA | 1396 | 4AC | C4-N4 | 3.34 | 1.44 | 1.39 |
| 27 | BA | 2610 | OMU | O4-C4 | -3.33 | 1.18 | 1.24 |
| 1 | Aa | 1276 | 5MC | O3'-C3' | 3.33 | 1.50 | 1.43 |
| 27 | BA | 799 | 4AC | C4-N4 | 3.31 | 1.44 | 1.39 |
| 27 | BA | 2992 | 4AC | C5-C4 | 3.29 | 1.47 | 1.40 |
| 27 | BA | 1375 | 4AC | C4-N4 | 3.29 | 1.44 | 1.39 |
| 1 | Aa | 446 | OMG | C2-N2 | 3.29 | 1.42 | 1.34 |
| 27 | BA | 2728 | OMG | C5-C4 | -3.29 | 1.34 | 1.43 |
| 27 | BA | 1319 | OMU | O4-C4 | -3.28 | 1.18 | 1.24 |
| 27 | BA | 2168 | OMG | C6-N1 | 3.28 | 1.42 | 1.37 |
| 27 | BA | 2047 | OMC | O2-C2 | -3.28 | 1.17 | 1.23 |
| 1 | Aa | 358 | 4AC | C5-C4 | 3.28 | 1.47 | 1.40 |
| 1 | Aa | 994 | OMG | C6-N1 | 3.28 | 1.42 | 1.37 |
| 27 | BA | 1810 | 4AC | C4-N4 | 3.28 | 1.44 | 1.39 |
| 27 | BA | 2528 | OMG | C2-N2 | 3.28 | 1.42 | 1.34 |
| 27 | BA | 124 | 4AC | C4-N4 | 3.27 | 1.44 | 1.39 |
| 1 | Aa | 41 | 4AC | C5-C4 | 3.26 | 1.47 | 1.40 |
| 27 | BA | 1820 | OMC | O2-C2 | -3.26 | 1.17 | 1.23 |
| 1 | Aa | 852 | OMG | O6-C6 | -3.26 | 1.16 | 1.23 |
| 27 | BA | 1517 | A2M | C5-C4 | -3.26 | 1.32 | 1.40 |
| 27 | BA | 1551 | OMU | O4-C4 | -3.25 | 1.18 | 1.24 |
| 27 | BA | 619 | OMU | O4-C4 | -3.25 | 1.18 | 1.24 |
| 1 | Aa | 320 | OMG | C2-N2 | 3.25 | 1.41 | 1.34 |
| 27 | BA | 2745 | OMG | C5-C4 | -3.25 | 1.34 | 1.43 |
| 27 | BA | 2159 | 4AC | C4-N4 | 3.25 | 1.44 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 1696 | 5MC | O2-C2 | -3.25 | 1.17 | 1.23 |
| 1 | Aa | 892 | OMG | C2-N2 | 3.24 | 1.41 | 1.34 |
| 27 | BA | 2010 | OMG | C2-N2 | 3.24 | 1.41 | 1.34 |
| 1 | Aa | 1025 | OMG | C2-N2 | 3.24 | 1.41 | 1.34 |
| 27 | BA | 488 | A2M | C5-C4 | -3.24 | 1.32 | 1.40 |
| 27 | BA | 1905 | 5MU | O2-C2 | -3.24 | 1.17 | 1.23 |
| 27 | BA | 2055 | 5MC | O2-C2 | -3.24 | 1.17 | 1.23 |
| 27 | BA | 561 | OMC | O2-C2 | -3.24 | 1.17 | 1.23 |
| 27 | BA | 2672 | OMG | C5-C4 | -3.24 | 1.34 | 1.43 |
| 27 | BA | 215 | OMG | C5-C4 | -3.24 | 1.34 | 1.43 |
| 27 | BA | 2656 | OMU | O4-C4 | -3.23 | 1.18 | 1.24 |
| 1 | Aa | 672 | 5MC | O2-C2 | -3.23 | 1.17 | 1.23 |
| 27 | BA | 1934 | 4AC | C4-N4 | 3.23 | 1.44 | 1.39 |
| 27 | BA | 2324 | OMG | C2-N2 | 3.23 | 1.41 | 1.34 |
| 27 | BA | 2384 | 5MU | O4-C4 | -3.23 | 1.17 | 1.23 |
| 27 | BA | 1953 | OMG | C5-C4 | -3.23 | 1.34 | 1.43 |
| 27 | BA | 1899 | 4AC | C4-N4 | 3.22 | 1.44 | 1.39 |
| 27 | BA | 34 | OMU | C4-N3 | 3.22 | 1.44 | 1.38 |
| 27 | BA | 2657 | OMG | C2-N2 | 3.22 | 1.41 | 1.34 |
| 27 | BA | 1398 | OMG | O6-C6 | -3.22 | 1.16 | 1.23 |
| 27 | BA | 34 | OMU | O2-C2 | -3.22 | 1.17 | 1.23 |
| 1 | Aa | 1459 | 4AC | O7-C7 | -3.22 | 1.16 | 1.23 |
| 27 | BA | 2955 | LHH | C2-N3 | 3.22 | 1.42 | 1.36 |
| 27 | BA | 2152 | OMG | O6-C6 | -3.21 | 1.16 | 1.23 |
| 1 | Aa | 854 | 5MC | O2-C2 | -3.21 | 1.17 | 1.23 |
| 27 | BA | 575 | OMG | C2-N2 | 3.21 | 1.41 | 1.34 |
| 1 | Aa | 240 | OMU | O4-C4 | -3.20 | 1.18 | 1.24 |
| 27 | BA | 433 | 4AC | C4-N4 | 3.20 | 1.44 | 1.39 |
| 27 | BA | 2075 | 5MC | O2-C2 | -3.19 | 1.17 | 1.23 |
| 27 | BA | 2630 | OMC | C4-N4 | 3.19 | 1.41 | 1.33 |
| 27 | BA | 872 | A2M | C5-C4 | -3.19 | 1.32 | 1.40 |
| 27 | BA | 849 | A2M | C5-C4 | -3.19 | 1.32 | 1.40 |
| 27 | BA | 201 | 4AC | C4-N4 | 3.19 | 1.44 | 1.39 |
| 1 | Aa | 1107 | OMG | C6-N1 | 3.19 | 1.42 | 1.37 |
| 27 | BA | 2688 | 5MU | O4-C4 | -3.18 | 1.17 | 1.23 |
| 27 | BA | 64 | OMG | C2-N2 | 3.18 | 1.41 | 1.34 |
| 27 | BA | 1750 | OMC | O2-C2 | -3.17 | 1.17 | 1.23 |
| 27 | BA | 2075 | 5MC | C4-N4 | 3.17 | 1.42 | 1.34 |
| 27 | BA | 2528 | OMG | O6-C6 | -3.17 | 1.16 | 1.23 |
| 1 | Aa | 1478 | 5MC | O2-C2 | -3.17 | 1.17 | 1.23 |
| 27 | BA | 833 | OMG | O6-C6 | -3.16 | 1.16 | 1.23 |
| 27 | BA | 756 | A2M | C5-C4 | -3.16 | 1.32 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Aa | 450 | OMG | C2-N2 | 3.16 | 1.41 | 1.34 |
| 27 | BA | 2553 | 4SU | O2-C2 | -3.16 | 1.17 | 1.23 |
| 27 | BA | 1790 | OMC | O2-C2 | -3.16 | 1.17 | 1.23 |
| 1 | Aa | 304 | OMU | O4-C4 | -3.16 | 1.18 | 1.24 |
| 27 | BA | 2527 | OMG | C5-C4 | -3.15 | 1.35 | 1.43 |
| 27 | BA | 1525 | OMG | C5-C4 | -3.15 | 1.35 | 1.43 |
| 27 | BA | 2797 | 4AC | C4-N4 | 3.15 | 1.44 | 1.39 |
| 1 | Aa | 296 | OMC | O2-C2 | -3.14 | 1.17 | 1.23 |
| 27 | BA | 2702 | A2M | C5-C4 | -3.14 | 1.32 | 1.40 |
| 27 | BA | 2605 | 5MC | O2-C2 | -3.14 | 1.17 | 1.23 |
| 27 | BA | 858 | 4AC | C4-N4 | 3.14 | 1.44 | 1.39 |
| 1 | Aa | 52 | OMU | O4-C4 | -3.13 | 1.18 | 1.24 |
| 27 | BA | 2016 | OMG | O6-C6 | -3.13 | 1.16 | 1.23 |
| 27 | BA | 2656 | OMU | O2-C2 | -3.13 | 1.17 | 1.23 |
| 27 | BA | 932 | A2M | C5-C4 | -3.13 | 1.32 | 1.40 |
| 1 | Aa | 532 | OMG | C5-C4 | -3.13 | 1.35 | 1.43 |
| 27 | BA | 778 | 4AC | C5-C4 | 3.13 | 1.47 | 1.40 |
| 1 | Aa | 1468 | MA6 | C5-C4 | -3.13 | 1.32 | 1.40 |
| 27 | BA | 879 | A2M | O5'-C5' | -3.13 | 1.37 | 1.44 |
| 27 | BA | 2121 | 4AC | C4-N4 | 3.13 | 1.44 | 1.39 |
| 27 | BA | 723 | OMG | C5-C4 | -3.13 | 1.35 | 1.43 |
| 27 | BA | 1548 | 5MU | O4-C4 | -3.12 | 1.17 | 1.23 |
| 27 | BA | 290 | OMG | C5-C4 | -3.12 | 1.35 | 1.43 |
| 1 | Aa | 682 | 4AC | C5-C4 | 3.11 | 1.47 | 1.40 |
| 27 | BA | 2016 | OMG | C2-N2 | 3.11 | 1.41 | 1.34 |
| 1 | Aa | 382 | OMG | C2-N2 | 3.11 | 1.41 | 1.34 |
| 27 | BA | 2379 | OMG | C5-C4 | -3.10 | 1.35 | 1.43 |
| 27 | BA | 768 | OMU | O4-C4 | -3.10 | 1.18 | 1.24 |
| 27 | BA | 1776 | OMU | C4-N3 | 3.10 | 1.44 | 1.38 |
| 27 | BA | 932 | A2M | O3'-C3' | -3.10 | 1.35 | 1.43 |
| 27 | BA | 1953 | OMG | O6-C6 | -3.10 | 1.17 | 1.23 |
| 1 | Aa | 1025 | OMG | C5-C4 | -3.09 | 1.35 | 1.43 |
| 27 | BA | 944 | 5MC | O2-C2 | -3.09 | 1.18 | 1.23 |
| 1 | Aa | 525 | 4AC | C4-N4 | 3.09 | 1.44 | 1.39 |
| 27 | BA | 376 | 4AC | C4-N4 | 3.09 | 1.44 | 1.39 |
| 27 | BA | 290 | OMG | C2-N2 | 3.09 | 1.41 | 1.34 |
| 27 | BA | 2016 | OMG | C5-C4 | -3.09 | 1.35 | 1.43 |
| 27 | BA | 2010 | OMG | C5-C4 | -3.08 | 1.35 | 1.43 |
| 27 | BA | 552 | OMG | C5-C4 | -3.08 | 1.35 | 1.43 |
| 27 | BA | 1427 | 4AC | C4-N4 | 3.08 | 1.44 | 1.39 |
| 27 | BA | 64 | OMG | C5-C4 | -3.08 | 1.35 | 1.43 |
| 27 | BA | 805 | 4AC | C4-N4 | 3.08 | 1.44 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Aa | 532 | OMG | C2-N2 | 3.08 | 1.41 | 1.34 |
| 1 | Aa | 8 | OMU | C4-N3 | 3.07 | 1.44 | 1.38 |
| 1 | Aa | 190 | OMC | O2-C2 | -3.07 | 1.18 | 1.23 |
| 27 | BA | 335 | 4AC | C5-C4 | 3.07 | 1.47 | 1.40 |
| 27 | BA | 2542 | OMU | O2-C2 | -3.07 | 1.17 | 1.23 |
| 27 | BA | 418 | 4AC | C5-C4 | 3.07 | 1.47 | 1.40 |
| 27 | BA | 1525 | OMG | O6-C6 | -3.06 | 1.17 | 1.23 |
| 1 | Aa | 913 | OMG | C6-N1 | 3.06 | 1.42 | 1.37 |
| 1 | Aa | 1276 | 5MC | O2-C2 | -3.06 | 1.18 | 1.23 |
| 1 | Aa | 5 | 4AC | C5-C4 | 3.06 | 1.47 | 1.40 |
| 27 | BA | 2745 | OMG | C2-N2 | 3.06 | 1.41 | 1.34 |
| 27 | BA | 2075 | 5MC | C6-N1 | 3.06 | 1.43 | 1.38 |
| 1 | Aa | 464 | 5MC | O2-C2 | -3.05 | 1.18 | 1.23 |
| 1 | Aa | 1358 | OMU | O2-C2 | -3.05 | 1.17 | 1.23 |
| 1 | Aa | 1434 | OMG | C2-N2 | 3.05 | 1.41 | 1.34 |
| 27 | BA | 290 | OMG | O6-C6 | -3.05 | 1.17 | 1.23 |
| 1 | Aa | 1434 | OMG | C5-C4 | -3.05 | 1.35 | 1.43 |
| 1 | Aa | 479 | OMU | O4-C4 | -3.05 | 1.18 | 1.24 |
| 27 | BA | 756 | A2M | O5'-C5' | -3.04 | 1.37 | 1.44 |
| 27 | BA | 526 | LHH | C4-N4 | 3.04 | 1.44 | 1.39 |
| 27 | BA | 1085 | 5MU | C6-C5 | 3.04 | 1.39 | 1.34 |
| 27 | BA | 657 | OMU | O2-C2 | -3.04 | 1.17 | 1.23 |
| 27 | BA | 912 | OMG | C2-N2 | 3.04 | 1.41 | 1.34 |
| 1 | Aa | 825 | OMC | O2-C2 | -3.04 | 1.18 | 1.23 |
| 27 | BA | 250 | OMC | O2-C2 | -3.04 | 1.18 | 1.23 |
| 1 | Aa | 852 | OMG | C5-C4 | -3.03 | 1.35 | 1.43 |
| 1 | Aa | 569 | 4AC | C5-C4 | 3.03 | 1.47 | 1.40 |
| 1 | Aa | 697 | 4AC | C5-C4 | 3.03 | 1.47 | 1.40 |
| 27 | BA | 1340 | OMU | O2-C2 | -3.03 | 1.17 | 1.23 |
| 27 | BA | 1776 | OMU | O2-C2 | -3.03 | 1.17 | 1.23 |
| 27 | BA | 2728 | OMG | O6-C6 | -3.03 | 1.17 | 1.23 |
| 27 | BA | 298 | 5MU | O2-C2 | -3.03 | 1.17 | 1.23 |
| 27 | BA | 2863 | 5MC | O2-C2 | -3.02 | 1.18 | 1.23 |
| 27 | BA | 2124 | OMC | O2-C2 | -3.02 | 1.18 | 1.23 |
| 27 | BA | 869 | OMC | O2-C2 | -3.01 | 1.18 | 1.23 |
| 1 | Aa | 246 | OMG | C2-N2 | 3.01 | 1.41 | 1.34 |
| 27 | BA | 833 | OMG | C5-C4 | -3.01 | 1.35 | 1.43 |
| 27 | BA | 2657 | OMG | C5-C4 | -3.01 | 1.35 | 1.43 |
| 27 | BA | 2955 | LHH | C4-N4 | 3.01 | 1.44 | 1.39 |
| 27 | BA | 2545 | OMC | C6-N1 | 3.00 | 1.45 | 1.38 |
| 27 | BA | 825 | A2M | O3'-C3' | -3.00 | 1.35 | 1.43 |
| 1 | Aa | 1217 | 4AC | C5-C4 | 3.00 | 1.47 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 1641 | 4AC | C5-C4 | 3.00 | 1.47 | 1.40 |
| 27 | BA | 2035 | 5MC | C3'-C4' | 3.00 | 1.60 | 1.53 |
| 27 | BA | 944 | 5MC | C4-N4 | 2.99 | 1.41 | 1.34 |
| 27 | BA | 2595 | OMC | O2-C2 | -2.99 | 1.18 | 1.23 |
| 27 | BA | 2527 | OMG | O6-C6 | -2.99 | 1.17 | 1.23 |
| 27 | BA | 2568 | OMG | C6-N1 | -2.99 | 1.33 | 1.37 |
| 27 | BA | 1799 | OMG | C5-C4 | -2.99 | 1.35 | 1.43 |
| 27 | BA | 1892 | OMG | C2-N2 | 2.98 | 1.41 | 1.34 |
| 27 | BA | 365 | OMG | C5-C4 | -2.98 | 1.35 | 1.43 |
| 27 | BA | 674 | OMG | C5-C4 | -2.98 | 1.35 | 1.43 |
| 1 | Aa | 525 | 4AC | C5-C4 | 2.98 | 1.47 | 1.40 |
| 27 | BA | 2997 | 4AC | C5-C4 | 2.98 | 1.47 | 1.40 |
| 27 | BA | 63 | OMG | O6-C6 | -2.97 | 1.17 | 1.23 |
| 27 | BA | 1480 | OMU | O2-C2 | -2.97 | 1.17 | 1.23 |
| 1 | Aa | 827 | 4AC | C5-C4 | 2.97 | 1.47 | 1.40 |
| 1 | Aa | 446 | OMG | C5-C4 | -2.97 | 1.35 | 1.43 |
| 27 | BA | 365 | OMG | C2-N2 | 2.97 | 1.41 | 1.34 |
| 27 | BA | 2528 | OMG | C5-C4 | -2.97 | 1.35 | 1.43 |
| 27 | BA | 552 | OMG | C5-C6 | 2.97 | 1.53 | 1.47 |
| 1 | Aa | 1354 | OMC | O2-C2 | -2.97 | 1.18 | 1.23 |
| 27 | BA | 2590 | 4AC | C5-C4 | 2.96 | 1.47 | 1.40 |
| 1 | Aa | 298 | 4AC | C5-C4 | 2.96 | 1.47 | 1.40 |
| 1 | Aa | 535 | OMC | O2-C2 | -2.96 | 1.18 | 1.23 |
| 27 | BA | 56 | 4AC | C5-C4 | 2.96 | 1.47 | 1.40 |
| 27 | BA | 763 | OMG | C2-N2 | 2.96 | 1.41 | 1.34 |
| 1 | Aa | 605 | 4AC | C5-C4 | 2.95 | 1.47 | 1.40 |
| 1 | Aa | 942 | 5MC | O2-C2 | -2.95 | 1.18 | 1.23 |
| 27 | BA | 879 | A2M | C5-C4 | -2.95 | 1.33 | 1.40 |
| 27 | BA | 1940 | OMG | C2-N2 | 2.95 | 1.41 | 1.34 |
| 1 | Aa | 752 | OMC | O2-C2 | -2.95 | 1.18 | 1.23 |
| 1 | Aa | 892 | OMG | C5-C4 | -2.95 | 1.35 | 1.43 |
| 27 | BA | 63 | OMG | C2-N2 | 2.95 | 1.41 | 1.34 |
| 1 | Aa | 818 | 4AC | C5-C4 | 2.94 | 1.47 | 1.40 |
| 27 | BA | 1558 | OMG | C2-N2 | 2.94 | 1.41 | 1.34 |
| 27 | BA | 2571 | OMC | O2-C2 | -2.94 | 1.18 | 1.23 |
| 27 | BA | 723 | OMG | O6-C6 | -2.93 | 1.17 | 1.23 |
| 27 | BA | 1940 | OMG | O6-C6 | -2.93 | 1.17 | 1.23 |
| 1 | Aa | 730 | 4AC | C5-C4 | 2.93 | 1.47 | 1.40 |
| 27 | BA | 2384 | 5MU | O2-C2 | -2.93 | 1.17 | 1.23 |
| 1 | Aa | 457 | 5MC | C3'-C4' | 2.93 | 1.60 | 1.53 |
| 1 | Aa | 382 | OMG | C5-C4 | -2.93 | 1.35 | 1.43 |
| 27 | BA | 2324 | OMG | C5-C4 | -2.93 | 1.35 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 1955 | 4AC | C4-N4 | 2.93 | 1.44 | 1.39 |
| 27 | BA | 1398 | OMG | C5-C4 | -2.92 | 1.35 | 1.43 |
| 27 | BA | 1265 | A2M | C5-C4 | -2.92 | 1.33 | 1.40 |
| 27 | BA | 488 | A2M | O2'-C2' | 2.91 | 1.50 | 1.42 |
| 1 | Aa | 246 | OMG | C5-C4 | -2.91 | 1.35 | 1.43 |
| 1 | Aa | 1352 | 5MC | O2-C2 | -2.91 | 1.18 | 1.23 |
| 1 | Aa | 501 | 4AC | C5-C4 | 2.91 | 1.47 | 1.40 |
| 1 | Aa | 1004 | 5MC | O2-C2 | -2.91 | 1.18 | 1.23 |
| 27 | BA | 1431 | 4AC | C5-C4 | 2.90 | 1.47 | 1.40 |
| 1 | Aa | 818 | 4AC | CM7-C7 | 2.90 | 1.56 | 1.50 |
| 27 | BA | 1525 | OMG | C2-N2 | 2.90 | 1.41 | 1.34 |
| 27 | BA | 2019 | OMG | O6-C6 | -2.90 | 1.17 | 1.23 |
| 27 | BA | 2521 | OMG | C5-C4 | -2.89 | 1.35 | 1.43 |
| 27 | BA | 1969 | OMU | O2-C2 | -2.89 | 1.17 | 1.23 |
| 1 | Aa | 381 | OMG | O6-C6 | -2.89 | 1.17 | 1.23 |
| 1 | Aa | 8 | OMU | O2-C2 | -2.89 | 1.17 | 1.23 |
| 1 | Aa | 498 | OMG | C5-C4 | -2.88 | 1.35 | 1.43 |
| 27 | BA | 1106 | OMG | O6-C6 | -2.88 | 1.17 | 1.23 |
| 27 | BA | 64 | OMG | O6-C6 | -2.88 | 1.17 | 1.23 |
| 27 | BA | 1940 | OMG | C5-C4 | -2.88 | 1.35 | 1.43 |
| 1 | Aa | 636 | OMG | C6-N1 | 2.87 | 1.42 | 1.37 |
| 27 | BA | 537 | 5MU | O2-C2 | -2.87 | 1.17 | 1.23 |
| 27 | BA | 875 | 5MU | O2-C2 | -2.86 | 1.17 | 1.23 |
| 27 | BA | 575 | OMG | C5-C6 | 2.86 | 1.53 | 1.47 |
| 27 | BA | 63 | OMG | C5-C4 | -2.86 | 1.35 | 1.43 |
| 27 | BA | 1106 | OMG | C5-C4 | -2.86 | 1.35 | 1.43 |
| 1 | Aa | 457 | 5MC | O2-C2 | -2.86 | 1.18 | 1.23 |
| 1 | Aa | 1025 | OMG | O6-C6 | -2.85 | 1.17 | 1.23 |
| 1 | Aa | 771 | OMG | C5-C4 | -2.85 | 1.35 | 1.43 |
| 27 | BA | 572 | 5MU | O2-C2 | -2.85 | 1.17 | 1.23 |
| 27 | BA | 3023 | 4AC | C5-C4 | 2.85 | 1.46 | 1.40 |
| 1 | Aa | 381 | OMG | C5-C4 | -2.85 | 1.35 | 1.43 |
| 27 | BA | 1106 | OMG | C2-N2 | 2.85 | 1.41 | 1.34 |
| 1 | Aa | 320 | OMG | O6-C6 | -2.85 | 1.17 | 1.23 |
| 27 | BA | 2527 | OMG | C2-N2 | 2.84 | 1.41 | 1.34 |
| 27 | BA | 2010 | OMG | O6-C6 | -2.84 | 1.17 | 1.23 |
| 1 | Aa | 1265 | OMG | C5-C4 | -2.84 | 1.35 | 1.43 |
| 27 | BA | 657 | OMU | C4-N3 | 2.83 | 1.43 | 1.38 |
| 27 | BA | 718 | OMC | O2-C2 | -2.83 | 1.18 | 1.23 |
| 27 | BA | 1400 | A2M | O3'-C3' | -2.83 | 1.36 | 1.43 |
| 1 | Aa | 498 | OMG | C6-N1 | 2.83 | 1.42 | 1.37 |
| 27 | BA | 2035 | 5MC | O2-C2 | -2.83 | 1.18 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 1106 | OMG | C6-N1 | 2.83 | 1.42 | 1.37 |
| 27 | BA | 501 | 4AC | O7-C7 | -2.83 | 1.16 | 1.23 |
| 1 | Aa | 382 | OMG | C6-N1 | 2.82 | 1.42 | 1.37 |
| 27 | BA | 2019 | OMG | C5-C4 | -2.82 | 1.35 | 1.43 |
| 27 | BA | 800 | OMG | C5-C4 | -2.82 | 1.35 | 1.43 |
| 1 | Aa | 532 | OMG | C6-N1 | 2.81 | 1.42 | 1.37 |
| 27 | BA | 353 | OMG | O6-C6 | -2.81 | 1.17 | 1.23 |
| 27 | BA | 879 | A2M | O3'-C3' | -2.81 | 1.36 | 1.43 |
| 1 | Aa | 876 | OMG | O6-C6 | -2.81 | 1.17 | 1.23 |
| 27 | BA | 1548 | 5MU | O2-C2 | -2.81 | 1.17 | 1.23 |
| 27 | BA | 1543 | 4AC | C5-C4 | 2.81 | 1.46 | 1.40 |
| 1 | Aa | 771 | OMG | O6-C6 | -2.81 | 1.17 | 1.23 |
| 27 | BA | 376 | 4AC | O7-C7 | -2.81 | 1.16 | 1.23 |
| 1 | Aa | 917 | 5MU | C4-N3 | -2.81 | 1.33 | 1.38 |
| 27 | BA | 1955 | 4AC | O7-C7 | -2.81 | 1.16 | 1.23 |
| 1 | Aa | 670 | 2MG | C5-C4 | -2.80 | 1.35 | 1.43 |
| 27 | BA | 2521 | OMG | O6-C6 | -2.80 | 1.17 | 1.23 |
| 27 | BA | 763 | OMG | C5-C4 | -2.80 | 1.35 | 1.43 |
| 27 | BA | 453 | OMU | O2-C2 | -2.80 | 1.17 | 1.23 |
| 27 | BA | 2610 | OMU | C6-N1 | 2.80 | 1.44 | 1.38 |
| 27 | BA | 488 | A2M | O3'-C3' | -2.80 | 1.36 | 1.43 |
| 1 | Aa | 1434 | OMG | C6-N1 | 2.80 | 1.42 | 1.37 |
| 27 | BA | 2581 | 4SU | O2-C2 | -2.80 | 1.17 | 1.23 |
| 27 | BA | 1892 | OMG | O6-C6 | -2.80 | 1.17 | 1.23 |
| 1 | Aa | 532 | OMG | O6-C6 | -2.80 | 1.17 | 1.23 |
| 1 | Aa | 1007 | 4AC | C4-N4 | -2.80 | 1.35 | 1.39 |
| 27 | BA | 730 | 4AC | C5-C4 | 2.80 | 1.46 | 1.40 |
| 1 | Aa | 913 | OMG | C5-C4 | -2.79 | 1.36 | 1.43 |
| 1 | Aa | 138 | OMG | O6-C6 | -2.79 | 1.17 | 1.23 |
| 27 | BA | 713 | 4AC | C5-C4 | 2.79 | 1.46 | 1.40 |
| 27 | BA | 353 | OMG | C5-C4 | -2.79 | 1.36 | 1.43 |
| 27 | BA | 1427 | 4AC | O7-C7 | -2.78 | 1.16 | 1.23 |
| 1 | Aa | 847 | 4AC | O7-C7 | -2.78 | 1.16 | 1.23 |
| 27 | BA | 2780 | 4AC | C5-C4 | 2.78 | 1.46 | 1.40 |
| 27 | BA | 800 | OMG | O6-C6 | -2.78 | 1.17 | 1.23 |
| 1 | Aa | 138 | OMG | C6-N1 | 2.78 | 1.42 | 1.37 |
| 1 | Aa | 1361 | OMC | O2-C2 | -2.78 | 1.18 | 1.23 |
| 27 | BA | 365 | OMG | O6-C6 | -2.78 | 1.17 | 1.23 |
| 1 | Aa | 1026 | OMG | C5-C4 | -2.78 | 1.36 | 1.43 |
| 27 | BA | 575 | OMG | C5-C4 | -2.77 | 1.36 | 1.43 |
| 27 | BA | 1551 | OMU | O2-C2 | -2.77 | 1.18 | 1.23 |
| 27 | BA | 2168 | OMG | C5-C4 | -2.77 | 1.36 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Aa | 913 | OMG | O6-C6 | -2.77 | 1.17 | 1.23 |
| 1 | Aa | 1265 | OMG | C6-N1 | 2.77 | 1.42 | 1.37 |
| 1 | Aa | 446 | OMG | O6-C6 | -2.77 | 1.17 | 1.23 |
| 1 | Aa | 876 | OMG | C5-C4 | -2.77 | 1.36 | 1.43 |
| 27 | BA | 2159 | 4AC | O7-C7 | -2.77 | 1.17 | 1.23 |
| 27 | BA | 723 | OMG | C5-C6 | 2.76 | 1.53 | 1.47 |
| 27 | BA | 1398 | OMG | C2-N2 | 2.76 | 1.40 | 1.34 |
| 1 | Aa | 373 | 4AC | C5-C4 | 2.76 | 1.46 | 1.40 |
| 27 | BA | 1375 | 4AC | C5-C4 | 2.76 | 1.46 | 1.40 |
| 1 | Aa | 892 | OMG | C6-N1 | 2.76 | 1.42 | 1.37 |
| 27 | BA | 925 | 4AC | C4-N4 | -2.76 | 1.35 | 1.39 |
| 1 | Aa | 450 | OMG | C5-C4 | -2.76 | 1.36 | 1.43 |
| 27 | BA | 2379 | OMG | C2-N2 | 2.76 | 1.40 | 1.34 |
| 27 | BA | 2688 | 5MU | O2-C2 | -2.76 | 1.18 | 1.23 |
| 27 | BA | 858 | 4AC | C5-C4 | 2.75 | 1.46 | 1.40 |
| 1 | Aa | 1434 | OMG | O6-C6 | -2.75 | 1.17 | 1.23 |
| 27 | BA | 2353 | OMG | O6-C6 | -2.75 | 1.17 | 1.23 |
| 27 | BA | 2121 | 4AC | C5-C4 | 2.75 | 1.46 | 1.40 |
| 27 | BA | 1934 | 4AC | O7-C7 | -2.74 | 1.17 | 1.23 |
| 27 | BA | 505 | A2M | O5'-C5' | -2.74 | 1.38 | 1.44 |
| 27 | BA | 825 | A2M | O5'-C5' | -2.74 | 1.38 | 1.44 |
| 1 | Aa | 1476 | 5MC | C3'-C4' | 2.74 | 1.60 | 1.53 |
| 1 | Aa | 730 | 4AC | CM7-C7 | 2.74 | 1.56 | 1.50 |
| 1 | Aa | 450 | OMG | O6-C6 | -2.74 | 1.17 | 1.23 |
| 27 | BA | 2353 | OMG | C2-N2 | 2.74 | 1.40 | 1.34 |
| 27 | BA | 2838 | 4AC | C5-C4 | 2.73 | 1.46 | 1.40 |
| 27 | BA | 2168 | OMG | C5-C6 | 2.73 | 1.53 | 1.47 |
| 27 | BA | 1319 | OMU | O2-C2 | -2.73 | 1.18 | 1.23 |
| 27 | BA | 1892 | OMG | C5-C4 | -2.73 | 1.36 | 1.43 |
| 1 | Aa | 847 | 4AC | C5-C4 | 2.72 | 1.46 | 1.40 |
| 1 | Aa | 659 | OMG | C5-C4 | -2.72 | 1.36 | 1.43 |
| 27 | BA | 2657 | OMG | O6-C6 | -2.72 | 1.17 | 1.23 |
| 1 | Aa | 1265 | OMG | O6-C6 | -2.72 | 1.17 | 1.23 |
| 27 | BA | 2124 | OMC | C6-N1 | 2.72 | 1.44 | 1.38 |
| 1 | Aa | 382 | OMG | O6-C6 | -2.72 | 1.17 | 1.23 |
| 1 | Aa | 730 | 4AC | O7-C7 | -2.72 | 1.17 | 1.23 |
| 1 | Aa | 1276 | 5MC | C3'-C4' | 2.71 | 1.59 | 1.53 |
| 27 | BA | 290 | OMG | C5-C6 | 2.71 | 1.52 | 1.47 |
| 27 | BA | 2121 | 4AC | O7-C7 | -2.71 | 1.17 | 1.23 |
| 27 | BA | 932 | A2M | C6-N6 | 2.71 | 1.43 | 1.34 |
| 27 | BA | 1641 | 4AC | O7-C7 | -2.71 | 1.17 | 1.23 |
| 27 | BA | 756 | A2M | O3'-C3' | -2.71 | 1.36 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 849 | A2M | C6-N6 | 2.71 | 1.43 | 1.34 |
| 27 | BA | 2353 | OMG | C5-C4 | -2.71 | 1.36 | 1.43 |
| 27 | BA | 1953 | OMG | C2-N2 | 2.71 | 1.40 | 1.34 |
| 1 | Aa | 1275 | OMG | C6-N1 | -2.70 | 1.33 | 1.37 |
| 27 | BA | 2521 | OMG | C2-N2 | 2.70 | 1.40 | 1.34 |
| 1 | Aa | 994 | OMG | C5-C6 | 2.70 | 1.52 | 1.47 |
| 1 | Aa | 876 | OMG | C6-N1 | 2.70 | 1.41 | 1.37 |
| 27 | BA | 1517 | A2M | C6-N6 | 2.70 | 1.43 | 1.34 |
| 27 | BA | 872 | A2M | O3'-C3' | -2.70 | 1.36 | 1.43 |
| 27 | BA | 2019 | OMG | C6-N1 | 2.70 | 1.41 | 1.37 |
| 1 | Aa | 138 | OMG | C5-C4 | -2.69 | 1.36 | 1.43 |
| 1 | Aa | 1026 | OMG | O6-C6 | -2.69 | 1.17 | 1.23 |
| 1 | Aa | 659 | OMG | C6-N1 | 2.69 | 1.41 | 1.37 |
| 1 | Aa | 320 | OMG | C5-C4 | -2.69 | 1.36 | 1.43 |
| 1 | Aa | 246 | OMG | O6-C6 | -2.69 | 1.17 | 1.23 |
| 27 | BA | 723 | OMG | C2-N2 | 2.68 | 1.40 | 1.34 |
| 27 | BA | 1558 | OMG | C5-C4 | -2.68 | 1.36 | 1.43 |
| 1 | Aa | 457 | 5MC | O4'-C4' | 2.68 | 1.51 | 1.45 |
