



Full wwPDB EM Validation Report ⓘ

Mar 6, 2025 – 02:52 pm GMT

PDB ID : 6TC3
EMDB ID : EMD-10458
Title : Cryo-EM structure of an Escherichia coli ribosome-SpeFL complex stalled in response to L-ornithine (Replicate 1)
Authors : Innis, C.A.; Herrero del Valle, A.
Deposited on : 2019-11-05
Resolution : 2.70 Å(reported)
Based on initial model : 4YBB

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 : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

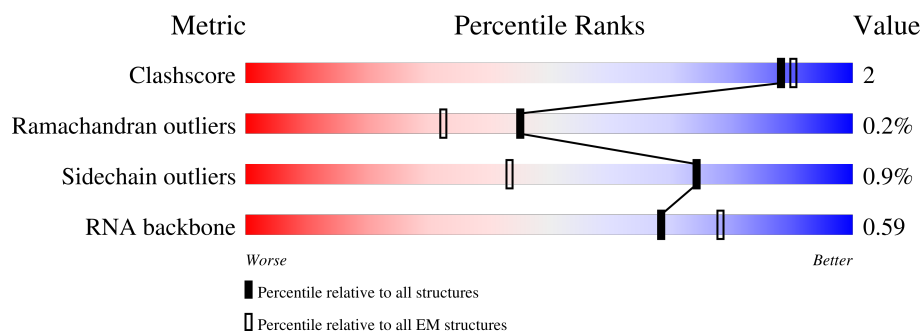
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

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



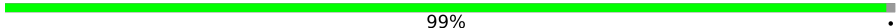



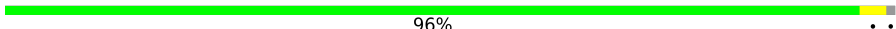

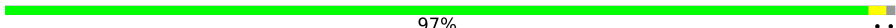
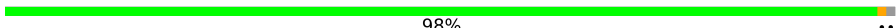
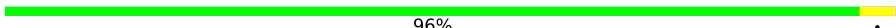
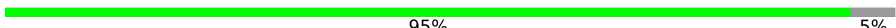


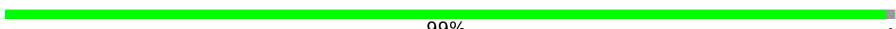



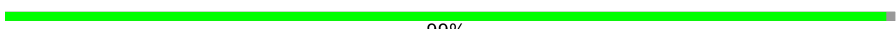
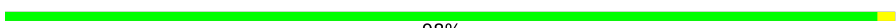
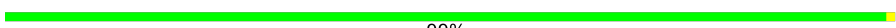
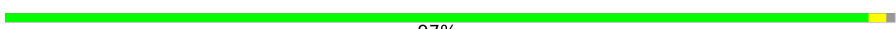
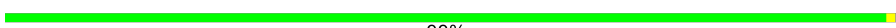




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |
| RNA backbone | 6643 | 2191 |

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 $\leq 5\%$.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 16S1 | 1534 | 64% 30% 5% |
| 2 | S021 | 241 | 90% 7% |
| 3 | S031 | 233 | 88% 12% |
| 4 | S041 | 206 | 98% . |
| 5 | S051 | 167 | 92% 7% |
| 6 | S061 | 135 | 78% 21% |
| 7 | S071 | 179 | 83% 16% |

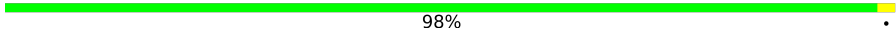
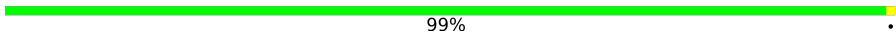

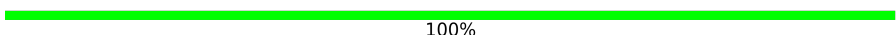
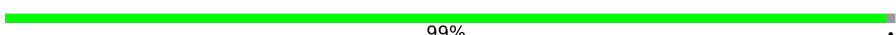
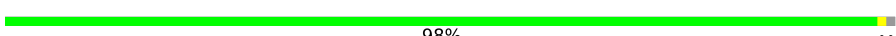
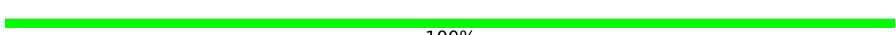






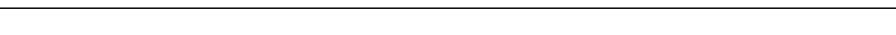

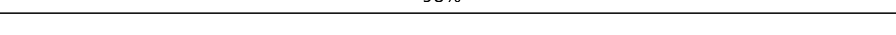
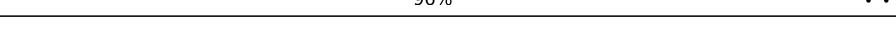
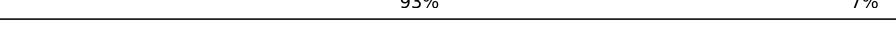
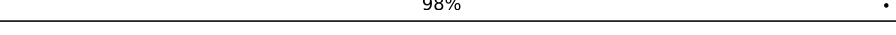
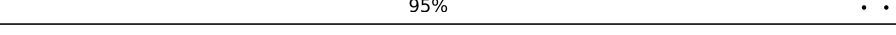
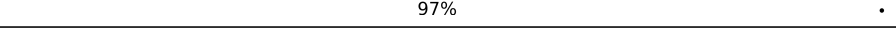


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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 8 | S081 | 130 |  99% . |
| 9 | S091 | 130 |  93% 5% .. |
| 10 | S101 | 103 |  88% 5% . . |
| 11 | S111 | 129 |  91% 9% |
| 12 | S121 | 124 |  96% . . |
| 13 | S131 | 118 |  91% 6% . |
| 14 | S141 | 102 |  97% . . |
| 15 | S151 | 89 |  98% . . |
| 16 | S161 | 82 |  96% . |
| 17 | S171 | 84 |  95% 5% |
| 18 | S181 | 75 |  71% . 27% |
| 19 | S191 | 92 |  86% . . 11% |
| 20 | S201 | 87 |  99% . |
| 21 | S211 | 71 |  75% . 21% |
| 22 | 23S1 | 2897 |  63% 31% 5% |
| 23 | 05S1 | 120 |  69% 28% . |
| 24 | L021 | 273 |  99% . |
| 25 | L031 | 209 |  98% . |
| 26 | L041 | 201 |  99% . |
| 27 | L051 | 179 |  97% . . |
| 28 | L061 | 177 |  99% . . |
| 29 | L091 | 149 |  92% 7% . |
| 30 | L311 | 70 |  93% . 6% |
| 31 | L131 | 142 |  99% . |
| 32 | L141 | 123 |  100% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 33 | L151 | 144 |  98% |
| 34 | L161 | 136 |  99% |
| 35 | L171 | 127 |  92% 7% |
| 36 | L181 | 117 |  100% |
| 37 | L191 | 115 |  99% |
| 38 | L201 | 118 |  98% |
| 39 | L211 | 103 |  100% |
| 40 | L221 | 110 |  99% |
| 41 | L231 | 100 |  93% 7% |
| 42 | L241 | 104 |  97% |
| 43 | L251 | 94 |  100% |
| 44 | L271 | 85 |  89% 11% |
| 45 | L281 | 78 |  96% |
| 46 | L291 | 63 |  98% |
| 47 | L301 | 59 |  98% |
| 48 | L321 | 57 |  96% |
| 49 | L331 | 55 |  93% 7% |
| 50 | L341 | 46 |  98% |
| 51 | L351 | 65 |  95% |
| 52 | L361 | 38 |  97% |
| 53 | SPE1 | 34 |  88% 12% |
| 54 | MRN1 | 7 |  29% 71% |
| 55 | PTR1 | 76 |  58% 34% 8% |

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 146672 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 |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 1 | 16S1 | 1534 | Total | C | N | O | P | 0 | 0 |
| | | | 32930 | 14694 | 6041 | 10661 | 1534 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2 | S021 | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1753 | 1109 | 315 | 321 | 8 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3 | S031 | 206 | Total | C | N | O | S | 0 | 0 |
| | | | 1624 | 1028 | 305 | 288 | 3 | | |

- Molecule 4 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4 | S041 | 205 | Total | C | N | O | S | 0 | 0 |
| | | | 1643 | 1026 | 315 | 298 | 4 | | |

- Molecule 5 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5 | S051 | 155 | Total | C | N | O | S | 0 | 0 |
| | | | 1144 | 711 | 216 | 211 | 6 | | |

- Molecule 6 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6 | S061 | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 862 | 545 | 156 | 154 | 7 | | |

- Molecule 7 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7 | S071 | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1181 | 735 | 227 | 215 | 4 | | |

- Molecule 8 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8 | S081 | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 979 | 616 | 173 | 184 | 6 | | |

- Molecule 9 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9 | S091 | 127 | Total | C | N | O | S | 0 | 0 |
| | | | 1022 | 634 | 206 | 179 | 3 | | |

- Molecule 10 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10 | S101 | 99 | Total | C | N | O | S | 0 | 0 |
| | | | 795 | 498 | 152 | 144 | 1 | | |

- Molecule 11 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11 | S111 | 117 | Total | C | N | O | S | 0 | 0 |
| | | | 877 | 540 | 174 | 160 | 3 | | |

- Molecule 12 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12 | S121 | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 957 | 591 | 196 | 165 | 5 | | |

- Molecule 13 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13 | S131 | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 883 | 546 | 178 | 156 | 3 | | |

- Molecule 14 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14 | S141 | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 799 | 498 | 165 | 133 | 3 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| S141 | 35 | ALA | - | insertion | UNP P0AG59 |

- Molecule 15 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15 | S151 | 88 | Total | C | N | O | S | 0 | 0 |
| | | | 714 | 439 | 144 | 130 | 1 | | |

- Molecule 16 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16 | S161 | 82 | Total | C | N | O | S | 0 | 0 |
| | | | 649 | 406 | 128 | 114 | 1 | | |

- Molecule 17 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17 | S171 | 80 | Total | C | N | O | S | 0 | 0 |
| | | | 648 | 411 | 121 | 113 | 3 | | |

- Molecule 18 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 18 | S181 | 55 | Total | C | N | O | 0 | 0 |
| | | | 455 | 288 | 86 | 81 | | |

- Molecule 19 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19 | S191 | 82 | Total | C | N | O | S | 0 | 0 |
| | | | 656 | 419 | 125 | 110 | 2 | | |

- Molecule 20 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20 | S201 | 86 | Total | C | N | O | S | 0 | 0 |
| | | | 670 | 414 | 138 | 115 | 3 | | |

- Molecule 21 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 21 | S211 | 56 | Total | C | N | O | S | 0 | 0 |
| | | | 465 | 290 | 96 | 78 | 1 | | |

- Molecule 22 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 22 | 23S1 | 2897 | Total | C | N | O | P | 0 | 0 |
| | | | 62209 | 27759 | 11446 | 20107 | 2897 | | |

- Molecule 23 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 23 | 05S1 | 120 | Total | C | N | O | P | 0 | 0 |
| | | | 2569 | 1144 | 468 | 837 | 120 | | |

- Molecule 24 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 24 | L021 | 271 | Total | C | N | O | S | 0 | 0 |
| | | | 2082 | 1288 | 423 | 364 | 7 | | |

- Molecule 25 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25 | L031 | 209 | Total | C | N | O | S | 0 | 0 |
| | | | 1566 | 980 | 288 | 294 | 4 | | |

- Molecule 26 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26 | L041 | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | |

- Molecule 27 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27 | L051 | 177 | Total | C | N | O | S | 0 | 0 |
| | | | 1410 | 899 | 249 | 256 | 6 | | |

- Molecule 28 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28 | L061 | 176 | Total | C | N | O | S | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | |

- Molecule 29 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29 | L091 | 149 | Total | C | N | O | S | 0 | 0 |
| | | | 1110 | 699 | 197 | 213 | 1 | | |

- Molecule 30 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 30 | L311 | 66 | Total | C | N | O | S | 0 | 0 |
| | | | 522 | 323 | 99 | 94 | 6 | | |

- Molecule 31 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31 | L131 | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | |

- Molecule 32 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32 | L141 | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 946 | 593 | 181 | 166 | 6 | | |

- Molecule 33 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33 | L151 | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1053 | 654 | 207 | 190 | 2 | | |

- Molecule 34 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34 | L161 | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1075 | 686 | 205 | 178 | 6 | | |

- Molecule 35 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35 | L171 | 118 | Total | C | N | O | S | 0 | 0 |
| | | | 945 | 585 | 194 | 161 | 5 | | |

- Molecule 36 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36 | L181 | 117 | Total | C | N | O | S | 0 | 0 |
| | | | 900 | 557 | 179 | 163 | 1 | | |

- Molecule 37 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37 | L191 | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 917 | 574 | 179 | 163 | 1 | | |

- Molecule 38 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 38 | L201 | 117 | Total | C | N | O | 0 | 0 |
| | | | 947 | 604 | 192 | 151 | | |

- Molecule 39 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39 | L211 | 103 | Total | C | N | O | S | 0 | 0 |
| | | | 816 | 516 | 153 | 145 | 2 | | |

- Molecule 40 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40 | L221 | 110 | Total | C | N | O | S | 0 | 0 |
| | | | 857 | 532 | 166 | 156 | 3 | | |

- Molecule 41 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41 | L231 | 93 | Total | C | N | O | S | 0 | 0 |
| | | | 738 | 466 | 139 | 131 | 2 | | |

- Molecule 42 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 42 | L241 | 102 | Total | C | N | O | | 0 | 0 |
| | | | 779 | 492 | 146 | 141 | | | |

- Molecule 43 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43 | L251 | 94 | Total | C | N | O | S | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | |

- Molecule 44 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44 | L271 | 76 | Total | C | N | O | S | 0 | 0 |
| | | | 580 | 359 | 117 | 103 | 1 | | |

- Molecule 45 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45 | L281 | 77 | Total | C | N | O | S | 0 | 0 |
| | | | 625 | 388 | 129 | 106 | 2 | | |

- Molecule 46 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 46 | L291 | 62 | Total | C | N | O | S | 0 | 0 |
| | | | 501 | 308 | 98 | 94 | 1 | | |

- Molecule 47 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 47 | L301 | 58 | Total | C | N | O | S | 0 | 0 |
| | | | 449 | 281 | 87 | 79 | 2 | | |

- Molecule 48 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 48 | L321 | 56 | Total | C | N | O | S | 0 | 0 |
| | | | 444 | 269 | 94 | 80 | 1 | | |

- Molecule 49 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|-------|
| 49 | L331 | 51 | Total | C | N | O | | 0 | 0 |
| | | | 414 | 266 | 76 | 72 | | | |

- Molecule 50 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 50 | L341 | 46 | Total | C | N | O | S | 0 | 0 |
| | | | 377 | 228 | 90 | 57 | 2 | | |

- Molecule 51 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 51 | L351 | 64 | Total | C | N | O | S | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | |

- Molecule 52 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 52 | L361 | 38 | Total | C | N | O | S | 0 | 0 |
| | | | 302 | 185 | 65 | 48 | 4 | | |

- Molecule 53 is a protein called SpeFL.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 53 | SPE1 | 34 | Total | C | N | O | S | 0 | 0 |
| | | | 300 | 187 | 62 | 48 | 3 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|----------------|
| SPE1 | 5 | SER | ASN | conflict | UNP A0A4S4NWS2 |
| SPE1 | 7 | THR | LEU | conflict | UNP A0A4S4NWS2 |

- Molecule 54 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 54 | MRN1 | 7 | Total | C | N | O | P | 0 | 0 |
| | | | 146 | 65 | 23 | 51 | 7 | | |

- Molecule 55 is a RNA chain called P-site Arg-tRNA.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 55 | PTR1 | 76 | Total | C | N | O | P | S | 0 | 0 |
| | | | 1627 | 727 | 294 | 528 | 76 | 2 | | |

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|-----|---------|
| 56 | 16S1 | 87 | Total | Mg | 0 |
| | | | 87 | 87 | |
| 56 | 23S1 | 249 | Total | Mg | 0 |
| | | | 249 | 249 | |
| 56 | L231 | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 56 | SPE1 | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 56 | PTR1 | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

- Molecule 57 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|-----|---------|
| 57 | 16S1 | 39 | Total | K | 0 |
| | | | 39 | 39 | |
| 57 | 23S1 | 106 | Total | K | 0 |
| | | | 106 | 106 | |
| 57 | 05S1 | 1 | Total | K | 0 |
| | | | 1 | 1 | |
| 57 | L031 | 1 | Total | K | 0 |
| | | | 1 | 1 | |

- Molecule 58 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|-----|---------|
| 58 | 16S1 | 145 | Total | X | 0 |
| | | | 145 | 145 | |
| 58 | S021 | 1 | Total | X | 0 |
| | | | 1 | 1 | |

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| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|--------------|----------|---------|
| 58 | S031 | 1 | Total 1 | X 1 | 0 |
| 58 | S081 | 1 | Total 1 | X 1 | 0 |
| 58 | S091 | 1 | Total 1 | X 1 | 0 |
| 58 | S111 | 2 | Total 2 | X 2 | 0 |
| 58 | S131 | 1 | Total 1 | X 1 | 0 |
| 58 | S171 | 1 | Total 1 | X 1 | 0 |
| 58 | 23S1 | 908 | Total 908 | X 908 | 0 |
| 58 | 05S1 | 9 | Total 9 | X 9 | 0 |
| 58 | L021 | 26 | Total 26 | X 26 | 0 |
| 58 | L031 | 17 | Total 17 | X 17 | 0 |
| 58 | L041 | 11 | Total 11 | X 11 | 0 |
| 58 | L131 | 6 | Total 6 | X 6 | 0 |
| 58 | L141 | 6 | Total 6 | X 6 | 0 |
| 58 | L151 | 5 | Total 5 | X 5 | 0 |
| 58 | L161 | 5 | Total 5 | X 5 | 0 |
| 58 | L171 | 5 | Total 5 | X 5 | 0 |
| 58 | L181 | 1 | Total 1 | X 1 | 0 |
| 58 | L191 | 4 | Total 4 | X 4 | 0 |
| 58 | L201 | 3 | Total 3 | X 3 | 0 |
| 58 | L211 | 1 | Total 1 | X 1 | 0 |
| 58 | L221 | 8 | Total 8 | X 8 | 0 |

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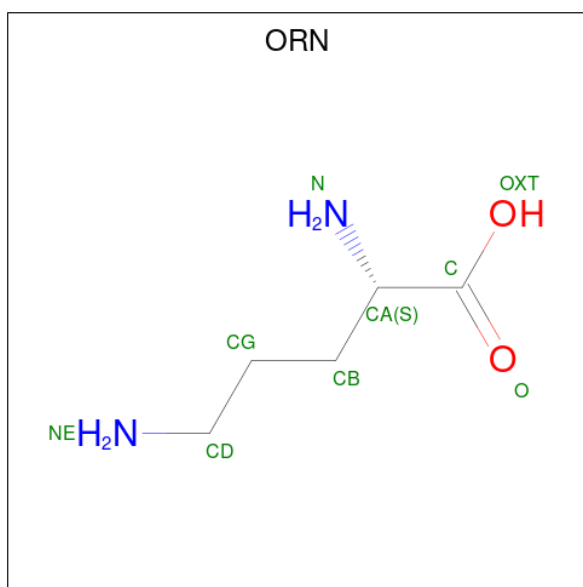
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| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|--------|---------|
| 58 | L231 | 1 | Total 1 | X 1 | 0 |
| 58 | L241 | 2 | Total 2 | X 2 | 0 |
| 58 | L251 | 1 | Total 1 | X 1 | 0 |
| 58 | L271 | 3 | Total 3 | X 3 | 0 |
| 58 | L281 | 2 | Total 2 | X 2 | 0 |
| 58 | L321 | 3 | Total 3 | X 3 | 0 |
| 58 | L331 | 1 | Total 1 | X 1 | 0 |
| 58 | L341 | 8 | Total 8 | X 8 | 0 |
| 58 | L351 | 3 | Total 3 | X 3 | 0 |
| 58 | SPE1 | 6 | Total 6 | X 6 | 0 |
| 58 | MRN1 | 1 | Total 1 | X 1 | 0 |
| 58 | PTR1 | 2 | Total 2 | X 2 | 0 |

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|---------|---------|
| 59 | S021 | 1 | Total 1 | Zn 1 | 0 |
| 59 | L311 | 1 | Total 1 | Zn 1 | 0 |
| 59 | L361 | 1 | Total 1 | Zn 1 | 0 |

- Molecule 60 is L-ornithine (three-letter code: ORN) (formula: C₅H₁₂N₂O₂).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 60 | 23S1 | 1 | Total | C | N | O | 0 |
| | | | 9 | 5 | 2 | 2 | |

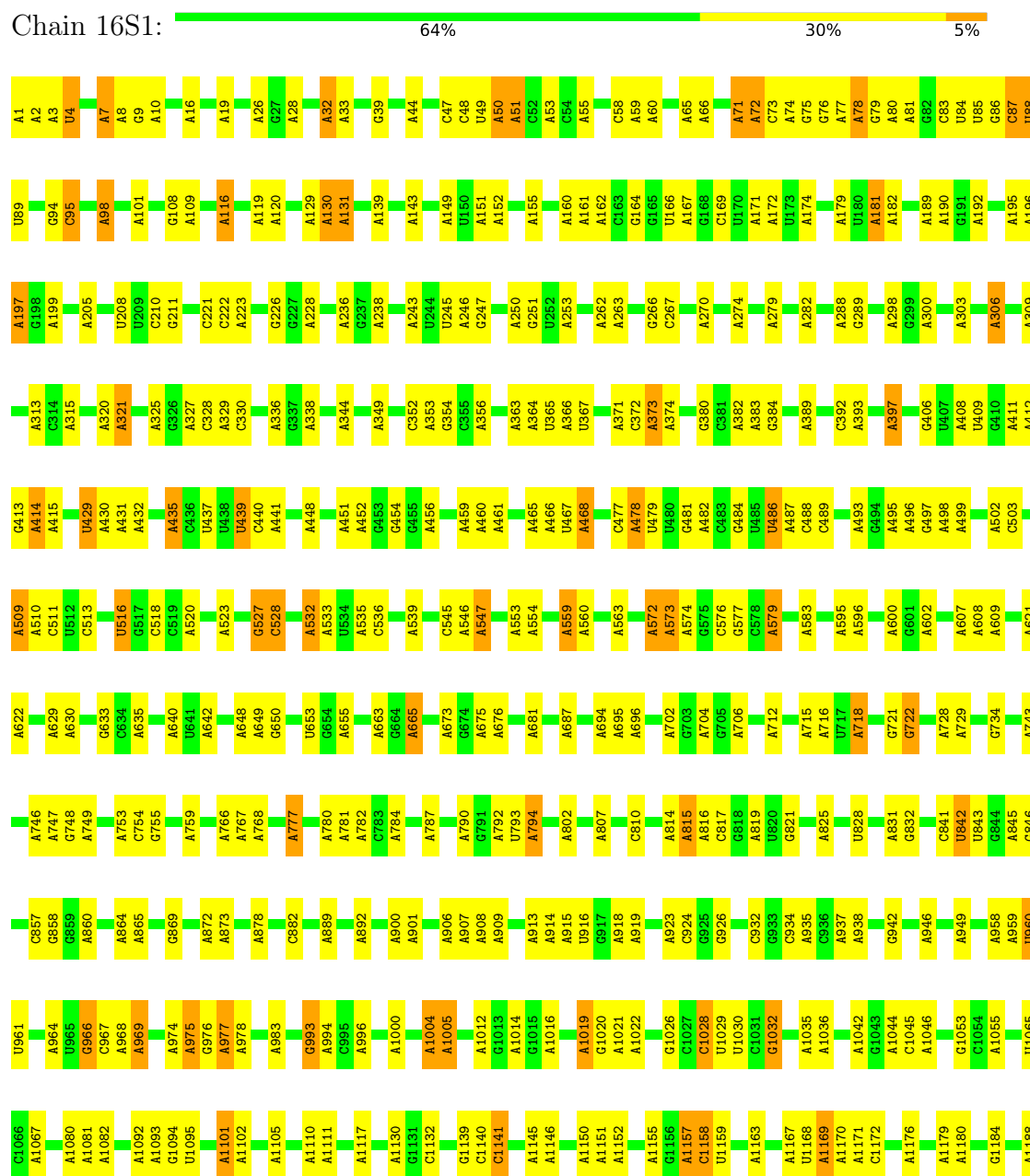
- Molecule 61 is water.