| 27 | BA | 2324 | OMG | O6-C6 | -2.68 | 1.17 | 1.23 |
| 27 | BA | 2019 | OMG | C5-C6 | 2.68 | 1.52 | 1.47 |
| 1 | Aa | 498 | OMG | O6-C6 | -2.68 | 1.17 | 1.23 |
| 1 | Aa | 190 | OMC | C6-N1 | 2.68 | 1.44 | 1.38 |
| 1 | Aa | 298 | 4AC | O7-C7 | -2.68 | 1.17 | 1.23 |
| 27 | BA | 768 | OMU | O2-C2 | -2.67 | 1.18 | 1.23 |
| 27 | BA | 27 | 4AC | C5-C4 | 2.67 | 1.46 | 1.40 |
| 1 | Aa | 659 | OMG | O6-C6 | -2.67 | 1.17 | 1.23 |
| 27 | BA | 1558 | OMG | C5-C6 | 2.67 | 1.52 | 1.47 |
| 27 | BA | 1400 | A2M | O2'-C2' | 2.66 | 1.49 | 1.42 |
| 27 | BA | 879 | A2M | C6-N6 | 2.66 | 1.43 | 1.34 |
| 27 | BA | 1357 | 4AC | C5-C4 | 2.65 | 1.46 | 1.40 |
| 27 | BA | 1955 | 4AC | C5-C4 | 2.65 | 1.46 | 1.40 |
| 1 | Aa | 246 | OMG | C6-N1 | 2.65 | 1.41 | 1.37 |
| 27 | BA | 872 | A2M | O5'-C5' | -2.65 | 1.38 | 1.44 |
| 27 | BA | 1470 | 4AC | O7-C7 | -2.65 | 1.17 | 1.23 |
| 1 | Aa | 1107 | OMG | C5-C6 | 2.64 | 1.52 | 1.47 |
| 1 | Aa | 670 | 2MG | O6-C6 | -2.64 | 1.17 | 1.23 |
| 27 | BA | 1265 | A2M | C6-N6 | 2.64 | 1.43 | 1.34 |
| 27 | BA | 1375 | 4AC | O7-C7 | -2.64 | 1.17 | 1.23 |
| 27 | BA | 1934 | 4AC | C5-C4 | 2.64 | 1.46 | 1.40 |
| 1 | Aa | 636 | OMG | C5-C6 | 2.63 | 1.52 | 1.47 |
| 1 | Aa | 670 | 2MG | C6-N1 | 2.63 | 1.41 | 1.37 |
| 27 | BA | 64 | OMG | C6-N1 | 2.63 | 1.41 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 674 | OMG | C5-C6 | 2.63 | 1.52 | 1.47 |
| 27 | BA | 2702 | A2M | O2'-C2' | 2.63 | 1.49 | 1.42 |
| 1 | Aa | 917 | 5MU | C6-C5 | 2.63 | 1.38 | 1.34 |
| 1 | Aa | 52 | OMU | O2-C2 | -2.62 | 1.18 | 1.23 |
| 1 | Aa | 450 | OMG | C6-N1 | 2.62 | 1.41 | 1.37 |
| 1 | Aa | 5 | 4AC | O7-C7 | -2.62 | 1.17 | 1.23 |
| 27 | BA | 1525 | OMG | C6-N1 | 2.62 | 1.41 | 1.37 |
| 1 | Aa | 1476 | 5MC | O4'-C4' | 2.62 | 1.50 | 1.45 |
| 27 | BA | 244 | 4AC | O7-C7 | -2.62 | 1.17 | 1.23 |
| 27 | BA | 833 | OMG | C2-N1 | 2.61 | 1.44 | 1.37 |
| 1 | Aa | 1107 | OMG | C5-C4 | -2.61 | 1.36 | 1.43 |
| 1 | Aa | 1026 | OMG | C6-N1 | 2.61 | 1.41 | 1.37 |
| 1 | Aa | 304 | OMU | O2-C2 | -2.61 | 1.18 | 1.23 |
| 27 | BA | 2571 | OMC | C6-N1 | 2.61 | 1.44 | 1.38 |
| 1 | Aa | 320 | OMG | C5-C6 | 2.61 | 1.52 | 1.47 |
| 27 | BA | 674 | OMG | C6-N1 | 2.60 | 1.41 | 1.37 |
| 27 | BA | 2353 | OMG | C6-N1 | 2.60 | 1.41 | 1.37 |
| 1 | Aa | 479 | OMU | C6-N1 | 2.60 | 1.44 | 1.38 |
| 27 | BA | 1265 | A2M | O2'-C2' | 2.60 | 1.49 | 1.42 |
| 27 | BA | 2997 | 4AC | O7-C7 | -2.60 | 1.17 | 1.23 |
| 27 | BA | 2672 | OMG | C2-N2 | 2.60 | 1.40 | 1.34 |
| 27 | BA | 718 | OMC | C6-N1 | 2.60 | 1.44 | 1.38 |
| 27 | BA | 3009 | 4AC | C5-C4 | 2.60 | 1.46 | 1.40 |
| 27 | BA | 756 | A2M | C6-N6 | 2.60 | 1.43 | 1.34 |
| 27 | BA | 619 | OMU | O2-C2 | -2.59 | 1.18 | 1.23 |
| 1 | Aa | 240 | OMU | O2-C2 | -2.59 | 1.18 | 1.23 |
| 27 | BA | 730 | 4AC | O7-C7 | -2.59 | 1.17 | 1.23 |
| 27 | BA | 1434 | 4AC | O7-C7 | -2.59 | 1.17 | 1.23 |
| 1 | Aa | 373 | 4AC | O7-C7 | -2.59 | 1.17 | 1.23 |
| 27 | BA | 2832 | 4AC | O7-C7 | -2.59 | 1.17 | 1.23 |
| 27 | BA | 488 | A2M | C6-N6 | 2.59 | 1.43 | 1.34 |
| 27 | BA | 2035 | 5MC | O4'-C4' | 2.59 | 1.50 | 1.45 |
| 1 | Aa | 636 | OMG | O6-C6 | -2.59 | 1.18 | 1.23 |
| 1 | Aa | 670 | 2MG | C5-C6 | 2.59 | 1.52 | 1.47 |
| 27 | BA | 2797 | 4AC | C5-C4 | 2.59 | 1.46 | 1.40 |
| 27 | BA | 3009 | 4AC | O7-C7 | -2.58 | 1.17 | 1.23 |
| 27 | BA | 2702 | A2M | C6-N6 | 2.58 | 1.43 | 1.34 |
| 27 | BA | 376 | 4AC | C5-C4 | 2.58 | 1.46 | 1.40 |
| 27 | BA | 1357 | 4AC | O7-C7 | -2.58 | 1.17 | 1.23 |
| 27 | BA | 56 | 4AC | O7-C7 | -2.58 | 1.17 | 1.23 |
| 1 | Aa | 852 | OMG | C2-N2 | 2.57 | 1.40 | 1.34 |
| 27 | BA | 1899 | 4AC | O7-C7 | -2.57 | 1.17 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Aa | 501 | 4AC | O7-C7 | -2.57 | 1.17 | 1.23 |
| 1 | Aa | 1276 | 5MC | O4'-C4' | 2.57 | 1.50 | 1.45 |
| 1 | Aa | 296 | OMC | C6-N1 | 2.57 | 1.44 | 1.38 |
| 1 | Aa | 771 | OMG | C6-N1 | 2.57 | 1.41 | 1.37 |
| 27 | BA | 2389 | OMU | C4-N3 | -2.57 | 1.34 | 1.38 |
| 1 | Aa | 752 | OMC | C6-N1 | 2.56 | 1.44 | 1.38 |
| 27 | BA | 754 | OMC | C6-N1 | 2.56 | 1.44 | 1.38 |
| 1 | Aa | 636 | OMG | C5-C4 | -2.56 | 1.36 | 1.43 |
| 1 | Aa | 1434 | OMG | C5-C6 | 2.56 | 1.52 | 1.47 |
| 1 | Aa | 381 | OMG | C6-N1 | 2.55 | 1.41 | 1.37 |
| 27 | BA | 2324 | OMG | C5-C6 | 2.55 | 1.52 | 1.47 |
| 27 | BA | 858 | 4AC | O7-C7 | -2.55 | 1.17 | 1.23 |
| 1 | Aa | 605 | 4AC | O7-C7 | -2.55 | 1.17 | 1.23 |
| 27 | BA | 879 | A2M | O2'-C2' | 2.54 | 1.49 | 1.42 |
| 27 | BA | 1396 | 4AC | C5-C4 | 2.54 | 1.46 | 1.40 |
| 1 | Aa | 446 | OMG | C6-N1 | 2.54 | 1.41 | 1.37 |
| 27 | BA | 1427 | 4AC | C5-C4 | 2.54 | 1.46 | 1.40 |
| 27 | BA | 1337 | 4AC | O7-C7 | -2.53 | 1.17 | 1.23 |
| 27 | BA | 800 | OMG | C2-N2 | 2.53 | 1.40 | 1.34 |
| 27 | BA | 353 | OMG | C2-N1 | 2.53 | 1.43 | 1.37 |
| 1 | Aa | 569 | 4AC | O7-C7 | -2.53 | 1.17 | 1.23 |
| 27 | BA | 2702 | A2M | O3'-C3' | -2.53 | 1.37 | 1.43 |
| 27 | BA | 2550 | OMG | C2-N2 | 2.53 | 1.40 | 1.34 |
| 27 | BA | 2745 | OMG | C5-C6 | 2.52 | 1.52 | 1.47 |
| 27 | BA | 723 | OMG | C6-N1 | 2.52 | 1.41 | 1.37 |
| 1 | Aa | 994 | OMG | C5-C4 | -2.52 | 1.36 | 1.43 |
| 1 | Aa | 304 | OMU | C6-N1 | 2.52 | 1.44 | 1.38 |
| 27 | BA | 335 | 4AC | O7-C7 | -2.52 | 1.17 | 1.23 |
| 1 | Aa | 892 | OMG | O6-C6 | -2.52 | 1.18 | 1.23 |
| 27 | BA | 505 | A2M | C6-N6 | 2.52 | 1.43 | 1.34 |
| 27 | BA | 833 | OMG | C5-C6 | 2.51 | 1.52 | 1.47 |
| 1 | Aa | 1107 | OMG | O6-C6 | -2.51 | 1.18 | 1.23 |
| 27 | BA | 501 | 4AC | C5-C4 | 2.51 | 1.46 | 1.40 |
| 1 | Aa | 535 | OMC | C6-N1 | 2.51 | 1.44 | 1.38 |
| 27 | BA | 2672 | OMG | C5-C6 | 2.51 | 1.52 | 1.47 |
| 27 | BA | 3023 | 4AC | O7-C7 | -2.50 | 1.17 | 1.23 |
| 27 | BA | 2832 | 4AC | C5-C4 | 2.50 | 1.46 | 1.40 |
| 27 | BA | 1470 | 4AC | C5-C4 | 2.50 | 1.46 | 1.40 |
| 27 | BA | 799 | 4AC | C5-C4 | 2.50 | 1.46 | 1.40 |
| 27 | BA | 1810 | 4AC | O7-C7 | -2.50 | 1.17 | 1.23 |
| 1 | Aa | 994 | OMG | O6-C6 | -2.50 | 1.18 | 1.23 |
| 27 | BA | 2070 | 5MC | C6-N1 | -2.50 | 1.33 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Aa | 52 | OMU | C6-N1 | 2.50 | 1.44 | 1.38 |
| 27 | BA | 2780 | 4AC | O7-C7 | -2.49 | 1.17 | 1.23 |
| 27 | BA | 2797 | 4AC | O7-C7 | -2.49 | 1.17 | 1.23 |
| 27 | BA | 1265 | A2M | O3'-C3' | -2.49 | 1.37 | 1.43 |
| 1 | Aa | 458 | 4AC | C4-N4 | -2.48 | 1.36 | 1.39 |
| 27 | BA | 2610 | OMU | O2-C2 | -2.48 | 1.18 | 1.23 |
| 27 | BA | 552 | OMG | C2-N2 | 2.48 | 1.40 | 1.34 |
| 1 | Aa | 240 | OMU | C6-N1 | 2.48 | 1.44 | 1.38 |
| 27 | BA | 124 | 4AC | O7-C7 | -2.47 | 1.17 | 1.23 |
| 1 | Aa | 682 | 4AC | O7-C7 | -2.47 | 1.17 | 1.23 |
| 27 | BA | 1551 | OMU | C6-N1 | 2.47 | 1.43 | 1.38 |
| 27 | BA | 763 | OMG | C5-C6 | 2.47 | 1.52 | 1.47 |
| 1 | Aa | 1025 | OMG | C6-N1 | 2.46 | 1.41 | 1.37 |
| 1 | Aa | 320 | OMG | C6-N1 | 2.46 | 1.41 | 1.37 |
| 27 | BA | 713 | 4AC | O7-C7 | -2.46 | 1.17 | 1.23 |
| 27 | BA | 778 | 4AC | O7-C7 | -2.45 | 1.17 | 1.23 |
| 1 | Aa | 1354 | OMC | C6-N1 | 2.45 | 1.43 | 1.38 |
| 27 | BA | 433 | 4AC | O7-C7 | -2.45 | 1.17 | 1.23 |
| 27 | BA | 1776 | OMU | C6-N1 | 2.45 | 1.43 | 1.38 |
| 27 | BA | 2590 | 4AC | O7-C7 | -2.45 | 1.17 | 1.23 |
| 27 | BA | 2728 | OMG | C5-C6 | 2.45 | 1.52 | 1.47 |
| 27 | BA | 433 | 4AC | C5-C4 | 2.45 | 1.46 | 1.40 |
| 27 | BA | 805 | 4AC | O7-C7 | -2.44 | 1.17 | 1.23 |
| 1 | Aa | 1265 | OMG | C5-C6 | 2.44 | 1.52 | 1.47 |
| 1 | Aa | 358 | 4AC | O7-C7 | -2.43 | 1.17 | 1.23 |
| 27 | BA | 1337 | 4AC | C5-C4 | 2.43 | 1.46 | 1.40 |
| 27 | BA | 201 | 4AC | O7-C7 | -2.42 | 1.17 | 1.23 |
| 27 | BA | 2630 | OMC | C6-N1 | 2.42 | 1.43 | 1.38 |
| 27 | BA | 2838 | 4AC | O7-C7 | -2.42 | 1.17 | 1.23 |
| 27 | BA | 505 | A2M | C4-N3 | -2.42 | 1.32 | 1.35 |
| 27 | BA | 2152 | OMG | C2-N2 | 2.42 | 1.40 | 1.34 |
| 1 | Aa | 1217 | 4AC | O7-C7 | -2.42 | 1.17 | 1.23 |
| 1 | Aa | 913 | OMG | C5-C6 | 2.41 | 1.52 | 1.47 |
| 27 | BA | 1517 | A2M | O3'-C3' | -2.41 | 1.37 | 1.43 |
| 1 | Aa | 1361 | OMC | C6-N1 | 2.41 | 1.43 | 1.38 |
| 27 | BA | 619 | OMU | C6-N1 | 2.41 | 1.43 | 1.38 |
| 27 | BA | 2595 | OMC | C6-N1 | 2.41 | 1.43 | 1.38 |
| 27 | BA | 932 | A2M | O5'-C5' | -2.40 | 1.38 | 1.44 |
| 1 | Aa | 659 | OMG | C5-C6 | 2.40 | 1.52 | 1.47 |
| 27 | BA | 800 | OMG | C5-C6 | 2.40 | 1.52 | 1.47 |
| 27 | BA | 34 | OMU | C6-N1 | 2.40 | 1.43 | 1.38 |
| 27 | BA | 825 | A2M | O2'-C2' | 2.40 | 1.48 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Aa | 532 | OMG | C5-C6 | 2.39 | 1.52 | 1.47 |
| 1 | Aa | 138 | OMG | C5-C6 | 2.39 | 1.52 | 1.47 |
| 1 | Aa | 854 | 5MC | C6-N1 | 2.39 | 1.42 | 1.38 |
| 1 | Aa | 917 | 5MU | C2-N3 | -2.39 | 1.33 | 1.38 |
| 1 | Aa | 450 | OMG | C5-C6 | 2.39 | 1.52 | 1.47 |
| 27 | BA | 1558 | OMG | O6-C6 | -2.39 | 1.18 | 1.23 |
| 27 | BA | 1820 | OMC | C6-N1 | 2.39 | 1.43 | 1.38 |
| 27 | BA | 2047 | OMC | C6-N1 | 2.38 | 1.43 | 1.38 |
| 27 | BA | 215 | OMG | C2-N1 | 2.38 | 1.43 | 1.37 |
| 27 | BA | 2553 | 4SU | C6-N1 | 2.37 | 1.43 | 1.38 |
| 27 | BA | 2168 | OMG | O6-C6 | -2.37 | 1.18 | 1.23 |
| 1 | Aa | 827 | 4AC | O7-C7 | -2.37 | 1.17 | 1.23 |
| 1 | Aa | 917 | 5MU | C6-N1 | -2.37 | 1.34 | 1.38 |
| 27 | BA | 1396 | 4AC | O7-C7 | -2.36 | 1.17 | 1.23 |
| 27 | BA | 1431 | 4AC | O7-C7 | -2.36 | 1.17 | 1.23 |
| 1 | Aa | 479 | OMU | O2-C2 | -2.36 | 1.18 | 1.23 |
| 1 | Aa | 246 | OMG | C5-C6 | 2.36 | 1.52 | 1.47 |
| 1 | Aa | 825 | OMC | C6-N1 | 2.36 | 1.43 | 1.38 |
| 1 | Aa | 818 | 4AC | O7-C7 | -2.36 | 1.17 | 1.23 |
| 27 | BA | 201 | 4AC | C5-C4 | 2.36 | 1.45 | 1.40 |
| 27 | BA | 2010 | OMG | C5-C6 | 2.35 | 1.52 | 1.47 |
| 27 | BA | 2992 | 4AC | O7-C7 | -2.35 | 1.17 | 1.23 |
| 27 | BA | 1892 | OMG | C6-N1 | 2.35 | 1.41 | 1.37 |
| 27 | BA | 27 | 4AC | O7-C7 | -2.35 | 1.17 | 1.23 |
| 27 | BA | 1810 | 4AC | C5-C4 | 2.35 | 1.45 | 1.40 |
| 27 | BA | 1525 | OMG | C5-C6 | 2.35 | 1.52 | 1.47 |
| 27 | BA | 1400 | A2M | C6-C5 | -2.35 | 1.34 | 1.43 |
| 27 | BA | 2657 | OMG | C6-N1 | 2.35 | 1.41 | 1.37 |
| 27 | BA | 1543 | 4AC | O7-C7 | -2.35 | 1.17 | 1.23 |
| 1 | Aa | 525 | 4AC | O7-C7 | -2.35 | 1.17 | 1.23 |
| 27 | BA | 244 | 4AC | C5-C4 | 2.35 | 1.45 | 1.40 |
| 27 | BA | 849 | A2M | O2'-C2' | 2.34 | 1.48 | 1.42 |
| 27 | BA | 1431 | 4AC | O2-C2 | -2.34 | 1.19 | 1.23 |
| 27 | BA | 872 | A2M | C6-N6 | 2.34 | 1.42 | 1.34 |
| 27 | BA | 768 | OMU | C6-N1 | 2.34 | 1.43 | 1.38 |
| 1 | Aa | 498 | OMG | C5-C6 | 2.34 | 1.52 | 1.47 |
| 27 | BA | 1480 | OMU | C6-N1 | 2.34 | 1.43 | 1.38 |
| 27 | BA | 799 | 4AC | O7-C7 | -2.34 | 1.18 | 1.23 |
| 1 | Aa | 913 | OMG | C2-N1 | 2.33 | 1.43 | 1.37 |
| 27 | BA | 2016 | OMG | C5-C6 | 2.33 | 1.52 | 1.47 |
| 27 | BA | 2389 | OMU | C2-N3 | -2.33 | 1.33 | 1.38 |
| 27 | BA | 353 | OMG | C6-N1 | 2.33 | 1.41 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Aa | 876 | OMG | C5-C6 | 2.33 | 1.52 | 1.47 |
| 1 | Aa | 8 | OMU | C6-N1 | 2.33 | 1.43 | 1.38 |
| 27 | BA | 2324 | OMG | C6-N1 | 2.33 | 1.41 | 1.37 |
| 1 | Aa | 1459 | 4AC | O2-C2 | -2.32 | 1.19 | 1.23 |
| 27 | BA | 418 | 4AC | O7-C7 | -2.32 | 1.18 | 1.23 |
| 27 | BA | 805 | 4AC | C5-C4 | 2.32 | 1.45 | 1.40 |
| 27 | BA | 290 | OMG | C6-N1 | 2.32 | 1.41 | 1.37 |
| 27 | BA | 2590 | 4AC | O2-C2 | -2.32 | 1.19 | 1.23 |
| 27 | BA | 2035 | 5MC | O2'-C2' | 2.32 | 1.48 | 1.43 |
| 1 | Aa | 994 | OMG | C2-N1 | 2.32 | 1.43 | 1.37 |
| 27 | BA | 869 | OMC | C6-N1 | 2.31 | 1.43 | 1.38 |
| 27 | BA | 2019 | OMG | C2-N1 | 2.31 | 1.43 | 1.37 |
| 27 | BA | 561 | OMC | C6-N1 | 2.31 | 1.43 | 1.38 |
| 1 | Aa | 457 | 5MC | O2'-C2' | 2.31 | 1.48 | 1.43 |
| 27 | BA | 365 | OMG | C6-N1 | 2.31 | 1.41 | 1.37 |
| 27 | BA | 1940 | OMG | C6-N1 | 2.30 | 1.41 | 1.37 |
| 1 | Aa | 697 | 4AC | O7-C7 | -2.30 | 1.18 | 1.23 |
| 27 | BA | 2542 | OMU | C6-N1 | 2.30 | 1.43 | 1.38 |
| 1 | Aa | 892 | OMG | C5-C6 | 2.30 | 1.52 | 1.47 |
| 27 | BA | 1517 | A2M | O2'-C2' | 2.30 | 1.48 | 1.42 |
| 27 | BA | 1400 | A2M | O5'-C5' | -2.30 | 1.39 | 1.44 |
| 27 | BA | 674 | OMG | O6-C6 | -2.29 | 1.18 | 1.23 |
| 27 | BA | 1899 | 4AC | C5-C4 | 2.29 | 1.45 | 1.40 |
| 27 | BA | 124 | 4AC | O2-C2 | -2.29 | 1.19 | 1.23 |
| 27 | BA | 2070 | 5MC | C6-C5 | 2.28 | 1.38 | 1.34 |
| 27 | BA | 1305 | 4AC | O7-C7 | -2.28 | 1.18 | 1.23 |
| 27 | BA | 2159 | 4AC | O2-C2 | -2.28 | 1.19 | 1.23 |
| 27 | BA | 488 | A2M | O5'-C5' | -2.27 | 1.39 | 1.44 |
| 27 | BA | 1892 | OMG | C5-C6 | 2.27 | 1.52 | 1.47 |
| 1 | Aa | 382 | OMG | C5-C6 | 2.27 | 1.52 | 1.47 |
| 27 | BA | 1969 | OMU | C6-N1 | 2.26 | 1.43 | 1.38 |
| 27 | BA | 2527 | OMG | C6-N1 | 2.25 | 1.41 | 1.37 |
| 27 | BA | 505 | A2M | O3'-C3' | -2.25 | 1.37 | 1.43 |
| 27 | BA | 763 | OMG | O6-C6 | -2.25 | 1.18 | 1.23 |
| 27 | BA | 872 | A2M | C6-C5 | -2.25 | 1.34 | 1.43 |
| 27 | BA | 1375 | 4AC | O2-C2 | -2.24 | 1.19 | 1.23 |
| 27 | BA | 2389 | OMU | C5-C4 | -2.24 | 1.38 | 1.43 |
| 1 | Aa | 1026 | OMG | C5-C6 | 2.24 | 1.52 | 1.47 |
| 1 | Aa | 446 | OMG | C5-C6 | 2.24 | 1.52 | 1.47 |
| 27 | BA | 1799 | OMG | C5-C6 | 2.24 | 1.51 | 1.47 |
| 27 | BA | 2656 | OMU | C6-N1 | 2.23 | 1.43 | 1.38 |
| 27 | BA | 1434 | 4AC | C5-C4 | 2.23 | 1.45 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Aa | 41 | 4AC | O7-C7 | -2.23 | 1.18 | 1.23 |
| 27 | BA | 124 | 4AC | C5-C4 | 2.23 | 1.45 | 1.40 |
| 27 | BA | 932 | A2M | O2'-C2' | 2.21 | 1.48 | 1.42 |
| 27 | BA | 2657 | OMG | C5-C6 | 2.21 | 1.51 | 1.47 |
| 1 | Aa | 1025 | OMG | C5-C6 | 2.21 | 1.51 | 1.47 |
| 1 | Aa | 352 | A2M | C5-C4 | 2.21 | 1.46 | 1.40 |
| 27 | BA | 799 | 4AC | O2-C2 | -2.20 | 1.19 | 1.23 |
| 1 | Aa | 136 | 4AC | O7-C7 | -2.20 | 1.18 | 1.23 |
| 27 | BA | 365 | OMG | C5-C6 | 2.20 | 1.51 | 1.47 |
| 27 | BA | 872 | A2M | O2'-C2' | 2.19 | 1.48 | 1.42 |
| 27 | BA | 805 | 4AC | O2-C2 | -2.19 | 1.19 | 1.23 |
| 1 | Aa | 771 | OMG | C5-C6 | 2.19 | 1.51 | 1.47 |
| 1 | Aa | 525 | 4AC | O2-C2 | -2.19 | 1.19 | 1.23 |
| 1 | Aa | 479 | OMU | C5-C4 | 2.19 | 1.48 | 1.43 |
| 27 | BA | 201 | 4AC | O2-C2 | -2.18 | 1.19 | 1.23 |
| 27 | BA | 290 | OMG | C2-N1 | 2.18 | 1.43 | 1.37 |
| 1 | Aa | 1107 | OMG | C2-N1 | 2.18 | 1.43 | 1.37 |
| 27 | BA | 1106 | OMG | C5-C6 | 2.18 | 1.51 | 1.47 |
| 27 | BA | 1953 | OMG | C5-C6 | 2.18 | 1.51 | 1.47 |
| 27 | BA | 1434 | 4AC | O2-C2 | -2.18 | 1.19 | 1.23 |
| 27 | BA | 825 | A2M | C6-C5 | -2.18 | 1.35 | 1.43 |
| 27 | BA | 2521 | OMG | C5-C6 | 2.17 | 1.51 | 1.47 |
| 27 | BA | 2550 | OMG | C5-C6 | 2.17 | 1.51 | 1.47 |
| 27 | BA | 2581 | 4SU | C6-N1 | 2.17 | 1.43 | 1.38 |
| 27 | BA | 872 | A2M | C5-N7 | -2.17 | 1.31 | 1.39 |
| 27 | BA | 849 | A2M | O5'-C5' | -2.17 | 1.39 | 1.44 |
| 27 | BA | 505 | A2M | C5-N7 | -2.17 | 1.31 | 1.39 |
| 1 | Aa | 381 | OMG | C5-C6 | 2.16 | 1.51 | 1.47 |
| 1 | Aa | 1276 | 5MC | O2'-C2' | 2.16 | 1.48 | 1.43 |
| 27 | BA | 1396 | 4AC | O2-C2 | -2.16 | 1.19 | 1.23 |
| 27 | BA | 1400 | A2M | C8-N7 | -2.15 | 1.30 | 1.34 |
| 27 | BA | 575 | OMG | O6-C6 | -2.15 | 1.18 | 1.23 |
| 1 | Aa | 730 | 4AC | O2-C2 | -2.15 | 1.19 | 1.23 |
| 27 | BA | 2018 | OMC | C6-N1 | 2.14 | 1.43 | 1.38 |
| 27 | BA | 617 | LHH | O7-C7 | -2.14 | 1.18 | 1.23 |
| 27 | BA | 723 | OMG | C2-N1 | 2.14 | 1.43 | 1.37 |
| 27 | BA | 212 | A2M | C5-C4 | 2.14 | 1.46 | 1.40 |
| 27 | BA | 912 | OMG | C2-N1 | 2.14 | 1.43 | 1.37 |
| 27 | BA | 756 | A2M | O2'-C2' | 2.14 | 1.48 | 1.42 |
| 27 | BA | 526 | LHH | O7-C7 | -2.14 | 1.18 | 1.23 |
| 27 | BA | 1400 | A2M | C5-N7 | -2.14 | 1.32 | 1.39 |
| 27 | BA | 2702 | A2M | C6-C5 | -2.14 | 1.35 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 912 | OMG | C5-C6 | 2.13 | 1.51 | 1.47 |
| 27 | BA | 2955 | LHH | O7-C7 | -2.13 | 1.18 | 1.23 |
| 27 | BA | 1400 | A2M | C6-N6 | 2.13 | 1.41 | 1.34 |
| 27 | BA | 1790 | OMC | C6-N1 | 2.12 | 1.43 | 1.38 |
| 27 | BA | 833 | OMG | C6-N1 | 2.12 | 1.41 | 1.37 |
| 27 | BA | 244 | 4AC | O2-C2 | -2.12 | 1.19 | 1.23 |
| 1 | Aa | 1476 | 5MC | O2'-C2' | 2.12 | 1.48 | 1.43 |
| 27 | BA | 2832 | 4AC | O2-C2 | -2.12 | 1.19 | 1.23 |
| 27 | BA | 825 | A2M | C6-N6 | 2.12 | 1.41 | 1.34 |
| 27 | BA | 849 | A2M | O3'-C3' | -2.11 | 1.38 | 1.43 |
| 27 | BA | 1953 | OMG | C2-N1 | 2.11 | 1.42 | 1.37 |
| 1 | Aa | 876 | OMG | C2-N1 | 2.11 | 1.42 | 1.37 |
| 27 | BA | 1319 | OMU | C6-N1 | 2.10 | 1.43 | 1.38 |
| 27 | BA | 2702 | A2M | C5-N7 | -2.10 | 1.32 | 1.39 |
| 27 | BA | 858 | 4AC | O2-C2 | -2.10 | 1.19 | 1.23 |
| 27 | BA | 353 | OMG | C5-C6 | 2.10 | 1.51 | 1.47 |
| 27 | BA | 1305 | 4AC | C6-N1 | 2.09 | 1.43 | 1.38 |
| 27 | BA | 1899 | 4AC | O2-C2 | -2.09 | 1.19 | 1.23 |
| 1 | Aa | 1467 | MA6 | C4-N3 | -2.09 | 1.32 | 1.35 |
| 27 | BA | 2457 | LHH | O7-C7 | -2.08 | 1.18 | 1.23 |
| 27 | BA | 1955 | 4AC | O2-C2 | -2.07 | 1.19 | 1.23 |
| 27 | BA | 3009 | 4AC | O2-C2 | -2.07 | 1.19 | 1.23 |
| 27 | BA | 1750 | OMC | C6-N1 | 2.07 | 1.43 | 1.38 |
| 1 | Aa | 1467 | MA6 | C5-N7 | -2.07 | 1.32 | 1.39 |
| 27 | BA | 1799 | OMG | O6-C6 | -2.07 | 1.19 | 1.23 |
| 27 | BA | 2121 | 4AC | O2-C2 | -2.07 | 1.19 | 1.23 |
| 27 | BA | 730 | 4AC | O2-C2 | -2.07 | 1.19 | 1.23 |
| 1 | Aa | 381 | OMG | C2-N1 | 2.07 | 1.42 | 1.37 |
| 1 | Aa | 5 | 4AC | O2-C2 | -2.07 | 1.19 | 1.23 |
| 27 | BA | 1357 | 4AC | O2-C2 | -2.07 | 1.19 | 1.23 |
| 27 | BA | 27 | 4AC | O2-C2 | -2.07 | 1.19 | 1.23 |
| 1 | Aa | 1020 | LHH | O7-C7 | -2.06 | 1.18 | 1.23 |
| 27 | BA | 453 | OMU | C6-N1 | 2.06 | 1.42 | 1.38 |
| 27 | BA | 1340 | OMU | C6-N1 | 2.05 | 1.42 | 1.38 |
| 1 | Aa | 1358 | OMU | C6-N1 | 2.05 | 1.42 | 1.38 |
| 27 | BA | 215 | OMG | C5-C6 | 2.05 | 1.51 | 1.47 |
| 27 | BA | 1810 | 4AC | O2-C2 | -2.05 | 1.19 | 1.23 |
| 27 | BA | 932 | A2M | C5-N7 | -2.05 | 1.32 | 1.39 |
| 27 | BA | 418 | 4AC | O2-C2 | -2.05 | 1.19 | 1.23 |
| 27 | BA | 825 | A2M | C5-N7 | -2.05 | 1.32 | 1.39 |
| 27 | BA | 2521 | OMG | C6-N1 | 2.04 | 1.40 | 1.37 |
| 27 | BA | 756 | A2M | C5-N7 | -2.04 | 1.32 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 2159 | 4AC | C5-C4 | 2.04 | 1.45 | 1.40 |
| 1 | Aa | 1276 | 5MC | O5'-C5' | -2.04 | 1.39 | 1.44 |
| 27 | BA | 552 | OMG | C2-N1 | 2.04 | 1.42 | 1.37 |
| 27 | BA | 2797 | 4AC | O2-C2 | -2.03 | 1.19 | 1.23 |
| 27 | BA | 849 | A2M | C5-N7 | -2.03 | 1.32 | 1.39 |
| 1 | Aa | 847 | 4AC | O2-C2 | -2.03 | 1.19 | 1.23 |
| 1 | Aa | 229 | LHH | O7-C7 | -2.03 | 1.18 | 1.23 |
| 27 | BA | 2702 | A2M | O5'-C5' | -2.03 | 1.39 | 1.44 |
| 27 | BA | 778 | 4AC | C6-N1 | 2.02 | 1.42 | 1.38 |
| 27 | BA | 2528 | OMG | C5-C6 | 2.02 | 1.51 | 1.47 |
| 27 | BA | 250 | OMC | C6-N1 | 2.02 | 1.42 | 1.38 |
| 27 | BA | 1799 | OMG | C2-N1 | 2.02 | 1.42 | 1.37 |
| 27 | BA | 2610 | OMU | C5-C4 | 2.01 | 1.48 | 1.43 |
| 27 | BA | 2992 | 4AC | C6-N1 | 2.01 | 1.42 | 1.38 |
| 1 | Aa | 659 | OMG | C2-N1 | 2.01 | 1.42 | 1.37 |
| 1 | Aa | 1265 | OMG | C2-N1 | 2.01 | 1.42 | 1.37 |
| 27 | BA | 1517 | A2M | O5'-C5' | -2.01 | 1.39 | 1.44 |
| 1 | Aa | 818 | 4AC | O2-C2 | -2.01 | 1.20 | 1.23 |
| 27 | BA | 1337 | 4AC | O2-C2 | -2.00 | 1.20 | 1.23 |
| 27 | BA | 488 | A2M | C5-N7 | -2.00 | 1.32 | 1.39 |

All (955) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | Aa | 1468 | MA6 | N1-C6-N6 | -13.10 | 103.27 | 117.06 |
| 27 | BA | 1905 | 5MU | C5-C4-N3 | 12.43 | 125.92 | 115.31 |
| 27 | BA | 537 | 5MU | C5-C4-N3 | 12.41 | 125.90 | 115.31 |
| 1 | Aa | 1467 | MA6 | N1-C6-N6 | -12.33 | 104.08 | 117.06 |
| 27 | BA | 1548 | 5MU | C5-C4-N3 | 12.23 | 125.75 | 115.31 |
| 27 | BA | 572 | 5MU | C5-C4-N3 | 12.21 | 125.73 | 115.31 |
| 27 | BA | 875 | 5MU | C5-C4-N3 | 12.16 | 125.69 | 115.31 |
| 27 | BA | 2384 | 5MU | C5-C4-N3 | 11.97 | 125.53 | 115.31 |
| 27 | BA | 298 | 5MU | C5-C4-N3 | 11.66 | 125.26 | 115.31 |
| 27 | BA | 2688 | 5MU | C5-C4-N3 | 11.34 | 124.99 | 115.31 |
| 27 | BA | 1085 | 5MU | C5-C6-N1 | -10.38 | 112.67 | 123.34 |
| 27 | BA | 505 | A2M | C5-C6-N6 | 10.33 | 136.05 | 120.35 |
| 27 | BA | 1265 | A2M | C5-C6-N6 | 10.11 | 135.72 | 120.35 |
| 27 | BA | 1085 | 5MU | C5-C4-N3 | 10.06 | 123.90 | 115.31 |
| 27 | BA | 849 | A2M | C5-C6-N6 | 9.70 | 135.10 | 120.35 |
| 27 | BA | 1085 | 5MU | C5M-C5-C6 | -9.63 | 109.99 | 122.85 |
| 27 | BA | 2688 | 5MU | C5-C6-N1 | -9.37 | 113.70 | 123.34 |
| 27 | BA | 879 | A2M | C5-C6-N6 | 8.96 | 133.96 | 120.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 1548 | 5MU | C5-C6-N1 | -8.94 | 114.14 | 123.34 |
| 27 | BA | 875 | 5MU | C5-C6-N1 | -8.93 | 114.15 | 123.34 |
| 27 | BA | 298 | 5MU | C5-C6-N1 | -8.92 | 114.16 | 123.34 |
| 27 | BA | 488 | A2M | C5-C6-N6 | 8.88 | 133.85 | 120.35 |
| 27 | BA | 872 | A2M | C5-C6-N6 | 8.87 | 133.83 | 120.35 |
| 27 | BA | 2384 | 5MU | C5-C6-N1 | -8.76 | 114.32 | 123.34 |
| 27 | BA | 756 | A2M | C5-C6-N6 | 8.63 | 133.47 | 120.35 |
| 27 | BA | 1517 | A2M | C5-C6-N6 | 8.50 | 133.27 | 120.35 |
| 27 | BA | 537 | 5MU | C5-C6-N1 | -8.45 | 114.65 | 123.34 |
| 27 | BA | 825 | A2M | C5-C6-N6 | 8.29 | 132.95 | 120.35 |
| 27 | BA | 1400 | A2M | C5-C6-N6 | 8.28 | 132.94 | 120.35 |
| 27 | BA | 419 | OMG | O6-C6-N1 | -8.05 | 111.14 | 120.65 |
| 27 | BA | 1085 | 5MU | C5M-C5-C4 | 8.02 | 127.59 | 118.77 |
| 27 | BA | 1905 | 5MU | C5-C6-N1 | -7.99 | 115.12 | 123.34 |
| 27 | BA | 419 | OMG | C2-N1-C6 | -7.82 | 110.70 | 125.10 |
| 27 | BA | 572 | 5MU | C5-C6-N1 | -7.81 | 115.31 | 123.34 |
| 27 | BA | 932 | A2M | C5-C6-N6 | 7.77 | 132.16 | 120.35 |
| 27 | BA | 2457 | LHH | CM7-C7-N4 | 7.76 | 128.72 | 115.29 |
| 27 | BA | 2702 | A2M | C5-C6-N6 | 7.62 | 131.93 | 120.35 |
| 27 | BA | 537 | 5MU | C5M-C5-C4 | 7.62 | 127.15 | 118.77 |
| 27 | BA | 2581 | 4SU | C4-N3-C2 | -7.57 | 119.98 | 127.34 |
| 27 | BA | 1265 | A2M | N6-C6-N1 | -7.49 | 103.03 | 118.57 |
| 27 | BA | 1905 | 5MU | C5M-C5-C4 | 7.46 | 126.98 | 118.77 |
| 27 | BA | 505 | A2M | N6-C6-N1 | -7.20 | 103.62 | 118.57 |
| 27 | BA | 419 | OMG | C5-C6-N1 | 7.12 | 126.52 | 113.95 |
| 27 | BA | 849 | A2M | N6-C6-N1 | -6.72 | 104.64 | 118.57 |
| 27 | BA | 2553 | 4SU | C4-N3-C2 | -6.60 | 120.92 | 127.34 |
| 27 | BA | 872 | A2M | N6-C6-N1 | -6.55 | 104.98 | 118.57 |
| 27 | BA | 572 | 5MU | C5M-C5-C4 | 6.53 | 125.95 | 118.77 |
| 27 | BA | 879 | A2M | N6-C6-N1 | -6.44 | 105.21 | 118.57 |
| 27 | BA | 488 | A2M | N6-C6-N1 | -6.38 | 105.34 | 118.57 |
| 27 | BA | 2384 | 5MU | C5M-C5-C4 | 6.32 | 125.73 | 118.77 |
| 27 | BA | 537 | 5MU | C5M-C5-C6 | -6.31 | 114.42 | 122.85 |
| 27 | BA | 419 | OMG | N2-C2-N3 | -6.28 | 107.51 | 119.74 |
| 1 | Aa | 1449 | 6MZ | C2-N1-C6 | 6.20 | 121.91 | 116.59 |
| 1 | Aa | 1358 | OMU | C4-N3-C2 | -6.19 | 118.42 | 126.58 |
| 27 | BA | 825 | A2M | N6-C6-N1 | -6.18 | 105.74 | 118.57 |
| 27 | BA | 1400 | A2M | N6-C6-N1 | -6.14 | 105.83 | 118.57 |
| 1 | Aa | 136 | 4AC | CM7-C7-N4 | 6.09 | 125.83 | 115.29 |
| 27 | BA | 756 | A2M | N6-C6-N1 | -6.05 | 106.01 | 118.57 |
| 27 | BA | 1517 | A2M | N6-C6-N1 | -6.01 | 106.11 | 118.57 |
| 1 | Aa | 41 | 4AC | CM7-C7-N4 | 5.99 | 125.66 | 115.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 2955 | LHH | CM7-C7-N4 | 5.96 | 125.60 | 115.29 |
| 27 | BA | 298 | 5MU | O4-C4-C5 | -5.95 | 118.00 | 124.90 |
| 27 | BA | 1905 | 5MU | C5M-C5-C6 | -5.92 | 114.94 | 122.85 |
| 27 | BA | 858 | 4AC | CM7-C7-N4 | 5.90 | 125.49 | 115.29 |
| 1 | Aa | 358 | 4AC | CM7-C7-N4 | 5.88 | 125.47 | 115.29 |
| 27 | BA | 2688 | 5MU | C5M-C5-C6 | -5.85 | 115.03 | 122.85 |
| 1 | Aa | 5 | 4AC | CM7-C7-N4 | 5.84 | 125.39 | 115.29 |
| 27 | BA | 572 | 5MU | O4-C4-C5 | -5.79 | 118.19 | 124.90 |
| 27 | BA | 1085 | 5MU | O4-C4-C5 | -5.78 | 118.20 | 124.90 |
| 27 | BA | 1434 | 4AC | CM7-C7-N4 | 5.78 | 125.29 | 115.29 |
| 1 | Aa | 697 | 4AC | CM7-C7-N4 | 5.71 | 125.17 | 115.29 |
| 1 | Aa | 525 | 4AC | N4-C4-N3 | 5.71 | 123.43 | 113.85 |
| 27 | BA | 1305 | 4AC | CM7-C7-N4 | 5.71 | 125.16 | 115.29 |
| 27 | BA | 201 | 4AC | CM7-C7-N4 | 5.70 | 125.15 | 115.29 |
| 27 | BA | 1085 | 5MU | C4-N3-C2 | -5.62 | 120.07 | 127.35 |
| 27 | BA | 617 | LHH | CM7-C7-N4 | 5.60 | 124.99 | 115.29 |
| 27 | BA | 2688 | 5MU | C5M-C5-C4 | 5.60 | 124.93 | 118.77 |
| 27 | BA | 2702 | A2M | N6-C6-N1 | -5.59 | 106.97 | 118.57 |
| 27 | BA | 932 | A2M | N6-C6-N1 | -5.54 | 107.08 | 118.57 |
| 1 | Aa | 229 | LHH | CM7-C7-N4 | 5.47 | 124.75 | 115.29 |
| 27 | BA | 2384 | 5MU | C5M-C5-C6 | -5.44 | 115.58 | 122.85 |
| 27 | BA | 2610 | OMU | C4-N3-C2 | -5.43 | 119.42 | 126.58 |
| 1 | Aa | 818 | 4AC | CM7-C7-N4 | 5.42 | 124.66 | 115.29 |
| 1 | Aa | 917 | 5MU | C4-N3-C2 | -5.40 | 120.36 | 127.35 |
| 27 | BA | 875 | 5MU | O4-C4-C5 | -5.39 | 118.65 | 124.90 |
| 27 | BA | 1400 | A2M | N3-C2-N1 | -5.39 | 120.25 | 128.68 |
| 27 | BA | 875 | 5MU | C5M-C5-C4 | 5.35 | 124.66 | 118.77 |
| 1 | Aa | 730 | 4AC | CM7-C7-N4 | 5.30 | 124.46 | 115.29 |
| 27 | BA | 572 | 5MU | C5M-C5-C6 | -5.30 | 115.78 | 122.85 |
| 27 | BA | 768 | OMU | C4-N3-C2 | -5.29 | 119.60 | 126.58 |
| 27 | BA | 2656 | OMU | C4-N3-C2 | -5.28 | 119.61 | 126.58 |
| 27 | BA | 1548 | 5MU | O4-C4-C5 | -5.25 | 118.81 | 124.90 |
| 1 | Aa | 917 | 5MU | N3-C2-N1 | 5.24 | 121.85 | 114.89 |
| 27 | BA | 1085 | 5MU | C6-C5-C4 | 5.24 | 122.41 | 118.03 |
| 1 | Aa | 479 | OMU | C4-N3-C2 | -5.23 | 119.69 | 126.58 |
| 27 | BA | 1517 | A2M | N3-C2-N1 | -5.20 | 120.55 | 128.68 |
| 1 | Aa | 1468 | MA6 | N3-C2-N1 | -5.17 | 120.60 | 128.68 |
| 1 | Aa | 304 | OMU | C4-N3-C2 | -5.16 | 119.77 | 126.58 |
| 27 | BA | 537 | 5MU | O4-C4-C5 | -5.16 | 118.92 | 124.90 |
| 27 | BA | 619 | OMU | C4-N3-C2 | -5.14 | 119.80 | 126.58 |
| 1 | Aa | 1020 | LHH | CM7-C7-N4 | 5.12 | 124.15 | 115.29 |
| 27 | BA | 875 | 5MU | C5M-C5-C6 | -5.11 | 116.02 | 122.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 2581 | 4SU | C5-C4-N3 | 5.10 | 119.42 | 114.69 |
| 1 | Aa | 240 | OMU | C4-N3-C2 | -5.09 | 119.86 | 126.58 |
| 27 | BA | 1319 | OMU | C4-N3-C2 | -5.09 | 119.86 | 126.58 |
| 27 | BA | 849 | A2M | N3-C2-N1 | -5.09 | 120.73 | 128.68 |
| 27 | BA | 825 | A2M | N3-C2-N1 | -5.07 | 120.75 | 128.68 |
| 27 | BA | 1548 | 5MU | C4-N3-C2 | -4.98 | 120.91 | 127.35 |
| 27 | BA | 298 | 5MU | C5M-C5-C6 | -4.95 | 116.24 | 122.85 |
| 27 | BA | 1340 | OMU | C4-N3-C2 | -4.94 | 120.07 | 126.58 |
| 27 | BA | 453 | OMU | C4-N3-C2 | -4.93 | 120.08 | 126.58 |
| 27 | BA | 2688 | 5MU | C4-N3-C2 | -4.88 | 121.03 | 127.35 |
| 27 | BA | 1085 | 5MU | N3-C2-N1 | 4.88 | 121.37 | 114.89 |
| 1 | Aa | 8 | OMU | C4-N3-C2 | -4.87 | 120.15 | 126.58 |
| 1 | Aa | 1467 | MA6 | N3-C2-N1 | -4.86 | 121.08 | 128.68 |
| 27 | BA | 1551 | OMU | C4-N3-C2 | -4.85 | 120.19 | 126.58 |
| 27 | BA | 872 | A2M | N3-C2-N1 | -4.84 | 121.11 | 128.68 |
| 27 | BA | 298 | 5MU | C4-N3-C2 | -4.84 | 121.09 | 127.35 |
| 27 | BA | 2384 | 5MU | N3-C2-N1 | 4.84 | 121.31 | 114.89 |
| 27 | BA | 298 | 5MU | C5M-C5-C4 | 4.84 | 124.09 | 118.77 |
| 27 | BA | 2384 | 5MU | C4-N3-C2 | -4.83 | 121.10 | 127.35 |
| 1 | Aa | 52 | OMU | C4-N3-C2 | -4.82 | 120.22 | 126.58 |
| 27 | BA | 34 | OMU | C4-N3-C2 | -4.80 | 120.25 | 126.58 |
| 1 | Aa | 605 | 4AC | CM7-C7-N4 | 4.80 | 123.59 | 115.29 |
| 27 | BA | 1905 | 5MU | O4-C4-C5 | -4.73 | 119.41 | 124.90 |
| 27 | BA | 1548 | 5MU | N3-C2-N1 | 4.72 | 121.16 | 114.89 |
| 27 | BA | 2702 | A2M | N3-C2-N1 | -4.72 | 121.31 | 128.68 |
| 27 | BA | 932 | A2M | N3-C2-N1 | -4.71 | 121.31 | 128.68 |
| 27 | BA | 2542 | OMU | C4-N3-C2 | -4.71 | 120.37 | 126.58 |
| 27 | BA | 1969 | OMU | C4-N3-C2 | -4.70 | 120.38 | 126.58 |
| 27 | BA | 1776 | OMU | C4-N3-C2 | -4.70 | 120.38 | 126.58 |
| 27 | BA | 1548 | 5MU | C5M-C5-C4 | 4.69 | 123.93 | 118.77 |
| 27 | BA | 912 | OMG | C5-C6-N1 | 4.69 | 122.22 | 113.95 |
| 1 | Aa | 1358 | OMU | N3-C2-N1 | 4.68 | 121.10 | 114.89 |
| 27 | BA | 2528 | OMG | C5-C6-N1 | 4.68 | 122.21 | 113.95 |
| 27 | BA | 1480 | OMU | C4-N3-C2 | -4.65 | 120.44 | 126.58 |
| 1 | Aa | 917 | 5MU | C5-C4-N3 | 4.65 | 119.28 | 115.31 |
| 27 | BA | 756 | A2M | N3-C2-N1 | -4.64 | 121.42 | 128.68 |
| 27 | BA | 2688 | 5MU | O4-C4-C5 | -4.63 | 119.53 | 124.90 |
| 27 | BA | 1265 | A2M | N3-C2-N1 | -4.63 | 121.44 | 128.68 |
| 27 | BA | 1085 | 5MU | C1'-N1-C2 | 4.61 | 125.91 | 117.57 |
| 1 | Aa | 1217 | 4AC | N4-C4-N3 | 4.60 | 121.58 | 113.85 |
| 27 | BA | 879 | A2M | N3-C2-N1 | -4.58 | 121.51 | 128.68 |
| 27 | BA | 353 | OMG | C5-C6-N1 | 4.56 | 122.01 | 113.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 537 | 5MU | C4-N3-C2 | -4.55 | 121.46 | 127.35 |
| 1 | Aa | 605 | 4AC | N4-C4-N3 | 4.54 | 121.48 | 113.85 |
| 27 | BA | 2379 | OMG | O6-C6-N1 | -4.53 | 115.30 | 120.65 |
| 1 | Aa | 525 | 4AC | CM7-C7-N4 | 4.49 | 123.06 | 115.29 |
| 27 | BA | 912 | OMG | O6-C6-N1 | -4.47 | 115.36 | 120.65 |
| 27 | BA | 215 | OMG | C5-C6-N1 | 4.46 | 121.83 | 113.95 |
| 27 | BA | 505 | A2M | N3-C2-N1 | -4.45 | 121.72 | 128.68 |
| 27 | BA | 298 | 5MU | N3-C2-N1 | 4.45 | 120.79 | 114.89 |
| 27 | BA | 1548 | 5MU | C5M-C5-C6 | -4.45 | 116.91 | 122.85 |
| 27 | BA | 572 | 5MU | C4-N3-C2 | -4.44 | 121.60 | 127.35 |
| 27 | BA | 875 | 5MU | C4-N3-C2 | -4.41 | 121.64 | 127.35 |
| 27 | BA | 2389 | OMU | C4-N3-C2 | -4.38 | 120.80 | 126.58 |
| 27 | BA | 2688 | 5MU | N3-C2-N1 | 4.38 | 120.70 | 114.89 |
| 27 | BA | 2581 | 4SU | C5-C4-S4 | -4.37 | 118.83 | 124.47 |
| 1 | Aa | 8 | OMU | N3-C2-N1 | 4.36 | 120.68 | 114.89 |
| 27 | BA | 1905 | 5MU | C4-N3-C2 | -4.35 | 121.72 | 127.35 |
| 27 | BA | 1953 | OMG | C5-C6-N1 | 4.34 | 121.62 | 113.95 |
| 1 | Aa | 917 | 5MU | O4-C4-C5 | -4.33 | 119.88 | 124.90 |
| 27 | BA | 2379 | OMG | C5-C6-N1 | 4.32 | 121.57 | 113.95 |
| 27 | BA | 63 | OMG | C5-C6-N1 | 4.31 | 121.56 | 113.95 |
| 27 | BA | 488 | A2M | N3-C2-N1 | -4.26 | 122.03 | 128.68 |
| 27 | BA | 215 | OMG | O6-C6-N1 | -4.25 | 115.63 | 120.65 |
| 27 | BA | 912 | OMG | C2-N1-C6 | -4.21 | 117.34 | 125.10 |
| 27 | BA | 2550 | OMG | C5-C6-N1 | 4.21 | 121.38 | 113.95 |
| 27 | BA | 419 | OMG | N2-C2-N1 | 4.19 | 125.64 | 116.71 |
| 27 | BA | 2019 | OMG | C5-C6-N1 | 4.17 | 121.32 | 113.95 |
| 27 | BA | 2159 | 4AC | N4-C4-N3 | 4.16 | 120.83 | 113.85 |
| 1 | Aa | 682 | 4AC | N4-C4-N3 | 4.11 | 120.75 | 113.85 |
| 27 | BA | 858 | 4AC | O7-C7-N4 | -4.10 | 115.18 | 121.82 |
| 27 | BA | 2955 | LHH | O3'-C3'-C2' | 4.08 | 122.76 | 111.17 |
| 27 | BA | 2780 | 4AC | N4-C4-N3 | 4.08 | 120.70 | 113.85 |
| 27 | BA | 1810 | 4AC | N4-C4-N3 | 4.07 | 120.69 | 113.85 |
| 27 | BA | 833 | OMG | C5-C6-N1 | 4.06 | 121.12 | 113.95 |
| 27 | BA | 2610 | OMU | N3-C2-N1 | 4.05 | 120.27 | 114.89 |
| 27 | BA | 526 | LHH | N4-C4-N3 | 4.03 | 120.62 | 113.85 |
| 1 | Aa | 913 | OMG | O3'-C3'-C2' | 4.03 | 122.61 | 111.17 |
| 27 | BA | 2553 | 4SU | N3-C2-N1 | 4.02 | 120.22 | 114.89 |
| 27 | BA | 2656 | OMU | N3-C2-N1 | 4.02 | 120.22 | 114.89 |
| 1 | Aa | 1459 | 4AC | N4-C4-N3 | 4.02 | 120.59 | 113.85 |
| 27 | BA | 833 | OMG | C2-N1-C6 | -4.01 | 117.72 | 125.10 |
| 27 | BA | 1776 | OMU | N3-C2-N1 | 4.00 | 120.20 | 114.89 |
| 27 | BA | 1085 | 5MU | C1'-N1-C6 | -3.97 | 114.51 | 121.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 2992 | 4AC | N4-C4-N3 | 3.97 | 120.52 | 113.85 |
| 27 | BA | 572 | 5MU | N3-C2-N1 | 3.97 | 120.16 | 114.89 |
| 1 | Aa | 240 | OMU | N3-C2-N1 | 3.96 | 120.15 | 114.89 |
| 27 | BA | 2672 | OMG | C5-C6-N1 | 3.96 | 120.94 | 113.95 |
| 1 | Aa | 298 | 4AC | N4-C4-N3 | 3.96 | 120.50 | 113.85 |
| 27 | BA | 768 | OMU | N3-C2-N1 | 3.96 | 120.14 | 114.89 |
| 1 | Aa | 298 | 4AC | CM7-C7-N4 | 3.94 | 122.11 | 115.29 |
| 27 | BA | 298 | 5MU | C1'-N1-C2 | 3.91 | 124.64 | 117.57 |
| 1 | Aa | 373 | 4AC | N4-C4-N3 | 3.91 | 120.41 | 113.85 |
| 27 | BA | 290 | OMG | C2-N1-C6 | -3.90 | 117.92 | 125.10 |
| 27 | BA | 2745 | OMG | C5-C6-N1 | 3.89 | 120.83 | 113.95 |
| 1 | Aa | 501 | 4AC | N4-C4-N3 | 3.89 | 120.38 | 113.85 |
| 27 | BA | 1525 | OMG | C5-C6-N1 | 3.88 | 120.80 | 113.95 |
| 27 | BA | 2457 | LHH | O7-C7-N4 | -3.88 | 115.54 | 121.82 |
| 27 | BA | 657 | OMU | C1'-N1-C2 | 3.88 | 124.59 | 117.57 |
| 27 | BA | 723 | OMG | CM2-O2'-C2' | -3.87 | 104.38 | 114.52 |
| 27 | BA | 215 | OMG | C2-N1-C6 | -3.86 | 117.99 | 125.10 |
| 27 | BA | 2672 | OMG | O6-C6-N1 | -3.86 | 116.09 | 120.65 |
| 27 | BA | 2672 | OMG | C2-N1-C6 | -3.85 | 118.00 | 125.10 |
| 27 | BA | 2016 | OMG | C5-C6-N1 | 3.85 | 120.75 | 113.95 |
| 27 | BA | 290 | OMG | C5-C6-N1 | 3.85 | 120.74 | 113.95 |
| 1 | Aa | 913 | OMG | C5-C6-N1 | 3.83 | 120.71 | 113.95 |
| 1 | Aa | 917 | 5MU | C5-C6-N1 | -3.83 | 119.40 | 123.34 |
| 27 | BA | 2528 | OMG | O6-C6-N1 | -3.83 | 116.13 | 120.65 |
| 27 | BA | 1551 | OMU | N3-C2-N1 | 3.80 | 119.94 | 114.89 |
| 27 | BA | 2550 | OMG | C2-N1-C6 | -3.80 | 118.11 | 125.10 |
| 27 | BA | 2019 | OMG | C2-N1-C6 | -3.79 | 118.12 | 125.10 |
| 27 | BA | 526 | LHH | CM7-C7-N4 | 3.79 | 121.85 | 115.29 |
| 27 | BA | 657 | OMU | C4-N3-C2 | -3.79 | 121.58 | 126.58 |
| 27 | BA | 2389 | OMU | C5-C4-N3 | 3.78 | 120.50 | 114.84 |
| 27 | BA | 925 | 4AC | CM7-C7-N4 | 3.78 | 121.83 | 115.29 |
| 27 | BA | 2955 | LHH | O3'-C3'-C4' | 3.76 | 121.92 | 111.05 |
| 27 | BA | 27 | 4AC | N4-C4-N3 | 3.76 | 120.16 | 113.85 |
| 27 | BA | 1905 | 5MU | C1'-N1-C2 | 3.75 | 124.36 | 117.57 |
| 27 | BA | 453 | OMU | O4-C4-C5 | -3.74 | 118.58 | 125.16 |
| 1 | Aa | 605 | 4AC | O7-C7-CM7 | -3.74 | 115.12 | 122.06 |
| 27 | BA | 501 | 4AC | N4-C4-N3 | 3.74 | 120.12 | 113.85 |
| 1 | Aa | 913 | OMG | O3'-C3'-C4' | 3.73 | 121.84 | 111.05 |
| 27 | BA | 1396 | 4AC | N4-C4-N3 | 3.73 | 120.11 | 113.85 |
| 27 | BA | 2389 | OMU | N3-C2-N1 | 3.72 | 119.83 | 114.89 |
| 27 | BA | 537 | 5MU | N3-C2-N1 | 3.72 | 119.83 | 114.89 |
| 27 | BA | 2545 | OMC | O3'-C3'-C2' | 3.72 | 121.73 | 111.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 2055 | 5MC | C5-C6-N1 | -3.71 | 119.53 | 123.34 |
| 27 | BA | 2070 | 5MC | C5-C6-N1 | -3.70 | 119.53 | 123.34 |
| 27 | BA | 875 | 5MU | N3-C2-N1 | 3.68 | 119.77 | 114.89 |
| 27 | BA | 1905 | 5MU | N3-C2-N1 | 3.68 | 119.77 | 114.89 |
| 27 | BA | 1431 | 4AC | N4-C4-N3 | 3.67 | 120.02 | 113.85 |
| 27 | BA | 2581 | 4SU | N3-C2-N1 | 3.67 | 119.76 | 114.89 |
| 1 | Aa | 304 | OMU | N3-C2-N1 | 3.67 | 119.76 | 114.89 |
| 27 | BA | 1953 | OMG | C2-N1-C6 | -3.67 | 118.34 | 125.10 |
| 1 | Aa | 730 | 4AC | C6-C5-C4 | 3.66 | 121.44 | 116.96 |
| 1 | Aa | 854 | 5MC | C5-C6-N1 | -3.65 | 119.58 | 123.34 |