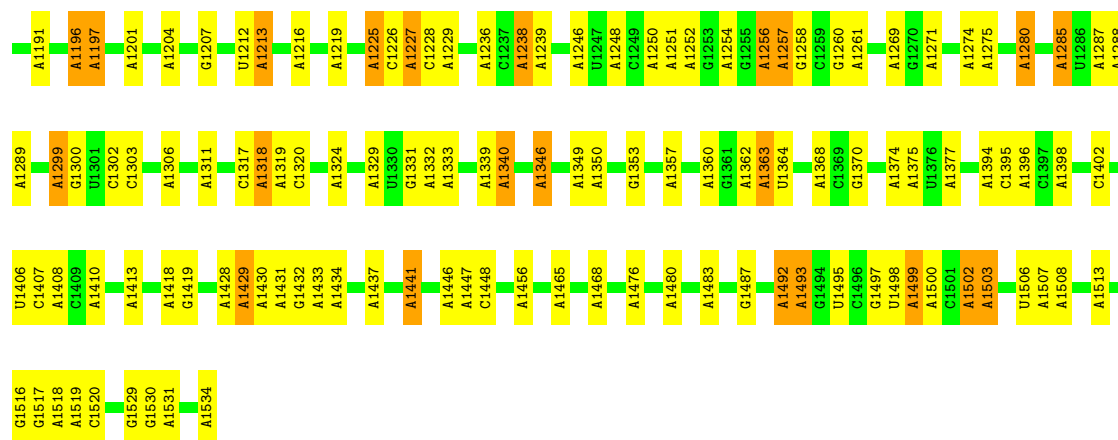
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|-----|---------|
| 61 | 16S1 | 167 | Total | O | 0 |
| | | | 167 | 167 | |
| 61 | S111 | 1 | Total | O | 0 |
| | | | 1 | 1 | |
| 61 | S131 | 2 | Total | O | 0 |
| | | | 2 | 2 | |
| 61 | S141 | 1 | Total | O | 0 |
| | | | 1 | 1 | |
| 61 | S171 | 1 | Total | O | 0 |
| | | | 1 | 1 | |
| 61 | 23S1 | 619 | Total | O | 0 |
| | | | 619 | 619 | |
| 61 | L021 | 3 | Total | O | 0 |
| | | | 3 | 3 | |
| 61 | L031 | 2 | Total | O | 0 |
| | | | 2 | 2 | |
| 61 | L151 | 2 | Total | O | 0 |
| | | | 2 | 2 | |
| 61 | L171 | 2 | Total | O | 0 |
| | | | 2 | 2 | |

3 Residue-property plots

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





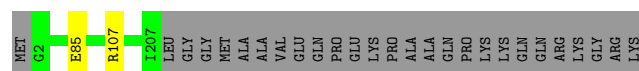
- Molecule 2: 30S ribosomal protein S2

Chain S021: 90% 7%



- Molecule 3: 30S ribosomal protein S3

Chain S031: 88% 12%



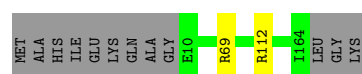
- Molecule 4: 30S ribosomal protein S4

Chain S041: 98%



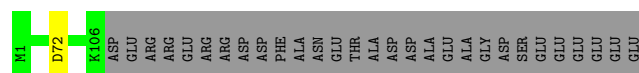
- Molecule 5: 30S ribosomal protein S5

Chain S051: 92% 7%




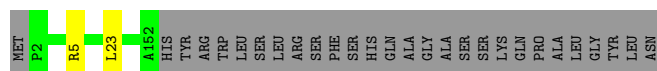
- Molecule 6: 30S ribosomal protein S6

Chain S061: 78% 21%



- Molecule 7: 30S ribosomal protein S7

Chain S071:  83% 16%



- Molecule 8: 30S ribosomal protein S8

Chain S081:  99%



- Molecule 9: 30S ribosomal protein S9

Chain S091:  93% 5%



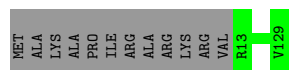
- Molecule 10: 30S ribosomal protein S10

Chain S101:  88% 5%



- Molecule 11: 30S ribosomal protein S11

Chain S111:  91% 9%



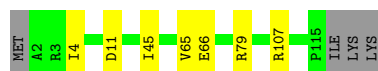
- Molecule 12: 30S ribosomal protein S12

Chain S121:  96%



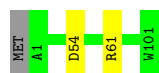
- Molecule 13: 30S ribosomal protein S13

Chain S131:  91% 6%



- Molecule 14: 30S ribosomal protein S14

Chain S141:  97% ..



- Molecule 15: 30S ribosomal protein S15

Chain S151:  98% ..



- Molecule 16: 30S ribosomal protein S16

Chain S161:  96% .




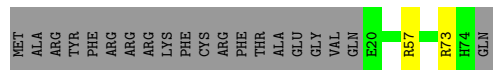
- Molecule 17: 30S ribosomal protein S17

Chain S171:  95% 5%




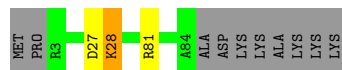
- Molecule 18: 30S ribosomal protein S18

Chain S181:  71% . 27%



- Molecule 19: 30S ribosomal protein S19

Chain S191:  86% .. 11%



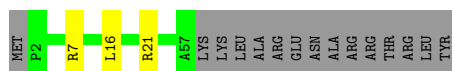
- Molecule 20: 30S ribosomal protein S20

Chain S201:  99% .



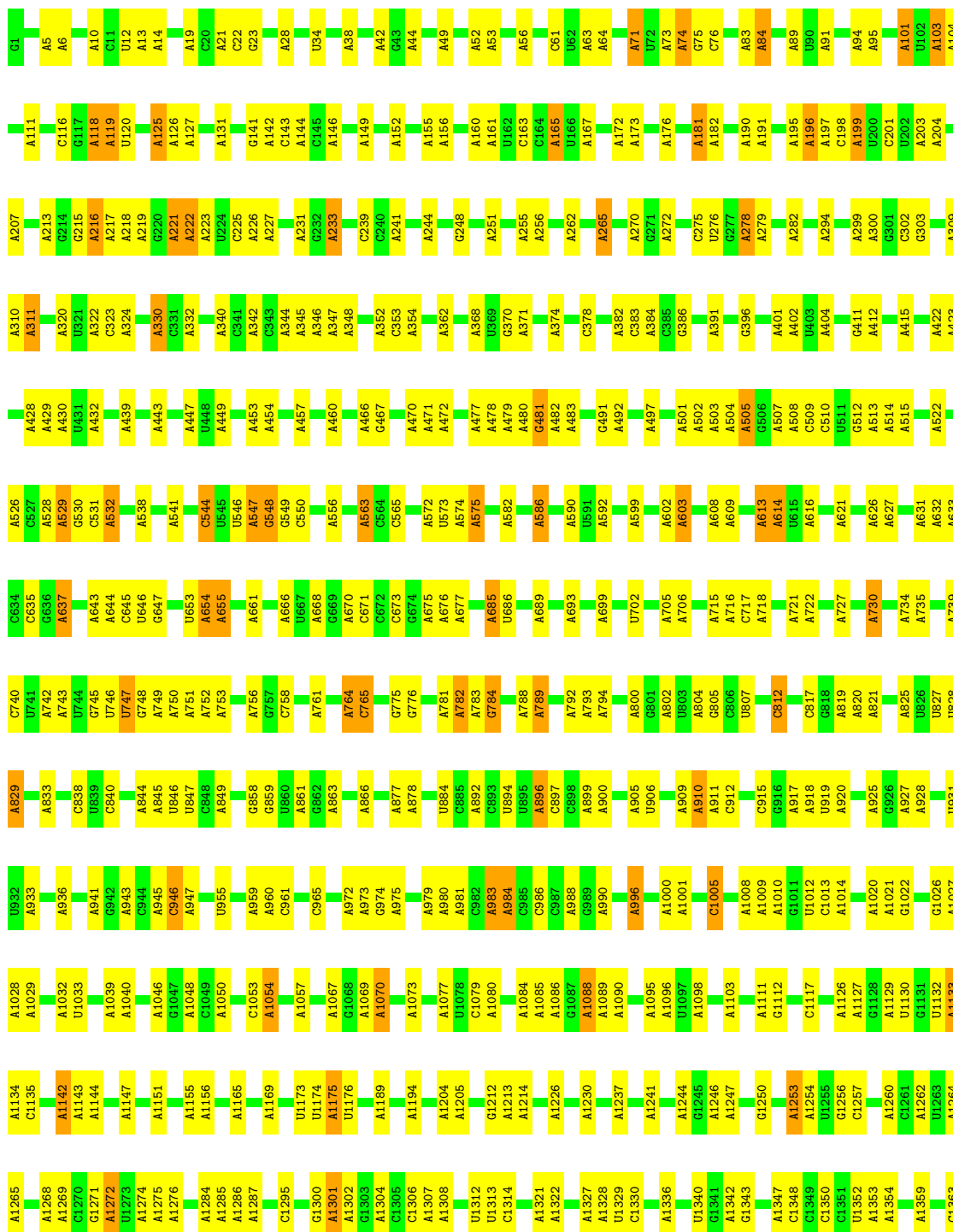
- Molecule 21: 30S ribosomal protein S21

Chain S211: 75% . 21%



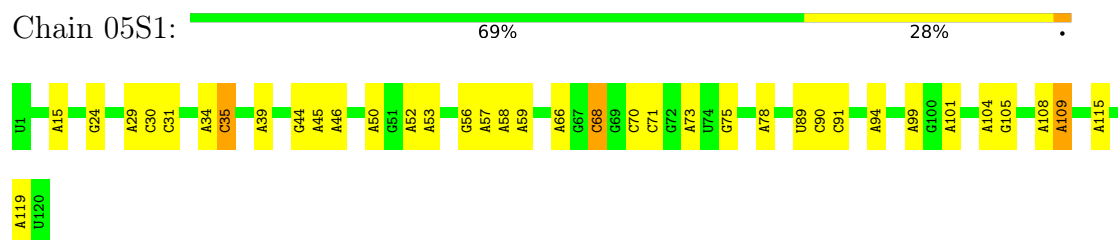
- Molecule 22: 23S rRNA

Chain 23S1:  63% 31% 5%



| | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| A2837 | A2733 | U2613 | A2503 | U2305 | U2182 | G2100 | A2013 | A1913 | G1792 | G1699 | C1607 | A1496 | G1364 |
| A2850 | A2734 | A2614 | U2504 | C2306 | A2183 | A2101 | A2015 | C1914 | C1793 | A1700 | A1608 | A1496 | A1365 |
| A2851 | G2735 | U2615 | G2505 | G2307 | A2184 | C2104 | A2016 | A1916 | A1794 | A1701 | A1609 | A1502 | A1366 |
| A2856 | A2736 | C2616 | C2510 | G2308 | U2189 | U2109 | A2019 | U1917 | C1800 | A1705 | C1611 | A1503 | A1367 |
| A2860 | G2737 | U2629 | A2513 | C2310 | G2190 | A2108 | A2020 | A1918 | A1801 | A1711 | A1614 | A1505 | A1373 |
| U2861 | A2738 | A2632 | A2516 | A2311 | U2191 | U2110 | A2023 | A1919 | A1802 | U1712 | C1615 | A1508 | C1376 |
| A2868 | U2739 | G2633 | C2517 | A2314 | U2195 | G2111 | C2023 | U1927 | C1804 | U1713 | A1616 | A1509 | G1377 |
| G2869 | A2740 | A2634 | A2518 | A2317 | U2198 | U2112 | G2027 | A1928 | A1805 | A1717 | C1617 | A1515 | U1379 |
| U2870 | G2741 | C2635 | A2529 | A2321 | A2198 | U2113 | A2030 | A1929 | A1808 | A1722 | A1626 | A1522 | A1383 |
| A2873 | A2742 | U2636 | A2530 | A2322 | A2199 | U2114 | A2031 | G1930 | A1809 | A1729 | A1630 | A1525 | A1384 |
| A2879 | U2743 | A2637 | A2531 | G2325 | G2204 | G2115 | G2032 | U1931 | A1803 | C1730 | G1632 | A1528 | C1386 |
| C2880 | A2744 | A2638 | A2534 | C2326 | A2205 | A2116 | A2033 | A1932 | A1804 | C1731 | A1634 | A1532 | A1387 |
| U2881 | G2745 | U2639 | A2541 | A2327 | A2211 | U2118 | A2037 | A1936 | A1815 | C1732 | G1633 | A1535 | A1392 |
| U2882 | A2746 | A2640 | A2542 | A2328 | A2212 | A2119 | A2042 | A1938 | C1816 | A1735 | A1635 | A1539 | A1393 |
| U2883 | A2747 | U2641 | A2547 | A2335 | A2225 | G2125 | C2044 | U1939 | U1820 | A1744 | U1636 | A1544 | U1394 |
| U2884 | U2748 | C2642 | A2552 | A2336 | C2226 | G2126 | A2051 | A1952 | A1821 | G1738 | A1637 | A1545 | A1395 |
| A2885 | A2749 | A2643 | U2553 | A2337 | A2227 | A2127 | A2052 | A1953 | C1822 | A1739 | A1640 | A1553 | C1398 |
| A2886 | A2750 | U2644 | A2560 | A2338 | G2238 | G2128 | G2053 | U1955 | A1829 | A1744 | A1641 | A1548 | A1403 |
| A2887 | G2751 | C2645 | A2561 | G2239 | U2240 | U2131 | A2054 | A1960 | G1835 | A1745 | C1644 | A1549 | A1413 |
| U2891 | A2752 | U2646 | U2562 | U2241 | G2242 | U2132 | C2055 | C1962 | C1836 | A1746 | U1647 | C1550 | A1416 |
| A2893 | A2753 | A2647 | A2563 | A2242 | U2243 | A2133 | G2056 | U1967 | A1847 | A1749 | U1648 | A1551 | A1427 |
| A2899 | U2754 | U2648 | A2564 | A2243 | U2244 | A2134 | A2058 | A1969 | A1848 | A1754 | G1649 | A1552 | C1428 |
| A2900 | A2755 | A2649 | A2565 | U2245 | A2247 | G2136 | A2059 | C1966 | A1853 | A1755 | A1650 | A1571 | A1431 |
| U2903 | A2756 | U2650 | A2566 | A2246 | G2251 | U2137 | G2060 | U1967 | G1756 | A1757 | G1651 | A1572 | A1437 |
| A2894 | A2757 | A2651 | A2567 | C2247 | G2252 | A2142 | A2061 | A1970 | A1854 | U1758 | G1652 | A1586 | U1438 |
| A2895 | U2758 | C2448 | A2572 | A2248 | C2260 | C2146 | C2062 | U1971 | A1858 | A1759 | A1654 | A1590 | A1439 |
| A2896 | A2759 | U2651 | C2573 | A2249 | A2261 | A2147 | C2063 | G1972 | A1866 | A1762 | C1658 | A1586 | G1452 |
| A2897 | U2760 | A2652 | A2577 | A2250 | A2266 | C2150 | A2070 | A1977 | A1871 | C1764 | A1664 | A1580 | A1433 |
| U2898 | A2761 | U2653 | G2578 | A2251 | A2267 | A2154 | C2071 | A1978 | G1872 | A1772 | A1665 | A1579 | A1434 |
| A2899 | A2762 | C2654 | U2580 | G2268 | A2268 | G2157 | C2072 | A1981 | C1873 | A1773 | A1668 | A1583 | U1437 |
| A2900 | U2763 | A2655 | C2368 | U2270 | A2273 | A2158 | C2073 | C1985 | G1874 | C1774 | A1669 | U1584 | A1439 |
| U2903 | A2764 | U2656 | A2369 | A2271 | A2274 | G2159 | A2077 | C1986 | A1875 | U1775 | A1670 | A1586 | G1452 |
| A2891 | A2765 | A2657 | A2376 | A2272 | A2275 | C2162 | A2080 | A1987 | A1876 | A1779 | U1671 | A1586 | A1453 |
| A2892 | U2766 | U2658 | A2377 | A2276 | A2278 | A2163 | A2082 | U1991 | A1885 | A1780 | G1672 | A1590 | A1469 |
| A2893 | A2767 | A2659 | A2378 | A2279 | A2281 | C2164 | A2088 | G1992 | A1889 | U1781 | G1673 | A1591 | A1470 |
| A2894 | U2768 | U2660 | A2381 | A2282 | G2282 | C2165 | C2089 | U1993 | A1890 | A1782 | A1674 | C1592 | A1477 |
| A2895 | A2769 | A2661 | U2382 | A2283 | U2284 | A2169 | A2090 | C1997 | A1899 | U1783 | A1675 | A1593 | A1482 |
| A2896 | U2770 | C2662 | C2383 | A2284 | A2285 | A2170 | G2093 | A1998 | A1899 | A1784 | A1676 | A1596 | A1490 |
| A2897 | A2771 | U2663 | A2384 | A2286 | A2287 | U2171 | A2094 | A2003 | A1901 | A1785 | A1677 | A1597 | A1494 |
| A2898 | U2772 | A2664 | U2385 | A2288 | A2289 | U2172 | A2095 | G2004 | G1906 | A1786 | A1678 | A1598 | A1495 |
| A2899 | A2773 | U2665 | A2386 | A2290 | A2291 | A2173 | C2096 | A2005 | U1911 | A1787 | A1679 | A1603 | |
| A2900 | U2774 | C2666 | A2387 | A2292 | A2293 | C2174 | U2097 | A2006 | C1788 | A1788 | A1689 | C1606 | |
| U2903 | A2775 | U2667 | A2388 | A2294 | A2295 | A2175 | U2098 | C2007 | C1789 | A1789 | A1690 | | |
| | A2776 | U2668 | A2389 | A2296 | A2297 | A2176 | U2099 | A2009 | A1912 | A1791 | A1698 | | |

- Molecule 23: 5S rRNA



- Molecule 24: 50S ribosomal protein L2



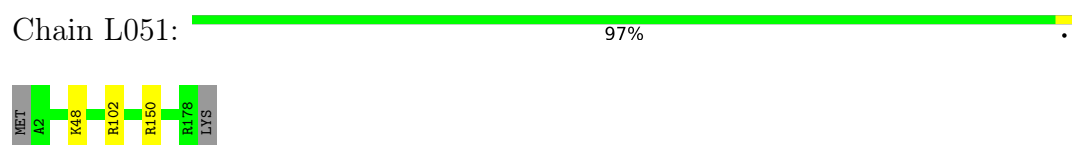
- Molecule 25: 50S ribosomal protein L3



- Molecule 26: 50S ribosomal protein L4



- Molecule 27: 50S ribosomal protein L5

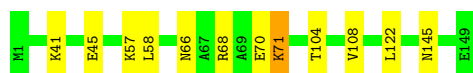


- Molecule 28: 50S ribosomal protein L6



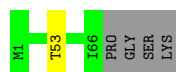
- Molecule 29: 50S ribosomal protein L9





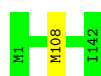
- Molecule 30: 50S ribosomal protein L31

Chain L311: 93% 6%



- Molecule 31: 50S ribosomal protein L13

Chain L131: 99%



- Molecule 32: 50S ribosomal protein L14

Chain L141: 100%

There are no outlier residues recorded for this chain.

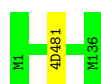
- Molecule 33: 50S ribosomal protein L15

Chain L151: 98%



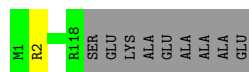
- Molecule 34: 50S ribosomal protein L16

Chain L161: 99%



- Molecule 35: 50S ribosomal protein L17

Chain L171: 92% 7%



- Molecule 36: 50S ribosomal protein L18

Chain L181: 100%

There are no outlier residues recorded for this chain.

- Molecule 37: 50S ribosomal protein L19

Chain L191:  99% .



- Molecule 38: 50S ribosomal protein L20

Chain L201:  98% ..



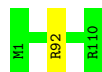
- Molecule 39: 50S ribosomal protein L21

Chain L211:  100%

There are no outlier residues recorded for this chain.

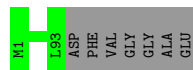
- Molecule 40: 50S ribosomal protein L22

Chain L221:  99% .



- Molecule 41: 50S ribosomal protein L23

Chain L231:  93% 7%



- Molecule 42: 50S ribosomal protein L24

Chain L241:  97% ..



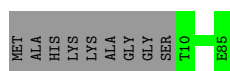
- Molecule 43: 50S ribosomal protein L25

Chain L251:  100%

There are no outlier residues recorded for this chain.

- Molecule 44: 50S ribosomal protein L27

Chain L271:  89% 11%



- Molecule 45: 50S ribosomal protein L28

Chain L281: 96% ..



- Molecule 46: 50S ribosomal protein L29

Chain L291: 98% .



- Molecule 47: 50S ribosomal protein L30

Chain L301: 98% .



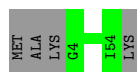
- Molecule 48: 50S ribosomal protein L32

Chain L321: 96% ..



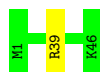
- Molecule 49: 50S ribosomal protein L33

Chain L331: 93% 7%



- Molecule 50: 50S ribosomal protein L34

Chain L341: 98% .



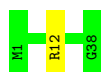
- Molecule 51: 50S ribosomal protein L35

Chain L351: 95% ..