| 27 | BA | 2550 | OMG | O6-C6-N1 | -3.65 | 116.34 | 120.65 |
| 27 | BA | 2384 | 5MU | O4-C4-C5 | -3.65 | 120.67 | 124.90 |
| 1 | Aa | 1358 | OMU | O3'-C3'-C4' | 3.64 | 121.59 | 111.05 |
| 27 | BA | 2075 | 5MC | C5-C6-N1 | -3.64 | 119.59 | 123.34 |
| 27 | BA | 2542 | OMU | N3-C2-N1 | 3.63 | 119.71 | 114.89 |
| 27 | BA | 2457 | LHH | C6-C5-C4 | 3.63 | 121.40 | 116.96 |
| 27 | BA | 572 | 5MU | C1'-N1-C2 | 3.62 | 124.13 | 117.57 |
| 27 | BA | 2553 | 4SU | C5-C4-N3 | 3.62 | 118.05 | 114.69 |
| 27 | BA | 1470 | 4AC | N4-C4-N3 | 3.62 | 119.93 | 113.85 |
| 1 | Aa | 913 | OMG | C2-N1-C6 | -3.62 | 118.44 | 125.10 |
| 27 | BA | 2838 | 4AC | N4-C4-N3 | 3.61 | 119.91 | 113.85 |
| 27 | BA | 2728 | OMG | C5-C6-N1 | 3.60 | 120.31 | 113.95 |
| 1 | Aa | 1478 | 5MC | C5-C6-N1 | -3.59 | 119.64 | 123.34 |
| 27 | BA | 1357 | 4AC | N4-C4-N3 | 3.59 | 119.87 | 113.85 |
| 1 | Aa | 1358 | OMU | O3'-C3'-C2' | 3.59 | 121.35 | 111.17 |
| 27 | BA | 2521 | OMG | C2-N1-C6 | -3.58 | 118.51 | 125.10 |
| 1 | Aa | 569 | 4AC | N4-C4-N3 | 3.58 | 119.86 | 113.85 |
| 27 | BA | 1969 | OMU | N3-C2-N1 | 3.57 | 119.63 | 114.89 |
| 27 | BA | 869 | OMC | C5-C4-N4 | -3.56 | 114.97 | 120.57 |
| 1 | Aa | 605 | 4AC | C6-C5-C4 | 3.55 | 121.30 | 116.96 |
| 1 | Aa | 464 | 5MC | CM5-C5-C6 | -3.54 | 118.12 | 122.85 |
| 27 | BA | 56 | 4AC | O3'-C3'-C4' | 3.54 | 121.29 | 111.05 |
| 27 | BA | 2745 | OMG | C2-N1-C6 | -3.53 | 118.59 | 125.10 |
| 27 | BA | 2016 | OMG | C2-N1-C6 | -3.53 | 118.60 | 125.10 |
| 27 | BA | 2542 | OMU | O4-C4-C5 | -3.53 | 118.95 | 125.16 |
| 27 | BA | 619 | OMU | N3-C2-N1 | 3.53 | 119.57 | 114.89 |
| 27 | BA | 799 | 4AC | N4-C4-N3 | 3.51 | 119.75 | 113.85 |
| 27 | BA | 723 | OMG | C2-N1-C6 | -3.51 | 118.63 | 125.10 |
| 27 | BA | 2521 | OMG | C5-C6-N1 | 3.50 | 120.14 | 113.95 |
| 27 | BA | 2745 | OMG | O6-C6-N1 | -3.50 | 116.52 | 120.65 |
| 27 | BA | 2152 | OMG | C5-C6-N1 | 3.49 | 120.11 | 113.95 |
| 27 | BA | 718 | OMC | C5-C4-N4 | -3.48 | 115.10 | 120.57 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 376 | 4AC | N4-C4-N3 | 3.48 | 119.69 | 113.85 |
| 1 | Aa | 1004 | 5MC | CM5-C5-C6 | -3.47 | 118.21 | 122.85 |
| 27 | BA | 1899 | 4AC | N4-C4-N3 | 3.47 | 119.68 | 113.85 |
| 27 | BA | 1375 | 4AC | N4-C4-N3 | 3.47 | 119.67 | 113.85 |
| 1 | Aa | 525 | 4AC | C5-C4-N4 | -3.46 | 116.90 | 122.92 |
| 27 | BA | 925 | 4AC | C6-C5-C4 | 3.46 | 121.20 | 116.96 |
| 1 | Aa | 479 | OMU | N3-C2-N1 | 3.46 | 119.49 | 114.89 |
| 27 | BA | 2610 | OMU | C5-C4-N3 | 3.46 | 120.02 | 114.84 |
| 1 | Aa | 298 | 4AC | O7-C7-CM7 | -3.45 | 115.66 | 122.06 |
| 1 | Aa | 52 | OMU | N3-C2-N1 | 3.43 | 119.44 | 114.89 |
| 27 | BA | 552 | OMG | C2-N1-C6 | -3.41 | 118.82 | 125.10 |
| 27 | BA | 2379 | OMG | C2-N1-C6 | -3.41 | 118.82 | 125.10 |
| 27 | BA | 1398 | OMG | C5-C6-N1 | 3.41 | 119.97 | 113.95 |
| 27 | BA | 2457 | LHH | O7-C7-CM7 | -3.40 | 115.73 | 122.06 |
| 27 | BA | 537 | 5MU | C1'-N1-C2 | 3.40 | 123.73 | 117.57 |
| 27 | BA | 723 | OMG | C5-C6-N1 | 3.40 | 119.96 | 113.95 |
| 27 | BA | 2010 | OMG | C5-C6-N1 | 3.40 | 119.95 | 113.95 |
| 27 | BA | 2657 | OMG | C5-C6-N1 | 3.40 | 119.95 | 113.95 |
| 27 | BA | 34 | OMU | N3-C2-N1 | 3.39 | 119.38 | 114.89 |
| 27 | BA | 944 | 5MC | CM5-C5-C6 | -3.38 | 118.33 | 122.85 |
| 27 | BA | 1340 | OMU | O4-C4-C5 | -3.38 | 119.22 | 125.16 |
| 1 | Aa | 501 | 4AC | CM7-C7-N4 | 3.38 | 121.14 | 115.29 |
| 27 | BA | 2832 | 4AC | N4-C4-N3 | 3.38 | 119.52 | 113.85 |
| 1 | Aa | 1358 | OMU | C5-C4-N3 | 3.38 | 119.89 | 114.84 |
| 1 | Aa | 994 | OMG | C5-C6-N1 | 3.37 | 119.89 | 113.95 |
| 27 | BA | 2728 | OMG | C2-N1-C6 | -3.36 | 118.91 | 125.10 |
| 27 | BA | 1525 | OMG | C2-N1-C6 | -3.35 | 118.93 | 125.10 |
| 1 | Aa | 1020 | LHH | C6-C5-C4 | 3.35 | 121.05 | 116.96 |
| 27 | BA | 619 | OMU | C5-C4-N3 | 3.34 | 119.84 | 114.84 |
| 27 | BA | 34 | OMU | C5-C4-N3 | 3.34 | 119.83 | 114.84 |
| 1 | Aa | 827 | 4AC | N4-C4-N3 | 3.33 | 119.44 | 113.85 |
| 27 | BA | 3023 | 4AC | N4-C4-N3 | 3.33 | 119.44 | 113.85 |
| 27 | BA | 2550 | OMG | O3'-C3'-C4' | 3.32 | 120.65 | 111.05 |
| 27 | BA | 212 | A2M | N3-C2-N1 | -3.32 | 123.49 | 128.68 |
| 1 | Aa | 229 | LHH | C6-C5-C4 | 3.32 | 121.02 | 116.96 |
| 27 | BA | 453 | OMU | N3-C2-N1 | 3.31 | 119.28 | 114.89 |
| 27 | BA | 433 | 4AC | N4-C4-N3 | 3.31 | 119.41 | 113.85 |
| 1 | Aa | 479 | OMU | C5-C4-N3 | 3.31 | 119.78 | 114.84 |
| 1 | Aa | 1020 | LHH | N4-C4-N3 | 3.30 | 119.40 | 113.85 |
| 27 | BA | 1810 | 4AC | C6-C5-C4 | 3.30 | 121.00 | 116.96 |
| 27 | BA | 1319 | OMU | N3-C2-N1 | 3.30 | 119.27 | 114.89 |
| 27 | BA | 2384 | 5MU | O4-C4-N3 | -3.30 | 113.80 | 120.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | Aa | 876 | OMG | C5-C6-N1 | 3.29 | 119.77 | 113.95 |
| 27 | BA | 526 | LHH | O7-C7-CM7 | -3.29 | 115.94 | 122.06 |
| 1 | Aa | 8 | OMU | CM2-O2'-C2' | -3.29 | 105.89 | 114.52 |
| 27 | BA | 1470 | 4AC | O3'-C3'-C4' | 3.29 | 120.56 | 111.05 |
| 1 | Aa | 672 | 5MC | C5-C6-N1 | -3.29 | 119.95 | 123.34 |
| 1 | Aa | 1265 | OMG | C5-C6-N1 | 3.29 | 119.76 | 113.95 |
| 27 | BA | 1340 | OMU | N3-C2-N1 | 3.28 | 119.25 | 114.89 |
| 1 | Aa | 381 | OMG | C5-C6-N1 | 3.28 | 119.75 | 113.95 |
| 1 | Aa | 1478 | 5MC | C5-C4-N4 | -3.28 | 116.57 | 121.48 |
| 1 | Aa | 457 | 5MC | C5-C6-N1 | -3.28 | 119.97 | 123.34 |
| 27 | BA | 2780 | 4AC | CM7-C7-N4 | 3.28 | 120.96 | 115.29 |
| 27 | BA | 2528 | OMG | C2-N1-C6 | -3.28 | 119.07 | 125.10 |
| 1 | Aa | 240 | OMU | O4-C4-C5 | -3.27 | 119.40 | 125.16 |
| 1 | Aa | 1217 | 4AC | C6-C5-C4 | 3.27 | 120.96 | 116.96 |
| 1 | Aa | 304 | OMU | C5-C4-N3 | 3.27 | 119.73 | 114.84 |
| 27 | BA | 1969 | OMU | O4-C4-C5 | -3.26 | 119.42 | 125.16 |
| 1 | Aa | 730 | 4AC | O7-C7-CM7 | -3.26 | 116.01 | 122.06 |
| 27 | BA | 730 | 4AC | N4-C4-N3 | 3.25 | 119.31 | 113.85 |
| 1 | Aa | 1358 | OMU | O4-C4-C5 | -3.25 | 119.44 | 125.16 |
| 27 | BA | 2035 | 5MC | C5-C6-N1 | -3.25 | 120.00 | 123.34 |
| 27 | BA | 2527 | OMG | C5-C6-N1 | 3.24 | 119.67 | 113.95 |
| 27 | BA | 1340 | OMU | C5-C4-N3 | 3.23 | 119.68 | 114.84 |
| 27 | BA | 1551 | OMU | O4-C4-C5 | -3.23 | 119.47 | 125.16 |
| 27 | BA | 1337 | 4AC | N4-C4-N3 | 3.23 | 119.28 | 113.85 |
| 27 | BA | 453 | OMU | C5-C4-N3 | 3.23 | 119.67 | 114.84 |
| 27 | BA | 2324 | OMG | C5-C6-N1 | 3.22 | 119.64 | 113.95 |
| 27 | BA | 501 | 4AC | C6-C5-C4 | 3.21 | 120.89 | 116.96 |
| 27 | BA | 2863 | 5MC | C1'-N1-C6 | -3.21 | 115.77 | 121.12 |
| 27 | BA | 2997 | 4AC | N4-C4-N3 | 3.21 | 119.24 | 113.85 |
| 27 | BA | 2528 | OMG | N2-C2-N3 | 3.20 | 125.96 | 119.74 |
| 27 | BA | 244 | 4AC | N4-C4-N3 | 3.19 | 119.21 | 113.85 |
| 1 | Aa | 352 | A2M | N3-C2-N1 | -3.19 | 123.69 | 128.68 |
| 27 | BA | 2780 | 4AC | C6-C5-C4 | 3.19 | 120.86 | 116.96 |
| 27 | BA | 1319 | OMU | O4-C4-C5 | -3.18 | 119.56 | 125.16 |
| 1 | Aa | 138 | OMG | C5-C6-N1 | 3.18 | 119.57 | 113.95 |
| 27 | BA | 2550 | OMG | O3'-C3'-C2' | 3.18 | 120.20 | 111.17 |
| 27 | BA | 2389 | OMU | O4-C4-C5 | -3.18 | 119.57 | 125.16 |
| 1 | Aa | 304 | OMU | O4-C4-C5 | -3.18 | 119.57 | 125.16 |
| 27 | BA | 1934 | 4AC | N4-C4-N3 | 3.18 | 119.18 | 113.85 |
| 27 | BA | 1398 | OMG | C2-N1-C6 | -3.18 | 119.25 | 125.10 |
| 27 | BA | 713 | 4AC | N4-C4-N3 | 3.17 | 119.18 | 113.85 |
| 1 | Aa | 569 | 4AC | CM7-C7-N4 | 3.17 | 120.77 | 115.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | Aa | 1020 | LHH | O4'-C1'-N1 | 3.16 | 115.59 | 108.36 |
| 27 | BA | 27 | 4AC | C6-C5-C4 | 3.16 | 120.83 | 116.96 |
| 27 | BA | 63 | OMG | O6-C6-N1 | -3.16 | 116.92 | 120.65 |
| 1 | Aa | 501 | 4AC | C6-C5-C4 | 3.16 | 120.82 | 116.96 |
| 1 | Aa | 320 | OMG | C5-C6-N1 | 3.15 | 119.52 | 113.95 |
| 27 | BA | 1480 | OMU | N3-C2-N1 | 3.15 | 119.07 | 114.89 |
| 1 | Aa | 1459 | 4AC | O7-C7-CM7 | -3.15 | 116.21 | 122.06 |
| 27 | BA | 2657 | OMG | C2-N1-C6 | -3.15 | 119.30 | 125.10 |
| 1 | Aa | 446 | OMG | C5-C6-N1 | 3.14 | 119.50 | 113.95 |
| 1 | Aa | 1459 | 4AC | C1'-N1-C2 | 3.14 | 125.42 | 118.42 |
| 27 | BA | 805 | 4AC | N4-C4-N3 | 3.13 | 119.11 | 113.85 |
| 27 | BA | 849 | A2M | C3'-C2'-C1' | 3.13 | 108.77 | 102.89 |
| 27 | BA | 1480 | OMU | C5-C4-N3 | 3.13 | 119.52 | 114.84 |
| 1 | Aa | 854 | 5MC | CM5-C5-C6 | -3.12 | 118.68 | 122.85 |
| 1 | Aa | 1449 | 6MZ | N3-C2-N1 | -3.12 | 123.80 | 128.68 |
| 1 | Aa | 240 | OMU | C5-C4-N3 | 3.12 | 119.51 | 114.84 |
| 1 | Aa | 1434 | OMG | C5-C6-N1 | 3.12 | 119.46 | 113.95 |
| 27 | BA | 2955 | LHH | C6-C5-C4 | 3.11 | 120.77 | 116.96 |
| 1 | Aa | 670 | 2MG | C5-C6-N1 | 3.11 | 119.44 | 113.95 |
| 1 | Aa | 1276 | 5MC | C5-C6-N1 | -3.11 | 120.14 | 123.34 |
| 1 | Aa | 771 | OMG | C5-C6-N1 | 3.11 | 119.44 | 113.95 |
| 1 | Aa | 636 | OMG | C5-C6-N1 | 3.10 | 119.43 | 113.95 |
| 27 | BA | 56 | 4AC | O3'-C3'-C2' | 3.10 | 121.86 | 111.82 |
| 1 | Aa | 847 | 4AC | N4-C4-N3 | 3.10 | 119.05 | 113.85 |
| 1 | Aa | 52 | OMU | C5-C4-N3 | 3.10 | 119.47 | 114.84 |
| 1 | Aa | 525 | 4AC | C6-C5-C4 | 3.10 | 120.75 | 116.96 |
| 1 | Aa | 229 | LHH | N4-C4-N3 | 3.09 | 119.04 | 113.85 |
| 27 | BA | 1470 | 4AC | O3'-C3'-C2' | 3.09 | 121.82 | 111.82 |
| 27 | BA | 2353 | OMG | O3'-C3'-C4' | 3.09 | 119.99 | 111.05 |
| 27 | BA | 657 | OMU | N3-C2-N1 | 3.09 | 118.99 | 114.89 |
| 1 | Aa | 1026 | OMG | C5-C6-N1 | 3.09 | 119.41 | 113.95 |
| 1 | Aa | 682 | 4AC | CM7-C7-N4 | 3.09 | 120.64 | 115.29 |
| 27 | BA | 768 | OMU | O4-C4-C5 | -3.09 | 119.73 | 125.16 |
| 27 | BA | 617 | LHH | C6-C5-C4 | 3.09 | 120.74 | 116.96 |
| 1 | Aa | 382 | OMG | C5-C6-N1 | 3.08 | 119.40 | 113.95 |
| 1 | Aa | 659 | OMG | C5-C6-N1 | 3.08 | 119.39 | 113.95 |
| 27 | BA | 250 | OMC | N4-C4-N3 | 3.07 | 123.36 | 117.97 |
| 1 | Aa | 298 | 4AC | C6-C5-C4 | 3.07 | 120.72 | 116.96 |
| 27 | BA | 1319 | OMU | C5-C4-N3 | 3.07 | 119.44 | 114.84 |
| 27 | BA | 2656 | OMU | C5-C4-N3 | 3.07 | 119.43 | 114.84 |
| 1 | Aa | 697 | 4AC | C6-C5-C4 | 3.07 | 120.71 | 116.96 |
| 1 | Aa | 358 | 4AC | O7-C7-CM7 | -3.07 | 116.36 | 122.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 1427 | 4AC | N4-C4-N3 | 3.06 | 118.99 | 113.85 |
| 27 | BA | 1434 | 4AC | C6-C5-C4 | 3.05 | 120.70 | 116.96 |
| 27 | BA | 768 | OMU | C5-C4-N3 | 3.05 | 119.40 | 114.84 |
| 27 | BA | 2152 | OMG | C2-N1-C6 | -3.05 | 119.48 | 125.10 |
| 27 | BA | 2545 | OMC | O3'-C3'-C4' | 3.05 | 119.86 | 111.05 |
| 27 | BA | 674 | OMG | C2-N1-C6 | -3.05 | 119.49 | 125.10 |
| 27 | BA | 2121 | 4AC | CM7-C7-N4 | 3.04 | 120.54 | 115.29 |
| 27 | BA | 1799 | OMG | O6-C6-C5 | -3.03 | 118.45 | 124.37 |
| 1 | Aa | 1025 | OMG | C5-C6-N1 | 3.03 | 119.31 | 113.95 |
| 27 | BA | 365 | OMG | C5-C6-N1 | 3.03 | 119.30 | 113.95 |
| 1 | Aa | 892 | OMG | C5-C6-N1 | 3.03 | 119.30 | 113.95 |
| 27 | BA | 1969 | OMU | C5-C4-N3 | 3.03 | 119.37 | 114.84 |
| 1 | Aa | 498 | OMG | C5-C6-N1 | 3.03 | 119.30 | 113.95 |
| 1 | Aa | 464 | 5MC | C5-C6-N1 | -3.03 | 120.22 | 123.34 |
| 27 | BA | 1641 | 4AC | N4-C4-N3 | 3.02 | 118.93 | 113.85 |
| 1 | Aa | 1476 | 5MC | C5-C6-N1 | -3.02 | 120.23 | 123.34 |
| 1 | Aa | 382 | OMG | C2-N1-C6 | -3.02 | 119.53 | 125.10 |
| 27 | BA | 526 | LHH | C1'-N1-C2 | 3.02 | 125.16 | 118.42 |
| 27 | BA | 1558 | OMG | O6-C6-C5 | -3.02 | 118.48 | 124.37 |
| 1 | Aa | 818 | 4AC | O7-C7-CM7 | -3.02 | 116.46 | 122.06 |
| 27 | BA | 619 | OMU | O4-C4-C5 | -3.01 | 119.86 | 125.16 |
| 27 | BA | 657 | OMU | O4-C4-C5 | -3.01 | 119.86 | 125.16 |
| 27 | BA | 1543 | 4AC | N4-C4-N3 | 3.01 | 118.90 | 113.85 |
| 27 | BA | 944 | 5MC | C5-C6-N1 | -3.01 | 120.24 | 123.34 |
| 1 | Aa | 1265 | OMG | C2-N1-C6 | -3.00 | 119.58 | 125.10 |
| 1 | Aa | 636 | OMG | C2-N1-C6 | -2.99 | 119.58 | 125.10 |
| 1 | Aa | 876 | OMG | C2-N1-C6 | -2.99 | 119.58 | 125.10 |
| 27 | BA | 526 | LHH | C6-C5-C4 | 2.99 | 120.62 | 116.96 |
| 27 | BA | 718 | OMC | N4-C4-N3 | 2.99 | 123.22 | 117.97 |
| 1 | Aa | 569 | 4AC | C6-C5-C4 | 2.99 | 120.62 | 116.96 |
| 1 | Aa | 682 | 4AC | C6-C5-C4 | 2.99 | 120.62 | 116.96 |
| 1 | Aa | 479 | OMU | O4-C4-C5 | -2.99 | 119.90 | 125.16 |
| 27 | BA | 1480 | OMU | O4-C4-C5 | -2.98 | 119.91 | 125.16 |
| 1 | Aa | 450 | OMG | C5-C6-N1 | 2.98 | 119.22 | 113.95 |
| 27 | BA | 1551 | OMU | C5-C4-N3 | 2.98 | 119.30 | 114.84 |
| 27 | BA | 124 | 4AC | N4-C4-N3 | 2.97 | 118.84 | 113.85 |
| 27 | BA | 1905 | 5MU | C1'-N1-C6 | -2.97 | 116.18 | 121.12 |
| 27 | BA | 2610 | OMU | O4-C4-C5 | -2.97 | 119.94 | 125.16 |
| 1 | Aa | 697 | 4AC | O7-C7-CM7 | -2.97 | 116.55 | 122.06 |
| 27 | BA | 353 | OMG | C2-N1-C6 | -2.97 | 119.64 | 125.10 |
| 1 | Aa | 320 | OMG | C2-N1-C6 | -2.96 | 119.64 | 125.10 |
| 1 | Aa | 1449 | 6MZ | C4-C5-N7 | -2.96 | 106.31 | 109.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 2384 | 5MU | O2-C2-N1 | -2.96 | 118.85 | 122.79 |
| 27 | BA | 2047 | OMC | O2-C2-N3 | -2.96 | 117.52 | 122.33 |
| 27 | BA | 298 | 5MU | C1'-N1-C6 | -2.96 | 116.20 | 121.12 |
| 1 | Aa | 246 | OMG | C5-C6-N1 | 2.95 | 119.17 | 113.95 |
| 27 | BA | 849 | A2M | C2'-C3'-C4' | -2.95 | 95.58 | 101.99 |
| 27 | BA | 1776 | OMU | O4-C4-C5 | -2.95 | 119.97 | 125.16 |
| 27 | BA | 1799 | OMG | N2-C2-N1 | 2.95 | 122.99 | 116.71 |
| 1 | Aa | 1434 | OMG | C2-N1-C6 | -2.95 | 119.67 | 125.10 |
| 27 | BA | 730 | 4AC | CM7-C7-N4 | 2.95 | 120.39 | 115.29 |
| 1 | Aa | 605 | 4AC | C5-C4-N3 | -2.95 | 117.85 | 122.59 |
| 1 | Aa | 52 | OMU | O4-C4-C5 | -2.94 | 119.98 | 125.16 |
| 1 | Aa | 1107 | OMG | C5-C6-N1 | 2.94 | 119.14 | 113.95 |
| 27 | BA | 1776 | OMU | C5-C4-N3 | 2.93 | 119.23 | 114.84 |
| 27 | BA | 2571 | OMC | O2-C2-N3 | -2.93 | 117.56 | 122.33 |
| 27 | BA | 1892 | OMG | C2-N1-C6 | -2.93 | 119.70 | 125.10 |
| 1 | Aa | 1217 | 4AC | CM7-C7-N4 | 2.93 | 120.36 | 115.29 |
| 1 | Aa | 1217 | 4AC | C5-C4-N3 | -2.93 | 117.88 | 122.59 |
| 1 | Aa | 446 | OMG | C2-N1-C6 | -2.92 | 119.72 | 125.10 |
| 27 | BA | 2955 | LHH | O7-C7-N4 | -2.92 | 117.09 | 121.82 |
| 1 | Aa | 41 | 4AC | O7-C7-CM7 | -2.91 | 116.65 | 122.06 |
| 1 | Aa | 373 | 4AC | C6-C5-C4 | 2.91 | 120.52 | 116.96 |
| 27 | BA | 1375 | 4AC | CM7-C7-N4 | 2.91 | 120.32 | 115.29 |
| 27 | BA | 201 | 4AC | C6-C5-C4 | 2.90 | 120.51 | 116.96 |
| 1 | Aa | 532 | OMG | C5-C6-N1 | 2.90 | 119.08 | 113.95 |
| 1 | Aa | 1459 | 4AC | C1'-N1-C6 | -2.90 | 114.52 | 120.84 |
| 27 | BA | 2010 | OMG | C2-N1-C6 | -2.90 | 119.76 | 125.10 |
| 27 | BA | 212 | A2M | C4-C5-N7 | -2.90 | 106.38 | 109.40 |
| 1 | Aa | 994 | OMG | C2-N1-C6 | -2.90 | 119.77 | 125.10 |
| 27 | BA | 1955 | 4AC | C6-C5-C4 | 2.89 | 120.50 | 116.96 |
| 1 | Aa | 458 | 4AC | C6-C5-C4 | 2.89 | 120.50 | 116.96 |
| 27 | BA | 1892 | OMG | C5-C6-N1 | 2.89 | 119.06 | 113.95 |
| 27 | BA | 2553 | 4SU | C5-C4-S4 | -2.89 | 120.74 | 124.47 |
| 27 | BA | 1470 | 4AC | C6-C5-C4 | 2.88 | 120.49 | 116.96 |
| 27 | BA | 2168 | OMG | C8-N7-C5 | 2.88 | 108.48 | 102.99 |
| 27 | BA | 2780 | 4AC | O7-C7-CM7 | -2.88 | 116.70 | 122.06 |
| 1 | Aa | 450 | OMG | C2-N1-C6 | -2.88 | 119.80 | 125.10 |
| 27 | BA | 713 | 4AC | C6-C5-C4 | 2.88 | 120.48 | 116.96 |
| 1 | Aa | 730 | 4AC | C5-C4-N3 | -2.87 | 117.97 | 122.59 |
| 27 | BA | 2016 | OMG | C8-N7-C5 | 2.87 | 108.45 | 102.99 |
| 27 | BA | 2581 | 4SU | O2-C2-N1 | -2.87 | 118.97 | 122.79 |
| 27 | BA | 2324 | OMG | C2-N1-C6 | -2.86 | 119.82 | 125.10 |
| 27 | BA | 763 | OMG | N2-C2-N1 | 2.86 | 122.80 | 116.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 124 | 4AC | C6-C5-C4 | 2.86 | 120.46 | 116.96 |
| 1 | Aa | 136 | 4AC | O7-C7-CM7 | -2.86 | 116.75 | 122.06 |
| 27 | BA | 1305 | 4AC | O7-C7-N4 | -2.86 | 117.19 | 121.82 |
| 27 | BA | 1696 | 5MC | C5-C6-N1 | -2.86 | 120.40 | 123.34 |
| 27 | BA | 505 | A2M | C1'-N9-C4 | -2.86 | 121.62 | 126.64 |
| 27 | BA | 1396 | 4AC | C1'-N1-C2 | 2.85 | 124.78 | 118.42 |
| 27 | BA | 1776 | OMU | C1'-N1-C2 | 2.85 | 122.73 | 117.57 |
| 27 | BA | 1934 | 4AC | CM7-C7-N4 | 2.85 | 120.22 | 115.29 |
| 27 | BA | 1905 | 5MU | O4-C4-N3 | -2.84 | 114.67 | 120.12 |
| 27 | BA | 552 | OMG | C8-N7-C5 | 2.84 | 108.40 | 102.99 |
| 27 | BA | 56 | 4AC | N4-C4-N3 | 2.84 | 118.62 | 113.85 |
| 27 | BA | 875 | 5MU | C1'-N1-C2 | 2.84 | 122.71 | 117.57 |
| 1 | Aa | 136 | 4AC | C6-C5-C4 | 2.84 | 120.43 | 116.96 |
| 27 | BA | 730 | 4AC | C6-C5-C4 | 2.84 | 120.43 | 116.96 |
| 1 | Aa | 659 | OMG | C2-N1-C6 | -2.83 | 119.88 | 125.10 |
| 1 | Aa | 381 | OMG | C2-N1-C6 | -2.83 | 119.89 | 125.10 |
| 27 | BA | 537 | 5MU | C1'-N1-C6 | -2.83 | 116.42 | 121.12 |
| 27 | BA | 1799 | OMG | C2-N1-C6 | -2.82 | 119.90 | 125.10 |
| 27 | BA | 3009 | 4AC | N4-C4-N3 | 2.82 | 118.59 | 113.85 |
| 27 | BA | 552 | OMG | O6-C6-C5 | -2.82 | 118.86 | 124.37 |
| 27 | BA | 2780 | 4AC | C1'-N1-C2 | 2.82 | 124.72 | 118.42 |
| 27 | BA | 2527 | OMG | C2-N1-C6 | -2.81 | 119.92 | 125.10 |
| 1 | Aa | 1004 | 5MC | C5-C6-N1 | -2.81 | 120.44 | 123.34 |
| 27 | BA | 453 | OMU | C1'-N1-C2 | 2.81 | 122.66 | 117.57 |
| 1 | Aa | 827 | 4AC | C6-C5-C4 | 2.81 | 120.40 | 116.96 |
| 27 | BA | 2992 | 4AC | C6-C5-C4 | 2.81 | 120.40 | 116.96 |
| 1 | Aa | 852 | OMG | C5-C6-N1 | 2.81 | 118.91 | 113.95 |
| 27 | BA | 1434 | 4AC | O7-C7-N4 | -2.80 | 117.28 | 121.82 |
| 27 | BA | 2353 | OMG | O3'-C3'-C2' | 2.79 | 119.10 | 111.17 |
| 1 | Aa | 942 | 5MC | CM5-C5-C6 | -2.79 | 119.12 | 122.85 |
| 27 | BA | 723 | OMG | C8-N7-C5 | 2.79 | 108.30 | 102.99 |
| 1 | Aa | 1478 | 5MC | C1'-N1-C6 | -2.78 | 116.49 | 121.12 |
| 1 | Aa | 229 | LHH | O7-C7-CM7 | -2.78 | 116.89 | 122.06 |
| 1 | Aa | 892 | OMG | C2-N1-C6 | -2.78 | 119.98 | 125.10 |
| 27 | BA | 799 | 4AC | C6-C5-C4 | 2.78 | 120.36 | 116.96 |
| 27 | BA | 805 | 4AC | CM7-C7-N4 | 2.78 | 120.10 | 115.29 |
| 27 | BA | 1953 | OMG | O6-C6-N1 | -2.77 | 117.38 | 120.65 |
| 1 | Aa | 1358 | OMU | O2-C2-N1 | -2.76 | 119.11 | 122.79 |
| 27 | BA | 376 | 4AC | CM7-C7-N4 | 2.76 | 120.07 | 115.29 |
| 27 | BA | 2542 | OMU | C5-C4-N3 | 2.76 | 118.97 | 114.84 |
| 27 | BA | 1955 | 4AC | CM7-C7-N4 | 2.76 | 120.06 | 115.29 |
| 27 | BA | 2168 | OMG | N2-C2-N1 | 2.76 | 122.58 | 116.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 1750 | OMC | C1'-N1-C2 | 2.76 | 124.57 | 118.42 |
| 27 | BA | 1558 | OMG | O6-C6-N1 | 2.75 | 123.90 | 120.65 |
| 1 | Aa | 498 | OMG | C2-N1-C6 | -2.75 | 120.03 | 125.10 |
| 1 | Aa | 1107 | OMG | C2-N1-C6 | -2.75 | 120.03 | 125.10 |
| 1 | Aa | 913 | OMG | C8-N7-C5 | 2.75 | 108.23 | 102.99 |
| 27 | BA | 2019 | OMG | C8-N7-C5 | 2.75 | 108.23 | 102.99 |
| 1 | Aa | 246 | OMG | C2-N1-C6 | -2.75 | 120.04 | 125.10 |
| 27 | BA | 418 | 4AC | N4-C4-N3 | 2.74 | 118.45 | 113.85 |
| 1 | Aa | 771 | OMG | C2-N1-C6 | -2.74 | 120.06 | 125.10 |
| 27 | BA | 1106 | OMG | C2-N1-C6 | -2.73 | 120.06 | 125.10 |
| 27 | BA | 1525 | OMG | C8-N7-C5 | 2.73 | 108.20 | 102.99 |
| 27 | BA | 1431 | 4AC | C6-C5-C4 | 2.73 | 120.30 | 116.96 |
| 1 | Aa | 138 | OMG | C2-N1-C6 | -2.73 | 120.07 | 125.10 |
| 27 | BA | 353 | OMG | O6-C6-N1 | -2.73 | 117.43 | 120.65 |
| 1 | Aa | 41 | 4AC | C6-C5-C4 | 2.73 | 120.30 | 116.96 |
| 1 | Aa | 1217 | 4AC | C1'-N1-C2 | 2.72 | 124.50 | 118.42 |
| 27 | BA | 617 | LHH | N4-C4-N3 | 2.72 | 118.41 | 113.85 |
| 27 | BA | 1357 | 4AC | CM7-C7-N4 | 2.72 | 119.99 | 115.29 |
| 27 | BA | 2595 | OMC | O2-C2-N3 | -2.72 | 117.91 | 122.33 |
| 1 | Aa | 5 | 4AC | O7-C7-CM7 | -2.72 | 117.01 | 122.06 |
| 27 | BA | 34 | OMU | O4-C4-C5 | -2.71 | 120.39 | 125.16 |
| 1 | Aa | 136 | 4AC | O7-C7-N4 | -2.71 | 117.42 | 121.82 |
| 1 | Aa | 1007 | 4AC | C6-C5-C4 | 2.71 | 120.28 | 116.96 |
| 27 | BA | 617 | LHH | O7-C7-CM7 | -2.71 | 117.02 | 122.06 |
| 1 | Aa | 1352 | 5MC | C5-C6-N1 | -2.71 | 120.55 | 123.34 |
| 1 | Aa | 917 | 5MU | O2-C2-N1 | -2.71 | 119.19 | 122.79 |
| 27 | BA | 2688 | 5MU | O2-C2-N1 | -2.71 | 119.19 | 122.79 |
| 27 | BA | 201 | 4AC | O7-C7-N4 | -2.71 | 117.44 | 121.82 |
| 1 | Aa | 1026 | OMG | C2-N1-C6 | -2.70 | 120.12 | 125.10 |
| 27 | BA | 1641 | 4AC | C6-C5-C4 | 2.70 | 120.26 | 116.96 |
| 27 | BA | 619 | OMU | CM2-O2'-C2' | 2.70 | 121.60 | 114.52 |
| 27 | BA | 2728 | OMG | O6-C6-N1 | -2.69 | 117.47 | 120.65 |
| 27 | BA | 1969 | OMU | C1'-N1-C2 | 2.68 | 122.43 | 117.57 |
| 27 | BA | 353 | OMG | N1-C2-N3 | -2.68 | 118.31 | 123.32 |
| 27 | BA | 1820 | OMC | N4-C4-N3 | 2.68 | 122.67 | 117.97 |
| 27 | BA | 1965 | 5MC | C5-C6-N1 | -2.68 | 120.58 | 123.34 |
| 27 | BA | 1955 | 4AC | N4-C4-N3 | 2.67 | 118.34 | 113.85 |
| 27 | BA | 1427 | 4AC | CM7-C7-N4 | 2.67 | 119.91 | 115.29 |
| 1 | Aa | 352 | A2M | C4-C5-N7 | -2.67 | 106.62 | 109.40 |
| 27 | BA | 869 | OMC | N4-C4-N3 | 2.67 | 122.65 | 117.97 |
| 27 | BA | 2688 | 5MU | C1'-N1-C2 | 2.67 | 122.40 | 117.57 |
| 1 | Aa | 818 | 4AC | C6-C5-C4 | 2.67 | 120.22 | 116.96 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 63 | OMG | N1-C2-N3 | -2.66 | 118.34 | 123.32 |
| 27 | BA | 1820 | OMC | C1'-N1-C2 | 2.66 | 124.36 | 118.42 |
| 27 | BA | 1427 | 4AC | C6-C5-C4 | 2.66 | 120.22 | 116.96 |
| 1 | Aa | 373 | 4AC | CM7-C7-N4 | 2.66 | 119.89 | 115.29 |
| 27 | BA | 944 | 5MC | O2-C2-N3 | -2.66 | 118.01 | 122.33 |
| 27 | BA | 2838 | 4AC | CM7-C7-N4 | 2.66 | 119.89 | 115.29 |
| 27 | BA | 2863 | 5MC | CM5-C5-C6 | -2.66 | 119.30 | 122.85 |
| 27 | BA | 2595 | OMC | C1'-N1-C6 | -2.65 | 115.05 | 120.84 |
| 27 | BA | 2152 | OMG | C8-N7-C5 | 2.65 | 108.05 | 102.99 |
| 1 | Aa | 1020 | LHH | C5-C4-N3 | -2.65 | 118.32 | 122.59 |
| 27 | BA | 2605 | 5MC | CM5-C5-C6 | -2.65 | 119.31 | 122.85 |
| 27 | BA | 290 | OMG | C8-N7-C5 | 2.65 | 108.04 | 102.99 |
| 27 | BA | 1434 | 4AC | N4-C4-N3 | 2.65 | 118.30 | 113.85 |
| 27 | BA | 674 | OMG | C8-N7-C5 | 2.65 | 108.04 | 102.99 |
| 1 | Aa | 569 | 4AC | O7-C7-CM7 | -2.65 | 117.14 | 122.06 |
| 27 | BA | 2542 | OMU | C1'-N1-C2 | 2.65 | 122.36 | 117.57 |
| 1 | Aa | 942 | 5MC | C5-C6-N1 | -2.64 | 120.62 | 123.34 |
| 27 | BA | 674 | OMG | N2-C2-N1 | 2.64 | 122.33 | 116.71 |
| 1 | Aa | 532 | OMG | C2-N1-C6 | -2.63 | 120.25 | 125.10 |
| 27 | BA | 3023 | 4AC | CM7-C7-N4 | 2.62 | 119.82 | 115.29 |
| 1 | Aa | 1352 | 5MC | CM5-C5-C6 | -2.61 | 119.36 | 122.85 |
| 27 | BA | 526 | LHH | C1'-N1-C6 | -2.61 | 115.15 | 120.84 |
| 1 | Aa | 1459 | 4AC | O7-C7-N4 | 2.61 | 126.04 | 121.82 |
| 27 | BA | 2457 | LHH | C5-C4-N3 | -2.61 | 118.39 | 122.59 |
| 1 | Aa | 5 | 4AC | O7-C7-N4 | -2.61 | 117.59 | 121.82 |
| 1 | Aa | 852 | OMG | C2-N1-C6 | -2.60 | 120.30 | 125.10 |
| 27 | BA | 1551 | OMU | C1'-N1-C2 | 2.60 | 122.28 | 117.57 |
| 27 | BA | 335 | 4AC | CM7-C7-N4 | 2.60 | 119.79 | 115.29 |
| 27 | BA | 365 | OMG | C2-N1-C6 | -2.60 | 120.31 | 125.10 |
| 27 | BA | 290 | OMG | O6-C6-N1 | -2.58 | 117.60 | 120.65 |
| 27 | BA | 1799 | OMG | C5-C6-N1 | 2.58 | 118.51 | 113.95 |
| 27 | BA | 1396 | 4AC | C1'-N1-C6 | -2.58 | 115.22 | 120.84 |
| 27 | BA | 2571 | OMC | O3'-C3'-C2' | 2.58 | 118.49 | 111.17 |
| 27 | BA | 763 | OMG | C8-N7-C5 | 2.58 | 107.90 | 102.99 |
| 27 | BA | 537 | 5MU | O4-C4-N3 | -2.58 | 115.18 | 120.12 |
| 27 | BA | 1337 | 4AC | C6-C5-C4 | 2.58 | 120.11 | 116.96 |
| 27 | BA | 1940 | OMG | C5-C6-N1 | 2.58 | 118.50 | 113.95 |
| 1 | Aa | 682 | 4AC | O7-C7-CM7 | -2.57 | 117.28 | 122.06 |
| 1 | Aa | 854 | 5MC | C5-C4-N4 | -2.57 | 117.63 | 121.48 |
| 1 | Aa | 8 | OMU | C5-C4-N3 | 2.57 | 118.68 | 114.84 |
| 1 | Aa | 1020 | LHH | O7-C7-CM7 | -2.57 | 117.29 | 122.06 |
| 27 | BA | 1396 | 4AC | O7-C7-CM7 | -2.57 | 117.29 | 122.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 2457 | LHH | O4'-C4'-C5' | 2.56 | 117.80 | 109.37 |
| 1 | Aa | 1459 | 4AC | C5-C4-N4 | -2.56 | 118.48 | 122.92 |
| 27 | BA | 2955 | LHH | O7-C7-CM7 | -2.56 | 117.31 | 122.06 |
| 27 | BA | 1265 | A2M | C3'-C2'-C1' | 2.55 | 107.68 | 102.89 |
| 27 | BA | 488 | A2M | C3'-C2'-C1' | 2.55 | 107.67 | 102.89 |
| 27 | BA | 2121 | 4AC | C6-C5-C4 | 2.55 | 120.08 | 116.96 |
| 1 | Aa | 41 | 4AC | O7-C7-N4 | -2.55 | 117.69 | 121.82 |
| 27 | BA | 617 | LHH | C5-C4-N3 | -2.54 | 118.50 | 122.59 |
| 27 | BA | 2997 | 4AC | CM7-C7-N4 | 2.54 | 119.69 | 115.29 |
| 27 | BA | 1319 | OMU | C1'-N1-C2 | 2.54 | 122.17 | 117.57 |
| 27 | BA | 575 | OMG | N2-C2-N1 | 2.54 | 122.12 | 116.71 |
| 27 | BA | 215 | OMG | C8-N7-C5 | 2.54 | 107.82 | 102.99 |
| 27 | BA | 1543 | 4AC | C1'-N1-C2 | 2.54 | 124.08 | 118.42 |
| 27 | BA | 778 | 4AC | N4-C4-N3 | 2.53 | 118.10 | 113.85 |
| 1 | Aa | 847 | 4AC | CM7-C7-N4 | 2.53 | 119.67 | 115.29 |
| 27 | BA | 572 | 5MU | C1'-N1-C6 | -2.53 | 116.92 | 121.12 |
| 27 | BA | 2018 | OMC | C1'-N1-C6 | -2.52 | 115.34 | 120.84 |
| 1 | Aa | 605 | 4AC | C5'-C4'-C3' | 2.52 | 124.64 | 115.18 |
| 1 | Aa | 501 | 4AC | C5-C4-N3 | -2.52 | 118.54 | 122.59 |
| 27 | BA | 1820 | OMC | C5-C4-N4 | -2.52 | 116.61 | 120.57 |
| 27 | BA | 925 | 4AC | C5-C4-N3 | -2.51 | 118.55 | 122.59 |
| 27 | BA | 1810 | 4AC | CM7-C7-N4 | 2.51 | 119.64 | 115.29 |
| 27 | BA | 2797 | 4AC | N4-C4-N3 | 2.51 | 118.07 | 113.85 |
| 27 | BA | 805 | 4AC | C6-C5-C4 | 2.51 | 120.03 | 116.96 |
| 27 | BA | 64 | OMG | C5-C6-N1 | 2.51 | 118.38 | 113.95 |
| 27 | BA | 1431 | 4AC | CM7-C7-N4 | 2.50 | 119.62 | 115.29 |
| 27 | BA | 1641 | 4AC | CM7-C7-N4 | 2.50 | 119.62 | 115.29 |
| 1 | Aa | 818 | 4AC | C5-C4-N3 | -2.50 | 118.57 | 122.59 |
| 27 | BA | 201 | 4AC | O7-C7-CM7 | -2.50 | 117.42 | 122.06 |
| 1 | Aa | 229 | LHH | C5-C4-N3 | -2.50 | 118.57 | 122.59 |
| 27 | BA | 2568 | OMG | C8-N7-C5 | 2.49 | 107.74 | 102.99 |
| 1 | Aa | 1265 | OMG | C8-N7-C5 | 2.49 | 107.74 | 102.99 |
| 27 | BA | 1434 | 4AC | O7-C7-CM7 | -2.49 | 117.43 | 122.06 |
| 27 | BA | 1106 | OMG | C5-C6-N1 | 2.49 | 118.35 | 113.95 |
| 1 | Aa | 5 | 4AC | C5-C4-N3 | -2.49 | 118.59 | 122.59 |
| 27 | BA | 250 | OMC | O2-C2-N3 | -2.49 | 118.29 | 122.33 |
| 27 | BA | 2019 | OMG | O6-C6-N1 | -2.49 | 117.71 | 120.65 |
| 27 | BA | 805 | 4AC | O7-C7-CM7 | -2.48 | 117.44 | 122.06 |
| 27 | BA | 674 | OMG | CM2-O2'-C2' | -2.48 | 108.02 | 114.52 |
| 27 | BA | 201 | 4AC | C5-C4-N3 | -2.48 | 118.61 | 122.59 |
| 1 | Aa | 5 | 4AC | C6-C5-C4 | 2.48 | 119.99 | 116.96 |
| 1 | Aa | 827 | 4AC | CM7-C7-N4 | 2.47 | 119.57 | 115.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | Aa | 1107 | OMG | C8-N7-C5 | 2.47 | 107.70 | 102.99 |
| 27 | BA | 1396 | 4AC | CM7-C7-N4 | 2.47 | 119.57 | 115.29 |
| 1 | Aa | 358 | 4AC | C6-C5-C4 | 2.47 | 119.98 | 116.96 |
| 27 | BA | 2832 | 4AC | C6-C5-C4 | 2.47 | 119.98 | 116.96 |
| 27 | BA | 912 | OMG | C8-N7-C5 | 2.47 | 107.69 | 102.99 |
| 1 | Aa | 458 | 4AC | N4-C4-N3 | 2.47 | 117.99 | 113.85 |
| 27 | BA | 3023 | 4AC | C1'-N1-C2 | 2.46 | 123.91 | 118.42 |
| 27 | BA | 879 | A2M | O5'-C5'-C4' | 2.46 | 117.36 | 108.99 |
| 27 | BA | 244 | 4AC | C6-C5-C4 | 2.46 | 119.97 | 116.96 |
| 27 | BA | 805 | 4AC | C1'-N1-C2 | 2.46 | 123.90 | 118.42 |
| 27 | BA | 2630 | OMC | C5-C4-N4 | -2.46 | 116.71 | 120.57 |
| 27 | BA | 2527 | OMG | C8-N7-C5 | 2.46 | 107.67 | 102.99 |
| 27 | BA | 833 | OMG | O6-C6-N1 | -2.45 | 117.75 | 120.65 |
| 27 | BA | 1431 | 4AC | O7-C7-CM7 | -2.45 | 117.50 | 122.06 |
| 1 | Aa | 994 | OMG | C8-N7-C5 | 2.45 | 107.66 | 102.99 |
| 1 | Aa | 501 | 4AC | O7-C7-CM7 | -2.45 | 117.51 | 122.06 |
| 27 | BA | 552 | OMG | O6-C6-N1 | 2.45 | 123.54 | 120.65 |
| 27 | BA | 2832 | 4AC | CM7-C7-N4 | 2.45 | 119.53 | 115.29 |
| 27 | BA | 2568 | OMG | C5-C6-N1 | 2.45 | 118.27 | 113.95 |
| 1 | Aa | 605 | 4AC | O4'-C4'-C5' | 2.45 | 117.42 | 109.37 |
| 27 | BA | 1548 | 5MU | O4-C4-N3 | -2.44 | 115.44 | 120.12 |
| 1 | Aa | 1478 | 5MC | N4-C4-N3 | 2.44 | 122.93 | 118.48 |
| 27 | BA | 2992 | 4AC | C5-C4-N3 | -2.44 | 118.67 | 122.59 |
| 1 | Aa | 697 | 4AC | C5-C4-N3 | -2.43 | 118.68 | 122.59 |
| 27 | BA | 2152 | OMG | O6-C6-N1 | -2.43 | 117.78 | 120.65 |
| 1 | Aa | 1025 | OMG | C2-N1-C6 | -2.43 | 120.62 | 125.10 |
| 27 | BA | 2688 | 5MU | O4-C4-N3 | -2.43 | 115.47 | 120.12 |
| 27 | BA | 1357 | 4AC | O7-C7-CM7 | -2.43 | 117.55 | 122.06 |
| 1 | Aa | 672 | 5MC | C5-C4-N4 | -2.42 | 117.85 | 121.48 |
| 27 | BA | 1400 | A2M | C1'-N9-C4 | -2.42 | 122.38 | 126.64 |
| 27 | BA | 353 | OMG | C8-N7-C5 | 2.42 | 107.59 | 102.99 |
| 1 | Aa | 847 | 4AC | C6-C5-C4 | 2.42 | 119.92 | 116.96 |
| 1 | Aa | 136 | 4AC | C5-C4-N3 | -2.41 | 118.71 | 122.59 |
| 27 | BA | 2159 | 4AC | C6-C5-C4 | 2.41 | 119.91 | 116.96 |
| 1 | Aa | 532 | OMG | C8-N7-C5 | 2.41 | 107.58 | 102.99 |
| 27 | BA | 335 | 4AC | N4-C4-N3 | 2.41 | 117.90 | 113.85 |
| 27 | BA | 2016 | OMG | O6-C6-N1 | -2.41 | 117.81 | 120.65 |
| 27 | BA | 1776 | OMU | C6-N1-C2 | -2.41 | 117.91 | 120.99 |
| 1 | Aa | 1051 | B8T | C6-C5-C4 | 2.41 | 119.91 | 116.96 |
| 27 | BA | 2521 | OMG | C8-N7-C5 | 2.41 | 107.57 | 102.99 |
| 27 | BA | 27 | 4AC | CM7-C7-N4 | 2.41 | 119.45 | 115.29 |
| 27 | BA | 418 | 4AC | CM7-C7-N4 | 2.41 | 119.45 | 115.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 2124 | OMC | C5-C4-N4 | -2.40 | 116.79 | 120.57 |
| 27 | BA | 1558 | OMG | C2-N1-C6 | -2.40 | 120.67 | 125.10 |
| 27 | BA | 419 | OMG | C8-N7-C5 | 2.40 | 107.56 | 102.99 |
| 27 | BA | 2688 | 5MU | C6-C5-C4 | 2.40 | 120.04 | 118.03 |
| 27 | BA | 800 | OMG | C5-C6-N1 | 2.40 | 118.18 | 113.95 |
| 27 | BA | 1357 | 4AC | C1'-N1-C2 | 2.40 | 123.77 | 118.42 |
| 27 | BA | 1934 | 4AC | C6-C5-C4 | 2.39 | 119.89 | 116.96 |
| 27 | BA | 674 | OMG | N2-C2-N3 | -2.39 | 115.08 | 119.74 |
| 1 | Aa | 1459 | 4AC | O2-C2-N3 | -2.39 | 118.44 | 122.33 |
| 1 | Aa | 41 | 4AC | C5-C4-N3 | -2.39 | 118.75 | 122.59 |
| 27 | BA | 1396 | 4AC | C6-C5-C4 | 2.39 | 119.88 | 116.96 |
| 27 | BA | 2324 | OMG | C8-N7-C5 | 2.38 | 107.53 | 102.99 |
| 27 | BA | 925 | 4AC | O2'-C2'-C3' | -2.38 | 104.12 | 111.82 |
| 27 | BA | 657 | OMU | C5-C4-N3 | 2.38 | 118.40 | 114.84 |
| 1 | Aa | 458 | 4AC | C5-C4-N3 | -2.38 | 118.77 | 122.59 |
| 27 | BA | 932 | A2M | C3'-C2'-C1' | 2.38 | 107.36 | 102.89 |
| 27 | BA | 925 | 4AC | N4-C4-N3 | 2.38 | 117.84 | 113.85 |
| 27 | BA | 1305 | 4AC | O7-C7-CM7 | -2.37 | 117.65 | 122.06 |
| 1 | Aa | 8 | OMU | O4-C4-C5 | -2.37 | 120.98 | 125.16 |
| 1 | Aa | 525 | 4AC | O2-C2-N3 | -2.37 | 118.47 | 122.33 |
| 27 | BA | 1548 | 5MU | C6-N1-C2 | -2.37 | 118.89 | 121.30 |
| 27 | BA | 2797 | 4AC | C6-C5-C4 | 2.37 | 119.86 | 116.96 |
| 27 | BA | 1375 | 4AC | C6-C5-C4 | 2.37 | 119.86 | 116.96 |
| 27 | BA | 1470 | 4AC | CM7-C7-N4 | 2.37 | 119.39 | 115.29 |
| 27 | BA | 617 | LHH | O7-C7-N4 | -2.36 | 117.99 | 121.82 |
| 27 | BA | 2672 | OMG | C8-N7-C5 | 2.36 | 107.49 | 102.99 |
| 1 | Aa | 1478 | 5MC | C1'-N1-C2 | 2.36 | 123.68 | 118.42 |