- Molecule 52: 50S ribosomal protein L36

Chain L361: 97%



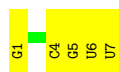
- Molecule 53: SpeFL

Chain SPE1: 88%



- Molecule 54: mRNA

Chain MRN1: 29%



- Molecule 55: P-site Arg-tRNA

Chain PTR1: 58%



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 68195 | 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 ($e^-/\text{\AA}^2$) | 30 | Depositor |
| Minimum defocus (nm) | -500 | Depositor |
| Maximum defocus (nm) | -1600 | Depositor |
| Magnification | 130000 | Depositor |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 4D4, OMU, UR3, D2T, OMG, K, MG, ZN, MEQ, RSP, G7M, 5MC, UNX, MA6, 2MA, ORN, 6MZ, OMC, 4SU, 5MU, 2MG, 3TD, 1MG, 4OC, FME, PSU

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 | 16S1 | 1.50 | 1056/36593 (2.9%) | 3.49 | 4371/57081 (7.7%) |
| 2 | S021 | 0.67 | 0/1784 | 0.69 | 2/2403 (0.1%) |
| 3 | S031 | 0.80 | 0/1651 | 0.63 | 0/2225 |
| 4 | S041 | 0.82 | 0/1665 | 0.54 | 0/2227 |
| 5 | S051 | 0.74 | 0/1157 | 0.67 | 1/1557 (0.1%) |
| 6 | S061 | 0.71 | 0/881 | 0.61 | 1/1189 (0.1%) |
| 7 | S071 | 0.87 | 0/1195 | 0.70 | 1/1602 (0.1%) |
| 8 | S081 | 0.70 | 0/989 | 0.54 | 0/1326 |
| 9 | S091 | 0.97 | 0/1034 | 0.82 | 3/1375 (0.2%) |
| 10 | S101 | 0.95 | 1/805 (0.1%) | 0.90 | 5/1089 (0.5%) |
| 11 | S111 | 0.81 | 0/893 | 0.58 | 0/1205 |
| 12 | S121 | 0.89 | 0/960 | 0.65 | 1/1286 (0.1%) |
| 13 | S131 | 0.92 | 0/892 | 0.84 | 3/1193 (0.3%) |
| 14 | S141 | 0.91 | 0/811 | 0.67 | 0/1081 |
| 15 | S151 | 0.87 | 0/722 | 0.53 | 1/964 (0.1%) |
| 16 | S161 | 0.87 | 0/659 | 0.67 | 1/884 (0.1%) |
| 17 | S171 | 0.76 | 0/657 | 0.57 | 0/881 |
| 18 | S181 | 0.88 | 0/462 | 0.49 | 0/621 |
| 19 | S191 | 0.83 | 0/672 | 0.75 | 1/904 (0.1%) |
| 20 | S201 | 0.74 | 0/676 | 0.56 | 0/895 |
| 21 | S211 | 1.02 | 0/472 | 0.78 | 3/627 (0.5%) |
| 22 | 23S1 | 1.58 | 1959/69120 (2.8%) | 3.57 | 8521/107824 (7.9%) |
| 23 | 05S1 | 1.36 | 69/2872 (2.4%) | 3.12 | 276/4478 (6.2%) |
| 24 | L021 | 0.85 | 0/2121 | 0.60 | 0/2852 |
| 25 | L031 | 0.70 | 0/1576 | 0.55 | 0/2119 |
| 26 | L041 | 0.71 | 0/1571 | 0.57 | 0/2113 |
| 27 | L051 | 0.78 | 0/1434 | 0.67 | 0/1926 |
| 28 | L061 | 0.68 | 0/1343 | 0.64 | 0/1816 |
| 29 | L091 | 0.71 | 0/1121 | 1.05 | 6/1515 (0.4%) |
| 30 | L311 | 0.79 | 0/531 | 0.91 | 0/709 |
| 31 | L131 | 0.76 | 1/1152 (0.1%) | 0.52 | 0/1551 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|--------------------|-------------|---------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 32 | L141 | 0.84 | 0/955 | 0.61 | 0/1279 |
| 33 | L151 | 0.82 | 0/1062 | 0.60 | 0/1413 |
| 34 | L161 | 0.80 | 0/1081 | 0.55 | 0/1443 |
| 35 | L171 | 0.95 | 0/958 | 0.61 | 0/1281 |
| 36 | L181 | 0.84 | 0/910 | 0.54 | 0/1219 |
| 37 | L191 | 0.85 | 0/929 | 0.58 | 0/1242 |
| 38 | L201 | 0.92 | 0/960 | 0.49 | 0/1278 |
| 39 | L211 | 0.75 | 0/829 | 0.61 | 0/1107 |
| 40 | L221 | 0.80 | 0/864 | 0.54 | 0/1156 |
| 41 | L231 | 0.75 | 0/744 | 0.63 | 0/994 |
| 42 | L241 | 0.67 | 0/787 | 0.56 | 1/1051 (0.1%) |
| 43 | L251 | 0.66 | 0/766 | 0.51 | 0/1025 |
| 44 | L271 | 0.84 | 0/587 | 0.50 | 0/776 |
| 45 | L281 | 0.92 | 0/635 | 0.53 | 0/848 |
| 46 | L291 | 0.76 | 0/502 | 0.51 | 0/667 |
| 47 | L301 | 0.83 | 0/453 | 0.56 | 0/605 |
| 48 | L321 | 0.90 | 0/450 | 0.69 | 1/599 (0.2%) |
| 49 | L331 | 0.65 | 0/421 | 0.62 | 0/561 |
| 50 | L341 | 1.14 | 0/380 | 0.65 | 0/498 |
| 51 | L351 | 0.78 | 0/513 | 0.64 | 0/676 |
| 52 | L361 | 0.91 | 0/303 | 0.62 | 0/397 |
| 53 | SPE1 | 0.93 | 0/299 | 0.69 | 0/399 |
| 54 | MRN1 | 0.77 | 0/161 | 1.39 | 1/248 (0.4%) |
| 55 | PTR1 | 1.66 | 56/1672 (3.3%) | 3.19 | 171/2598 (6.6%) |
| All | All | 1.37 | 3142/155692 (2.0%) | 3.05 | 13371/232878 (5.7%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2 | S021 | 0 | 2 |
| 3 | S031 | 0 | 1 |
| 10 | S101 | 0 | 5 |
| 13 | S131 | 0 | 3 |
| 19 | S191 | 0 | 3 |
| 26 | L041 | 0 | 1 |
| 29 | L091 | 0 | 5 |
| 30 | L311 | 0 | 1 |
| 33 | L151 | 0 | 1 |
| 51 | L351 | 0 | 1 |
| All | All | 0 | 23 |