| 27 | BA | 2018 | OMC | C1'-N1-C2 | 2.36 | 123.68 | 118.42 |
| 1 | Aa | 246 | OMG | C8-N7-C5 | 2.35 | 107.48 | 102.99 |
| 1 | Aa | 1275 | OMG | C5-C6-N1 | 2.35 | 118.11 | 113.95 |
| 27 | BA | 376 | 4AC | C1'-N1-C2 | 2.35 | 123.67 | 118.42 |
| 27 | BA | 2657 | OMG | C8-N7-C5 | 2.35 | 107.47 | 102.99 |
| 27 | BA | 800 | OMG | C2-N1-C6 | -2.35 | 120.77 | 125.10 |
| 1 | Aa | 373 | 4AC | C1'-N1-C2 | 2.35 | 123.66 | 118.42 |
| 27 | BA | 1750 | OMC | C5-C4-N4 | -2.35 | 116.88 | 120.57 |
| 27 | BA | 365 | OMG | N2-C2-N1 | 2.34 | 121.70 | 116.71 |
| 27 | BA | 505 | A2M | C3'-C2'-C1' | 2.34 | 107.29 | 102.89 |
| 27 | BA | 1305 | 4AC | C5-C4-N3 | -2.34 | 118.83 | 122.59 |
| 1 | Aa | 670 | 2MG | C8-N7-C5 | 2.34 | 107.45 | 102.99 |
| 27 | BA | 2590 | 4AC | N4-C4-N3 | 2.34 | 117.78 | 113.85 |
| 27 | BA | 2838 | 4AC | C6-C5-C4 | 2.33 | 119.82 | 116.96 |
| 27 | BA | 2728 | OMG | C8-N7-C5 | 2.33 | 107.43 | 102.99 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 3023 | 4AC | C6-C5-C4 | 2.33 | 119.81 | 116.96 |
| 27 | BA | 418 | 4AC | C6-C5-C4 | 2.33 | 119.81 | 116.96 |
| 1 | Aa | 682 | 4AC | C5-C4-N3 | -2.32 | 118.85 | 122.59 |
| 27 | BA | 1750 | OMC | N4-C4-N3 | 2.32 | 122.05 | 117.97 |
| 27 | BA | 124 | 4AC | C5-C4-N3 | -2.32 | 118.85 | 122.59 |
| 27 | BA | 1558 | OMG | C8-N7-C5 | 2.32 | 107.42 | 102.99 |
| 27 | BA | 875 | 5MU | O4-C4-N3 | -2.32 | 115.66 | 120.12 |
| 27 | BA | 2590 | 4AC | C6-C5-C4 | 2.32 | 119.80 | 116.96 |
| 27 | BA | 572 | 5MU | C6-N1-C2 | -2.32 | 118.95 | 121.30 |
| 27 | BA | 2595 | OMC | C1'-N1-C2 | 2.31 | 123.59 | 118.42 |
| 27 | BA | 2992 | 4AC | CM7-C7-N4 | 2.31 | 119.30 | 115.29 |
| 27 | BA | 1357 | 4AC | C6-C5-C4 | 2.31 | 119.79 | 116.96 |
| 1 | Aa | 382 | OMG | C8-N7-C5 | 2.31 | 107.39 | 102.99 |
| 27 | BA | 1375 | 4AC | O7-C7-CM7 | -2.31 | 117.77 | 122.06 |
| 1 | Aa | 498 | OMG | C8-N7-C5 | 2.31 | 107.38 | 102.99 |
| 1 | Aa | 1352 | 5MC | C1'-N1-C6 | -2.31 | 117.29 | 121.12 |
| 27 | BA | 2457 | LHH | C5'-C4'-C3' | 2.30 | 123.81 | 115.18 |
| 27 | BA | 1820 | OMC | O2-C2-N3 | -2.30 | 118.59 | 122.33 |
| 27 | BA | 925 | 4AC | O7-C7-CM7 | -2.30 | 117.79 | 122.06 |
| 27 | BA | 250 | OMC | C5-C4-N4 | -2.29 | 116.97 | 120.57 |
| 1 | Aa | 1434 | OMG | C8-N7-C5 | 2.29 | 107.36 | 102.99 |
| 27 | BA | 2997 | 4AC | C6-C5-C4 | 2.29 | 119.77 | 116.96 |
| 27 | BA | 1431 | 4AC | C1'-N1-C2 | 2.29 | 123.53 | 118.42 |
| 1 | Aa | 479 | OMU | O2-C2-N1 | -2.29 | 119.74 | 122.79 |
| 1 | Aa | 320 | OMG | C8-N7-C5 | 2.29 | 107.35 | 102.99 |
| 27 | BA | 575 | OMG | C2-N1-C6 | -2.29 | 120.89 | 125.10 |
| 27 | BA | 2745 | OMG | C8-N7-C5 | 2.28 | 107.34 | 102.99 |
| 1 | Aa | 876 | OMG | C8-N7-C5 | 2.28 | 107.34 | 102.99 |
| 1 | Aa | 1107 | OMG | CM2-O2'-C2' | 2.28 | 120.52 | 114.52 |
| 27 | BA | 2121 | 4AC | N4-C4-N3 | 2.28 | 117.69 | 113.85 |
| 27 | BA | 2780 | 4AC | C5-C4-N3 | -2.28 | 118.92 | 122.59 |
| 27 | BA | 2353 | OMG | C2-N1-C6 | -2.28 | 120.90 | 125.10 |
| 1 | Aa | 446 | OMG | C8-N7-C5 | 2.28 | 107.33 | 102.99 |
| 27 | BA | 2838 | 4AC | O7-C7-CM7 | -2.28 | 117.82 | 122.06 |
| 27 | BA | 833 | OMG | C8-N7-C5 | 2.28 | 107.33 | 102.99 |
| 27 | BA | 1940 | OMG | C2-N1-C6 | -2.28 | 120.90 | 125.10 |
| 1 | Aa | 697 | 4AC | N4-C4-N3 | 2.27 | 117.67 | 113.85 |
| 27 | BA | 1434 | 4AC | C5-C4-N3 | -2.27 | 118.94 | 122.59 |
| 27 | BA | 575 | OMG | C8-N7-C5 | 2.27 | 107.32 | 102.99 |
| 27 | BA | 376 | 4AC | O7-C7-CM7 | -2.27 | 117.84 | 122.06 |
| 27 | BA | 64 | OMG | C2-N1-C6 | -2.27 | 120.92 | 125.10 |
| 27 | BA | 1548 | 5MU | O2-C2-N1 | -2.26 | 119.78 | 122.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 1934 | 4AC | O7-C7-CM7 | -2.26 | 117.86 | 122.06 |
| 27 | BA | 1899 | 4AC | C6-C5-C4 | 2.26 | 119.73 | 116.96 |
| 1 | Aa | 1025 | OMG | C8-N7-C5 | 2.26 | 107.30 | 102.99 |
| 27 | BA | 2550 | OMG | C8-N7-C5 | 2.26 | 107.29 | 102.99 |
| 27 | BA | 3009 | 4AC | CM7-C7-N4 | 2.26 | 119.19 | 115.29 |
| 1 | Aa | 358 | 4AC | O7-C7-N4 | -2.26 | 118.17 | 121.82 |
| 27 | BA | 1431 | 4AC | C5-C4-N3 | -2.26 | 118.96 | 122.59 |
| 27 | BA | 1965 | 5MC | O2-C2-N3 | -2.25 | 118.66 | 122.33 |
| 1 | Aa | 138 | OMG | C8-N7-C5 | 2.25 | 107.28 | 102.99 |
| 27 | BA | 27 | 4AC | C5-C4-N3 | -2.25 | 118.97 | 122.59 |
| 27 | BA | 298 | 5MU | C6-N1-C2 | -2.25 | 119.02 | 121.30 |
| 27 | BA | 718 | OMC | O2-C2-N3 | -2.25 | 118.67 | 122.33 |
| 1 | Aa | 373 | 4AC | O7-C7-CM7 | -2.25 | 117.88 | 122.06 |
| 27 | BA | 575 | OMG | O6-C6-C5 | -2.25 | 119.98 | 124.37 |
| 27 | BA | 335 | 4AC | C6-C5-C4 | 2.25 | 119.71 | 116.96 |
| 27 | BA | 1892 | OMG | C8-N7-C5 | 2.25 | 107.27 | 102.99 |
| 1 | Aa | 1276 | 5MC | CM5-C5-C6 | -2.25 | 119.85 | 122.85 |
| 27 | BA | 2384 | 5MU | O4'-C4'-C5' | 2.25 | 116.76 | 109.37 |
| 27 | BA | 63 | OMG | C2-N1-C6 | -2.24 | 120.97 | 125.10 |
| 27 | BA | 2797 | 4AC | CM7-C7-N4 | 2.24 | 119.17 | 115.29 |
| 27 | BA | 875 | 5MU | O2-C2-N1 | -2.24 | 119.81 | 122.79 |
| 1 | Aa | 358 | 4AC | C5-C4-N3 | -2.24 | 118.99 | 122.59 |
| 27 | BA | 501 | 4AC | C5-C4-N3 | -2.24 | 118.99 | 122.59 |
| 27 | BA | 2590 | 4AC | O2-C2-N3 | -2.24 | 118.69 | 122.33 |
| 27 | BA | 805 | 4AC | C1'-N1-C6 | -2.23 | 115.97 | 120.84 |
| 27 | BA | 2384 | 5MU | C6-N1-C2 | -2.23 | 119.04 | 121.30 |
| 27 | BA | 1106 | OMG | O6-C6-C5 | -2.23 | 120.01 | 124.37 |
| 27 | BA | 2389 | OMU | O3'-C3'-C4' | -2.23 | 104.60 | 111.05 |
| 1 | Aa | 1007 | 4AC | C2'-C1'-N1 | -2.23 | 106.91 | 113.22 |
| 27 | BA | 2590 | 4AC | C5-C4-N3 | -2.23 | 119.01 | 122.59 |
| 27 | BA | 1790 | OMC | CM2-O2'-C2' | -2.23 | 108.68 | 114.52 |
| 27 | BA | 2571 | OMC | O2-C2-N1 | 2.22 | 123.48 | 118.89 |
| 27 | BA | 357 | B8T | C6-C5-C4 | 2.22 | 119.68 | 116.96 |
| 1 | Aa | 1459 | 4AC | C6-C5-C4 | 2.22 | 119.67 | 116.96 |
| 27 | BA | 433 | 4AC | CM7-C7-N4 | 2.22 | 119.13 | 115.29 |
| 1 | Aa | 1262 | B8T | C6-C5-C4 | 2.22 | 119.67 | 116.96 |
| 1 | Aa | 1275 | OMG | C8-N7-C5 | 2.22 | 107.21 | 102.99 |
| 27 | BA | 63 | OMG | C8-N7-C5 | 2.21 | 107.21 | 102.99 |
| 27 | BA | 778 | 4AC | CM7-C7-N4 | 2.20 | 119.11 | 115.29 |
| 27 | BA | 505 | A2M | O2'-C2'-C1' | -2.20 | 104.72 | 109.09 |
| 27 | BA | 1525 | OMG | O6-C6-N1 | -2.20 | 118.05 | 120.65 |
| 27 | BA | 212 | A2M | O2'-C2'-C1' | 2.20 | 113.45 | 109.09 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | BA | 27 | 4AC | O7-C7-CM7 | -2.20 | 117.97 | 122.06 |
| 1 | Aa | 373 | 4AC | C5-C4-N3 | -2.20 | 119.06 | 122.59 |
| 27 | BA | 2010 | OMG | C8-N7-C5 | 2.19 | 107.17 | 102.99 |
| 1 | Aa | 913 | OMG | O6-C6-C5 | -2.19 | 120.09 | 124.37 |
| 1 | Aa | 697 | 4AC | O7-C7-N4 | -2.19 | 118.28 | 121.82 |
| 27 | BA | 657 | OMU | C6-N1-C2 | -2.19 | 118.20 | 120.99 |
| 27 | BA | 1558 | OMG | N2-C2-N1 | 2.18 | 121.36 | 116.71 |
| 27 | BA | 849 | A2M | O4'-C1'-C2' | -2.18 | 102.80 | 106.59 |
| 27 | BA | 572 | 5MU | O2-C2-N1 | -2.18 | 119.89 | 122.79 |
| 27 | BA | 1470 | 4AC | O7-C7-CM7 | -2.18 | 118.01 | 122.06 |
| 1 | Aa | 659 | OMG | C8-N7-C5 | 2.18 | 107.14 | 102.99 |
| 27 | BA | 619 | OMU | C1'-N1-C2 | 2.17 | 121.50 | 117.57 |
| 27 | BA | 756 | A2M | C3'-C2'-C1' | 2.17 | 106.97 | 102.89 |
| 27 | BA | 2124 | OMC | O2-C2-N3 | -2.17 | 118.80 | 122.33 |
| 27 | BA | 2389 | OMU | O2'-C2'-C1' | 2.17 | 113.31 | 109.08 |
| 27 | BA | 2168 | OMG | O6-C6-C5 | -2.16 | 120.15 | 124.37 |
| 27 | BA | 526 | LHH | O2-C2-N3 | -2.16 | 118.82 | 122.33 |
| 1 | Aa | 854 | 5MC | N4-C4-N3 | 2.16 | 122.41 | 118.48 |
| 27 | BA | 1810 | 4AC | O7-C7-CM7 | -2.16 | 118.05 | 122.06 |
| 1 | Aa | 1026 | OMG | C8-N7-C5 | 2.16 | 107.10 | 102.99 |
| 1 | Aa | 730 | 4AC | N4-C4-N3 | 2.16 | 117.47 | 113.85 |
| 1 | Aa | 1476 | 5MC | CM5-C5-C6 | -2.15 | 119.97 | 122.85 |
| 1 | Aa | 525 | 4AC | O7-C7-CM7 | -2.15 | 118.06 | 122.06 |
| 27 | BA | 2528 | OMG | C8-N7-C5 | 2.15 | 107.09 | 102.99 |
| 27 | BA | 799 | 4AC | CM7-C7-N4 | 2.15 | 119.02 | 115.29 |
| 27 | BA | 872 | A2M | C3'-C2'-C1' | 2.15 | 106.93 | 102.89 |
| 27 | BA | 244 | 4AC | C1'-N1-C2 | 2.15 | 123.22 | 118.42 |
| 27 | BA | 2590 | 4AC | CM7-C7-N4 | 2.15 | 119.01 | 115.29 |
| 27 | BA | 56 | 4AC | C6-C5-C4 | 2.15 | 119.59 | 116.96 |
| 27 | BA | 1543 | 4AC | C6-C5-C4 | 2.15 | 119.59 | 116.96 |
| 1 | Aa | 296 | OMC | O2-C2-N3 | -2.15 | 118.84 | 122.33 |
| 1 | Aa | 298 | 4AC | C5-C4-N3 | -2.15 | 119.14 | 122.59 |
| 1 | Aa | 1026 | OMG | O6-C6-C5 | -2.14 | 120.19 | 124.37 |
| 1 | Aa | 229 | LHH | O7-C7-N4 | -2.14 | 118.36 | 121.82 |
| 27 | BA | 2702 | A2M | C3'-C2'-C1' | 2.14 | 106.90 | 102.89 |
| 27 | BA | 1750 | OMC | C1'-N1-C6 | -2.13 | 116.19 | 120.84 |
| 27 | BA | 800 | OMG | C8-N7-C5 | 2.13 | 107.05 | 102.99 |
| 1 | Aa | 771 | OMG | C8-N7-C5 | 2.13 | 107.05 | 102.99 |
| 27 | BA | 763 | OMG | O6-C6-C5 | -2.13 | 120.21 | 124.37 |
| 27 | BA | 1750 | OMC | O2-C2-N3 | -2.13 | 118.88 | 122.33 |
| 27 | BA | 244 | 4AC | C5-C4-N3 | -2.12 | 119.18 | 122.59 |
| 27 | BA | 805 | 4AC | C5-C4-N3 | -2.12 | 119.18 | 122.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | Aa | 892 | OMG | C8-N7-C5 | 2.12 | 107.03 | 102.99 |
| 1 | Aa | 827 | 4AC | C5-C4-N3 | -2.12 | 119.19 | 122.59 |
| 27 | BA | 376 | 4AC | C6-C5-C4 | 2.12 | 119.55 | 116.96 |
| 1 | Aa | 569 | 4AC | C5-C4-N3 | -2.12 | 119.19 | 122.59 |
| 27 | BA | 2571 | OMC | O3'-C3'-C4' | 2.12 | 117.17 | 111.05 |
| 27 | BA | 2630 | OMC | O2-C2-N3 | -2.12 | 118.89 | 122.33 |
| 1 | Aa | 771 | OMG | O6-C6-C5 | -2.12 | 120.24 | 124.37 |
| 1 | Aa | 1478 | 5MC | O2-C2-N3 | -2.11 | 118.89 | 122.33 |
| 27 | BA | 1641 | 4AC | O2-C2-N3 | -2.11 | 118.89 | 122.33 |
| 1 | Aa | 636 | OMG | C8-N7-C5 | 2.11 | 107.01 | 102.99 |
| 27 | BA | 800 | OMG | N2-C2-N1 | 2.11 | 121.20 | 116.71 |
| 27 | BA | 2168 | OMG | C2-N1-C6 | -2.11 | 121.22 | 125.10 |
| 27 | BA | 572 | 5MU | O4-C4-N3 | -2.11 | 116.08 | 120.12 |
| 1 | Aa | 1007 | 4AC | N4-C4-N3 | 2.10 | 117.38 | 113.85 |
| 27 | BA | 1305 | 4AC | C6-C5-C4 | 2.10 | 119.53 | 116.96 |
| 27 | BA | 1543 | 4AC | C1'-N1-C6 | -2.10 | 116.27 | 120.84 |
| 27 | BA | 2379 | OMG | C8-N7-C5 | 2.10 | 106.98 | 102.99 |
| 1 | Aa | 876 | OMG | O6-C6-C5 | -2.10 | 120.28 | 124.37 |
| 27 | BA | 2353 | OMG | C5-C6-N1 | 2.09 | 117.65 | 113.95 |
| 27 | BA | 1305 | 4AC | N4-C4-N3 | 2.09 | 117.36 | 113.85 |
| 27 | BA | 2159 | 4AC | O7-C7-CM7 | -2.09 | 118.18 | 122.06 |
| 27 | BA | 56 | 4AC | C5-C4-N3 | -2.09 | 119.23 | 122.59 |
| 27 | BA | 1427 | 4AC | O7-C7-CM7 | -2.09 | 118.18 | 122.06 |
| 27 | BA | 1357 | 4AC | C1'-N1-C6 | -2.09 | 116.29 | 120.84 |
| 27 | BA | 1641 | 4AC | C5-C4-N3 | -2.09 | 119.23 | 122.59 |
| 1 | Aa | 381 | OMG | C8-N7-C5 | 2.09 | 106.97 | 102.99 |
| 27 | BA | 561 | OMC | O2-C2-N3 | -2.08 | 118.94 | 122.33 |
| 27 | BA | 250 | OMC | C1'-N1-C2 | 2.08 | 123.07 | 118.42 |
| 27 | BA | 1398 | OMG | C8-N7-C5 | 2.08 | 106.95 | 102.99 |
| 27 | BA | 1810 | 4AC | C5-C4-N3 | -2.08 | 119.25 | 122.59 |
| 27 | BA | 674 | OMG | C5-C6-N1 | 2.08 | 117.62 | 113.95 |
| 27 | BA | 674 | OMG | O6-C6-C5 | -2.08 | 120.32 | 124.37 |
| 27 | BA | 1558 | OMG | C5-C6-N1 | 2.08 | 117.62 | 113.95 |
| 1 | Aa | 1354 | OMC | N4-C4-N3 | 2.07 | 121.61 | 117.97 |
| 27 | BA | 2168 | OMG | CM2-O2'-C2' | -2.07 | 109.10 | 114.52 |
| 27 | BA | 552 | OMG | C5-C6-N1 | 2.07 | 117.60 | 113.95 |
| 27 | BA | 1696 | 5MC | CM5-C5-C6 | -2.07 | 120.09 | 122.85 |
| 1 | Aa | 752 | OMC | C5-C4-N4 | -2.06 | 117.33 | 120.57 |
| 27 | BA | 418 | 4AC | C5-C4-N3 | -2.06 | 119.27 | 122.59 |
| 27 | BA | 1085 | 5MU | O2-C2-N1 | -2.06 | 120.05 | 122.79 |
| 27 | BA | 2121 | 4AC | O7-C7-CM7 | -2.06 | 118.23 | 122.06 |
| 27 | BA | 1899 | 4AC | CM7-C7-N4 | 2.06 | 118.86 | 115.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | Aa | 1020 | LHH | C2'-C1'-N1 | 2.06 | 118.22 | 114.22 |
| 27 | BA | 763 | OMG | C5-C6-N1 | 2.06 | 117.59 | 113.95 |
| 27 | BA | 2832 | 4AC | C1'-N1-C2 | 2.06 | 123.01 | 118.42 |
| 27 | BA | 1953 | OMG | C8-N7-C5 | 2.06 | 106.91 | 102.99 |
| 27 | BA | 2656 | OMU | O4-C4-C5 | -2.06 | 121.55 | 125.16 |
| 27 | BA | 1340 | OMU | C1'-N1-C2 | 2.05 | 121.29 | 117.57 |
| 27 | BA | 2168 | OMG | C5-C6-N1 | 2.05 | 117.57 | 113.95 |
| 27 | BA | 2863 | 5MC | O2-C2-N3 | -2.05 | 119.00 | 122.33 |
| 27 | BA | 2780 | 4AC | C1'-N1-C6 | -2.05 | 116.38 | 120.84 |
| 27 | BA | 718 | OMC | O2-C2-N1 | 2.05 | 123.12 | 118.89 |
| 27 | BA | 2018 | OMC | O2-C2-N3 | -2.05 | 119.00 | 122.33 |
| 27 | BA | 2124 | OMC | C1'-N1-C2 | 2.05 | 122.98 | 118.42 |
| 1 | Aa | 8 | OMU | C6-N1-C2 | -2.04 | 118.38 | 120.99 |
| 27 | BA | 2035 | 5MC | CM5-C5-C6 | -2.04 | 120.12 | 122.85 |
| 1 | Aa | 994 | OMG | O6-C6-C5 | -2.04 | 120.38 | 124.37 |
| 27 | BA | 3023 | 4AC | O7-C7-CM7 | -2.04 | 118.27 | 122.06 |
| 1 | Aa | 854 | 5MC | C1'-N1-C6 | -2.04 | 117.73 | 121.12 |
| 27 | BA | 64 | OMG | O6-C6-C5 | -2.04 | 120.39 | 124.37 |
| 27 | BA | 1899 | 4AC | O7-C7-CM7 | -2.04 | 118.27 | 122.06 |
| 1 | Aa | 450 | OMG | C8-N7-C5 | 2.04 | 106.88 | 102.99 |
| 1 | Aa | 818 | 4AC | N4-C4-N3 | 2.04 | 117.28 | 113.85 |
| 1 | Aa | 852 | OMG | C8-N7-C5 | 2.04 | 106.87 | 102.99 |
| 27 | BA | 2553 | 4SU | O2-C2-N1 | -2.04 | 120.08 | 122.79 |
| 27 | BA | 3009 | 4AC | C5-C4-N3 | -2.04 | 119.32 | 122.59 |
| 27 | BA | 2384 | 5MU | C5'-C4'-C3' | 2.04 | 122.81 | 115.18 |
| 27 | BA | 2863 | 5MC | C1'-N1-C2 | 2.04 | 122.96 | 118.42 |
| 27 | BA | 2070 | 5MC | C2'-C1'-N1 | -2.03 | 107.45 | 113.22 |
| 27 | BA | 3023 | 4AC | C1'-N1-C6 | -2.03 | 116.41 | 120.84 |
| 27 | BA | 201 | 4AC | N4-C4-N3 | 2.03 | 117.27 | 113.85 |
| 27 | BA | 1337 | 4AC | CM7-C7-N4 | 2.03 | 118.81 | 115.29 |
| 27 | BA | 2070 | 5MC | C5-C4-N3 | -2.03 | 119.48 | 121.67 |
| 27 | BA | 730 | 4AC | O7-C7-CM7 | -2.03 | 118.28 | 122.06 |
| 27 | BA | 730 | 4AC | O2-C2-N3 | -2.03 | 119.03 | 122.33 |
| 27 | BA | 3023 | 4AC | C5-C4-N3 | -2.03 | 119.33 | 122.59 |
| 27 | BA | 1799 | OMG | O6-C6-N1 | 2.03 | 123.04 | 120.65 |
| 27 | BA | 1940 | OMG | O6-C6-C5 | -2.03 | 120.42 | 124.37 |
| 27 | BA | 1955 | 4AC | C5-C4-N3 | -2.03 | 119.33 | 122.59 |
| 27 | BA | 875 | 5MU | O2'-C2'-C3' | 2.02 | 118.37 | 111.82 |
| 27 | BA | 433 | 4AC | C6-C5-C4 | 2.02 | 119.44 | 116.96 |
| 27 | BA | 2159 | 4AC | CM7-C7-N4 | 2.02 | 118.79 | 115.29 |
| 1 | Aa | 1358 | OMU | C1'-N1-C6 | 2.02 | 125.25 | 120.84 |
| 27 | BA | 1820 | OMC | C1'-N1-C6 | -2.02 | 116.44 | 120.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | Aa | 381 | OMG | O6-C6-C5 | -2.02 | 120.43 | 124.37 |
| 1 | Aa | 1007 | 4AC | C5-C4-N3 | -2.02 | 119.35 | 122.59 |
| 1 | Aa | 446 | OMG | O6-C6-C5 | -2.01 | 120.44 | 124.37 |
| 1 | Aa | 1020 | LHH | O7-C7-N4 | -2.01 | 118.56 | 121.82 |
| 1 | Aa | 1217 | 4AC | C1'-N1-C6 | -2.01 | 116.45 | 120.84 |
| 27 | BA | 250 | OMC | C6-C5-C4 | 2.01 | 120.75 | 117.50 |
| 27 | BA | 2159 | 4AC | C5-C4-N4 | -2.01 | 119.43 | 122.92 |
| 27 | BA | 2992 | 4AC | C1'-N1-C2 | 2.01 | 122.91 | 118.42 |
| 1 | Aa | 659 | OMG | O6-C6-C5 | -2.01 | 120.45 | 124.37 |
| 27 | BA | 1905 | 5MU | O2-C2-N1 | -2.01 | 120.12 | 122.79 |
| 1 | Aa | 1354 | OMC | C5-C4-N4 | -2.00 | 117.42 | 120.57 |
| 1 | Aa | 8 | OMU | O2-C2-N1 | -2.00 | 120.13 | 122.79 |
| 1 | Aa | 8 | OMU | O2'-C2'-C1' | 2.00 | 112.98 | 109.08 |

There are no chirality outliers.

All (235) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 1 | Aa | 52 | OMU | C3'-C4'-C5'-O5' |
| 1 | Aa | 52 | OMU | O4'-C4'-C5'-O5' |
| 1 | Aa | 352 | A2M | C1'-C2'-O2'-CM' |
| 1 | Aa | 382 | OMG | O4'-C4'-C5'-O5' |
| 1 | Aa | 446 | OMG | O4'-C4'-C5'-O5' |
| 1 | Aa | 446 | OMG | C3'-C4'-C5'-O5' |
| 1 | Aa | 458 | 4AC | O7-C7-N4-C4 |
| 1 | Aa | 458 | 4AC | CM7-C7-N4-C4 |
| 1 | Aa | 525 | 4AC | O4'-C1'-N1-C2 |
| 1 | Aa | 525 | 4AC | O4'-C1'-N1-C6 |
| 1 | Aa | 876 | OMG | O4'-C4'-C5'-O5' |
| 1 | Aa | 876 | OMG | C3'-C4'-C5'-O5' |
| 1 | Aa | 917 | 5MU | C3'-C4'-C5'-O5' |
| 1 | Aa | 917 | 5MU | O4'-C4'-C5'-O5' |
| 1 | Aa | 1107 | OMG | C3'-C2'-O2'-CM2 |
| 1 | Aa | 1217 | 4AC | C3'-C4'-C5'-O5' |
| 1 | Aa | 1275 | OMG | C1'-C2'-O2'-CM2 |
| 1 | Aa | 1352 | 5MC | O4'-C4'-C5'-O5' |
| 1 | Aa | 1352 | 5MC | C3'-C4'-C5'-O5' |
| 1 | Aa | 1354 | OMC | C3'-C4'-C5'-O5' |
| 1 | Aa | 1354 | OMC | O4'-C4'-C5'-O5' |
| 1 | Aa | 1358 | OMU | O4'-C4'-C5'-O5' |
| 1 | Aa | 1468 | MA6 | O4'-C4'-C5'-O5' |
| 27 | BA | 27 | 4AC | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 27 | BA | 27 | 4AC | C3'-C4'-C5'-O5' |
| 27 | BA | 34 | OMU | C1'-C2'-O2'-CM2 |
| 27 | BA | 212 | A2M | C1'-C2'-O2'-CM' |
| 27 | BA | 215 | OMG | O4'-C4'-C5'-O5' |
| 27 | BA | 353 | OMG | O4'-C4'-C5'-O5' |
| 27 | BA | 353 | OMG | C3'-C4'-C5'-O5' |
| 27 | BA | 488 | A2M | C3'-C2'-O2'-CM' |
| 27 | BA | 619 | OMU | C1'-C2'-O2'-CM2 |
| 27 | BA | 657 | OMU | C1'-C2'-O2'-CM2 |
| 27 | BA | 754 | OMC | C3'-C4'-C5'-O5' |
| 27 | BA | 849 | A2M | C3'-C4'-C5'-O5' |
| 27 | BA | 1480 | OMU | O4'-C4'-C5'-O5' |
| 27 | BA | 1517 | A2M | C3'-C2'-O2'-CM' |
| 27 | BA | 1525 | OMG | O4'-C4'-C5'-O5' |
| 27 | BA | 1525 | OMG | C3'-C4'-C5'-O5' |
| 27 | BA | 1543 | 4AC | C3'-C4'-C5'-O5' |
| 27 | BA | 1548 | 5MU | C3'-C4'-C5'-O5' |
| 27 | BA | 1551 | OMU | C1'-C2'-O2'-CM2 |
| 27 | BA | 2018 | OMC | O4'-C4'-C5'-O5' |
| 27 | BA | 2019 | OMG | C3'-C4'-C5'-O5' |
| 27 | BA | 2055 | 5MC | O4'-C4'-C5'-O5' |
| 27 | BA | 2152 | OMG | O4'-C4'-C5'-O5' |
| 27 | BA | 2152 | OMG | C3'-C4'-C5'-O5' |
| 27 | BA | 2353 | OMG | O4'-C4'-C5'-O5' |
| 27 | BA | 2353 | OMG | C3'-C4'-C5'-O5' |
| 27 | BA | 2389 | OMU | C3'-C4'-C5'-O5' |
| 27 | BA | 2457 | LHH | C3'-C4'-C5'-O5' |
| 27 | BA | 2457 | LHH | O4'-C4'-C5'-O5' |
| 27 | BA | 2550 | OMG | O4'-C4'-C5'-O5' |
| 27 | BA | 2568 | OMG | C3'-C4'-C5'-O5' |
| 27 | BA | 2581 | 4SU | O4'-C4'-C5'-O5' |
| 27 | BA | 2838 | 4AC | C3'-C4'-C5'-O5' |
| 27 | BA | 2955 | LHH | C1'-C2'-O2'-C1 |
| 27 | BA | 2992 | 4AC | O4'-C4'-C5'-O5' |
| 27 | BA | 2992 | 4AC | C3'-C4'-C5'-O5' |
| 27 | BA | 3023 | 4AC | O4'-C4'-C5'-O5' |
| 1 | Aa | 382 | OMG | C3'-C4'-C5'-O5' |
| 1 | Aa | 457 | 5MC | O4'-C4'-C5'-O5' |
| 1 | Aa | 457 | 5MC | C3'-C4'-C5'-O5' |
| 1 | Aa | 458 | 4AC | O4'-C4'-C5'-O5' |
| 1 | Aa | 532 | OMG | O4'-C4'-C5'-O5' |
| 1 | Aa | 532 | OMG | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 1 | Aa | 892 | OMG | O4'-C4'-C5'-O5' |
| 1 | Aa | 892 | OMG | C3'-C4'-C5'-O5' |
| 1 | Aa | 1007 | 4AC | O4'-C4'-C5'-O5' |
| 1 | Aa | 1276 | 5MC | C3'-C4'-C5'-O5' |
| 1 | Aa | 1358 | OMU | C3'-C4'-C5'-O5' |
| 1 | Aa | 1468 | MA6 | C3'-C4'-C5'-O5' |
| 27 | BA | 64 | OMG | C3'-C4'-C5'-O5' |
| 27 | BA | 215 | OMG | C3'-C4'-C5'-O5' |
| 27 | BA | 419 | OMG | O4'-C4'-C5'-O5' |
| 27 | BA | 875 | 5MU | C3'-C4'-C5'-O5' |
| 27 | BA | 875 | 5MU | O4'-C4'-C5'-O5' |
| 27 | BA | 1375 | 4AC | O4'-C4'-C5'-O5' |
| 27 | BA | 1480 | OMU | C3'-C4'-C5'-O5' |
| 27 | BA | 1543 | 4AC | O4'-C4'-C5'-O5' |
| 27 | BA | 1810 | 4AC | O4'-C4'-C5'-O5' |
| 27 | BA | 1940 | OMG | O4'-C4'-C5'-O5' |
| 27 | BA | 1955 | 4AC | O4'-C4'-C5'-O5' |
| 27 | BA | 2018 | OMC | C3'-C4'-C5'-O5' |
| 27 | BA | 2019 | OMG | O4'-C4'-C5'-O5' |
| 27 | BA | 2055 | 5MC | C3'-C4'-C5'-O5' |
| 27 | BA | 2379 | OMG | O4'-C4'-C5'-O5' |
| 27 | BA | 2379 | OMG | C3'-C4'-C5'-O5' |
| 27 | BA | 2550 | OMG | C3'-C4'-C5'-O5' |
| 27 | BA | 2581 | 4SU | C3'-C4'-C5'-O5' |
| 27 | BA | 2595 | OMC | O4'-C4'-C5'-O5' |
| 27 | BA | 2610 | OMU | C3'-C4'-C5'-O5' |
| 27 | BA | 3023 | 4AC | C3'-C4'-C5'-O5' |
| 1 | Aa | 697 | 4AC | O4'-C4'-C5'-O5' |
| 1 | Aa | 1004 | 5MC | O4'-C4'-C5'-O5' |
| 1 | Aa | 1007 | 4AC | C3'-C4'-C5'-O5' |
| 27 | BA | 64 | OMG | O4'-C4'-C5'-O5' |
| 27 | BA | 419 | OMG | C3'-C4'-C5'-O5' |
| 27 | BA | 488 | A2M | O4'-C4'-C5'-O5' |
| 27 | BA | 754 | OMC | O4'-C4'-C5'-O5' |
| 27 | BA | 849 | A2M | O4'-C4'-C5'-O5' |
| 27 | BA | 1265 | A2M | O4'-C4'-C5'-O5' |
| 27 | BA | 1337 | 4AC | O4'-C4'-C5'-O5' |
| 27 | BA | 1375 | 4AC | C3'-C4'-C5'-O5' |
| 27 | BA | 1396 | 4AC | O4'-C4'-C5'-O5' |
| 27 | BA | 1548 | 5MU | O4'-C4'-C5'-O5' |
| 27 | BA | 1810 | 4AC | C3'-C4'-C5'-O5' |
| 27 | BA | 1940 | OMG | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 27 | BA | 1953 | OMG | C3'-C4'-C5'-O5' |
| 27 | BA | 1955 | 4AC | C3'-C4'-C5'-O5' |
| 27 | BA | 2389 | OMU | O4'-C4'-C5'-O5' |
| 27 | BA | 2527 | OMG | O4'-C4'-C5'-O5' |
| 27 | BA | 2595 | OMC | C3'-C4'-C5'-O5' |
| 27 | BA | 2610 | OMU | O4'-C4'-C5'-O5' |
| 27 | BA | 2838 | 4AC | O4'-C4'-C5'-O5' |
| 1 | Aa | 458 | 4AC | C3'-C4'-C5'-O5' |
| 27 | BA | 1953 | OMG | O4'-C4'-C5'-O5' |
| 27 | BA | 2568 | OMG | O4'-C4'-C5'-O5' |
| 1 | Aa | 1004 | 5MC | C3'-C4'-C5'-O5' |
| 1 | Aa | 1107 | OMG | C3'-C4'-C5'-O5' |
| 1 | Aa | 1217 | 4AC | O4'-C4'-C5'-O5' |
| 27 | BA | 575 | OMG | C3'-C4'-C5'-O5' |
| 27 | BA | 1265 | A2M | C3'-C4'-C5'-O5' |
| 27 | BA | 1396 | 4AC | C3'-C4'-C5'-O5' |
| 1 | Aa | 605 | 4AC | O4'-C4'-C5'-O5' |
| 1 | Aa | 697 | 4AC | C3'-C4'-C5'-O5' |
| 1 | Aa | 913 | OMG | C3'-C4'-C5'-O5' |
| 27 | BA | 575 | OMG | O4'-C4'-C5'-O5' |
| 27 | BA | 2527 | OMG | C3'-C4'-C5'-O5' |
| 1 | Aa | 5 | 4AC | O4'-C4'-C5'-O5' |
| 1 | Aa | 1107 | OMG | O4'-C4'-C5'-O5' |
| 27 | BA | 1337 | 4AC | C3'-C4'-C5'-O5' |
| 27 | BA | 3009 | 4AC | O4'-C4'-C5'-O5' |
| 27 | BA | 505 | A2M | O4'-C4'-C5'-O5' |
| 27 | BA | 1790 | OMC | O4'-C4'-C5'-O5' |
| 27 | BA | 617 | LHH | O4'-C4'-C5'-O5' |
| 27 | BA | 869 | OMC | O4'-C4'-C5'-O5' |
| 1 | Aa | 5 | 4AC | O7-C7-N4-C4 |
| 1 | Aa | 5 | 4AC | CM7-C7-N4-C4 |
| 1 | Aa | 41 | 4AC | O7-C7-N4-C4 |
| 1 | Aa | 41 | 4AC | CM7-C7-N4-C4 |
| 1 | Aa | 136 | 4AC | O7-C7-N4-C4 |
| 1 | Aa | 136 | 4AC | CM7-C7-N4-C4 |
| 1 | Aa | 229 | LHH | CM7-C7-N4-C4 |
| 1 | Aa | 229 | LHH | O7-C7-N4-C4 |
| 1 | Aa | 358 | 4AC | O7-C7-N4-C4 |
| 1 | Aa | 358 | 4AC | CM7-C7-N4-C4 |
| 1 | Aa | 525 | 4AC | O7-C7-N4-C4 |
| 1 | Aa | 525 | 4AC | CM7-C7-N4-C4 |
| 1 | Aa | 697 | 4AC | O7-C7-N4-C4 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 1 | Aa | 697 | 4AC | CM7-C7-N4-C4 |
| 1 | Aa | 730 | 4AC | O7-C7-N4-C4 |
| 1 | Aa | 730 | 4AC | CM7-C7-N4-C4 |
| 1 | Aa | 818 | 4AC | O7-C7-N4-C4 |
| 1 | Aa | 818 | 4AC | CM7-C7-N4-C4 |
| 1 | Aa | 1020 | LHH | CM7-C7-N4-C4 |
| 1 | Aa | 1020 | LHH | O7-C7-N4-C4 |
| 27 | BA | 201 | 4AC | O7-C7-N4-C4 |
| 27 | BA | 201 | 4AC | CM7-C7-N4-C4 |
| 27 | BA | 617 | LHH | CM7-C7-N4-C4 |
| 27 | BA | 617 | LHH | O7-C7-N4-C4 |
| 27 | BA | 858 | 4AC | O7-C7-N4-C4 |
| 27 | BA | 858 | 4AC | CM7-C7-N4-C4 |
| 27 | BA | 925 | 4AC | O7-C7-N4-C4 |
| 27 | BA | 925 | 4AC | CM7-C7-N4-C4 |
| 27 | BA | 1305 | 4AC | O7-C7-N4-C4 |
| 27 | BA | 1305 | 4AC | CM7-C7-N4-C4 |
| 27 | BA | 1434 | 4AC | O7-C7-N4-C4 |
| 27 | BA | 1434 | 4AC | CM7-C7-N4-C4 |
| 27 | BA | 2457 | LHH | CM7-C7-N4-C4 |
| 27 | BA | 2457 | LHH | O7-C7-N4-C4 |
| 27 | BA | 2955 | LHH | CM7-C7-N4-C4 |
| 27 | BA | 2955 | LHH | O7-C7-N4-C4 |
| 1 | Aa | 190 | OMC | O4'-C4'-C5'-O5' |
| 1 | Aa | 636 | OMG | O4'-C4'-C5'-O5' |
| 27 | BA | 453 | OMU | O4'-C4'-C5'-O5' |
| 27 | BA | 2571 | OMC | C3'-C4'-C5'-O5' |
| 27 | BA | 2568 | OMG | C1'-C2'-O2'-CM2 |
| 1 | Aa | 1478 | 5MC | O4'-C1'-N1-C6 |
| 1 | Aa | 994 | OMG | C4'-C5'-O5'-P |
| 1 | Aa | 913 | OMG | O4'-C4'-C5'-O5' |
| 1 | Aa | 1276 | 5MC | O4'-C4'-C5'-O5' |
| 1 | Aa | 892 | OMG | C3'-C2'-O2'-CM2 |
| 1 | Aa | 458 | 4AC | N3-C4-N4-C7 |
| 1 | Aa | 458 | 4AC | C5-C4-N4-C7 |
| 1 | Aa | 525 | 4AC | N3-C4-N4-C7 |
| 27 | BA | 2379 | OMG | C4'-C5'-O5'-P |
| 27 | BA | 1641 | 4AC | O4'-C4'-C5'-O5' |
| 27 | BA | 1641 | 4AC | C3'-C4'-C5'-O5' |
| 27 | BA | 1799 | OMG | O4'-C4'-C5'-O5' |
| 27 | BA | 2571 | OMC | O4'-C4'-C5'-O5' |
| 1 | Aa | 1478 | 5MC | O4'-C1'-N1-C2 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 27 | BA | 2545 | OMC | C4'-C5'-O5'-P |
| 1 | Aa | 479 | OMU | C3'-C2'-O2'-CM2 |
| 27 | BA | 617 | LHH | C3'-C2'-O2'-C1 |
| 27 | BA | 1799 | OMG | C3'-C2'-O2'-CM2 |
| 27 | BA | 2702 | A2M | C3'-C2'-O2'-CM' |
| 27 | BA | 488 | A2M | C3'-C4'-C5'-O5' |
| 27 | BA | 1892 | OMG | C3'-C4'-C5'-O5' |
| 1 | Aa | 1025 | OMG | C4'-C5'-O5'-P |
| 27 | BA | 505 | A2M | C3'-C2'-O2'-CM' |
| 27 | BA | 1400 | A2M | C3'-C2'-O2'-CM' |
| 1 | Aa | 1217 | 4AC | C2'-C1'-N1-C6 |
| 27 | BA | 365 | OMG | O4'-C4'-C5'-O5' |
| 1 | Aa | 5 | 4AC | C3'-C4'-C5'-O5' |
| 1 | Aa | 1026 | OMG | O4'-C4'-C5'-O5' |
| 27 | BA | 244 | 4AC | O4'-C4'-C5'-O5' |
| 27 | BA | 1790 | OMC | C3'-C4'-C5'-O5' |
| 27 | BA | 1799 | OMG | C3'-C4'-C5'-O5' |
| 27 | BA | 2832 | 4AC | O4'-C4'-C5'-O5' |
| 27 | BA | 3009 | 4AC | C3'-C4'-C5'-O5' |
| 1 | Aa | 1217 | 4AC | C2'-C1'-N1-C2 |
| 27 | BA | 1551 | OMU | C2'-C1'-N1-C2 |
| 1 | Aa | 1434 | OMG | O4'-C4'-C5'-O5' |
| 1 | Aa | 304 | OMU | C2'-C1'-N1-C2 |
| 1 | Aa | 1358 | OMU | C2'-C1'-N1-C2 |
| 27 | BA | 2610 | OMU | C2'-C1'-N1-C2 |
| 27 | BA | 453 | OMU | C3'-C4'-C5'-O5' |
| 27 | BA | 617 | LHH | C3'-C4'-C5'-O5' |
| 27 | BA | 869 | OMC | C3'-C4'-C5'-O5' |
| 1 | Aa | 1478 | 5MC | C2'-C1'-N1-C2 |
| 27 | BA | 2992 | 4AC | C2'-C1'-N1-C2 |
| 27 | BA | 723 | OMG | C4'-C5'-O5'-P |
| 1 | Aa | 8 | OMU | O4'-C4'-C5'-O5' |
| 1 | Aa | 190 | OMC | C3'-C4'-C5'-O5' |
| 1 | Aa | 636 | OMG | C3'-C4'-C5'-O5' |
| 1 | Aa | 8 | OMU | C2'-C1'-N1-C6 |
| 1 | Aa | 229 | LHH | N3-C4-N4-C7 |
| 1 | Aa | 1020 | LHH | C5-C4-N4-C7 |
| 1 | Aa | 1020 | LHH | N3-C4-N4-C7 |
| 27 | BA | 526 | LHH | N3-C4-N4-C7 |
| 27 | BA | 1543 | 4AC | C2'-C1'-N1-C2 |
| 27 | BA | 1551 | OMU | C4'-C5'-O5'-P |
| 1 | Aa | 8 | OMU | O4'-C1'-N1-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 1 | Aa | 854 | 5MC | C3'-C4'-C5'-O5' |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