All (3142) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 55 | PTR1 | 20 | U | C5-C6 | 23.29 | 1.55 | 1.34 |
| 55 | PTR1 | 17 | U | C5-C6 | 22.31 | 1.54 | 1.34 |
| 22 | 23S1 | 2449 | U | C5-C6 | 21.06 | 1.53 | 1.34 |
| 55 | PTR1 | 17 | U | N1-C6 | 10.30 | 1.47 | 1.38 |
| 55 | PTR1 | 20 | U | N1-C6 | 10.08 | 1.47 | 1.38 |
| 22 | 23S1 | 2451 | A | C8-N7 | 9.55 | 1.38 | 1.31 |
| 1 | 16S1 | 412 | A | C8-N7 | 9.46 | 1.38 | 1.31 |
| 55 | PTR1 | 20 | U | C4-C5 | 9.19 | 1.51 | 1.43 |
| 1 | 16S1 | 152 | A | C8-N7 | 8.43 | 1.37 | 1.31 |
| 22 | 23S1 | 2449 | U | N1-C6 | 8.32 | 1.45 | 1.38 |
| 22 | 23S1 | 2101 | A | C8-N7 | 8.19 | 1.37 | 1.31 |
| 22 | 23S1 | 2566 | A | C5-C4 | -8.12 | 1.33 | 1.38 |
| 1 | 16S1 | 431 | A | C8-N7 | 8.08 | 1.37 | 1.31 |
| 22 | 23S1 | 2872 | A | C8-N7 | 8.07 | 1.37 | 1.31 |
| 22 | 23S1 | 142 | A | C5-C4 | -8.05 | 1.33 | 1.38 |
| 22 | 23S1 | 1583 | A | C8-N7 | 8.05 | 1.37 | 1.31 |
| 22 | 23S1 | 1028 | A | C5-C4 | -8.05 | 1.33 | 1.38 |
| 55 | PTR1 | 20 | U | C2-N3 | 8.05 | 1.43 | 1.37 |
| 55 | PTR1 | 51 | A | C8-N7 | 8.04 | 1.37 | 1.31 |
| 22 | 23S1 | 142 | A | N3-C4 | 7.92 | 1.39 | 1.34 |
| 22 | 23S1 | 1434 | A | C8-N7 | 7.88 | 1.37 | 1.31 |
| 22 | 23S1 | 1090 | A | C8-N7 | 7.87 | 1.37 | 1.31 |
| 22 | 23S1 | 195 | A | C8-N7 | 7.83 | 1.37 | 1.31 |
| 22 | 23S1 | 547 | A | C8-N7 | 7.80 | 1.37 | 1.31 |
| 22 | 23S1 | 1095 | A | C8-N7 | 7.78 | 1.36 | 1.31 |
| 22 | 23S1 | 508 | A | C8-N7 | 7.76 | 1.36 | 1.31 |
| 1 | 16S1 | 554 | A | C8-N7 | 7.72 | 1.36 | 1.31 |
| 1 | 16S1 | 978 | A | C8-N7 | 7.72 | 1.36 | 1.31 |
| 1 | 16S1 | 845 | A | C8-N7 | 7.72 | 1.36 | 1.31 |
| 22 | 23S1 | 2602 | A | C8-N7 | 7.71 | 1.36 | 1.31 |
| 22 | 23S1 | 161 | A | C8-N7 | 7.70 | 1.36 | 1.31 |
| 22 | 23S1 | 2154 | A | C8-N7 | 7.69 | 1.36 | 1.31 |
| 22 | 23S1 | 2741 | A | C5-C4 | -7.67 | 1.33 | 1.38 |
| 1 | 16S1 | 1493 | A | C8-N7 | 7.67 | 1.36 | 1.31 |
| 22 | 23S1 | 1077 | A | C8-N7 | 7.65 | 1.36 | 1.31 |
| 22 | 23S1 | 2572 | A | C5-C4 | -7.65 | 1.33 | 1.38 |
| 22 | 23S1 | 2837 | A | C5-C4 | -7.65 | 1.33 | 1.38 |
| 22 | 23S1 | 354 | A | C8-N7 | 7.64 | 1.36 | 1.31 |
| 22 | 23S1 | 2211 | A | C8-N7 | 7.64 | 1.36 | 1.31 |
| 22 | 23S1 | 1535 | A | C8-N7 | 7.63 | 1.36 | 1.31 |
| 22 | 23S1 | 2183 | A | C8-N7 | 7.62 | 1.36 | 1.31 |
| 55 | PTR1 | 34 | I | N3-C4 | 7.61 | 1.51 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 1046 | A | C8-N7 | 7.61 | 1.36 | 1.31 |
| 1 | 16S1 | 414 | A | C8-N7 | 7.60 | 1.36 | 1.31 |
| 22 | 23S1 | 84 | A | C8-N7 | 7.60 | 1.36 | 1.31 |
| 22 | 23S1 | 2147 | A | C8-N7 | 7.56 | 1.36 | 1.31 |
| 22 | 23S1 | 1419 | A | C8-N7 | 7.55 | 1.36 | 1.31 |
| 55 | PTR1 | 17 | U | C2-N3 | 7.55 | 1.43 | 1.37 |
| 22 | 23S1 | 2184 | A | C8-N7 | 7.53 | 1.36 | 1.31 |
| 22 | 23S1 | 1069 | A | C8-N7 | 7.53 | 1.36 | 1.31 |
| 22 | 23S1 | 1966 | A | C5-C4 | -7.52 | 1.33 | 1.38 |
| 1 | 16S1 | 74 | A | C8-N7 | 7.52 | 1.36 | 1.31 |
| 22 | 23S1 | 582 | A | C5-C4 | -7.52 | 1.33 | 1.38 |
| 22 | 23S1 | 1810 | A | N7-C5 | -7.51 | 1.34 | 1.39 |
| 1 | 16S1 | 478 | A | N3-C4 | 7.51 | 1.39 | 1.34 |
| 1 | 16S1 | 1441 | A | C8-N7 | 7.49 | 1.36 | 1.31 |
| 55 | PTR1 | 58 | A | C8-N7 | 7.49 | 1.36 | 1.31 |
| 1 | 16S1 | 815 | A | C5-C4 | -7.49 | 1.33 | 1.38 |
| 22 | 23S1 | 1057 | A | C8-N7 | 7.49 | 1.36 | 1.31 |
| 1 | 16S1 | 151 | A | C8-N7 | 7.48 | 1.36 | 1.31 |
| 1 | 16S1 | 1005 | A | C8-N7 | 7.48 | 1.36 | 1.31 |
| 22 | 23S1 | 574 | A | C5-C4 | -7.47 | 1.33 | 1.38 |
| 22 | 23S1 | 1080 | A | C8-N7 | 7.47 | 1.36 | 1.31 |
| 22 | 23S1 | 1096 | A | C8-N7 | 7.47 | 1.36 | 1.31 |
| 22 | 23S1 | 2173 | A | C8-N7 | 7.47 | 1.36 | 1.31 |
| 1 | 16S1 | 1213 | A | C8-N7 | 7.46 | 1.36 | 1.31 |
| 1 | 16S1 | 583 | A | C8-N7 | 7.46 | 1.36 | 1.31 |
| 22 | 23S1 | 282 | A | C8-N7 | 7.44 | 1.36 | 1.31 |
| 1 | 16S1 | 1035 | A | C8-N7 | 7.44 | 1.36 | 1.31 |
| 22 | 23S1 | 586 | A | C5-C4 | -7.44 | 1.33 | 1.38 |
| 22 | 23S1 | 821 | A | C5-C4 | -7.43 | 1.33 | 1.38 |
| 55 | PTR1 | 17 | U | C4-C5 | 7.43 | 1.50 | 1.43 |
| 22 | 23S1 | 119 | A | C8-N7 | 7.42 | 1.36 | 1.31 |
| 22 | 23S1 | 896 | A | C8-N7 | 7.42 | 1.36 | 1.31 |
| 1 | 16S1 | 716 | A | C5-C4 | -7.41 | 1.33 | 1.38 |
| 22 | 23S1 | 1871 | A | C8-N7 | 7.41 | 1.36 | 1.31 |
| 1 | 16S1 | 1239 | A | C8-N7 | 7.41 | 1.36 | 1.31 |
| 22 | 23S1 | 878 | A | C8-N7 | 7.41 | 1.36 | 1.31 |
| 22 | 23S1 | 2449 | U | C4-C5 | 7.41 | 1.50 | 1.43 |
| 55 | PTR1 | 23 | A | C8-N7 | 7.40 | 1.36 | 1.31 |
| 22 | 23S1 | 1144 | A | C5-C4 | -7.40 | 1.33 | 1.38 |
| 22 | 23S1 | 1509 | A | C8-N7 | 7.40 | 1.36 | 1.31 |
| 22 | 23S1 | 507 | A | C8-N7 | 7.40 | 1.36 | 1.31 |
| 22 | 23S1 | 2826 | A | C5-C4 | -7.39 | 1.33 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 2117 | A | C8-N7 | 7.39 | 1.36 | 1.31 |
| 22 | 23S1 | 10 | A | C8-N7 | 7.37 | 1.36 | 1.31 |
| 22 | 23S1 | 504 | A | C8-N7 | 7.37 | 1.36 | 1.31 |
| 22 | 23S1 | 1515 | A | C8-N7 | 7.37 | 1.36 | 1.31 |
| 22 | 23S1 | 207 | A | C5-C4 | -7.37 | 1.33 | 1.38 |
| 22 | 23S1 | 165 | A | C8-N7 | 7.36 | 1.36 | 1.31 |
| 1 | 16S1 | 16 | A | C5-C4 | -7.35 | 1.33 | 1.38 |
| 1 | 16S1 | 116 | A | C5-C4 | -7.35 | 1.33 | 1.38 |
| 1 | 16S1 | 1257 | A | C8-N7 | 7.35 | 1.36 | 1.31 |
| 22 | 23S1 | 1175 | A | C8-N7 | 7.35 | 1.36 | 1.31 |
| 22 | 23S1 | 2820 | A | C8-N7 | 7.35 | 1.36 | 1.31 |
| 22 | 23S1 | 613 | A | N3-C4 | 7.35 | 1.39 | 1.34 |
| 22 | 23S1 | 2020 | A | C5-C4 | -7.35 | 1.33 | 1.38 |
| 22 | 23S1 | 2134 | A | C8-N7 | 7.35 | 1.36 | 1.31 |
| 22 | 23S1 | 2170 | A | C8-N7 | 7.33 | 1.36 | 1.31 |
| 1 | 16S1 | 468 | A | C8-N7 | 7.33 | 1.36 | 1.31 |
| 22 | 23S1 | 1089 | A | C8-N7 | 7.33 | 1.36 | 1.31 |
| 22 | 23S1 | 2163 | A | N3-C4 | 7.32 | 1.39 | 1.34 |
| 22 | 23S1 | 1070 | A | C8-N7 | 7.31 | 1.36 | 1.31 |
| 22 | 23S1 | 563 | A | C5-C4 | -7.30 | 1.33 | 1.38 |
| 55 | PTR1 | 38 | A | C5-C4 | -7.30 | 1.33 | 1.38 |
| 22 | 23S1 | 693 | A | C5-C4 | -7.29 | 1.33 | 1.38 |
| 22 | 23S1 | 877 | A | C8-N7 | 7.29 | 1.36 | 1.31 |
| 1 | 16S1 | 179 | A | C8-N7 | 7.28 | 1.36 | 1.31 |
| 22 | 23S1 | 1952 | A | C5-C4 | -7.28 | 1.33 | 1.38 |
| 22 | 23S1 | 1650 | A | C5-C4 | -7.27 | 1.33 | 1.38 |
| 22 | 23S1 | 2158 | A | N3-C4 | 7.27 | 1.39 | 1.34 |
| 1 | 16S1 | 996 | A | C8-N7 | 7.27 | 1.36 | 1.31 |
| 22 | 23S1 | 1395 | A | C8-N7 | 7.26 | 1.36 | 1.31 |
| 1 | 16S1 | 300 | A | N7-C5 | -7.25 | 1.34 | 1.39 |
| 22 | 23S1 | 1175 | A | N3-C4 | 7.25 | 1.39 | 1.34 |
| 1 | 16S1 | 782 | A | C5-C4 | -7.24 | 1.33 | 1.38 |
| 22 | 23S1 | 2108 | A | C8-N7 | 7.23 | 1.36 | 1.31 |
| 1 | 16S1 | 1101 | A | C8-N7 | 7.23 | 1.36 | 1.31 |
| 1 | 16S1 | 1 | A | C8-N7 | 7.22 | 1.36 | 1.31 |
| 1 | 16S1 | 279 | A | C8-N7 | 7.22 | 1.36 | 1.31 |
| 22 | 23S1 | 845 | A | N3-C4 | 7.21 | 1.39 | 1.34 |
| 22 | 23S1 | 2163 | A | C8-N7 | 7.21 | 1.36 | 1.31 |
| 22 | 23S1 | 1570 | A | C5-C4 | -7.20 | 1.33 | 1.38 |
| 1 | 16S1 | 1145 | A | C8-N7 | 7.20 | 1.36 | 1.31 |
| 22 | 23S1 | 1354 | A | C5-C4 | -7.20 | 1.33 | 1.38 |
| 22 | 23S1 | 1420 | A | C8-N7 | 7.20 | 1.36 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 16S1 | 456 | A | C8-N7 | 7.19 | 1.36 | 1.31 |
| 22 | 23S1 | 2095 | A | C8-N7 | 7.19 | 1.36 | 1.31 |
| 22 | 23S1 | 2682 | A | C5-C4 | -7.19 | 1.33 | 1.38 |
| 1 | 16S1 | 167 | A | C8-N7 | 7.19 | 1.36 | 1.31 |
| 22 | 23S1 | 1809 | A | C5-C4 | -7.19 | 1.33 | 1.38 |
| 1 | 16S1 | 1150 | A | C8-N7 | 7.19 | 1.36 | 1.31 |
| 22 | 23S1 | 1088 | A | C8-N7 | 7.18 | 1.36 | 1.31 |
| 1 | 16S1 | 704 | A | C8-N7 | 7.18 | 1.36 | 1.31 |
| 22 | 23S1 | 1503 | A | C8-N7 | 7.18 | 1.36 | 1.31 |
| 23 | 05S1 | 66 | A | C8-N7 | 7.18 | 1.36 | 1.31 |
| 1 | 16S1 | 461 | A | C8-N7 | 7.17 | 1.36 | 1.31 |
| 1 | 16S1 | 1044 | A | C8-N7 | 7.17 | 1.36 | 1.31 |
| 22 | 23S1 | 514 | A | C5-C4 | -7.17 | 1.33 | 1.38 |
| 22 | 23S1 | 2750 | A | C8-N7 | 7.17 | 1.36 | 1.31 |
| 1 | 16S1 | 195 | A | C8-N7 | 7.17 | 1.36 | 1.31 |
| 22 | 23S1 | 515 | A | C5-C4 | -7.17 | 1.33 | 1.38 |
| 1 | 16S1 | 553 | A | C5-C4 | -7.17 | 1.33 | 1.38 |
| 22 | 23S1 | 1532 | A | C8-N7 | 7.17 | 1.36 | 1.31 |
| 22 | 23S1 | 2090 | A | C5-C4 | -7.17 | 1.33 | 1.38 |
| 1 | 16S1 | 435 | A | C8-N7 | 7.16 | 1.36 | 1.31 |
| 22 | 23S1 | 1067 | A | C8-N7 | 7.16 | 1.36 | 1.31 |
| 22 | 23S1 | 125 | A | C8-N7 | 7.16 | 1.36 | 1.31 |
| 1 | 16S1 | 274 | A | C8-N7 | 7.15 | 1.36 | 1.31 |
| 1 | 16S1 | 1216 | A | C8-N7 | 7.15 | 1.36 | 1.31 |
| 22 | 23S1 | 2173 | A | N3-C4 | 7.14 | 1.39 | 1.34 |
| 22 | 23S1 | 2031 | A | C5-C4 | -7.14 | 1.33 | 1.38 |
| 1 | 16S1 | 1092 | A | C8-N7 | 7.13 | 1.36 | 1.31 |
| 22 | 23S1 | 1571 | A | C5-C4 | -7.13 | 1.33 | 1.38 |
| 22 | 23S1 | 825 | A | C5-C4 | -7.13 | 1.33 | 1.38 |
| 22 | 23S1 | 1505 | A | C8-N7 | 7.13 | 1.36 | 1.31 |
| 55 | PTR1 | 59 | A | C8-N7 | 7.13 | 1.36 | 1.31 |
| 22 | 23S1 | 802 | A | C5-C4 | -7.12 | 1.33 | 1.38 |
| 55 | PTR1 | 3 | A | C8-N7 | 7.12 | 1.36 | 1.31 |
| 1 | 16S1 | 19 | A | C5-C4 | -7.12 | 1.33 | 1.38 |
| 1 | 16S1 | 81 | A | C8-N7 | 7.12 | 1.36 | 1.31 |
| 22 | 23S1 | 2013 | A | C5-C4 | -7.11 | 1.33 | 1.38 |
| 22 | 23S1 | 1073 | A | C8-N7 | 7.09 | 1.36 | 1.31 |
| 22 | 23S1 | 2497 | A | C5-C4 | -7.09 | 1.33 | 1.38 |
| 23 | 05S1 | 29 | A | C8-N7 | 7.09 | 1.36 | 1.31 |
| 22 | 23S1 | 792 | A | C5-C4 | -7.09 | 1.33 | 1.38 |
| 1 | 16S1 | 1447 | A | C8-N7 | 7.08 | 1.36 | 1.31 |
| 22 | 23S1 | 892 | A | C8-N7 | 7.08 | 1.36 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 352 | A | C8-N7 | 7.08 | 1.36 | 1.31 |
| 22 | 23S1 | 1676 | A | C5-C4 | -7.08 | 1.33 | 1.38 |
| 22 | 23S1 | 1789 | A | C5-C4 | -7.08 | 1.33 | 1.38 |
| 1 | 16S1 | 816 | A | C5-C4 | -7.08 | 1.33 | 1.38 |
| 1 | 16S1 | 131 | A | C8-N7 | 7.07 | 1.36 | 1.31 |
| 22 | 23S1 | 2758 | A | C8-N7 | 7.07 | 1.36 | 1.31 |
| 23 | 05S1 | 119 | A | C8-N7 | 7.07 | 1.36 | 1.31 |
| 1 | 16S1 | 411 | A | C8-N7 | 7.07 | 1.36 | 1.31 |
| 22 | 23S1 | 457 | A | C5-C4 | -7.07 | 1.33 | 1.38 |
| 22 | 23S1 | 1383 | A | C8-N7 | 7.07 | 1.36 | 1.31 |
| 1 | 16S1 | 129 | A | C8-N7 | 7.07 | 1.36 | 1.31 |
| 22 | 23S1 | 1237 | A | C5-C4 | -7.06 | 1.33 | 1.38 |
| 22 | 23S1 | 1264 | A | C5-C4 | -7.06 | 1.33 | 1.38 |
| 1 | 16S1 | 466 | A | C8-N7 | 7.06 | 1.36 | 1.31 |
| 22 | 23S1 | 1286 | A | C5-C4 | -7.06 | 1.33 | 1.38 |
| 1 | 16S1 | 197 | A | C8-N7 | 7.05 | 1.36 | 1.31 |
| 22 | 23S1 | 936 | A | C5-C4 | -7.05 | 1.33 | 1.38 |
| 1 | 16S1 | 749 | A | C8-N7 | 7.05 | 1.36 | 1.31 |
| 22 | 23S1 | 428 | A | C5-C4 | -7.05 | 1.33 | 1.38 |
| 23 | 05S1 | 57 | A | C8-N7 | 7.05 | 1.36 | 1.31 |
| 22 | 23S1 | 2740 | A | C5-C4 | -7.05 | 1.33 | 1.38 |
| 55 | PTR1 | 34 | I | C5-C6 | 7.05 | 1.53 | 1.39 |
| 1 | 16S1 | 1534 | A | C8-N7 | 7.04 | 1.36 | 1.31 |
| 22 | 23S1 | 1655 | A | C5-C4 | -7.04 | 1.33 | 1.38 |
| 22 | 23S1 | 1000 | A | C5-C4 | -7.04 | 1.33 | 1.38 |
| 1 | 16S1 | 465 | A | C8-N7 | 7.03 | 1.36 | 1.31 |
| 22 | 23S1 | 1268 | A | C5-C4 | -7.03 | 1.33 | 1.38 |
| 22 | 23S1 | 1302 | A | C5-C4 | -7.03 | 1.33 | 1.38 |
| 22 | 23S1 | 2247 | A | C5-C4 | -7.03 | 1.33 | 1.38 |
| 22 | 23S1 | 979 | A | C5-C4 | -7.03 | 1.33 | 1.38 |
| 1 | 16S1 | 223 | A | C8-N7 | 7.02 | 1.36 | 1.31 |
| 22 | 23S1 | 1089 | A | N3-C4 | 7.02 | 1.39 | 1.34 |
| 22 | 23S1 | 1652 | A | C5-C4 | -7.02 | 1.33 | 1.38 |
| 1 | 16S1 | 573 | A | C5-C4 | -7.02 | 1.33 | 1.38 |
| 22 | 23S1 | 800 | A | C5-C4 | -7.02 | 1.33 | 1.38 |
| 1 | 16S1 | 205 | A | C8-N7 | 7.01 | 1.36 | 1.31 |
| 22 | 23S1 | 2014 | A | C5-C4 | -7.01 | 1.33 | 1.38 |
| 22 | 23S1 | 2158 | A | C8-N7 | 7.01 | 1.36 | 1.31 |
| 22 | 23S1 | 1453 | A | C8-N7 | 7.01 | 1.36 | 1.31 |
| 22 | 23S1 | 2516 | A | C5-C4 | -7.00 | 1.33 | 1.38 |
| 22 | 23S1 | 1342 | A | C5-C4 | -7.00 | 1.33 | 1.38 |
| 23 | 05S1 | 46 | A | C8-N7 | 7.00 | 1.36 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 16S1 | 1408 | A | C8-N7 | 7.00 | 1.36 | 1.31 |
| 1 | 16S1 | 563 | A | C5-C4 | -7.00 | 1.33 | 1.38 |
| 22 | 23S1 | 2883 | A | C5-C4 | -6.99 | 1.33 | 1.38 |
| 1 | 16S1 | 1492 | A | C8-N7 | 6.99 | 1.36 | 1.31 |
| 22 | 23S1 | 1784 | A | C5-C4 | -6.99 | 1.33 | 1.38 |
| 22 | 23S1 | 1916 | A | C8-N7 | 6.99 | 1.36 | 1.31 |
| 23 | 05S1 | 108 | A | C5-C4 | -6.99 | 1.33 | 1.38 |
| 22 | 23S1 | 1677 | A | C5-C4 | -6.98 | 1.33 | 1.38 |
| 1 | 16S1 | 171 | A | C8-N7 | 6.98 | 1.36 | 1.31 |
| 22 | 23S1 | 2097 | A | C8-N7 | 6.98 | 1.36 | 1.31 |
| 1 | 16S1 | 729 | A | C5-C4 | -6.98 | 1.33 | 1.38 |
| 1 | 16S1 | 915 | A | C5-C4 | -6.98 | 1.33 | 1.38 |
| 22 | 23S1 | 675 | A | C5-C4 | -6.98 | 1.33 | 1.38 |
| 22 | 23S1 | 1783 | A | C5-C4 | -6.98 | 1.33 | 1.38 |
| 22 | 23S1 | 2126 | A | C8-N7 | 6.98 | 1.36 | 1.31 |
| 22 | 23S1 | 2386 | A | C5-C4 | -6.98 | 1.33 | 1.38 |
| 22 | 23S1 | 1630 | A | C5-C4 | -6.97 | 1.33 | 1.38 |
| 22 | 23S1 | 1525 | A | C8-N7 | 6.97 | 1.36 | 1.31 |
| 1 | 16S1 | 327 | A | C5-C4 | -6.97 | 1.33 | 1.38 |
| 22 | 23S1 | 1086 | A | N3-C4 | 6.97 | 1.39 | 1.34 |
| 22 | 23S1 | 1254 | A | C5-C4 | -6.97 | 1.33 | 1.38 |
| 1 | 16S1 | 1434 | A | C5-C4 | -6.97 | 1.33 | 1.38 |
| 22 | 23S1 | 1084 | A | C8-N7 | 6.97 | 1.36 | 1.31 |
| 22 | 23S1 | 892 | A | N3-C4 | 6.96 | 1.39 | 1.34 |
| 22 | 23S1 | 2600 | A | C5-C4 | -6.96 | 1.33 | 1.38 |
| 1 | 16S1 | 787 | A | C5-C4 | -6.96 | 1.33 | 1.38 |
| 22 | 23S1 | 1678 | A | C5-C4 | -6.96 | 1.33 | 1.38 |
| 1 | 16S1 | 1042 | A | C8-N7 | 6.96 | 1.36 | 1.31 |
| 22 | 23S1 | 2748 | A | C8-N7 | 6.96 | 1.36 | 1.31 |
| 22 | 23S1 | 504 | A | C5-C4 | -6.96 | 1.33 | 1.38 |
| 1 | 16S1 | 794 | A | C5-C4 | -6.95 | 1.33 | 1.38 |
| 22 | 23S1 | 479 | A | C5-C4 | -6.95 | 1.33 | 1.38 |
| 22 | 23S1 | 900 | A | C8-N7 | 6.95 | 1.36 | 1.31 |
| 22 | 23S1 | 2590 | A | C5-C4 | -6.95 | 1.33 | 1.38 |
| 22 | 23S1 | 960 | A | N7-C5 | -6.95 | 1.35 | 1.39 |
| 1 | 16S1 | 1274 | A | C8-N7 | 6.95 | 1.36 | 1.31 |
| 22 | 23S1 | 412 | A | C5-C4 | -6.95 | 1.33 | 1.38 |
| 22 | 23S1 | 668 | A | C5-C4 | -6.94 | 1.33 | 1.38 |
| 22 | 23S1 | 1735 | A | C8-N7 | 6.94 | 1.36 | 1.31 |
| 22 | 23S1 | 861 | A | C5-C4 | -6.94 | 1.33 | 1.38 |
| 1 | 16S1 | 8 | A | C5-C4 | -6.94 | 1.33 | 1.38 |
| 22 | 23S1 | 689 | A | C5-C4 | -6.94 | 1.33 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 2733 | A | C8-N7 | 6.94 | 1.36 | 1.31 |
| 22 | 23S1 | 2670 | A | C8-N7 | 6.94 | 1.36 | 1.31 |
| 22 | 23S1 | 1050 | A | C8-N7 | 6.94 | 1.36 | 1.31 |
| 22 | 23S1 | 2019 | A | C5-C4 | -6.94 | 1.33 | 1.38 |
| 22 | 23S1 | 1981 | A | C5-C4 | -6.93 | 1.33 | 1.38 |
| 1 | 16S1 | 747 | A | C8-N7 | 6.93 | 1.36 | 1.31 |
| 22 | 23S1 | 111 | A | C8-N7 | 6.93 | 1.36 | 1.31 |
| 1 | 16S1 | 1019 | A | C8-N7 | 6.93 | 1.36 | 1.31 |
| 22 | 23S1 | 344 | A | C8-N7 | 6.93 | 1.36 | 1.31 |
| 1 | 16S1 | 80 | A | C8-N7 | 6.92 | 1.36 | 1.31 |
| 22 | 23S1 | 756 | A | C5-C4 | -6.92 | 1.33 | 1.38 |
| 22 | 23S1 | 1431 | A | C5-C4 | -6.92 | 1.33 | 1.38 |
| 1 | 16S1 | 143 | A | C8-N7 | 6.92 | 1.36 | 1.31 |
| 22 | 23S1 | 144 | A | C8-N7 | 6.92 | 1.36 | 1.31 |
| 22 | 23S1 | 804 | A | C5-C4 | -6.92 | 1.33 | 1.38 |
| 22 | 23S1 | 1701 | A | C5-C4 | -6.92 | 1.33 | 1.38 |
| 1 | 16S1 | 1261 | A | C8-N7 | 6.92 | 1.36 | 1.31 |
| 22 | 23S1 | 2675 | A | C5-C4 | -6.92 | 1.33 | 1.38 |
| 1 | 16S1 | 1289 | A | C8-N7 | 6.91 | 1.36 | 1.31 |
| 22 | 23S1 | 781 | A | C5-C4 | -6.91 | 1.33 | 1.38 |
| 22 | 23S1 | 1504 | A | C8-N7 | 6.91 | 1.36 | 1.31 |
| 22 | 23S1 | 1890 | A | C5-C4 | -6.91 | 1.33 | 1.38 |
| 22 | 23S1 | 1304 | A | C5-C4 | -6.91 | 1.33 | 1.38 |
| 1 | 16S1 | 461 | A | N3-C4 | 6.91 | 1.39 | 1.34 |
| 1 | 16S1 | 1238 | A | C8-N7 | 6.91 | 1.36 | 1.31 |
| 22 | 23S1 | 614 | A | C8-N7 | 6.91 | 1.36 | 1.31 |
| 1 | 16S1 | 1346 | A | C8-N7 | 6.90 | 1.36 | 1.31 |
| 1 | 16S1 | 44 | A | C8-N7 | 6.90 | 1.36 | 1.31 |
| 1 | 16S1 | 1012 | A | C8-N7 | 6.90 | 1.36 | 1.31 |
| 22 | 23S1 | 676 | A | C5-C4 | -6.90 | 1.33 | 1.38 |
| 1 | 16S1 | 1204 | A | C8-N7 | 6.90 | 1.36 | 1.31 |
| 22 | 23S1 | 751 | A | C5-C4 | -6.90 | 1.33 | 1.38 |
| 22 | 23S1 | 2114 | A | C8-N7 | 6.90 | 1.36 | 1.31 |
| 1 | 16S1 | 914 | A | C5-C4 | -6.90 | 1.33 | 1.38 |
| 22 | 23S1 | 204 | A | C5-C4 | -6.90 | 1.33 | 1.38 |
| 1 | 16S1 | 460 | A | C8-N7 | 6.90 | 1.36 | 1.31 |
| 22 | 23S1 | 1129 | A | C5-C4 | -6.90 | 1.33 | 1.38 |
| 22 | 23S1 | 2052 | A | C5-C4 | -6.90 | 1.33 | 1.38 |
| 22 | 23S1 | 28 | A | C5-C4 | -6.89 | 1.33 | 1.38 |
| 1 | 16S1 | 1130 | A | C8-N7 | 6.89 | 1.36 | 1.31 |
| 22 | 23S1 | 613 | A | C8-N7 | 6.89 | 1.36 | 1.31 |
| 22 | 23S1 | 1672 | A | C5-C4 | -6.89 | 1.33 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 1495 | A | C8-N7 | 6.89 | 1.36 | 1.31 |
| 1 | 16S1 | 172 | A | C8-N7 | 6.88 | 1.36 | 1.31 |
| 1 | 16S1 | 1332 | A | C8-N7 | 6.88 | 1.36 | 1.31 |
| 22 | 23S1 | 2328 | A | C5-C4 | -6.88 | 1.33 | 1.38 |
| 1 | 16S1 | 189 | A | C8-N7 | 6.88 | 1.36 | 1.31 |
| 22 | 23S1 | 2147 | A | N3-C4 | 6.88 | 1.39 | 1.34 |
| 1 | 16S1 | 532 | A | C8-N7 | 6.88 | 1.36 | 1.31 |
| 1 | 16S1 | 649 | A | C8-N7 | 6.88 | 1.36 | 1.31 |
| 22 | 23S1 | 2054 | A | C5-C4 | -6.88 | 1.33 | 1.38 |
| 1 | 16S1 | 80 | A | N3-C4 | 6.88 | 1.39 | 1.34 |
| 1 | 16S1 | 408 | A | C8-N7 | 6.88 | 1.36 | 1.31 |
| 1 | 16S1 | 1396 | A | C5-C4 | -6.87 | 1.33 | 1.38 |
| 1 | 16S1 | 1410 | A | C8-N7 | 6.87 | 1.36 | 1.31 |
| 22 | 23S1 | 2388 | A | C5-C4 | -6.87 | 1.33 | 1.38 |
| 1 | 16S1 | 139 | A | C8-N7 | 6.87 | 1.36 | 1.31 |
| 22 | 23S1 | 2142 | A | N3-C4 | 6.87 | 1.39 | 1.34 |
| 22 | 23S1 | 947 | A | C5-C4 | -6.87 | 1.33 | 1.38 |
| 1 | 16S1 | 1021 | A | C8-N7 | 6.87 | 1.36 | 1.31 |
| 22 | 23S1 | 1544 | A | C8-N7 | 6.86 | 1.36 | 1.31 |
| 1 | 16S1 | 746 | A | C8-N7 | 6.86 | 1.36 | 1.31 |
| 22 | 23S1 | 2589 | A | C5-C4 | -6.86 | 1.33 | 1.38 |
| 1 | 16S1 | 60 | A | C8-N7 | 6.86 | 1.36 | 1.31 |
| 22 | 23S1 | 1147 | A | C8-N7 | 6.86 | 1.36 | 1.31 |
| 1 | 16S1 | 1176 | A | C8-N7 | 6.85 | 1.36 | 1.31 |
| 22 | 23S1 | 2114 | A | N3-C4 | 6.85 | 1.39 | 1.34 |
| 1 | 16S1 | 1333 | A | C8-N7 | 6.85 | 1.36 | 1.31 |
| 1 | 16S1 | 495 | A | C8-N7 | 6.85 | 1.36 | 1.31 |
| 1 | 16S1 | 665 | A | C5-C4 | -6.85 | 1.33 | 1.38 |
| 1 | 16S1 | 196 | A | C8-N7 | 6.85 | 1.36 | 1.31 |
| 22 | 23S1 | 1085 | A | C8-N7 | 6.85 | 1.36 | 1.31 |
| 22 | 23S1 | 2577 | A | C5-C4 | -6.85 | 1.33 | 1.38 |
| 22 | 23S1 | 2587 | A | C5-C4 | -6.85 | 1.33 | 1.38 |
| 1 | 16S1 | 149 | A | C8-N7 | 6.84 | 1.36 | 1.31 |
| 22 | 23S1 | 172 | A | C8-N7 | 6.84 | 1.36 | 1.31 |
| 22 | 23S1 | 1490 | A | N3-C4 | 6.84 | 1.39 | 1.34 |
| 22 | 23S1 | 156 | A | C8-N7 | 6.84 | 1.36 | 1.31 |
| 22 | 23S1 | 1275 | A | C5-C4 | -6.84 | 1.33 | 1.38 |
| 22 | 23S1 | 10 | A | C5-C4 | -6.83 | 1.33 | 1.38 |
| 1 | 16S1 | 1016 | A | C8-N7 | 6.83 | 1.36 | 1.31 |
| 22 | 23S1 | 1098 | A | N3-C4 | 6.83 | 1.39 | 1.34 |
| 22 | 23S1 | 1427 | A | C8-N7 | 6.83 | 1.36 | 1.31 |
| 23 | 05S1 | 45 | A | C5-C4 | -6.83 | 1.33 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 16S1 | 814 | A | C5-C4 | -6.83 | 1.33 | 1.38 |
| 22 | 23S1 | 2476 | A | C5-C4 | -6.83 | 1.33 | 1.38 |
| 1 | 16S1 | 192 | A | C8-N7 | 6.83 | 1.36 | 1.31 |
| 22 | 23S1 | 761 | A | C5-C4 | -6.83 | 1.33 | 1.38 |
| 1 | 16S1 | 825 | A | C5-C4 | -6.83 | 1.33 | 1.38 |
| 22 | 23S1 | 2660 | A | C8-N7 | 6.83 | 1.36 | 1.31 |
| 22 | 23S1 | 1067 | A | N3-C4 | 6.82 | 1.39 | 1.34 |
| 22 | 23S1 | 2381 | A | C5-C4 | -6.82 | 1.33 | 1.38 |
| 1 | 16S1 | 298 | A | C5-C4 | -6.82 | 1.33 | 1.38 |
| 1 | 16S1 | 766 | A | C5-C4 | -6.82 | 1.33 | 1.38 |
| 1 | 16S1 | 1468 | A | C5-C4 | -6.82 | 1.33 | 1.38 |
| 22 | 23S1 | 1847 | A | C8-N7 | 6.82 | 1.36 | 1.31 |
| 23 | 05S1 | 34 | A | C8-N7 | 6.82 | 1.36 | 1.31 |
| 22 | 23S1 | 1155 | A | C5-C4 | -6.82 | 1.33 | 1.38 |
| 22 | 23S1 | 2459 | A | C5-C4 | -6.82 | 1.33 | 1.38 |
| 22 | 23S1 | 2070 | A | C5-C4 | -6.81 | 1.33 | 1.38 |
| 22 | 23S1 | 975 | A | C5-C4 | -6.81 | 1.33 | 1.38 |
| 22 | 23S1 | 661 | A | C5-C4 | -6.81 | 1.33 | 1.38 |
| 22 | 23S1 | 1247 | A | C5-C4 | -6.81 | 1.33 | 1.38 |
| 22 | 23S1 | 466 | A | C5-C4 | -6.81 | 1.33 | 1.38 |
| 22 | 23S1 | 1853 | A | C5-C4 | -6.81 | 1.33 | 1.38 |
| 55 | PTR1 | 26 | A | C8-N7 | 6.81 | 1.36 | 1.31 |
| 1 | 16S1 | 923 | A | C5-C4 | -6.81 | 1.33 | 1.38 |
| 22 | 23S1 | 1057 | A | N3-C4 | 6.81 | 1.39 | 1.34 |
| 22 | 23S1 | 941 | A | C5-C4 | -6.81 | 1.33 | 1.38 |
| 22 | 23S1 | 1711 | A | C5-C4 | -6.80 | 1.33 | 1.38 |
| 22 | 23S1 | 2119 | A | C8-N7 | 6.80 | 1.36 | 1.31 |
| 22 | 23S1 | 2212 | A | C5-C4 | -6.80 | 1.33 | 1.38 |
| 1 | 16S1 | 622 | A | C8-N7 | 6.80 | 1.36 | 1.31 |
| 1 | 16S1 | 702 | A | C8-N7 | 6.80 | 1.36 | 1.31 |
| 22 | 23S1 | 608 | A | C5-C4 | -6.80 | 1.33 | 1.38 |
| 22 | 23S1 | 1593 | A | C8-N7 | 6.80 | 1.36 | 1.31 |
| 22 | 23S1 | 1953 | A | C5-C4 | -6.80 | 1.33 | 1.38 |
| 22 | 23S1 | 829 | A | C5-C4 | -6.80 | 1.33 | 1.38 |
| 1 | 16S1 | 715 | A | C5-C4 | -6.80 | 1.33 | 1.38 |
| 1 | 16S1 | 1000 | A | C8-N7 | 6.80 | 1.36 | 1.31 |
| 1 | 16S1 | 1036 | A | C8-N7 | 6.80 | 1.36 | 1.31 |
| 22 | 23S1 | 2311 | A | C5-C4 | -6.80 | 1.33 | 1.38 |
| 22 | 23S1 | 705 | A | C5-C4 | -6.79 | 1.33 | 1.38 |
| 22 | 23S1 | 1970 | A | C5-C4 | -6.79 | 1.33 | 1.38 |
| 1 | 16S1 | 520 | A | C8-N7 | 6.79 | 1.36 | 1.31 |
| 1 | 16S1 | 306 | A | C8-N7 | 6.79 | 1.36 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 279 | A | C8-N7 | 6.79 | 1.36 | 1.31 |
| 22 | 23S1 | 749 | A | C5-C4 | -6.79 | 1.33 | 1.38 |
| 22 | 23S1 | 1508 | A | C8-N7 | 6.79 | 1.36 | 1.31 |
| 22 | 23S1 | 2432 | A | C5-C4 | -6.79 | 1.33 | 1.38 |
| 22 | 23S1 | 2726 | A | C8-N7 | 6.79 | 1.36 | 1.31 |
| 1 | 16S1 | 1151 | A | C8-N7 | 6.79 | 1.36 | 1.31 |
| 22 | 23S1 | 2042 | A | C5-C4 | -6.79 | 1.33 | 1.38 |
| 22 | 23S1 | 529 | A | C8-N7 | 6.79 | 1.36 | 1.31 |
| 23 | 05S1 | 78 | A | C5-C4 | -6.79 | 1.33 | 1.38 |
| 22 | 23S1 | 91 | A | C8-N7 | 6.78 | 1.36 | 1.31 |
| 22 | 23S1 | 1366 | A | C5-C4 | -6.78 | 1.34 | 1.38 |
| 22 | 23S1 | 2135 | A | N3-C4 | 6.78 | 1.39 | 1.34 |
| 22 | 23S1 | 2700 | A | C5-C4 | -6.78 | 1.34 | 1.38 |
| 22 | 23S1 | 2800 | A | C8-N7 | 6.78 | 1.36 | 1.31 |
| 1 | 16S1 | 1246 | A | C8-N7 | 6.78 | 1.36 | 1.31 |
| 22 | 23S1 | 191 | A | C5-C4 | -6.78 | 1.34 | 1.38 |
| 22 | 23S1 | 1494 | A | C8-N7 | 6.78 | 1.36 | 1.31 |
| 22 | 23S1 | 2154 | A | N3-C4 | 6.78 | 1.39 | 1.34 |
| 22 | 23S1 | 5 | A | C8-N7 | 6.77 | 1.36 | 1.31 |
| 22 | 23S1 | 64 | A | C8-N7 | 6.77 | 1.36 | 1.31 |
| 22 | 23S1 | 160 | A | C8-N7 | 6.77 | 1.36 | 1.31 |
| 22 | 23S1 | 2281 | A | C5-C4 | -6.77 | 1.34 | 1.38 |
| 22 | 23S1 | 1086 | A | C8-N7 | 6.77 | 1.36 | 1.31 |
| 22 | 23S1 | 2887 | A | C5-C4 | -6.77 | 1.34 | 1.38 |
| 22 | 23S1 | 2406 | A | C8-N7 | 6.77 | 1.36 | 1.31 |
| 22 | 23S1 | 1213 | A | C5-C4 | -6.76 | 1.34 | 1.38 |
| 22 | 23S1 | 1253 | A | C5-C4 | -6.76 | 1.34 | 1.38 |
| 1 | 16S1 | 1280 | A | C8-N7 | 6.76 | 1.36 | 1.31 |
| 22 | 23S1 | 1054 | A | C8-N7 | 6.76 | 1.36 | 1.31 |
| 1 | 16S1 | 1311 | A | C8-N7 | 6.76 | 1.36 | 1.31 |
| 22 | 23S1 | 1214 | A | C5-C4 | -6.76 | 1.34 | 1.38 |
| 1 | 16S1 | 228 | A | C8-N7 | 6.76 | 1.36 | 1.31 |
| 1 | 16S1 | 1456 | A | C8-N7 | 6.76 | 1.36 | 1.31 |
| 22 | 23S1 | 2792 | A | C8-N7 | 6.76 | 1.36 | 1.31 |
| 1 | 16S1 | 270 | A | C8-N7 | 6.76 | 1.36 | 1.31 |
| 22 | 23S1 | 1772 | A | C5-C4 | -6.76 | 1.34 | 1.38 |
| 22 | 23S1 | 2469 | A | C5-C4 | -6.76 | 1.34 | 1.38 |
| 22 | 23S1 | 2541 | A | C5-C4 | -6.76 | 1.34 | 1.38 |
| 22 | 23S1 | 1665 | A | C5-C4 | -6.75 | 1.34 | 1.38 |
| 22 | 23S1 | 1786 | A | C5-C4 | -6.75 | 1.34 | 1.38 |
| 1 | 16S1 | 1513 | A | C5-C4 | -6.75 | 1.34 | 1.38 |
| 22 | 23S1 | 1579 | A | C8-N7 | 6.75 | 1.36 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 742 | A | C5-C4 | -6.75 | 1.34 | 1.38 |
| 22 | 23S1 | 2426 | A | C5-C4 | -6.75 | 1.34 | 1.38 |
| 1 | 16S1 | 78 | A | N3-C4 | 6.75 | 1.38 | 1.34 |
| 1 | 16S1 | 250 | A | C8-N7 | 6.75 | 1.36 | 1.31 |
| 22 | 23S1 | 655 | A | C8-N7 | 6.75 | 1.36 | 1.31 |
| 22 | 23S1 | 1039 | A | C8-N7 | 6.75 | 1.36 | 1.31 |
| 22 | 23S1 | 1327 | A | C5-C4 | -6.75 | 1.34 | 1.38 |
| 1 | 16S1 | 596 | A | C8-N7 | 6.74 | 1.36 | 1.31 |
| 1 | 16S1 | 1507 | A | C5-C4 | -6.74 | 1.34 | 1.38 |
| 22 | 23S1 | 899 | A | C8-N7 | 6.74 | 1.36 | 1.31 |
| 22 | 23S1 | 2171 | A | C8-N7 | 6.74 | 1.36 | 1.31 |
| 1 | 16S1 | 845 | A | N3-C4 | 6.74 | 1.38 | 1.34 |
| 1 | 16S1 | 958 | A | C5-C4 | -6.74 | 1.34 | 1.38 |
| 22 | 23S1 | 654 | A | C8-N7 | 6.74 | 1.36 | 1.31 |
| 22 | 23S1 | 1913 | A | C8-N7 | 6.74 | 1.36 | 1.31 |
| 23 | 05S1 | 39 | A | C8-N7 | 6.74 | 1.36 | 1.31 |
| 22 | 23S1 | 1020 | A | C5-C4 | -6.74 | 1.34 | 1.38 |
| 22 | 23S1 | 1566 | A | C5-C4 | -6.74 | 1.34 | 1.38 |
| 1 | 16S1 | 1256 | A | C8-N7 | 6.74 | 1.36 | 1.31 |
| 22 | 23S1 | 1938 | A | C5-C4 | -6.74 | 1.34 | 1.38 |
| 22 | 23S1 | 2060 | A | C5-C4 | -6.74 | 1.34 | 1.38 |
| 22 | 23S1 | 2598 | A | C5-C4 | -6.74 | 1.34 | 1.38 |
| 55 | PTR1 | 9 | A | C8-N7 | 6.73 | 1.36 | 1.31 |
| 22 | 23S1 | 2542 | A | C5-C4 | -6.73 | 1.34 | 1.38 |
| 22 | 23S1 | 750 | A | C5-C4 | -6.73 | 1.34 | 1.38 |
| 22 | 23S1 | 1088 | A | N3-C4 | 6.73 | 1.38 | 1.34 |
| 22 | 23S1 | 1885 | A | C8-N7 | 6.73 | 1.36 | 1.31 |
| 1 | 16S1 | 98 | A | C8-N7 | 6.73 | 1.36 | 1.31 |
| 22 | 23S1 | 1204 | A | C8-N7 | 6.73 | 1.36 | 1.31 |
| 22 | 23S1 | 863 | A | C5-C4 | -6.73 | 1.34 | 1.38 |
| 1 | 16S1 | 412 | A | N3-C4 | 6.72 | 1.38 | 1.34 |
| 22 | 23S1 | 1805 | A | C5-C4 | -6.72 | 1.34 | 1.38 |
| 10 | S101 | 53 | ILE | C-N | -6.72 | 1.18 | 1.34 |
| 22 | 23S1 | 925 | A | C5-C4 | -6.72 | 1.34 | 1.38 |
| 1 | 16S1 | 371 | A | C8-N7 | 6.72 | 1.36 | 1.31 |
| 22 | 23S1 | 233 | A | C5-C4 | -6.72 | 1.34 | 1.38 |
| 22 | 23S1 | 730 | A | C5-C4 | -6.71 | 1.34 | 1.38 |
| 22 | 23S1 | 2037 | A | C5-C4 | -6.71 | 1.34 | 1.38 |
| 22 | 23S1 | 2009 | A | C5-C4 | -6.71 | 1.34 | 1.38 |
| 22 | 23S1 | 2015 | A | C5-C4 | -6.71 | 1.34 | 1.38 |
| 1 | 16S1 | 1093 | A | C5-C4 | -6.71 | 1.34 | 1.38 |
| 1 | 16S1 | 1271 | A | C8-N7 | 6.71 | 1.36 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 1403 | A | C5-C4 | -6.71 | 1.34 | 1.38 |
| 1 | 16S1 | 872 | A | C8-N7 | 6.71 | 1.36 | 1.31 |
| 22 | 23S1 | 715 | A | C8-N7 | 6.71 | 1.36 | 1.31 |
| 22 | 23S1 | 1614 | A | C5-C4 | -6.71 | 1.34 | 1.38 |
| 22 | 23S1 | 371 | A | C8-N7 | 6.70 | 1.36 | 1.31 |
| 22 | 23S1 | 2632 | A | C5-C4 | -6.70 | 1.34 | 1.38 |
| 1 | 16S1 | 864 | A | C5-C4 | -6.70 | 1.34 | 1.38 |
| 1 | 16S1 | 681 | A | C8-N7 | 6.70 | 1.36 | 1.31 |
| 1 | 16S1 | 983 | A | N3-C4 | 6.70 | 1.38 | 1.34 |
| 22 | 23S1 | 1668 | A | C5-C4 | -6.70 | 1.34 | 1.38 |
| 22 | 23S1 | 1791 | A | C5-C4 | -6.70 | 1.34 | 1.38 |
| 22 | 23S1 | 794 | A | C5-C4 | -6.70 | 1.34 | 1.38 |
| 22 | 23S1 | 2309 | A | C8-N7 | 6.70 | 1.36 | 1.31 |
| 22 | 23S1 | 2565 | A | C5-C4 | -6.70 | 1.34 | 1.38 |
| 1 | 16S1 | 909 | A | C8-N7 | 6.70 | 1.36 | 1.31 |
| 1 | 16S1 | 478 | A | C8-N7 | 6.70 | 1.36 | 1.31 |
| 1 | 16S1 | 1431 | A | C5-C4 | -6.69 | 1.34 | 1.38 |
| 22 | 23S1 | 2753 | A | C8-N7 | 6.69 | 1.36 | 1.31 |
| 22 | 23S1 | 735 | A | C5-C4 | -6.69 | 1.34 | 1.38 |
| 22 | 23S1 | 1596 | A | C8-N7 | 6.69 | 1.36 | 1.31 |
| 22 | 23S1 | 2298 | A | C5-C4 | -6.69 | 1.34 | 1.38 |
| 22 | 23S1 | 2711 | A | C5-C4 | -6.69 | 1.34 | 1.38 |
| 1 | 16S1 | 496 | A | C8-N7 | 6.69 | 1.36 | 1.31 |
| 22 | 23S1 | 685 | A | C5-C4 | -6.69 | 1.34 | 1.38 |
| 22 | 23S1 | 2721 | A | C5-C4 | -6.69 | 1.34 | 1.38 |
| 23 | 05S1 | 53 | A | C8-N7 | 6.69 | 1.36 | 1.31 |
| 22 | 23S1 | 272 | A | C8-N7 | 6.69 | 1.36 | 1.31 |
| 1 | 16S1 | 72 | A | N3-C4 | 6.69 | 1.38 | 1.34 |
| 1 | 16S1 | 432 | A | C8-N7 | 6.69 | 1.36 | 1.31 |
| 1 | 16S1 | 1250 | A | C8-N7 | 6.69 | 1.36 | 1.31 |
| 1 | 16S1 | 1499 | A | C5-C4 | -6.69 | 1.34 | 1.38 |
| 22 | 23S1 | 278 | A | C8-N7 | 6.69 | 1.36 | 1.31 |
| 22 | 23S1 | 1630 | A | C8-N7 | 6.69 | 1.36 | 1.31 |
| 1 | 16S1 | 1299 | A | C8-N7 | 6.69 | 1.36 | 1.31 |
| 22 | 23S1 | 226 | A | C5-C4 | -6.69 | 1.34 | 1.38 |
| 22 | 23S1 | 439 | A | C8-N7 | 6.69 | 1.36 | 1.31 |
| 22 | 23S1 | 1308 | A | C5-C4 | -6.69 | 1.34 | 1.38 |
| 22 | 23S1 | 1977 | A | C5-C4 | -6.69 | 1.34 | 1.38 |
| 22 | 23S1 | 2134 | A | N3-C4 | 6.69 | 1.38 | 1.34 |
| 22 | 23S1 | 227 | A | C5-C4 | -6.68 | 1.34 | 1.38 |
| 22 | 23S1 | 1262 | A | C5-C4 | -6.68 | 1.34 | 1.38 |
| 22 | 23S1 | 1819 | A | C5-C4 | -6.68 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 752 | A | C8-N7 | 6.68 | 1.36 | 1.31 |
| 22 | 23S1 | 2142 | A | C8-N7 | 6.68 | 1.36 | 1.31 |
| 22 | 23S1 | 19 | A | C5-C4 | -6.68 | 1.34 | 1.38 |
| 22 | 23S1 | 1359 | A | C8-N7 | 6.68 | 1.36 | 1.31 |
| 22 | 23S1 | 2005 | A | C5-C4 | -6.68 | 1.34 | 1.38 |
| 1 | 16S1 | 130 | A | C5-C4 | -6.68 | 1.34 | 1.38 |
| 22 | 23S1 | 2734 | A | C5-C4 | -6.68 | 1.34 | 1.38 |
| 22 | 23S1 | 167 | A | C8-N7 | 6.67 | 1.36 | 1.31 |
| 1 | 16S1 | 718 | A | C8-N7 | 6.67 | 1.36 | 1.31 |
| 22 | 23S1 | 119 | A | C5-C4 | -6.67 | 1.34 | 1.38 |
| 22 | 23S1 | 155 | A | C8-N7 | 6.67 | 1.36 | 1.31 |
| 22 | 23S1 | 1353 | A | C5-C4 | -6.67 | 1.34 | 1.38 |
| 1 | 16S1 | 768 | A | C5-C4 | -6.67 | 1.34 | 1.38 |
| 1 | 16S1 | 900 | A | C5-C4 | -6.67 | 1.34 | 1.38 |
| 22 | 23S1 | 176 | A | C5-C4 | -6.67 | 1.34 | 1.38 |
| 1 | 16S1 | 1534 | A | N3-C4 | 6.67 | 1.38 | 1.34 |
| 22 | 23S1 | 53 | A | C5-C4 | -6.67 | 1.34 | 1.38 |
| 22 | 23S1 | 1367 | A | C5-C4 | -6.67 | 1.34 | 1.38 |
| 1 | 16S1 | 802 | A | C5-C4 | -6.67 | 1.34 | 1.38 |
| 22 | 23S1 | 833 | A | C5-C4 | -6.67 | 1.34 | 1.38 |
| 1 | 16S1 | 53 | A | C5-C4 | -6.66 | 1.34 | 1.38 |
| 1 | 16S1 | 784 | A | C5-C4 | -6.66 | 1.34 | 1.38 |
| 1 | 16S1 | 1275 | A | C8-N7 | 6.66 | 1.36 | 1.31 |
| 22 | 23S1 | 654 | A | N3-C4 | 6.66 | 1.38 | 1.34 |
| 22 | 23S1 | 1591 | A | C8-N7 | 6.66 | 1.36 | 1.31 |
| 22 | 23S1 | 1744 | A | C8-N7 | 6.66 | 1.36 | 1.31 |
| 22 | 23S1 | 2003 | A | C5-C4 | -6.66 | 1.34 | 1.38 |
| 1 | 16S1 | 389 | A | N3-C4 | 6.66 | 1.38 | 1.34 |
| 22 | 23S1 | 2448 | A | C5-C4 | -6.66 | 1.34 | 1.38 |