## 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.

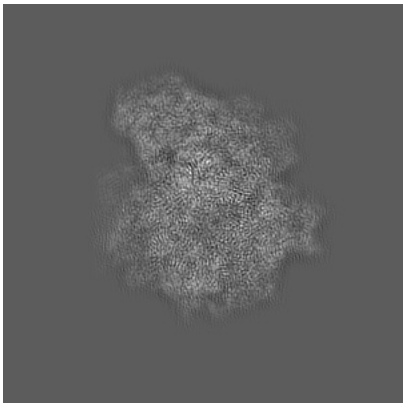
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10223. These allow visual inspection of the internal detail of the map and identification of artifacts.

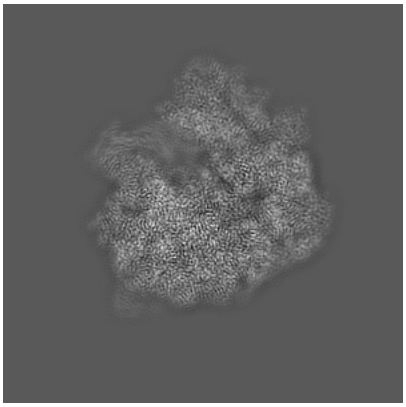
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

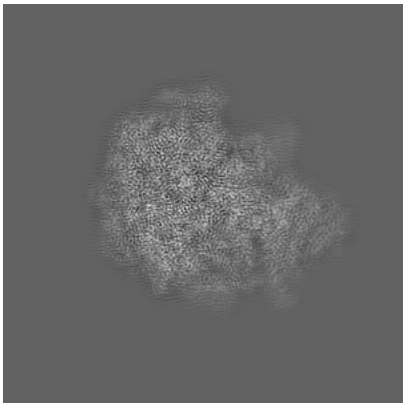
### 6.1.1 Primary map



X



Y

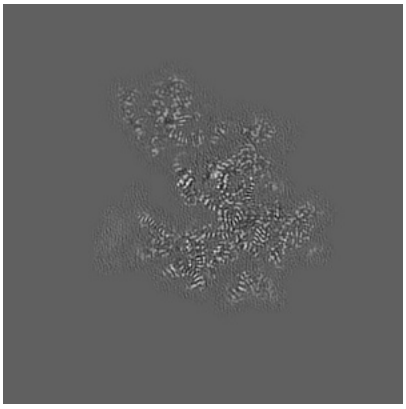


Z

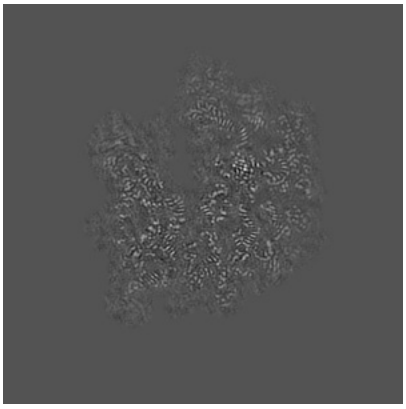
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

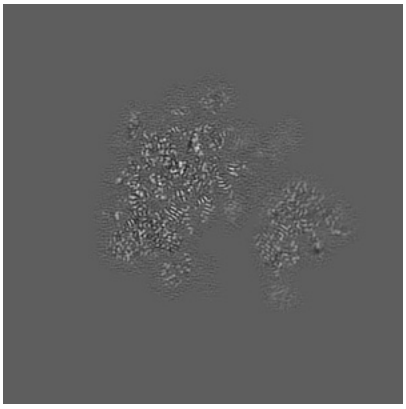
### 6.2.1 Primary map



X Index: 240



Y Index: 240

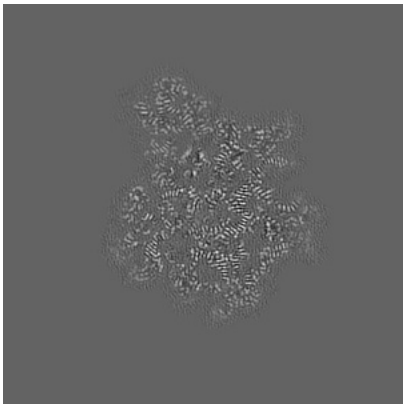


Z Index: 240

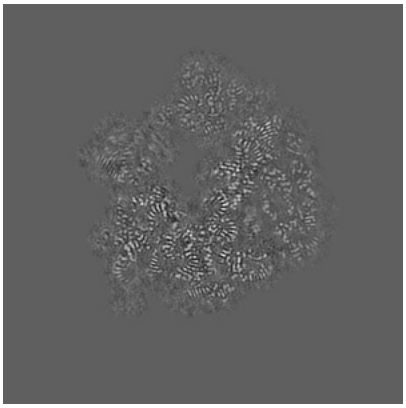
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

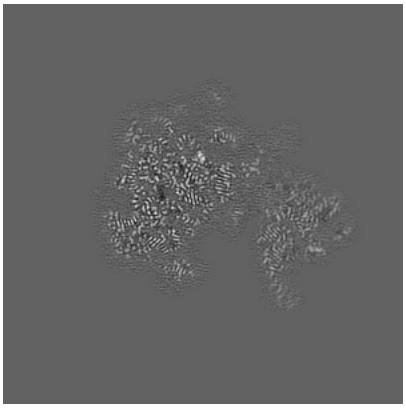
### 6.3.1 Primary map



X Index: 213



Y Index: 224

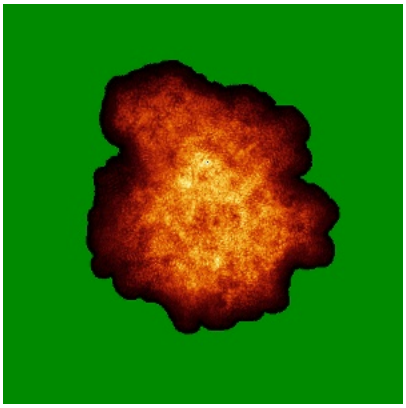


Z Index: 247

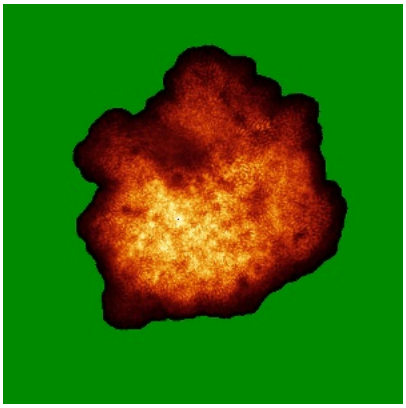
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) (i)

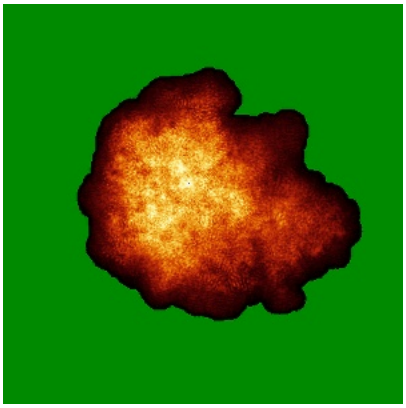
### 6.4.1 Primary map



X



Y

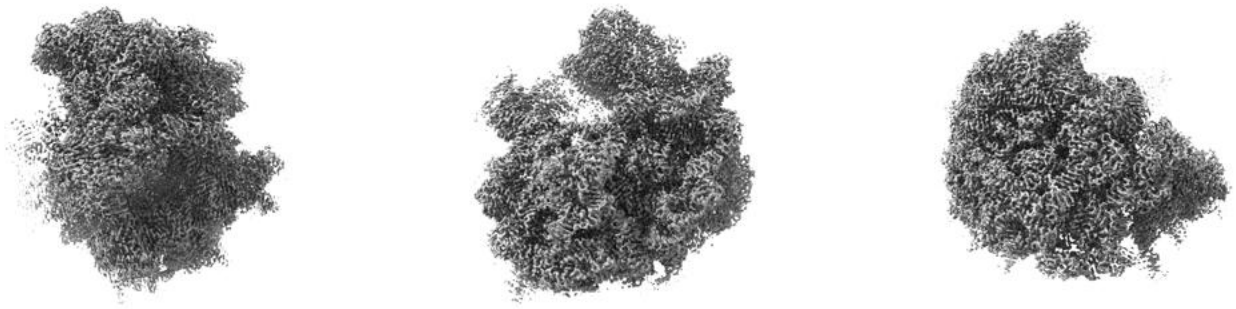


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

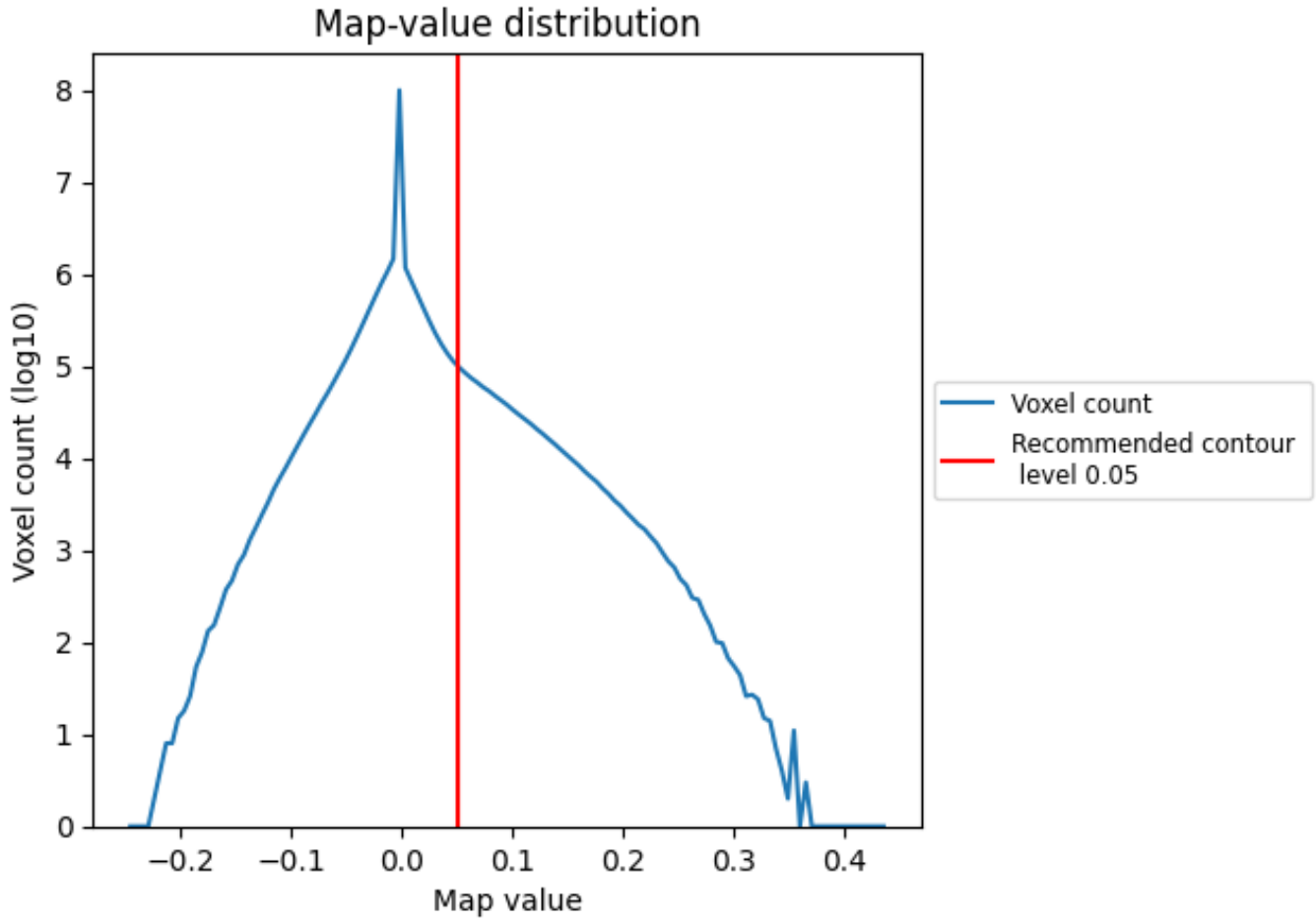
## 6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

# 7 Map analysis

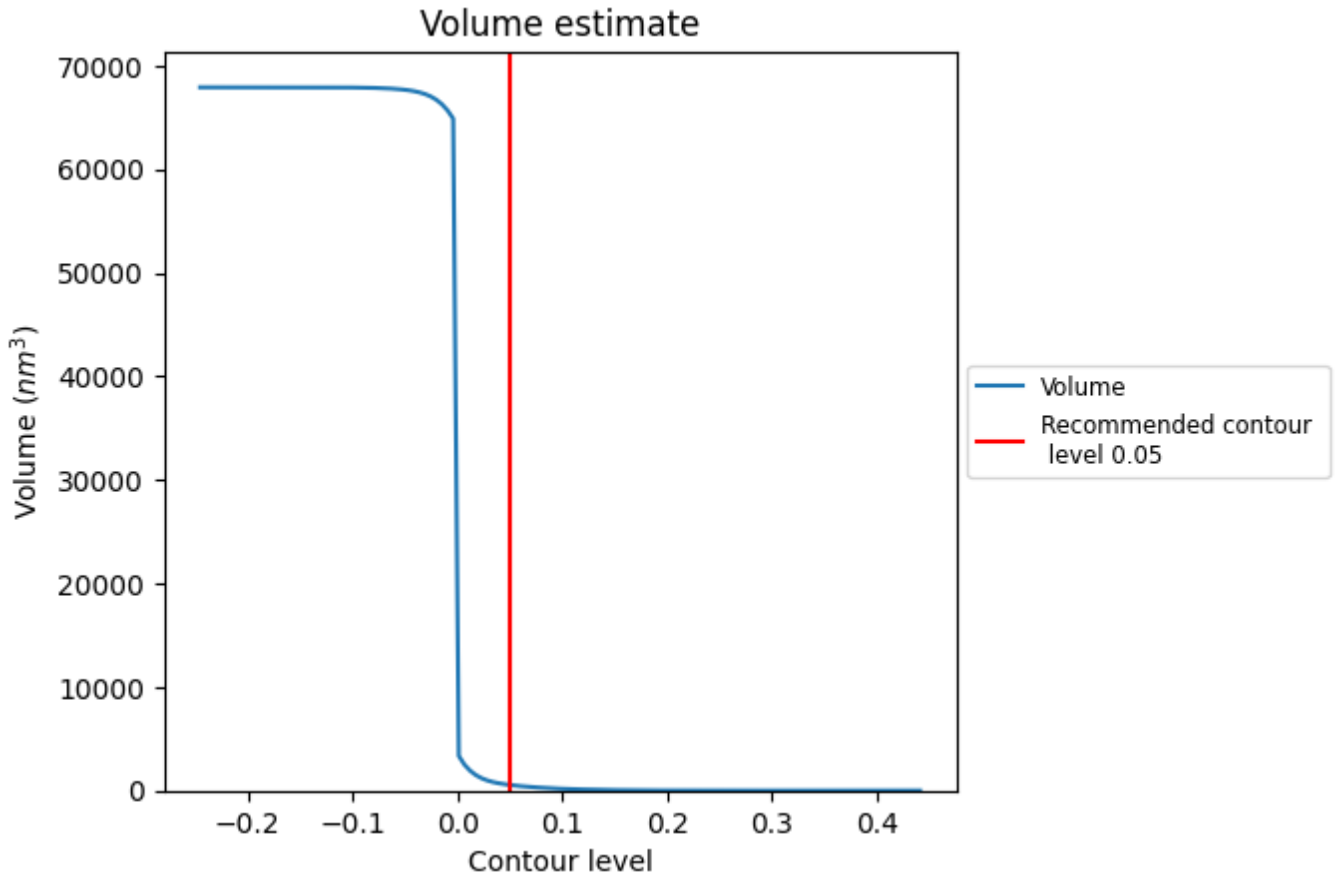
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

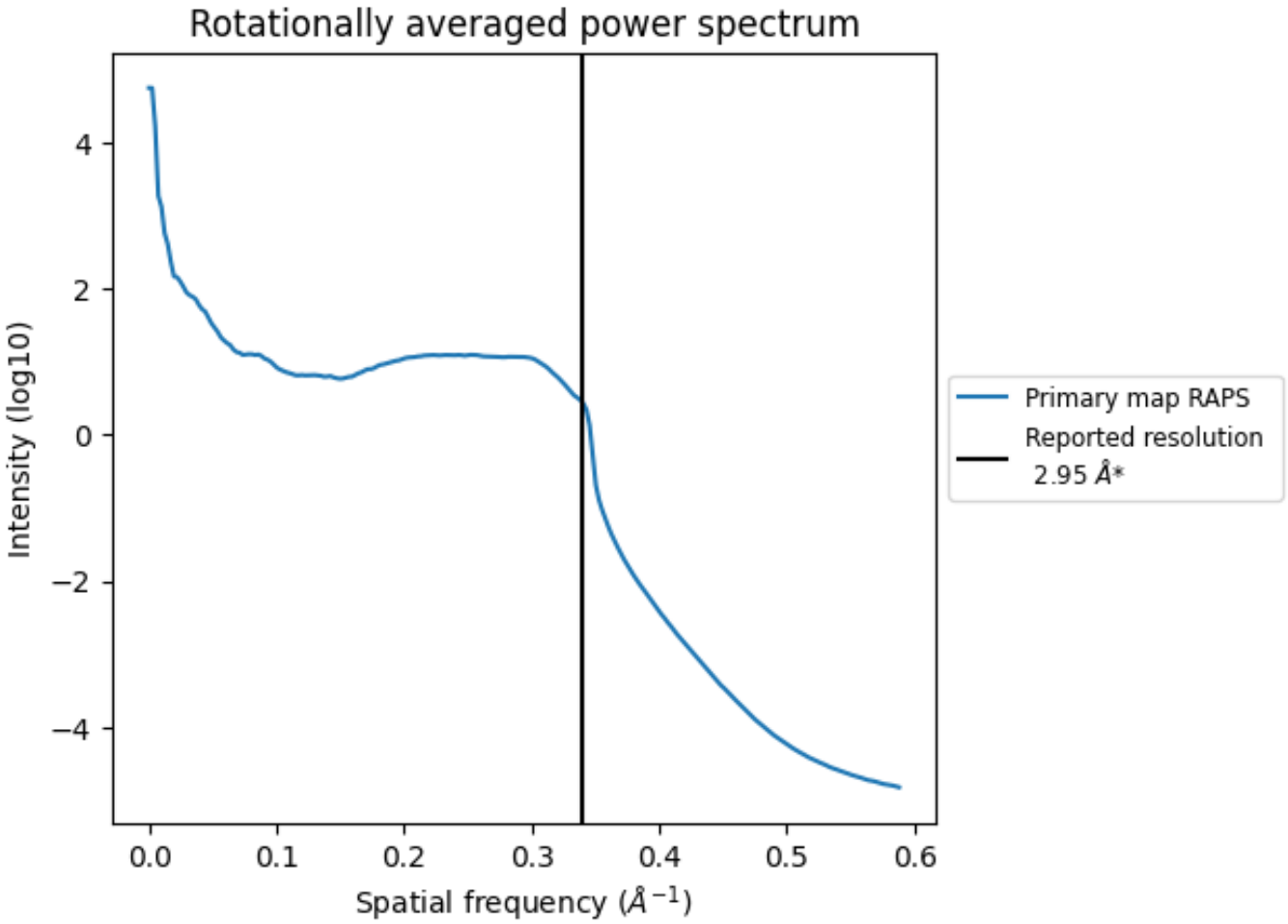
## 7.2 Volume estimate




The volume at the recommended contour level is 541 $nm^3$; this corresponds to an approximate mass of 488 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

## 7.3 Rotationally averaged power spectrum (i)




*Reported resolution corresponds to spatial frequency of 0.339 Å$^{-1}$

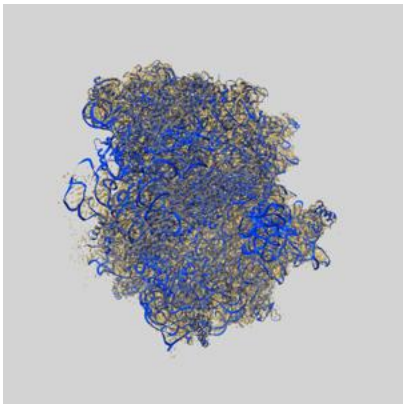
# 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

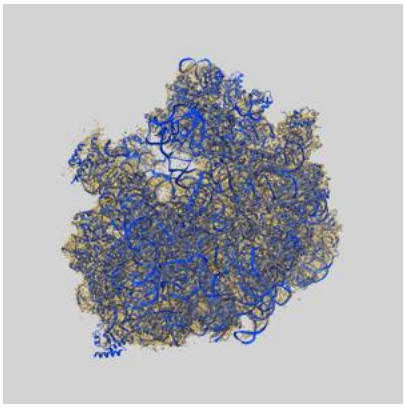
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10223 and PDB model 6SKF. Per-residue inclusion information can be found in section 3 on page 19.

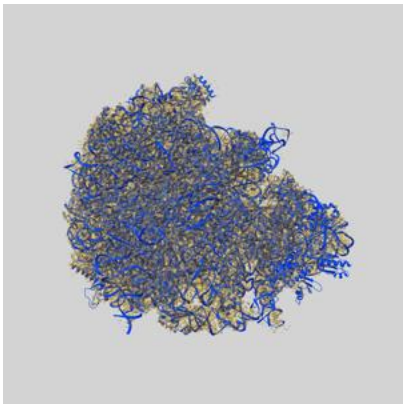
## 9.1 Map-model overlay



X



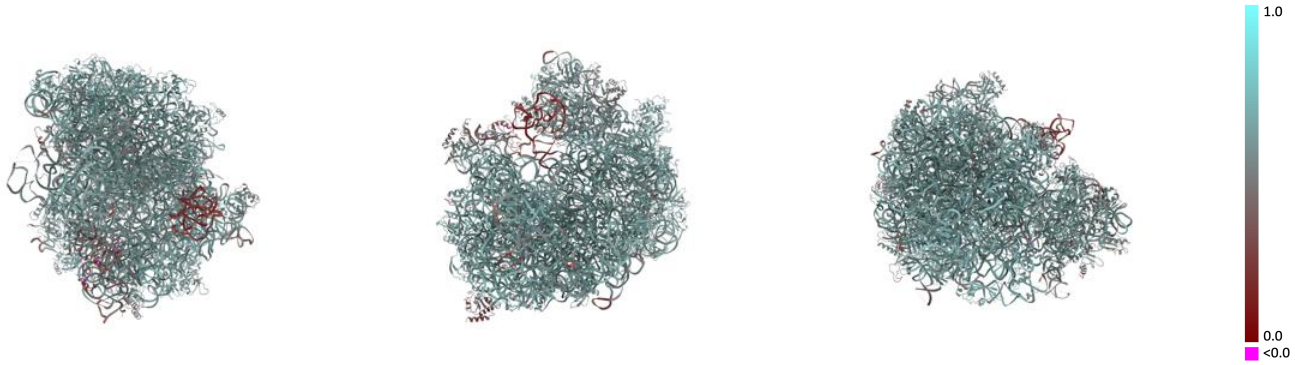
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

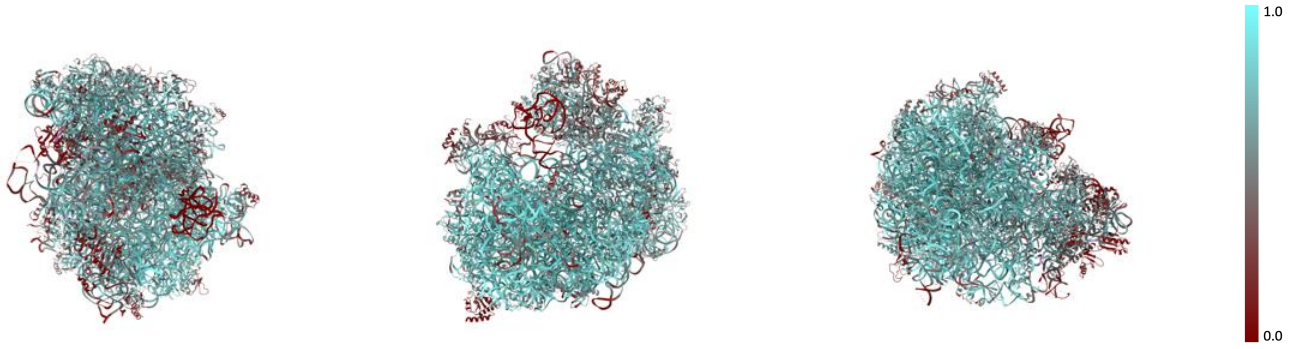
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

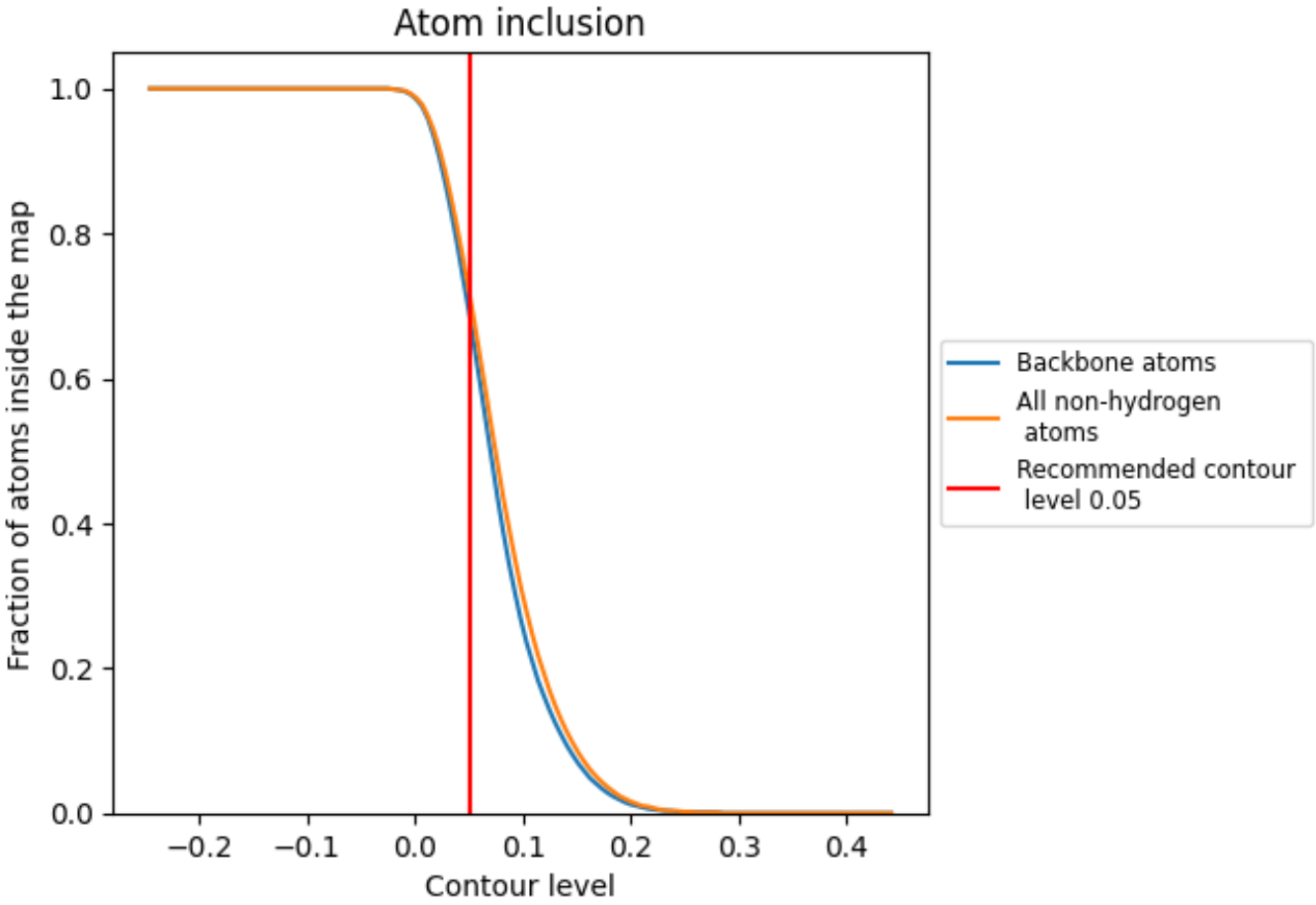
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

## 9.4 Atom inclusion (i)




At the recommended contour level, 69% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.7210 | 0.5970 |
| Aa | 0.7520 | 0.6120 |
| Ab | 0.5250 | 0.5890 |
| Ac | 0.2440 | 0.5210 |
| Ad | 0.5150 | 0.5720 |
| Ae | 0.6270 | 0.5960 |
| Af | 0.6610 | 0.6140 |
| Ag | 0.6510 | 0.6090 |
| Ah | 0.3630 | 0.5600 |
| Ai | 0.4980 | 0.5560 |
| Aj | 0.6690 | 0.6090 |
| Ak | 0.6120 | 0.5980 |
| Al | 0.4230 | 0.5680 |
| Am | 0.2060 | 0.5180 |
| An | 0.5510 | 0.5760 |
| Ao | 0.5930 | 0.6110 |
| Ap | 0.5280 | 0.5540 |
| Aq | 0.6230 | 0.5870 |
| Ar | 0.4590 | 0.5780 |
| As | 0.6270 | 0.6170 |
| At | 0.1600 | 0.4910 |
| Au | 0.4610 | 0.5730 |
| Av | 0.5550 | 0.5690 |
| Aw | 0.5730 | 0.5920 |
| Ax | 0.5000 | 0.5810 |
| Ay | 0.4370 | 0.5440 |
| Az | 0.5820 | 0.6170 |
| BA | 0.8210 | 0.6050 |
| BB | 0.6120 | 0.5320 |
| BC | 0.7770 | 0.6200 |
| BD | 0.7810 | 0.6230 |
| BE | 0.7630 | 0.6170 |
| BF | 0.1560 | 0.3000 |
| BG | 0.6630 | 0.5920 |
| BH | 0.5050 | 0.5590 |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| Chain | Atom inclusion | Q-score |
|---|---|---|
| BI | 0.0620 | 0.3640 |
| BJ | 0.7310 | 0.6020 |
| BK | 0.7460 | 0.6140 |
| BL | 0.7410 | 0.6150 |
| BM | 0.5940 | 0.5770 |
| BN | 0.5420 | 0.5580 |
| BO | 0.6000 | 0.5700 |
| BP | 0.8300 | 0.6350 |
| BQ | 0.4810 | 0.5340 |
| BR | 0.7480 | 0.6110 |
| BS | 0.7240 | 0.5990 |
| BT | 0.6150 | 0.5890 |
| BU | 0.8010 | 0.6300 |
| BV | 0.7830 | 0.6250 |
| BW | 0.6840 | 0.5900 |
| BX | 0.7410 | 0.6110 |
| BY | 0.8090 | 0.6270 |
| BZ | 0.5620 | 0.5550 |
| Ba | 0.7610 | 0.6100 |
| Bb | 0.6200 | 0.5610 |
| Bc | 0.7110 | 0.5980 |
| Bd | 0.7670 | 0.6230 |
| Be | 0.7390 | 0.6080 |
| Bg | 0.7510 | 0.6160 |
| Bh | 0.8750 | 0.6460 |
| Bi | 0.7910 | 0.6290 |
| Bj | 0.7470 | 0.6170 |
| Bk | 0.8900 | 0.6250 |
| Bl | 0.7300 | 0.6170 |