| 22 | 23S1 | 63 | A | C8-N7 | 6.66 | 1.36 | 1.31 |
| 22 | 23S1 | 1165 | A | C5-C4 | -6.66 | 1.34 | 1.38 |
| 22 | 23S1 | 310 | A | C8-N7 | 6.66 | 1.36 | 1.31 |
| 22 | 23S1 | 739 | A | C5-C4 | -6.66 | 1.34 | 1.38 |
| 1 | 16S1 | 1329 | A | C8-N7 | 6.65 | 1.36 | 1.31 |
| 22 | 23S1 | 920 | A | C5-C4 | -6.65 | 1.34 | 1.38 |
| 1 | 16S1 | 205 | A | N3-C4 | 6.65 | 1.38 | 1.34 |
| 22 | 23S1 | 2450 | A | C5-C4 | -6.65 | 1.34 | 1.38 |
| 23 | 05S1 | 15 | A | C8-N7 | 6.65 | 1.36 | 1.31 |
| 22 | 23S1 | 718 | A | C8-N7 | 6.65 | 1.36 | 1.31 |
| 22 | 23S1 | 1322 | A | C5-C4 | -6.65 | 1.34 | 1.38 |
| 22 | 23S1 | 2071 | A | C5-C4 | -6.65 | 1.34 | 1.38 |
| 22 | 23S1 | 1328 | A | C5-C4 | -6.65 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 2764 | A | C5-C4 | -6.65 | 1.34 | 1.38 |
| 22 | 23S1 | 1749 | A | C8-N7 | 6.65 | 1.36 | 1.31 |
| 22 | 23S1 | 251 | A | N7-C5 | -6.64 | 1.35 | 1.39 |
| 22 | 23S1 | 2171 | A | N3-C4 | 6.64 | 1.38 | 1.34 |
| 1 | 16S1 | 1179 | A | C8-N7 | 6.64 | 1.36 | 1.31 |
| 1 | 16S1 | 1285 | A | C8-N7 | 6.64 | 1.36 | 1.31 |
| 22 | 23S1 | 727 | A | C5-C4 | -6.64 | 1.34 | 1.38 |
| 22 | 23S1 | 1552 | A | C5-C4 | -6.64 | 1.34 | 1.38 |
| 22 | 23S1 | 2736 | A | C8-N7 | 6.64 | 1.36 | 1.31 |
| 22 | 23S1 | 2749 | A | C8-N7 | 6.64 | 1.36 | 1.31 |
| 22 | 23S1 | 706 | A | C5-C4 | -6.64 | 1.34 | 1.38 |
| 1 | 16S1 | 938 | A | C5-C4 | -6.64 | 1.34 | 1.38 |
| 22 | 23S1 | 1912 | A | C5-C4 | -6.63 | 1.34 | 1.38 |
| 22 | 23S1 | 599 | A | C5-C4 | -6.63 | 1.34 | 1.38 |
| 22 | 23S1 | 1532 | A | N3-C4 | 6.63 | 1.38 | 1.34 |
| 22 | 23S1 | 197 | A | C5-C4 | -6.63 | 1.34 | 1.38 |
| 1 | 16S1 | 602 | A | C8-N7 | 6.63 | 1.36 | 1.31 |
| 22 | 23S1 | 342 | A | C8-N7 | 6.63 | 1.36 | 1.31 |
| 22 | 23S1 | 2088 | A | C5-C4 | -6.63 | 1.34 | 1.38 |
| 22 | 23S1 | 1244 | A | C5-C4 | -6.62 | 1.34 | 1.38 |
| 22 | 23S1 | 1900 | A | C5-C4 | -6.62 | 1.34 | 1.38 |
| 1 | 16S1 | 1035 | A | N3-C4 | 6.62 | 1.38 | 1.34 |
| 22 | 23S1 | 492 | A | C5-C4 | -6.62 | 1.34 | 1.38 |
| 22 | 23S1 | 2270 | A | C5-C4 | -6.62 | 1.34 | 1.38 |
| 1 | 16S1 | 321 | A | C5-C4 | -6.62 | 1.34 | 1.38 |
| 22 | 23S1 | 616 | A | C8-N7 | 6.62 | 1.36 | 1.31 |
| 22 | 23S1 | 1616 | A | C5-C4 | -6.62 | 1.34 | 1.38 |
| 22 | 23S1 | 1858 | A | C8-N7 | 6.62 | 1.36 | 1.31 |
| 1 | 16S1 | 26 | A | C5-C4 | -6.62 | 1.34 | 1.38 |
| 1 | 16S1 | 935 | A | C8-N7 | 6.62 | 1.36 | 1.31 |
| 1 | 16S1 | 1169 | A | C8-N7 | 6.62 | 1.36 | 1.31 |
| 22 | 23S1 | 1640 | A | C8-N7 | 6.62 | 1.36 | 1.31 |
| 22 | 23S1 | 2850 | A | C5-C4 | -6.62 | 1.34 | 1.38 |
| 55 | PTR1 | 21 | A | C8-N7 | 6.62 | 1.36 | 1.31 |
| 1 | 16S1 | 120 | A | C8-N7 | 6.61 | 1.36 | 1.31 |
| 22 | 23S1 | 1307 | A | C5-C4 | -6.61 | 1.34 | 1.38 |
| 22 | 23S1 | 2657 | A | C8-N7 | 6.61 | 1.36 | 1.31 |
| 1 | 16S1 | 595 | A | C8-N7 | 6.61 | 1.36 | 1.31 |
| 1 | 16S1 | 1349 | A | C5-C4 | -6.61 | 1.34 | 1.38 |
| 22 | 23S1 | 789 | A | C5-C4 | -6.61 | 1.34 | 1.38 |
| 22 | 23S1 | 943 | A | C5-C4 | -6.61 | 1.34 | 1.38 |
| 22 | 23S1 | 1272 | A | C5-C4 | -6.61 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 2346 | A | C5-C4 | -6.61 | 1.34 | 1.38 |
| 1 | 16S1 | 397 | A | C5-C4 | -6.61 | 1.34 | 1.38 |
| 1 | 16S1 | 648 | A | C8-N7 | 6.61 | 1.36 | 1.31 |
| 1 | 16S1 | 767 | A | C5-C4 | -6.61 | 1.34 | 1.38 |
| 22 | 23S1 | 603 | A | C8-N7 | 6.60 | 1.36 | 1.31 |
| 22 | 23S1 | 633 | A | C5-C4 | -6.60 | 1.34 | 1.38 |
| 1 | 16S1 | 694 | A | C5-C4 | -6.60 | 1.34 | 1.38 |
| 22 | 23S1 | 1590 | A | C8-N7 | 6.60 | 1.36 | 1.31 |
| 22 | 23S1 | 2564 | A | C5-C4 | -6.60 | 1.34 | 1.38 |
| 1 | 16S1 | 101 | A | C8-N7 | 6.60 | 1.36 | 1.31 |
| 22 | 23S1 | 1866 | A | C8-N7 | 6.60 | 1.36 | 1.31 |
| 22 | 23S1 | 972 | A | C5-C4 | -6.59 | 1.34 | 1.38 |
| 22 | 23S1 | 1808 | A | C8-N7 | 6.59 | 1.36 | 1.31 |
| 22 | 23S1 | 2882 | A | C5-C4 | -6.59 | 1.34 | 1.38 |
| 1 | 16S1 | 539 | A | C8-N7 | 6.59 | 1.36 | 1.31 |
| 1 | 16S1 | 583 | A | C5-C4 | -6.59 | 1.34 | 1.38 |
| 22 | 23S1 | 497 | A | C8-N7 | 6.59 | 1.36 | 1.31 |
| 22 | 23S1 | 2471 | A | C8-N7 | 6.59 | 1.36 | 1.31 |
| 1 | 16S1 | 792 | A | C5-C4 | -6.59 | 1.34 | 1.38 |
| 22 | 23S1 | 1205 | A | C8-N7 | 6.59 | 1.36 | 1.31 |
| 22 | 23S1 | 1392 | A | C5-C4 | -6.59 | 1.34 | 1.38 |
| 22 | 23S1 | 14 | A | C5-C4 | -6.59 | 1.34 | 1.38 |
| 22 | 23S1 | 609 | A | C5-C4 | -6.59 | 1.34 | 1.38 |
| 22 | 23S1 | 2727 | A | C5-C4 | -6.59 | 1.34 | 1.38 |
| 22 | 23S1 | 346 | A | C8-N7 | 6.59 | 1.36 | 1.31 |
| 22 | 23S1 | 1276 | A | C5-C4 | -6.59 | 1.34 | 1.38 |
| 1 | 16S1 | 1022 | A | C8-N7 | 6.58 | 1.36 | 1.31 |
| 22 | 23S1 | 2882 | A | C8-N7 | 6.58 | 1.36 | 1.31 |
| 22 | 23S1 | 1635 | A | C5-C4 | -6.58 | 1.34 | 1.38 |
| 22 | 23S1 | 2358 | A | C5-C4 | -6.58 | 1.34 | 1.38 |
| 1 | 16S1 | 155 | A | C8-N7 | 6.58 | 1.36 | 1.31 |
| 1 | 16S1 | 28 | A | C5-C4 | -6.58 | 1.34 | 1.38 |
| 1 | 16S1 | 1146 | A | C8-N7 | 6.58 | 1.36 | 1.31 |
| 1 | 16S1 | 1201 | A | C8-N7 | 6.58 | 1.36 | 1.31 |
| 1 | 16S1 | 1254 | A | C8-N7 | 6.58 | 1.36 | 1.31 |
| 22 | 23S1 | 631 | A | C5-C4 | -6.58 | 1.34 | 1.38 |
| 22 | 23S1 | 1070 | A | N3-C4 | 6.58 | 1.38 | 1.34 |
| 22 | 23S1 | 1762 | A | C5-C4 | -6.58 | 1.34 | 1.38 |
| 1 | 16S1 | 1441 | A | N3-C4 | 6.58 | 1.38 | 1.34 |
| 22 | 23S1 | 677 | A | C5-C4 | -6.58 | 1.34 | 1.38 |
| 23 | 05S1 | 109 | A | C8-N7 | 6.57 | 1.36 | 1.31 |
| 1 | 16S1 | 253 | A | C8-N7 | 6.57 | 1.36 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 16S1 | 1446 | A | C8-N7 | 6.57 | 1.36 | 1.31 |
| 22 | 23S1 | 1151 | A | C5-C4 | -6.57 | 1.34 | 1.38 |
| 1 | 16S1 | 3 | A | C8-N7 | 6.57 | 1.36 | 1.31 |
| 22 | 23S1 | 1413 | A | N3-C4 | 6.57 | 1.38 | 1.34 |
| 22 | 23S1 | 1189 | A | C5-C4 | -6.57 | 1.34 | 1.38 |
| 22 | 23S1 | 1413 | A | C8-N7 | 6.57 | 1.36 | 1.31 |
| 22 | 23S1 | 2765 | A | C5-C4 | -6.57 | 1.34 | 1.38 |
| 22 | 23S1 | 322 | A | C5-C4 | -6.56 | 1.34 | 1.38 |
| 22 | 23S1 | 1609 | A | C8-N7 | 6.56 | 1.36 | 1.31 |
| 22 | 23S1 | 2184 | A | N3-C4 | 6.56 | 1.38 | 1.34 |
| 1 | 16S1 | 572 | A | C5-C4 | -6.56 | 1.34 | 1.38 |
| 22 | 23S1 | 300 | A | C5-C4 | -6.56 | 1.34 | 1.38 |
| 22 | 23S1 | 753 | A | C5-C4 | -6.56 | 1.34 | 1.38 |
| 1 | 16S1 | 728 | A | C5-C4 | -6.56 | 1.34 | 1.38 |
| 22 | 23S1 | 1439 | A | C5-C4 | -6.56 | 1.34 | 1.38 |
| 1 | 16S1 | 712 | A | C8-N7 | 6.56 | 1.36 | 1.31 |
| 22 | 23S1 | 222 | A | C5-C4 | -6.56 | 1.34 | 1.38 |
| 1 | 16S1 | 1531 | A | C8-N7 | 6.56 | 1.36 | 1.31 |
| 22 | 23S1 | 1304 | A | C8-N7 | 6.56 | 1.36 | 1.31 |
| 22 | 23S1 | 1502 | A | C8-N7 | 6.56 | 1.36 | 1.31 |
| 1 | 16S1 | 1196 | A | C5-C4 | -6.55 | 1.34 | 1.38 |
| 22 | 23S1 | 2333 | A | C5-C4 | -6.55 | 1.34 | 1.38 |
| 1 | 16S1 | 364 | A | C5-C4 | -6.55 | 1.34 | 1.38 |
| 22 | 23S1 | 990 | A | C5-C4 | -6.55 | 1.34 | 1.38 |
| 1 | 16S1 | 1433 | A | C5-C4 | -6.55 | 1.34 | 1.38 |
| 1 | 16S1 | 192 | A | N3-C4 | 6.55 | 1.38 | 1.34 |
| 1 | 16S1 | 574 | A | C5-C4 | -6.55 | 1.34 | 1.38 |
| 1 | 16S1 | 1429 | A | C5-C4 | -6.55 | 1.34 | 1.38 |
| 22 | 23S1 | 345 | A | C8-N7 | 6.55 | 1.36 | 1.31 |
| 22 | 23S1 | 547 | A | N3-C4 | 6.55 | 1.38 | 1.34 |
| 1 | 16S1 | 807 | A | C5-C4 | -6.54 | 1.34 | 1.38 |
| 22 | 23S1 | 322 | A | C8-N7 | 6.54 | 1.36 | 1.31 |
| 1 | 16S1 | 777 | A | C5-C4 | -6.54 | 1.34 | 1.38 |
| 22 | 23S1 | 56 | A | C5-C4 | -6.54 | 1.34 | 1.38 |
| 22 | 23S1 | 221 | A | C5-C4 | -6.54 | 1.34 | 1.38 |
| 22 | 23S1 | 844 | A | C5-C4 | -6.54 | 1.34 | 1.38 |
| 22 | 23S1 | 1419 | A | C5-C4 | -6.54 | 1.34 | 1.38 |
| 22 | 23S1 | 101 | A | N3-C4 | 6.54 | 1.38 | 1.34 |
| 1 | 16S1 | 320 | A | C5-C4 | -6.54 | 1.34 | 1.38 |
| 1 | 16S1 | 1105 | A | C5-C4 | -6.54 | 1.34 | 1.38 |
| 1 | 16S1 | 1500 | A | C5-C4 | -6.54 | 1.34 | 1.38 |
| 22 | 23S1 | 2851 | A | C5-C4 | -6.54 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 16S1 | 906 | A | C5-C4 | -6.54 | 1.34 | 1.38 |
| 22 | 23S1 | 1802 | A | C5-C4 | -6.54 | 1.34 | 1.38 |
| 1 | 16S1 | 72 | A | C8-N7 | 6.53 | 1.36 | 1.31 |
| 1 | 16S1 | 246 | A | C5-C4 | -6.53 | 1.34 | 1.38 |
| 22 | 23S1 | 2634 | A | C5-C4 | -6.53 | 1.34 | 1.38 |
| 22 | 23S1 | 1347 | A | C5-C4 | -6.53 | 1.34 | 1.38 |
| 1 | 16S1 | 696 | A | C5-C4 | -6.53 | 1.34 | 1.38 |
| 22 | 23S1 | 905 | A | C8-N7 | 6.53 | 1.36 | 1.31 |
| 22 | 23S1 | 988 | A | C5-C4 | -6.53 | 1.34 | 1.38 |
| 22 | 23S1 | 1496 | A | C5-C4 | -6.53 | 1.34 | 1.38 |
| 22 | 23S1 | 1937 | A | C8-N7 | 6.53 | 1.36 | 1.31 |
| 22 | 23S1 | 404 | A | C8-N7 | 6.53 | 1.36 | 1.31 |
| 1 | 16S1 | 629 | A | C8-N7 | 6.53 | 1.36 | 1.31 |
| 1 | 16S1 | 1055 | A | C5-C4 | -6.53 | 1.34 | 1.38 |
| 1 | 16S1 | 1067 | A | C5-C4 | -6.53 | 1.34 | 1.38 |
| 22 | 23S1 | 368 | A | C8-N7 | 6.53 | 1.36 | 1.31 |
| 1 | 16S1 | 743 | A | C5-C4 | -6.52 | 1.34 | 1.38 |
| 22 | 23S1 | 1032 | A | C5-C4 | -6.52 | 1.34 | 1.38 |
| 22 | 23S1 | 1705 | A | C5-C4 | -6.52 | 1.34 | 1.38 |
| 1 | 16S1 | 781 | A | C5-C4 | -6.52 | 1.34 | 1.38 |
| 22 | 23S1 | 788 | A | C5-C4 | -6.52 | 1.34 | 1.38 |
| 1 | 16S1 | 389 | A | C8-N7 | 6.52 | 1.36 | 1.31 |
| 22 | 23S1 | 2736 | A | C5-C4 | -6.52 | 1.34 | 1.38 |
| 22 | 23S1 | 2823 | A | C5-C4 | -6.52 | 1.34 | 1.38 |
| 22 | 23S1 | 505 | A | C5-C4 | -6.52 | 1.34 | 1.38 |
| 22 | 23S1 | 1226 | A | C5-C4 | -6.52 | 1.34 | 1.38 |
| 22 | 23S1 | 1378 | A | C5-C4 | -6.52 | 1.34 | 1.38 |
| 22 | 23S1 | 1522 | A | C8-N7 | 6.52 | 1.36 | 1.31 |
| 22 | 23S1 | 1654 | A | C5-C4 | -6.52 | 1.34 | 1.38 |
| 1 | 16S1 | 1280 | A | C5-C4 | -6.51 | 1.34 | 1.38 |
| 1 | 16S1 | 1360 | A | C8-N7 | 6.51 | 1.36 | 1.31 |
| 1 | 16S1 | 1377 | A | C8-N7 | 6.51 | 1.36 | 1.31 |
| 22 | 23S1 | 2227 | A | C5-C4 | -6.51 | 1.34 | 1.38 |
| 55 | PTR1 | 69 | A | C8-N7 | 6.51 | 1.36 | 1.31 |
| 1 | 16S1 | 510 | A | C5-C4 | -6.51 | 1.34 | 1.38 |
| 22 | 23S1 | 761 | A | C8-N7 | 6.51 | 1.36 | 1.31 |
| 22 | 23S1 | 2169 | A | C8-N7 | 6.51 | 1.36 | 1.31 |
| 1 | 16S1 | 1196 | A | C8-N7 | 6.51 | 1.36 | 1.31 |
| 1 | 16S1 | 1287 | A | C5-C4 | -6.51 | 1.34 | 1.38 |
| 22 | 23S1 | 190 | A | C5-C4 | -6.51 | 1.34 | 1.38 |
| 22 | 23S1 | 1073 | A | N3-C4 | 6.51 | 1.38 | 1.34 |
| 22 | 23S1 | 2392 | A | C5-C4 | -6.51 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 1014 | A | C5-C4 | -6.51 | 1.34 | 1.38 |
| 22 | 23S1 | 1048 | A | C8-N7 | 6.51 | 1.36 | 1.31 |
| 22 | 23S1 | 1246 | A | C5-C4 | -6.51 | 1.34 | 1.38 |
| 22 | 23S1 | 1260 | A | C5-C4 | -6.51 | 1.34 | 1.38 |
| 22 | 23S1 | 2033 | A | C5-C4 | -6.51 | 1.34 | 1.38 |
| 22 | 23S1 | 2418 | A | C5-C4 | -6.50 | 1.34 | 1.38 |
| 1 | 16S1 | 1288 | A | C5-C4 | -6.50 | 1.34 | 1.38 |
| 1 | 16S1 | 411 | A | C5-C4 | -6.50 | 1.34 | 1.38 |
| 1 | 16S1 | 502 | A | C5-C4 | -6.50 | 1.34 | 1.38 |
| 1 | 16S1 | 600 | A | C8-N7 | 6.50 | 1.36 | 1.31 |
| 1 | 16S1 | 1340 | A | C8-N7 | 6.50 | 1.36 | 1.31 |
| 22 | 23S1 | 219 | A | C5-C4 | -6.50 | 1.34 | 1.38 |
| 22 | 23S1 | 1469 | A | C5-C4 | -6.50 | 1.34 | 1.38 |
| 23 | 05S1 | 109 | A | C5-C4 | -6.50 | 1.34 | 1.38 |
| 1 | 16S1 | 498 | A | C8-N7 | 6.50 | 1.36 | 1.31 |
| 22 | 23S1 | 74 | A | C8-N7 | 6.50 | 1.36 | 1.31 |
| 22 | 23S1 | 1490 | A | C8-N7 | 6.50 | 1.36 | 1.31 |
| 1 | 16S1 | 315 | A | C5-C4 | -6.49 | 1.34 | 1.38 |
| 22 | 23S1 | 362 | A | N3-C4 | 6.49 | 1.38 | 1.34 |
| 22 | 23S1 | 21 | A | C5-C4 | -6.49 | 1.34 | 1.38 |
| 22 | 23S1 | 460 | A | C5-C4 | -6.49 | 1.34 | 1.38 |
| 22 | 23S1 | 1032 | A | C8-N7 | 6.49 | 1.36 | 1.31 |
| 22 | 23S1 | 167 | A | C5-C4 | -6.49 | 1.34 | 1.38 |
| 1 | 16S1 | 1394 | A | C5-C4 | -6.49 | 1.34 | 1.38 |
| 22 | 23S1 | 340 | A | C8-N7 | 6.49 | 1.36 | 1.31 |
| 22 | 23S1 | 1978 | A | C5-C4 | -6.49 | 1.34 | 1.38 |
| 22 | 23S1 | 42 | A | C8-N7 | 6.48 | 1.36 | 1.31 |
| 22 | 23S1 | 637 | A | C8-N7 | 6.48 | 1.36 | 1.31 |
| 22 | 23S1 | 1084 | A | N3-C4 | 6.48 | 1.38 | 1.34 |
| 22 | 23S1 | 2198 | A | C5-C4 | -6.48 | 1.34 | 1.38 |
| 1 | 16S1 | 1163 | A | N3-C4 | 6.48 | 1.38 | 1.34 |
| 22 | 23S1 | 95 | A | C8-N7 | 6.48 | 1.36 | 1.31 |
| 22 | 23S1 | 1069 | A | N3-C4 | 6.48 | 1.38 | 1.34 |
| 22 | 23S1 | 1287 | A | C5-C4 | -6.48 | 1.34 | 1.38 |
| 22 | 23S1 | 2566 | A | C8-N7 | 6.48 | 1.36 | 1.31 |
| 1 | 16S1 | 946 | A | C5-C4 | -6.48 | 1.34 | 1.38 |
| 22 | 23S1 | 1551 | A | C5-C4 | -6.48 | 1.34 | 1.38 |
| 22 | 23S1 | 324 | A | C5-C4 | -6.48 | 1.34 | 1.38 |
| 1 | 16S1 | 482 | A | C8-N7 | 6.47 | 1.36 | 1.31 |
| 22 | 23S1 | 1749 | A | C5-C4 | -6.47 | 1.34 | 1.38 |
| 1 | 16S1 | 602 | A | C5-C4 | -6.47 | 1.34 | 1.38 |
| 1 | 16S1 | 673 | A | C5-C4 | -6.47 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 16S1 | 182 | A | C8-N7 | 6.47 | 1.36 | 1.31 |
| 1 | 16S1 | 958 | A | C8-N7 | 6.47 | 1.36 | 1.31 |
| 55 | PTR1 | 42 | A | C8-N7 | 6.47 | 1.36 | 1.31 |
| 22 | 23S1 | 699 | A | C5-C4 | -6.47 | 1.34 | 1.38 |
| 22 | 23S1 | 270 | A | C8-N7 | 6.47 | 1.36 | 1.31 |
| 22 | 23S1 | 1545 | A | C8-N7 | 6.47 | 1.36 | 1.31 |
| 1 | 16S1 | 560 | A | C5-C4 | -6.46 | 1.34 | 1.38 |
| 1 | 16S1 | 1306 | A | C5-C4 | -6.46 | 1.34 | 1.38 |
| 22 | 23S1 | 2135 | A | C8-N7 | 6.46 | 1.36 | 1.31 |
| 1 | 16S1 | 1005 | A | N3-C4 | 6.46 | 1.38 | 1.34 |
| 22 | 23S1 | 1230 | A | C5-C4 | -6.46 | 1.34 | 1.38 |
| 22 | 23S1 | 2311 | A | C8-N7 | 6.46 | 1.36 | 1.31 |
| 1 | 16S1 | 640 | A | C8-N7 | 6.46 | 1.36 | 1.31 |
| 1 | 16S1 | 766 | A | C8-N7 | 6.46 | 1.36 | 1.31 |
| 22 | 23S1 | 575 | A | C5-C4 | -6.46 | 1.34 | 1.38 |
| 22 | 23S1 | 621 | A | C5-C4 | -6.46 | 1.34 | 1.38 |
| 22 | 23S1 | 1096 | A | N3-C4 | 6.46 | 1.38 | 1.34 |
| 22 | 23S1 | 1603 | A | C5-C4 | -6.46 | 1.34 | 1.38 |
| 22 | 23S1 | 2062 | A | C8-N7 | 6.46 | 1.36 | 1.31 |
| 22 | 23S1 | 2322 | A | C5-C4 | -6.46 | 1.34 | 1.38 |
| 22 | 23S1 | 181 | A | C8-N7 | 6.46 | 1.36 | 1.31 |
| 22 | 23S1 | 1960 | A | C8-N7 | 6.46 | 1.36 | 1.31 |
| 1 | 16S1 | 831 | A | C8-N7 | 6.46 | 1.36 | 1.31 |
| 22 | 23S1 | 734 | A | C5-C4 | -6.46 | 1.34 | 1.38 |
| 22 | 23S1 | 1477 | A | C8-N7 | 6.46 | 1.36 | 1.31 |
| 22 | 23S1 | 270 | A | C5-C4 | -6.45 | 1.34 | 1.38 |
| 22 | 23S1 | 1551 | A | C8-N7 | 6.45 | 1.36 | 1.31 |
| 1 | 16S1 | 33 | A | C5-C4 | -6.45 | 1.34 | 1.38 |
| 23 | 05S1 | 46 | A | C5-C4 | -6.45 | 1.34 | 1.38 |
| 55 | PTR1 | 76 | A | C5-C4 | -6.45 | 1.34 | 1.38 |
| 1 | 16S1 | 1155 | A | C8-N7 | 6.45 | 1.36 | 1.31 |
| 22 | 23S1 | 1785 | A | C5-C4 | -6.45 | 1.34 | 1.38 |
| 22 | 23S1 | 2706 | A | C5-C4 | -6.45 | 1.34 | 1.38 |
| 1 | 16S1 | 199 | A | C8-N7 | 6.45 | 1.36 | 1.31 |
| 1 | 16S1 | 374 | A | C8-N7 | 6.45 | 1.36 | 1.31 |
| 1 | 16S1 | 325 | A | C8-N7 | 6.45 | 1.36 | 1.31 |
| 1 | 16S1 | 363 | A | C8-N7 | 6.45 | 1.36 | 1.31 |
| 1 | 16S1 | 622 | A | C5-C4 | -6.45 | 1.34 | 1.38 |
| 1 | 16S1 | 675 | A | C5-C4 | -6.45 | 1.34 | 1.38 |
| 22 | 23S1 | 1169 | A | C8-N7 | 6.45 | 1.36 | 1.31 |
| 22 | 23S1 | 2482 | A | C5-C4 | -6.45 | 1.34 | 1.38 |
| 1 | 16S1 | 665 | A | C8-N7 | 6.44 | 1.36 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 16S1 | 1502 | A | C5-C4 | -6.44 | 1.34 | 1.38 |
| 22 | 23S1 | 866 | A | C5-C4 | -6.44 | 1.34 | 1.38 |
| 22 | 23S1 | 1284 | A | C8-N7 | 6.44 | 1.36 | 1.31 |
| 23 | 05S1 | 115 | A | C8-N7 | 6.44 | 1.36 | 1.31 |
| 22 | 23S1 | 282 | A | N3-C4 | 6.44 | 1.38 | 1.34 |
| 22 | 23S1 | 804 | A | C8-N7 | 6.44 | 1.36 | 1.31 |
| 1 | 16S1 | 162 | A | N7-C5 | -6.44 | 1.35 | 1.39 |
| 22 | 23S1 | 782 | A | C5-C4 | -6.44 | 1.34 | 1.38 |
| 1 | 16S1 | 1362 | A | C5-C4 | -6.44 | 1.34 | 1.38 |
| 1 | 16S1 | 315 | A | C8-N7 | 6.43 | 1.36 | 1.31 |
| 1 | 16S1 | 509 | A | C5-C4 | -6.43 | 1.34 | 1.38 |
| 22 | 23S1 | 526 | A | C5-C4 | -6.43 | 1.34 | 1.38 |
| 22 | 23S1 | 632 | A | C5-C4 | -6.43 | 1.34 | 1.38 |
| 22 | 23S1 | 783 | A | N3-C4 | 6.43 | 1.38 | 1.34 |
| 22 | 23S1 | 2761 | A | C8-N7 | 6.43 | 1.36 | 1.31 |
| 22 | 23S1 | 1960 | A | C5-C4 | -6.43 | 1.34 | 1.38 |
| 22 | 23S1 | 959 | A | C5-C4 | -6.43 | 1.34 | 1.38 |
| 22 | 23S1 | 1385 | A | C8-N7 | 6.43 | 1.36 | 1.31 |
| 1 | 16S1 | 1287 | A | C8-N7 | 6.43 | 1.36 | 1.31 |
| 22 | 23S1 | 241 | A | C5-C4 | -6.43 | 1.34 | 1.38 |
| 22 | 23S1 | 1205 | A | C5-C4 | -6.43 | 1.34 | 1.38 |
| 22 | 23S1 | 1754 | A | C5-C4 | -6.43 | 1.34 | 1.38 |
| 23 | 05S1 | 50 | A | C8-N7 | 6.43 | 1.36 | 1.31 |
| 23 | 05S1 | 108 | A | C8-N7 | 6.43 | 1.36 | 1.31 |
| 1 | 16S1 | 496 | A | N3-C4 | 6.43 | 1.38 | 1.34 |
| 22 | 23S1 | 2560 | A | C5-C4 | -6.43 | 1.34 | 1.38 |
| 1 | 16S1 | 493 | A | C8-N7 | 6.43 | 1.36 | 1.31 |
| 1 | 16S1 | 1117 | A | C8-N7 | 6.43 | 1.36 | 1.31 |
| 1 | 16S1 | 1250 | A | C5-C4 | -6.43 | 1.34 | 1.38 |
| 22 | 23S1 | 432 | A | C5-C4 | -6.43 | 1.34 | 1.38 |
| 22 | 23S1 | 1014 | A | C8-N7 | 6.43 | 1.36 | 1.31 |
| 22 | 23S1 | 1194 | A | C5-C4 | -6.43 | 1.34 | 1.38 |
| 22 | 23S1 | 2101 | A | N3-C4 | 6.43 | 1.38 | 1.34 |
| 1 | 16S1 | 1248 | A | C8-N7 | 6.42 | 1.36 | 1.31 |
| 22 | 23S1 | 309 | A | C5-C4 | -6.42 | 1.34 | 1.38 |
| 22 | 23S1 | 1285 | A | C5-C4 | -6.42 | 1.34 | 1.38 |
| 22 | 23S1 | 2899 | A | C5-C4 | -6.42 | 1.34 | 1.38 |
| 1 | 16S1 | 1413 | A | C5-C4 | -6.42 | 1.34 | 1.38 |
| 22 | 23S1 | 265 | A | C8-N7 | 6.42 | 1.36 | 1.31 |
| 22 | 23S1 | 621 | A | C8-N7 | 6.42 | 1.36 | 1.31 |
| 22 | 23S1 | 655 | A | C5-C4 | -6.42 | 1.34 | 1.38 |
| 22 | 23S1 | 900 | A | N3-C4 | 6.42 | 1.38 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 1040 | A | C8-N7 | 6.42 | 1.36 | 1.31 |
| 22 | 23S1 | 2835 | A | C5-C4 | -6.42 | 1.34 | 1.38 |
| 1 | 16S1 | 1408 | A | C5-C4 | -6.42 | 1.34 | 1.38 |
| 1 | 16S1 | 344 | A | C8-N7 | 6.42 | 1.36 | 1.31 |
| 1 | 16S1 | 353 | A | C8-N7 | 6.42 | 1.36 | 1.31 |
| 22 | 23S1 | 1717 | A | C5-C4 | -6.42 | 1.34 | 1.38 |
| 22 | 23S1 | 2813 | A | C5-C4 | -6.42 | 1.34 | 1.38 |
| 1 | 16S1 | 65 | A | C8-N7 | 6.42 | 1.36 | 1.31 |
| 22 | 23S1 | 155 | A | C5-C4 | -6.42 | 1.34 | 1.38 |
| 1 | 16S1 | 1229 | A | C8-N7 | 6.41 | 1.36 | 1.31 |
| 22 | 23S1 | 89 | A | C5-C4 | -6.41 | 1.34 | 1.38 |
| 22 | 23S1 | 5 | A | N3-C4 | 6.41 | 1.38 | 1.34 |
| 1 | 16S1 | 1080 | A | C5-C4 | -6.41 | 1.34 | 1.38 |
| 22 | 23S1 | 980 | A | C5-C4 | -6.41 | 1.34 | 1.38 |
| 22 | 23S1 | 878 | A | N3-C4 | 6.41 | 1.38 | 1.34 |
| 22 | 23S1 | 1336 | A | C5-C4 | -6.41 | 1.34 | 1.38 |
| 23 | 05S1 | 58 | A | C8-N7 | 6.41 | 1.36 | 1.31 |
| 1 | 16S1 | 77 | A | C8-N7 | 6.41 | 1.36 | 1.31 |
| 22 | 23S1 | 2335 | A | C5-C4 | -6.41 | 1.34 | 1.38 |
| 1 | 16S1 | 336 | A | C5-C4 | -6.41 | 1.34 | 1.38 |
| 1 | 16S1 | 1180 | A | C8-N7 | 6.41 | 1.36 | 1.31 |
| 22 | 23S1 | 2205 | A | C8-N7 | 6.41 | 1.36 | 1.31 |
| 22 | 23S1 | 2434 | A | C5-C4 | -6.41 | 1.34 | 1.38 |
| 1 | 16S1 | 535 | A | C5-C4 | -6.40 | 1.34 | 1.38 |
| 22 | 23S1 | 1359 | A | C5-C4 | -6.40 | 1.34 | 1.38 |
| 22 | 23S1 | 1301 | A | C5-C4 | -6.40 | 1.34 | 1.38 |
| 22 | 23S1 | 1634 | A | C8-N7 | 6.40 | 1.36 | 1.31 |
| 1 | 16S1 | 120 | A | C5-C4 | -6.40 | 1.34 | 1.38 |
| 1 | 16S1 | 819 | A | C5-C4 | -6.40 | 1.34 | 1.38 |
| 1 | 16S1 | 1022 | A | N3-C4 | 6.40 | 1.38 | 1.34 |
| 22 | 23S1 | 1597 | A | C5-C4 | -6.40 | 1.34 | 1.38 |
| 1 | 16S1 | 1021 | A | N3-C4 | 6.40 | 1.38 | 1.34 |
| 22 | 23S1 | 1040 | A | C5-C4 | -6.40 | 1.34 | 1.38 |
| 23 | 05S1 | 104 | A | C8-N7 | 6.40 | 1.36 | 1.31 |
| 22 | 23S1 | 1927 | A | C5-C4 | -6.40 | 1.34 | 1.38 |
| 1 | 16S1 | 919 | A | C5-C4 | -6.39 | 1.34 | 1.38 |
| 1 | 16S1 | 1476 | A | C5-C4 | -6.39 | 1.34 | 1.38 |
| 22 | 23S1 | 332 | A | C8-N7 | 6.39 | 1.36 | 1.31 |
| 22 | 23S1 | 2108 | A | N3-C4 | 6.39 | 1.38 | 1.34 |
| 22 | 23S1 | 2530 | A | C5-C4 | -6.39 | 1.34 | 1.38 |
| 1 | 16S1 | 1004 | A | C8-N7 | 6.39 | 1.36 | 1.31 |
| 22 | 23S1 | 1597 | A | C8-N7 | 6.39 | 1.36 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 2094 | A | C8-N7 | 6.39 | 1.36 | 1.31 |
| 22 | 23S1 | 2471 | A | C5-C4 | -6.39 | 1.34 | 1.38 |
| 1 | 16S1 | 1465 | A | C8-N7 | 6.39 | 1.36 | 1.31 |
| 22 | 23S1 | 522 | A | C5-C4 | -6.39 | 1.34 | 1.38 |
| 22 | 23S1 | 299 | A | C5-C4 | -6.39 | 1.34 | 1.38 |
| 22 | 23S1 | 382 | A | C5-C4 | -6.39 | 1.34 | 1.38 |
| 22 | 23S1 | 2435 | A | C5-C4 | -6.39 | 1.34 | 1.38 |
| 22 | 23S1 | 2809 | A | C8-N7 | 6.39 | 1.36 | 1.31 |
| 1 | 16S1 | 50 | A | N3-C4 | 6.39 | 1.38 | 1.34 |
| 1 | 16S1 | 1398 | A | C8-N7 | 6.39 | 1.36 | 1.31 |
| 22 | 23S1 | 820 | A | C5-C4 | -6.39 | 1.34 | 1.38 |
| 22 | 23S1 | 213 | A | C8-N7 | 6.38 | 1.36 | 1.31 |
| 1 | 16S1 | 913 | A | C8-N7 | 6.38 | 1.36 | 1.31 |
| 1 | 16S1 | 1167 | A | C8-N7 | 6.38 | 1.36 | 1.31 |
| 22 | 23S1 | 217 | A | C5-C4 | -6.38 | 1.34 | 1.38 |
| 22 | 23S1 | 262 | A | C8-N7 | 6.38 | 1.36 | 1.31 |
| 1 | 16S1 | 1319 | A | C8-N7 | 6.38 | 1.36 | 1.31 |
| 22 | 23S1 | 627 | A | C5-C4 | -6.38 | 1.34 | 1.38 |
| 22 | 23S1 | 1496 | A | C8-N7 | 6.38 | 1.36 | 1.31 |
| 22 | 23S1 | 1794 | A | C5-C4 | -6.38 | 1.34 | 1.38 |
| 1 | 16S1 | 1236 | A | C8-N7 | 6.38 | 1.36 | 1.31 |
| 22 | 23S1 | 332 | A | C5-C4 | -6.38 | 1.34 | 1.38 |
| 22 | 23S1 | 219 | A | C8-N7 | 6.38 | 1.36 | 1.31 |
| 22 | 23S1 | 1746 | A | C8-N7 | 6.38 | 1.36 | 1.31 |
| 22 | 23S1 | 2060 | A | C8-N7 | 6.38 | 1.36 | 1.31 |
| 22 | 23S1 | 917 | A | C5-C4 | -6.37 | 1.34 | 1.38 |
| 22 | 23S1 | 1698 | A | C5-C4 | -6.37 | 1.34 | 1.38 |
| 22 | 23S1 | 1700 | A | C5-C4 | -6.37 | 1.34 | 1.38 |
| 22 | 23S1 | 2119 | A | N3-C4 | 6.37 | 1.38 | 1.34 |
| 22 | 23S1 | 146 | A | C8-N7 | 6.37 | 1.36 | 1.31 |
| 22 | 23S1 | 221 | A | C8-N7 | 6.37 | 1.36 | 1.31 |
| 22 | 23S1 | 2761 | A | C5-C4 | -6.37 | 1.34 | 1.38 |
| 1 | 16S1 | 171 | A | C5-C4 | -6.37 | 1.34 | 1.38 |
| 1 | 16S1 | 353 | A | C5-C4 | -6.37 | 1.34 | 1.38 |
| 1 | 16S1 | 383 | A | N7-C5 | -6.37 | 1.35 | 1.39 |
| 22 | 23S1 | 2679 | A | C5-C4 | -6.37 | 1.34 | 1.38 |
| 1 | 16S1 | 109 | A | C5-C4 | -6.37 | 1.34 | 1.38 |
| 22 | 23S1 | 1321 | A | C8-N7 | 6.37 | 1.36 | 1.31 |
| 22 | 23S1 | 103 | A | C8-N7 | 6.37 | 1.36 | 1.31 |
| 22 | 23S1 | 2297 | A | C8-N7 | 6.37 | 1.36 | 1.31 |
| 1 | 16S1 | 66 | A | C8-N7 | 6.36 | 1.36 | 1.31 |
| 22 | 23S1 | 1237 | A | C8-N7 | 6.36 | 1.36 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 16S1 | 969 | A | C8-N7 | 6.36 | 1.36 | 1.31 |
| 22 | 23S1 | 2531 | A | C8-N7 | 6.36 | 1.36 | 1.31 |
| 22 | 23S1 | 2800 | A | C5-C4 | -6.36 | 1.34 | 1.38 |
| 23 | 05S1 | 115 | A | C5-C4 | -6.36 | 1.34 | 1.38 |
| 1 | 16S1 | 7 | A | C8-N7 | 6.36 | 1.36 | 1.31 |
| 1 | 16S1 | 498 | A | N3-C4 | 6.36 | 1.38 | 1.34 |
| 22 | 23S1 | 453 | A | C5-C4 | -6.36 | 1.34 | 1.38 |
| 22 | 23S1 | 1787 | A | C5-C4 | -6.36 | 1.34 | 1.38 |
| 22 | 23S1 | 1876 | A | C8-N7 | 6.36 | 1.36 | 1.31 |
| 1 | 16S1 | 250 | A | N3-C4 | 6.36 | 1.38 | 1.34 |
| 22 | 23S1 | 508 | A | N3-C4 | 6.36 | 1.38 | 1.34 |
| 22 | 23S1 | 1609 | A | C5-C4 | -6.36 | 1.34 | 1.38 |
| 22 | 23S1 | 2725 | A | C5-C4 | -6.36 | 1.34 | 1.38 |
| 22 | 23S1 | 1918 | A | C8-N7 | 6.35 | 1.35 | 1.31 |
| 22 | 23S1 | 1569 | A | C5-C4 | -6.35 | 1.34 | 1.38 |
| 23 | 05S1 | 73 | A | N3-C4 | 6.35 | 1.38 | 1.34 |
| 1 | 16S1 | 535 | A | C8-N7 | 6.35 | 1.35 | 1.31 |
| 1 | 16S1 | 1157 | A | C8-N7 | 6.35 | 1.35 | 1.31 |
| 22 | 23S1 | 819 | A | C5-C4 | -6.35 | 1.34 | 1.38 |
| 22 | 23S1 | 1009 | A | C5-C4 | -6.35 | 1.34 | 1.38 |
| 22 | 23S1 | 1899 | A | C5-C4 | -6.35 | 1.34 | 1.38 |
| 22 | 23S1 | 1987 | A | C5-C4 | -6.35 | 1.34 | 1.38 |
| 22 | 23S1 | 262 | A | C5-C4 | -6.35 | 1.34 | 1.38 |
| 22 | 23S1 | 721 | A | C8-N7 | 6.35 | 1.35 | 1.31 |
| 22 | 23S1 | 2821 | A | C5-C4 | -6.35 | 1.34 | 1.38 |
| 22 | 23S1 | 1265 | A | C5-C4 | -6.35 | 1.34 | 1.38 |
| 1 | 16S1 | 459 | A | N3-C4 | 6.34 | 1.38 | 1.34 |
| 1 | 16S1 | 1428 | A | C5-C4 | -6.34 | 1.34 | 1.38 |
| 22 | 23S1 | 213 | A | N3-C4 | 6.34 | 1.38 | 1.34 |
| 22 | 23S1 | 347 | A | C8-N7 | 6.34 | 1.35 | 1.31 |
| 22 | 23S1 | 478 | A | C5-C4 | -6.34 | 1.34 | 1.38 |
| 22 | 23S1 | 616 | A | C5-C4 | -6.34 | 1.34 | 1.38 |
| 22 | 23S1 | 1586 | A | C8-N7 | 6.34 | 1.35 | 1.31 |
| 22 | 23S1 | 1001 | A | C5-C4 | -6.34 | 1.34 | 1.38 |
| 22 | 23S1 | 2814 | A | C5-C4 | -6.34 | 1.34 | 1.38 |
| 1 | 16S1 | 71 | A | C8-N7 | 6.34 | 1.35 | 1.31 |
| 1 | 16S1 | 1252 | A | N3-C4 | 6.34 | 1.38 | 1.34 |
| 22 | 23S1 | 1269 | A | C5-C4 | -6.34 | 1.34 | 1.38 |
| 22 | 23S1 | 1384 | A | C5-C4 | -6.34 | 1.34 | 1.38 |
| 23 | 05S1 | 94 | A | C5-C4 | -6.34 | 1.34 | 1.38 |
| 1 | 16S1 | 860 | A | C8-N7 | 6.34 | 1.35 | 1.31 |
| 1 | 16S1 | 499 | A | C5-C4 | -6.34 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 16S1 | 889 | A | C8-N7 | 6.34 | 1.35 | 1.31 |
| 1 | 16S1 | 1227 | A | C8-N7 | 6.34 | 1.35 | 1.31 |
| 22 | 23S1 | 21 | A | C8-N7 | 6.34 | 1.35 | 1.31 |
| 22 | 23S1 | 2080 | A | C5-C4 | -6.34 | 1.34 | 1.38 |
| 22 | 23S1 | 2468 | A | C5-C4 | -6.34 | 1.34 | 1.38 |
| 1 | 16S1 | 1117 | A | C5-C4 | -6.33 | 1.34 | 1.38 |
| 1 | 16S1 | 309 | A | C8-N7 | 6.33 | 1.35 | 1.31 |
| 1 | 16S1 | 349 | A | C8-N7 | 6.33 | 1.35 | 1.31 |
| 1 | 16S1 | 547 | A | C8-N7 | 6.33 | 1.35 | 1.31 |
| 1 | 16S1 | 1000 | A | N3-C4 | 6.33 | 1.38 | 1.34 |
| 22 | 23S1 | 513 | A | N7-C5 | -6.33 | 1.35 | 1.39 |
| 22 | 23S1 | 2314 | A | C8-N7 | 6.33 | 1.35 | 1.31 |
| 22 | 23S1 | 84 | A | C5-C4 | -6.33 | 1.34 | 1.38 |
| 22 | 23S1 | 371 | A | C5-C4 | -6.33 | 1.34 | 1.38 |
| 22 | 23S1 | 401 | A | C5-C4 | -6.33 | 1.34 | 1.38 |
| 22 | 23S1 | 1080 | A | N3-C4 | 6.33 | 1.38 | 1.34 |
| 1 | 16S1 | 1503 | A | C5-C4 | -6.33 | 1.34 | 1.38 |
| 22 | 23S1 | 2453 | A | C5-C4 | -6.33 | 1.34 | 1.38 |
| 22 | 23S1 | 231 | A | C8-N7 | 6.33 | 1.35 | 1.31 |
| 22 | 23S1 | 311 | A | C8-N7 | 6.33 | 1.35 | 1.31 |
| 22 | 23S1 | 1103 | A | N3-C4 | 6.33 | 1.38 | 1.34 |
| 1 | 16S1 | 892 | A | C5-C4 | -6.32 | 1.34 | 1.38 |
| 1 | 16S1 | 1082 | A | C5-C4 | -6.32 | 1.34 | 1.38 |
| 22 | 23S1 | 1385 | A | C5-C4 | -6.32 | 1.34 | 1.38 |
| 22 | 23S1 | 2268 | A | C5-C4 | -6.32 | 1.34 | 1.38 |
| 22 | 23S1 | 2433 | A | C5-C4 | -6.32 | 1.34 | 1.38 |
| 22 | 23S1 | 2448 | A | C8-N7 | 6.32 | 1.35 | 1.31 |
| 1 | 16S1 | 1191 | A | C8-N7 | 6.32 | 1.35 | 1.31 |
| 22 | 23S1 | 1745 | A | C8-N7 | 6.32 | 1.35 | 1.31 |
| 1 | 16S1 | 1163 | A | C8-N7 | 6.32 | 1.35 | 1.31 |
| 1 | 16S1 | 1483 | A | C5-C4 | -6.32 | 1.34 | 1.38 |
| 22 | 23S1 | 422 | A | C5-C4 | -6.32 | 1.34 | 1.38 |
| 22 | 23S1 | 2176 | A | N3-C4 | 6.32 | 1.38 | 1.34 |
| 22 | 23S1 | 2317 | A | C8-N7 | 6.32 | 1.35 | 1.31 |
| 22 | 23S1 | 2635 | A | C8-N7 | 6.32 | 1.35 | 1.31 |
| 1 | 16S1 | 303 | A | C5-C4 | -6.32 | 1.34 | 1.38 |
| 1 | 16S1 | 393 | A | C8-N7 | 6.32 | 1.35 | 1.31 |
| 1 | 16S1 | 969 | A | C5-C4 | -6.32 | 1.34 | 1.38 |
| 1 | 16S1 | 1225 | A | C8-N7 | 6.32 | 1.35 | 1.31 |
| 22 | 23S1 | 244 | A | C5-C4 | -6.32 | 1.34 | 1.38 |
| 22 | 23S1 | 2212 | A | C8-N7 | 6.32 | 1.35 | 1.31 |
| 1 | 16S1 | 338 | A | C5-C4 | -6.32 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 541 | A | C8-N7 | 6.31 | 1.35 | 1.31 |
| 1 | 16S1 | 780 | A | C5-C4 | -6.31 | 1.34 | 1.38 |
| 1 | 16S1 | 908 | A | C5-C4 | -6.31 | 1.34 | 1.38 |
| 1 | 16S1 | 1437 | A | C5-C4 | -6.31 | 1.34 | 1.38 |
| 22 | 23S1 | 176 | A | C8-N7 | 6.31 | 1.35 | 1.31 |
| 22 | 23S1 | 382 | A | C8-N7 | 6.31 | 1.35 | 1.31 |
| 22 | 23S1 | 1103 | A | C8-N7 | 6.31 | 1.35 | 1.31 |
| 22 | 23S1 | 2469 | A | C8-N7 | 6.31 | 1.35 | 1.31 |
| 1 | 16S1 | 676 | A | C8-N7 | 6.31 | 1.35 | 1.31 |
| 1 | 16S1 | 1418 | A | C5-C4 | -6.31 | 1.34 | 1.38 |
| 1 | 16S1 | 1437 | A | C8-N7 | 6.31 | 1.35 | 1.31 |
| 22 | 23S1 | 1525 | A | C5-C4 | -6.31 | 1.34 | 1.38 |
| 22 | 23S1 | 1773 | A | C5-C4 | -6.31 | 1.34 | 1.38 |
| 22 | 23S1 | 2176 | A | C8-N7 | 6.31 | 1.35 | 1.31 |
| 55 | PTR1 | 73 | A | C8-N7 | 6.31 | 1.35 | 1.31 |
| 22 | 23S1 | 513 | A | C5-C4 | -6.30 | 1.34 | 1.38 |
| 22 | 23S1 | 2829 | A | C5-C4 | -6.30 | 1.34 | 1.38 |
| 22 | 23S1 | 2461 | A | C5-C4 | -6.30 | 1.34 | 1.38 |
| 22 | 23S1 | 483 | A | C8-N7 | 6.30 | 1.35 | 1.31 |
| 22 | 23S1 | 996 | A | C5-C4 | -6.30 | 1.34 | 1.38 |
| 22 | 23S1 | 1156 | A | C5-C4 | -6.30 | 1.34 | 1.38 |
| 22 | 23S1 | 1901 | A | C5-C4 | -6.30 | 1.34 | 1.38 |
| 22 | 23S1 | 2225 | A | C5-C4 | -6.30 | 1.34 | 1.38 |
| 22 | 23S1 | 1504 | A | C5-C4 | -6.30 | 1.34 | 1.38 |
| 22 | 23S1 | 1522 | A | C5-C4 | -6.30 | 1.34 | 1.38 |
| 22 | 23S1 | 1858 | A | C5-C4 | -6.30 | 1.34 | 1.38 |
| 22 | 23S1 | 2542 | A | C8-N7 | 6.30 | 1.35 | 1.31 |
| 22 | 23S1 | 2734 | A | C8-N7 | 6.30 | 1.35 | 1.31 |
| 1 | 16S1 | 889 | A | C5-C4 | -6.29 | 1.34 | 1.38 |
| 22 | 23S1 | 218 | A | C5-C4 | -6.29 | 1.34 | 1.38 |
| 22 | 23S1 | 2781 | A | C5-C4 | -6.29 | 1.34 | 1.38 |
| 1 | 16S1 | 913 | A | C5-C4 | -6.29 | 1.34 | 1.38 |
| 1 | 16S1 | 968 | A | C5-C4 | -6.29 | 1.34 | 1.38 |
| 22 | 23S1 | 925 | A | N3-C4 | 6.29 | 1.38 | 1.34 |
| 22 | 23S1 | 1134 | A | C5-C4 | -6.29 | 1.34 | 1.38 |
| 22 | 23S1 | 1134 | A | C8-N7 | 6.29 | 1.35 | 1.31 |
| 22 | 23S1 | 2376 | A | C8-N7 | 6.29 | 1.35 | 1.31 |
| 1 | 16S1 | 50 | A | C8-N7 | 6.29 | 1.35 | 1.31 |
| 22 | 23S1 | 144 | A | N3-C4 | 6.29 | 1.38 | 1.34 |
| 22 | 23S1 | 497 | A | C5-C4 | -6.29 | 1.34 | 1.38 |
| 22 | 23S1 | 2366 | A | C8-N7 | 6.29 | 1.35 | 1.31 |
| 22 | 23S1 | 2439 | A | C5-C4 | -6.29 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 2639 | A | C8-N7 | 6.29 | 1.35 | 1.31 |
| 1 | 16S1 | 26 | A | C8-N7 | 6.29 | 1.35 | 1.31 |
| 22 | 23S1 | 1690 | A | C5-C4 | -6.29 | 1.34 | 1.38 |
| 1 | 16S1 | 1251 | A | C5-C4 | -6.29 | 1.34 | 1.38 |
| 22 | 23S1 | 1127 | A | C5-C4 | -6.29 | 1.34 | 1.38 |
| 22 | 23S1 | 2033 | A | C8-N7 | 6.29 | 1.35 | 1.31 |
| 22 | 23S1 | 2082 | A | C5-C4 | -6.29 | 1.34 | 1.38 |
| 1 | 16S1 | 831 | A | C5-C4 | -6.28 | 1.34 | 1.38 |
| 1 | 16S1 | 1465 | A | C5-C4 | -6.28 | 1.34 | 1.38 |
| 22 | 23S1 | 256 | A | C5-C4 | -6.28 | 1.34 | 1.38 |
| 22 | 23S1 | 1803 | A | C5-C4 | -6.28 | 1.34 | 1.38 |
| 22 | 23S1 | 2513 | A | C5-C4 | -6.28 | 1.34 | 1.38 |
| 1 | 16S1 | 383 | A | N3-C4 | 6.28 | 1.38 | 1.34 |
| 22 | 23S1 | 44 | A | C8-N7 | 6.28 | 1.35 | 1.31 |
| 22 | 23S1 | 294 | A | C8-N7 | 6.28 | 1.35 | 1.31 |
| 22 | 23S1 | 1759 | A | C5-C4 | -6.28 | 1.34 | 1.38 |
| 22 | 23S1 | 2077 | A | C5-C4 | -6.28 | 1.34 | 1.38 |
| 22 | 23S1 | 2288 | A | C8-N7 | 6.28 | 1.35 | 1.31 |
| 1 | 16S1 | 1101 | A | C5-C4 | -6.28 | 1.34 | 1.38 |
| 22 | 23S1 | 391 | A | C5-C4 | -6.28 | 1.34 | 1.38 |
| 22 | 23S1 | 721 | A | C5-C4 | -6.28 | 1.34 | 1.38 |
| 22 | 23S1 | 1336 | A | C8-N7 | 6.28 | 1.35 | 1.31 |
| 22 | 23S1 | 2632 | A | C8-N7 | 6.28 | 1.35 | 1.31 |
| 22 | 23S1 | 2657 | A | C5-C4 | -6.28 | 1.34 | 1.38 |
| 22 | 23S1 | 2810 | A | C8-N7 | 6.28 | 1.35 | 1.31 |
| 22 | 23S1 | 2191 | A | C8-N7 | 6.27 | 1.35 | 1.31 |
| 22 | 23S1 | 443 | A | C5-C4 | -6.27 | 1.34 | 1.38 |
| 22 | 23S1 | 2478 | A | C8-N7 | 6.27 | 1.35 | 1.31 |
| 1 | 16S1 | 937 | A | C5-C4 | -6.27 | 1.34 | 1.38 |
| 22 | 23S1 | 909 | A | C8-N7 | 6.27 | 1.35 | 1.31 |
| 22 | 23S1 | 1821 | A | C5-C4 | -6.27 | 1.34 | 1.38 |
| 22 | 23S1 | 626 | A | C8-N7 | 6.27 | 1.35 | 1.31 |
| 22 | 23S1 | 910 | A | C5-C4 | -6.27 | 1.34 | 1.38 |
| 22 | 23S1 | 1932 | A | C5-C4 | -6.27 | 1.34 | 1.38 |
| 22 | 23S1 | 196 | A | C5-C4 | -6.27 | 1.34 | 1.38 |
| 22 | 23S1 | 241 | A | N3-C4 | 6.27 | 1.38 | 1.34 |
| 1 | 16S1 | 608 | A | C5-C4 | -6.27 | 1.34 | 1.38 |
| 22 | 23S1 | 71 | A | C8-N7 | 6.27 | 1.35 | 1.31 |
| 1 | 16S1 | 2 | A | C8-N7 | 6.26 | 1.35 | 1.31 |
| 22 | 23S1 | 503 | A | C5-C4 | -6.26 | 1.34 | 1.38 |
| 22 | 23S1 | 2478 | A | C5-C4 | -6.26 | 1.34 | 1.38 |
| 22 | 23S1 | 2835 | A | C8-N7 | 6.26 | 1.35 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 16S1 | 935 | A | C5-C4 | -6.26 | 1.34 | 1.38 |
| 22 | 23S1 | 1077 | A | N3-C4 | 6.26 | 1.38 | 1.34 |
| 1 | 16S1 | 937 | A | C8-N7 | 6.26 | 1.35 | 1.31 |
| 22 | 23S1 | 849 | A | C5-C4 | -6.26 | 1.34 | 1.38 |
| 22 | 23S1 | 2518 | A | C5-C4 | -6.26 | 1.34 | 1.38 |
| 22 | 23S1 | 2614 | A | C8-N7 | 6.26 | 1.35 | 1.31 |
| 22 | 23S1 | 2856 | A | C8-N7 | 6.26 | 1.35 | 1.31 |
| 1 | 16S1 | 1374 | A | C5-C4 | -6.26 | 1.34 | 1.38 |
| 1 | 16S1 | 1429 | A | C8-N7 | 6.26 | 1.35 | 1.31 |
| 22 | 23S1 | 477 | A | C5-C4 | -6.26 | 1.34 | 1.38 |
| 22 | 23S1 | 1133 | A | C5-C4 | -6.26 | 1.34 | 1.38 |
| 1 | 16S1 | 1413 | A | C8-N7 | 6.26 | 1.35 | 1.31 |
| 22 | 23S1 | 430 | A | C8-N7 | 6.26 | 1.35 | 1.31 |
| 22 | 23S1 | 984 | A | C5-C4 | -6.26 | 1.34 | 1.38 |
| 1 | 16S1 | 918 | A | C5-C4 | -6.25 | 1.34 | 1.38 |
| 22 | 23S1 | 1579 | A | C5-C4 | -6.25 | 1.34 | 1.38 |
| 22 | 23S1 | 324 | A | C8-N7 | 6.25 | 1.35 | 1.31 |
| 23 | 05S1 | 34 | A | C5-C4 | -6.25 | 1.34 | 1.38 |
| 1 | 16S1 | 1197 | A | C5-C4 | -6.25 | 1.34 | 1.38 |
| 22 | 23S1 | 752 | A | C5-C4 | -6.25 | 1.34 | 1.38 |
| 22 | 23S1 | 2267 | A | C5-C4 | -6.25 | 1.34 | 1.38 |
| 1 | 16S1 | 975 | A | C5-C4 | -6.25 | 1.34 | 1.38 |
| 22 | 23S1 | 501 | A | C8-N7 | 6.25 | 1.35 | 1.31 |
| 1 | 16S1 | 51 | A | C5-C4 | -6.25 | 1.34 | 1.38 |
| 1 | 16S1 | 382 | A | C8-N7 | 6.25 | 1.35 | 1.31 |
| 1 | 16S1 | 298 | A | C8-N7 | 6.24 | 1.35 | 1.31 |
| 1 | 16S1 | 1251 | A | C8-N7 | 6.24 | 1.35 | 1.31 |
| 22 | 23S1 | 470 | A | C5-C4 | -6.24 | 1.34 | 1.38 |
| 22 | 23S1 | 1020 | A | C8-N7 | 6.24 | 1.35 | 1.31 |
| 22 | 23S1 | 454 | A | C5-C4 | -6.24 | 1.34 | 1.38 |
| 22 | 23S1 | 265 | A | C5-C4 | -6.24 | 1.34 | 1.38 |
| 22 | 23S1 | 1378 | A | C8-N7 | 6.24 | 1.35 | 1.31 |
| 22 | 23S1 | 1420 | A | N3-C4 | 6.24 | 1.38 | 1.34 |
| 22 | 23S1 | 2860 | A | C5-C4 | -6.24 | 1.34 | 1.38 |
| 23 | 05S1 | 52 | A | N3-C4 | 6.24 | 1.38 | 1.34 |
| 22 | 23S1 | 156 | A | N3-C4 | 6.24 | 1.38 | 1.34 |
| 1 | 16S1 | 78 | A | C8-N7 | 6.24 | 1.35 | 1.31 |
| 1 | 16S1 | 1368 | A | C8-N7 | 6.24 | 1.35 | 1.31 |
| 22 | 23S1 | 233 | A | C8-N7 | 6.24 | 1.35 | 1.31 |
| 22 | 23S1 | 1877 | A | C8-N7 | 6.24 | 1.35 | 1.31 |
| 22 | 23S1 | 2199 | A | C5-C4 | -6.24 | 1.34 | 1.38 |
| 22 | 23S1 | 320 | A | C5-C4 | -6.23 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 1111 | A | C8-N7 | 6.23 | 1.35 | 1.31 |
| 1 | 16S1 | 901 | A | C5-C4 | -6.23 | 1.34 | 1.38 |
| 22 | 23S1 | 1591 | A | N3-C4 | 6.23 | 1.38 | 1.34 |
| 22 | 23S1 | 447 | A | C5-C4 | -6.23 | 1.34 | 1.38 |
| 22 | 23S1 | 927 | A | C8-N7 | 6.23 | 1.35 | 1.31 |
| 22 | 23S1 | 2799 | A | N3-C4 | 6.23 | 1.38 | 1.34 |
| 22 | 23S1 | 2829 | A | C8-N7 | 6.23 | 1.35 | 1.31 |
| 22 | 23S1 | 1815 | A | C5-C4 | -6.23 | 1.34 | 1.38 |
| 1 | 16S1 | 1201 | A | C5-C4 | -6.23 | 1.34 | 1.38 |
| 22 | 23S1 | 429 | A | C8-N7 | 6.23 | 1.35 | 1.31 |
| 22 | 23S1 | 2288 | A | C5-C4 | -6.23 | 1.34 | 1.38 |
| 1 | 16S1 | 28 | A | C8-N7 | 6.23 | 1.35 | 1.31 |
| 22 | 23S1 | 2639 | A | C5-C4 | -6.23 | 1.34 | 1.38 |
| 55 | PTR1 | 23 | A | N3-C4 | 6.23 | 1.38 | 1.34 |
| 1 | 16S1 | 452 | A | C8-N7 | 6.22 | 1.35 | 1.31 |
| 22 | 23S1 | 528 | A | C5-C4 | -6.22 | 1.34 | 1.38 |
| 22 | 23S1 | 2327 | A | C5-C4 | -6.22 | 1.34 | 1.38 |
| 1 | 16S1 | 1117 | A | N3-C4 | 6.22 | 1.38 | 1.34 |
| 22 | 23S1 | 2191 | A | N3-C4 | 6.22 | 1.38 | 1.34 |
| 1 | 16S1 | 1349 | A | C8-N7 | 6.22 | 1.35 | 1.31 |
| 22 | 23S1 | 1126 | A | C5-C4 | -6.22 | 1.34 | 1.38 |
| 1 | 16S1 | 415 | A | C8-N7 | 6.22 | 1.35 | 1.31 |
| 22 | 23S1 | 743 | A | C5-C4 | -6.22 | 1.34 | 1.38 |
| 1 | 16S1 | 448 | A | C8-N7 | 6.22 | 1.35 | 1.31 |
| 1 | 16S1 | 487 | A | C8-N7 | 6.22 | 1.35 | 1.31 |
| 1 | 16S1 | 288 | A | C8-N7 | 6.22 | 1.35 | 1.31 |
| 1 | 16S1 | 753 | A | C8-N7 | 6.22 | 1.35 | 1.31 |
| 22 | 23S1 | 866 | A | C8-N7 | 6.22 | 1.35 | 1.31 |
| 22 | 23S1 | 1610 | A | C8-N7 | 6.22 | 1.35 | 1.31 |
| 1 | 16S1 | 1430 | A | C8-N7 | 6.21 | 1.35 | 1.31 |
| 22 | 23S1 | 294 | A | C5-C4 | -6.21 | 1.34 | 1.38 |
| 22 | 23S1 | 532 | A | C5-C4 | -6.21 | 1.34 | 1.38 |
| 22 | 23S1 | 1365 | A | C8-N7 | 6.21 | 1.35 | 1.31 |
| 1 | 16S1 | 907 | A | C5-C4 | -6.21 | 1.34 | 1.38 |
| 22 | 23S1 | 449 | A | C5-C4 | -6.21 | 1.34 | 1.38 |
| 1 | 16S1 | 1171 | A | C8-N7 | 6.21 | 1.35 | 1.31 |
| 22 | 23S1 | 541 | A | C5-C4 | -6.21 | 1.34 | 1.38 |
| 22 | 23S1 | 1502 | A | C5-C4 | -6.21 | 1.34 | 1.38 |
| 22 | 23S1 | 1548 | A | C8-N7 | 6.21 | 1.35 | 1.31 |
| 1 | 16S1 | 460 | A | N3-C4 | 6.21 | 1.38 | 1.34 |
| 22 | 23S1 | 2376 | A | C5-C4 | -6.21 | 1.34 | 1.38 |
| 1 | 16S1 | 119 | A | C8-N7 | 6.21 | 1.35 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 666 | A | C5-C4 | -6.21 | 1.34 | 1.38 |
| 22 | 23S1 | 1669 | A | N3-C4 | 6.21 | 1.38 | 1.34 |
| 1 | 16S1 | 873 | A | C5-C4 | -6.21 | 1.34 | 1.38 |
| 1 | 16S1 | 238 | A | C8-N7 | 6.20 | 1.35 | 1.31 |
| 22 | 23S1 | 181 | A | N3-C4 | 6.20 | 1.38 | 1.34 |
| 1 | 16S1 | 465 | A | N3-C4 | 6.20 | 1.38 | 1.34 |
| 23 | 05S1 | 15 | A | C5-C4 | -6.20 | 1.34 | 1.38 |
| 1 | 16S1 | 160 | A | C8-N7 | 6.20 | 1.35 | 1.31 |
| 22 | 23S1 | 195 | A | C5-C4 | -6.20 | 1.34 | 1.38 |
| 22 | 23S1 | 529 | A | C5-C4 | -6.20 | 1.34 | 1.38 |
| 22 | 23S1 | 203 | A | C5-C4 | -6.20 | 1.34 | 1.38 |
| 22 | 23S1 | 348 | A | C8-N7 | 6.20 | 1.35 | 1.31 |
| 22 | 23S1 | 1535 | A | N3-C4 | 6.20 | 1.38 | 1.34 |
| 22 | 23S1 | 2377 | A | C8-N7 | 6.20 | 1.35 | 1.31 |
| 1 | 16S1 | 174 | A | C5-C4 | -6.20 | 1.34 | 1.38 |
| 1 | 16S1 | 1350 | A | C8-N7 | 6.20 | 1.35 | 1.31 |
| 22 | 23S1 | 1253 | A | C8-N7 | 6.20 | 1.35 | 1.31 |
| 22 | 23S1 | 1470 | A | C5-C4 | -6.20 | 1.34 | 1.38 |
| 1 | 16S1 | 238 | A | C5-C4 | -6.19 | 1.34 | 1.38 |
| 23 | 05S1 | 52 | A | C8-N7 | 6.19 | 1.35 | 1.31 |
| 1 | 16S1 | 1434 | A | C8-N7 | 6.19 | 1.35 | 1.31 |
| 22 | 23S1 | 2766 | A | N3-C4 | 6.19 | 1.38 | 1.34 |
| 1 | 16S1 | 236 | A | C8-N7 | 6.19 | 1.35 | 1.31 |
| 22 | 23S1 | 1590 | A | N3-C4 | 6.19 | 1.38 | 1.34 |
| 22 | 23S1 | 2590 | A | C8-N7 | 6.19 | 1.35 | 1.31 |
| 1 | 16S1 | 546 | A | C8-N7 | 6.18 | 1.35 | 1.31 |
| 1 | 16S1 | 1151 | A | C5-C4 | -6.18 | 1.34 | 1.38 |
| 22 | 23S1 | 844 | A | C8-N7 | 6.18 | 1.35 | 1.31 |
| 22 | 23S1 | 2547 | A | C5-C4 | -6.18 | 1.34 | 1.38 |
| 1 | 16S1 | 777 | A | C8-N7 | 6.18 | 1.35 | 1.31 |
| 22 | 23S1 | 2183 | A | N3-C4 | 6.18 | 1.38 | 1.34 |
| 1 | 16S1 | 10 | A | C8-N7 | 6.18 | 1.35 | 1.31 |
| 23 | 05S1 | 119 | A | N3-C4 | 6.18 | 1.38 | 1.34 |
| 22 | 23S1 | 722 | A | N3-C4 | 6.18 | 1.38 | 1.34 |
| 1 | 16S1 | 59 | A | C8-N7 | 6.18 | 1.35 | 1.31 |
| 1 | 16S1 | 759 | A | C8-N7 | 6.18 | 1.35 | 1.31 |
| 1 | 16S1 | 243 | A | C8-N7 | 6.17 | 1.35 | 1.31 |
| 1 | 16S1 | 262 | A | C5-C4 | -6.17 | 1.34 | 1.38 |
| 22 | 23S1 | 2297 | A | C5-C4 | -6.17 | 1.34 | 1.38 |
| 22 | 23S1 | 2820 | A | N3-C4 | 6.17 | 1.38 | 1.34 |
| 1 | 16S1 | 349 | A | C5-C4 | -6.17 | 1.34 | 1.38 |
| 1 | 16S1 | 468 | A | N3-C4 | 6.17 | 1.38 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 2241 | A | C5-C4 | -6.17 | 1.34 | 1.38 |
| 1 | 16S1 | 687 | A | C5-C4 | -6.17 | 1.34 | 1.38 |
| 22 | 23S1 | 2530 | A | C8-N7 | 6.17 | 1.35 | 1.31 |
| 1 | 16S1 | 523 | A | C8-N7 | 6.17 | 1.35 | 1.31 |
| 1 | 16S1 | 1046 | A | C8-N7 | 6.17 | 1.35 | 1.31 |
| 1 | 16S1 | 149 | A | N3-C4 | 6.17 | 1.38 | 1.34 |
| 1 | 16S1 | 306 | A | C5-C4 | -6.17 | 1.34 | 1.38 |
| 1 | 16S1 | 1019 | A | N3-C4 | 6.17 | 1.38 | 1.34 |
| 22 | 23S1 | 502 | A | C8-N7 | 6.17 | 1.35 | 1.31 |
| 22 | 23S1 | 722 | A | C5-C4 | -6.17 | 1.34 | 1.38 |
| 22 | 23S1 | 213 | A | C5-C4 | -6.17 | 1.34 | 1.38 |
| 22 | 23S1 | 927 | A | C5-C4 | -6.17 | 1.34 | 1.38 |
| 23 | 05S1 | 59 | A | C8-N7 | 6.17 | 1.35 | 1.31 |
| 1 | 16S1 | 459 | A | C8-N7 | 6.17 | 1.35 | 1.31 |
| 1 | 16S1 | 901 | A | N7-C5 | -6.16 | 1.35 | 1.39 |
| 1 | 16S1 | 1238 | A | C5-C4 | -6.16 | 1.34 | 1.38 |
| 1 | 16S1 | 1333 | A | C5-C4 | -6.16 | 1.34 | 1.38 |
| 22 | 23S1 | 374 | A | C5-C4 | -6.16 | 1.34 | 1.38 |
| 22 | 23S1 | 2378 | A | C8-N7 | 6.16 | 1.35 | 1.31 |
| 22 | 23S1 | 2572 | A | C8-N7 | 6.16 | 1.35 | 1.31 |
| 22 | 23S1 | 231 | A | C5-C4 | -6.16 | 1.34 | 1.38 |
| 1 | 16S1 | 1105 | A | C8-N7 | 6.16 | 1.35 | 1.31 |
| 22 | 23S1 | 981 | A | C5-C4 | -6.16 | 1.34 | 1.38 |
| 22 | 23S1 | 1384 | A | C8-N7 | 6.16 | 1.35 | 1.31 |
| 22 | 23S1 | 1757 | A | C5-C4 | -6.16 | 1.34 | 1.38 |
| 22 | 23S1 | 602 | A | C5-C4 | -6.16 | 1.34 | 1.38 |
| 22 | 23S1 | 1010 | A | C5-C4 | -6.16 | 1.34 | 1.38 |
| 22 | 23S1 | 2170 | A | N3-C4 | 6.16 | 1.38 | 1.34 |
| 22 | 23S1 | 538 | A | C8-N7 | 6.16 | 1.35 | 1.31 |
| 1 | 16S1 | 635 | A | C8-N7 | 6.15 | 1.35 | 1.31 |
| 22 | 23S1 | 423 | A | C8-N7 | 6.15 | 1.35 | 1.31 |
| 22 | 23S1 | 526 | A | C8-N7 | 6.15 | 1.35 | 1.31 |
| 22 | 23S1 | 2900 | A | C8-N7 | 6.15 | 1.35 | 1.31 |
| 22 | 23S1 | 1027 | A | C5-C4 | -6.15 | 1.34 | 1.38 |
| 22 | 23S1 | 1050 | A | N3-C4 | 6.15 | 1.38 | 1.34 |
| 22 | 23S1 | 2340 | A | C8-N7 | 6.15 | 1.35 | 1.31 |
| 22 | 23S1 | 592 | A | C5-C4 | -6.15 | 1.34 | 1.38 |
| 22 | 23S1 | 1755 | A | C5-C4 | -6.15 | 1.34 | 1.38 |
| 22 | 23S1 | 2278 | A | C5-C4 | -6.15 | 1.34 | 1.38 |
| 1 | 16S1 | 363 | A | C5-C4 | -6.14 | 1.34 | 1.38 |
| 22 | 23S1 | 1021 | A | C5-C4 | -6.14 | 1.34 | 1.38 |
| 22 | 23S1 | 1586 | A | N3-C4 | 6.14 | 1.38 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 23 | 05S1 | 50 | A | C5-C4 | -6.14 | 1.34 | 1.38 |
| 1 | 16S1 | 1299 | A | N3-C4 | 6.14 | 1.38 | 1.34 |
| 22 | 23S1 | 222 | A | C8-N7 | 6.14 | 1.35 | 1.31 |
| 22 | 23S1 | 483 | A | C5-C4 | -6.14 | 1.34 | 1.38 |
| 22 | 23S1 | 637 | A | C5-C4 | -6.14 | 1.34 | 1.38 |
| 22 | 23S1 | 1901 | A | C8-N7 | 6.14 | 1.35 | 1.31 |
| 23 | 05S1 | 39 | A | C5-C4 | -6.14 | 1.34 | 1.38 |
| 1 | 16S1 | 949 | A | C5-C4 | -6.14 | 1.34 | 1.38 |
| 1 | 16S1 | 1145 | A | C5-C4 | -6.14 | 1.34 | 1.38 |
| 1 | 16S1 | 1431 | A | C8-N7 | 6.14 | 1.35 | 1.31 |
| 22 | 23S1 | 1711 | A | C8-N7 | 6.14 | 1.35 | 1.31 |
| 1 | 16S1 | 356 | A | C5-C4 | -6.14 | 1.34 | 1.38 |
| 1 | 16S1 | 313 | A | C5-C4 | -6.13 | 1.34 | 1.38 |
| 1 | 16S1 | 994 | A | C8-N7 | 6.13 | 1.35 | 1.31 |
| 1 | 16S1 | 1363 | A | C8-N7 | 6.13 | 1.35 | 1.31 |
| 22 | 23S1 | 118 | A | C5-C4 | -6.13 | 1.34 | 1.38 |
| 22 | 23S1 | 933 | A | C5-C4 | -6.13 | 1.34 | 1.38 |
| 22 | 23S1 | 2126 | A | N3-C4 | 6.13 | 1.38 | 1.34 |
| 1 | 16S1 | 430 | A | C8-N7 | 6.13 | 1.35 | 1.31 |
| 1 | 16S1 | 441 | A | N3-C4 | 6.13 | 1.38 | 1.34 |
| 22 | 23S1 | 1969 | A | C5-C4 | -6.13 | 1.34 | 1.38 |
| 22 | 23S1 | 2726 | A | C5-C4 | -6.13 | 1.34 | 1.38 |
| 1 | 16S1 | 1 | A | N3-C4 | 6.13 | 1.38 | 1.34 |
| 22 | 23S1 | 2430 | A | N7-C5 | -6.13 | 1.35 | 1.39 |
| 1 | 16S1 | 743 | A | C8-N7 | 6.13 | 1.35 | 1.31 |
| 22 | 23S1 | 983 | A | C5-C4 | -6.13 | 1.34 | 1.38 |
| 22 | 23S1 | 1054 | A | N3-C4 | 6.13 | 1.38 | 1.34 |
| 22 | 23S1 | 127 | A | C5-C4 | -6.12 | 1.34 | 1.38 |
| 1 | 16S1 | 77 | A | N3-C4 | 6.12 | 1.38 | 1.34 |
| 1 | 16S1 | 151 | A | C5-C4 | -6.12 | 1.34 | 1.38 |
| 1 | 16S1 | 1171 | A | N3-C4 | 6.12 | 1.38 | 1.34 |
| 22 | 23S1 | 670 | A | C5-C4 | -6.12 | 1.34 | 1.38 |
| 1 | 16S1 | 1082 | A | C8-N7 | 6.12 | 1.35 | 1.31 |
| 22 | 23S1 | 152 | A | C5-C4 | -6.12 | 1.34 | 1.38 |
| 22 | 23S1 | 216 | A | C5-C4 | -6.12 | 1.34 | 1.38 |
| 22 | 23S1 | 255 | A | C5-C4 | -6.12 | 1.34 | 1.38 |
| 22 | 23S1 | 83 | A | C8-N7 | 6.12 | 1.35 | 1.31 |
| 1 | 16S1 | 10 | A | C5-C4 | -6.12 | 1.34 | 1.38 |
| 1 | 16S1 | 1163 | A | C5-C4 | -6.12 | 1.34 | 1.38 |
| 1 | 16S1 | 1180 | A | C5-C4 | -6.12 | 1.34 | 1.38 |
| 22 | 23S1 | 216 | A | C8-N7 | 6.12 | 1.35 | 1.31 |
| 22 | 23S1 | 471 | A | C5-C4 | -6.12 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 1637 | A | C5-C4 | -6.12 | 1.34 | 1.38 |
| 22 | 23S1 | 1632 | A | C5-C4 | -6.12 | 1.34 | 1.38 |
| 23 | 05S1 | 104 | A | C5-C4 | -6.12 | 1.34 | 1.38 |
| 22 | 23S1 | 311 | A | C5-C4 | -6.11 | 1.34 | 1.38 |
| 22 | 23S1 | 1387 | A | C8-N7 | 6.11 | 1.35 | 1.31 |
| 1 | 16S1 | 554 | A | C5-C4 | -6.11 | 1.34 | 1.38 |
| 22 | 23S1 | 1046 | A | N3-C4 | 6.11 | 1.38 | 1.34 |
| 22 | 23S1 | 1932 | A | C8-N7 | 6.11 | 1.35 | 1.31 |
| 1 | 16S1 | 753 | A | C5-C4 | -6.11 | 1.34 | 1.38 |
| 1 | 16S1 | 1480 | A | C8-N7 | 6.11 | 1.35 | 1.31 |
| 22 | 23S1 | 1373 | A | C5-C4 | -6.11 | 1.34 | 1.38 |
| 22 | 23S1 | 2051 | A | C5-C4 | -6.11 | 1.34 | 1.38 |
| 22 | 23S1 | 199 | A | C5-C4 | -6.11 | 1.34 | 1.38 |
| 22 | 23S1 | 2198 | A | C8-N7 | 6.11 | 1.35 | 1.31 |
| 1 | 16S1 | 263 | A | C5-C4 | -6.11 | 1.34 | 1.38 |
| 1 | 16S1 | 974 | A | C8-N7 | 6.11 | 1.35 | 1.31 |
| 22 | 23S1 | 6 | A | C8-N7 | 6.11 | 1.35 | 1.31 |
| 22 | 23S1 | 270 | A | N3-C4 | 6.11 | 1.38 | 1.34 |
| 22 | 23S1 | 2740 | A | C8-N7 | 6.11 | 1.35 | 1.31 |
| 55 | PTR1 | 3 | A | N3-C4 | 6.11 | 1.38 | 1.34 |
| 1 | 16S1 | 181 | A | C8-N7 | 6.11 | 1.35 | 1.31 |
| 1 | 16S1 | 282 | A | C8-N7 | 6.11 | 1.35 | 1.31 |
| 22 | 23S1 | 49 | A | C5-C4 | -6.11 | 1.34 | 1.38 |
| 22 | 23S1 | 502 | A | C5-C4 | -6.11 | 1.34 | 1.38 |
| 22 | 23S1 | 1885 | A | C5-C4 | -6.11 | 1.34 | 1.38 |
| 22 | 23S1 | 2097 | A | N3-C4 | 6.11 | 1.38 | 1.34 |
| 22 | 23S1 | 2856 | A | C5-C4 | -6.11 | 1.34 | 1.38 |
| 22 | 23S1 | 2333 | A | C8-N7 | 6.10 | 1.35 | 1.31 |
| 1 | 16S1 | 1257 | A | N3-C4 | 6.10 | 1.38 | 1.34 |
| 1 | 16S1 | 1410 | A | C5-C4 | -6.10 | 1.34 | 1.38 |
| 22 | 23S1 | 310 | A | C5-C4 | -6.10 | 1.34 | 1.38 |
| 22 | 23S1 | 472 | A | C5-C4 | -6.10 | 1.34 | 1.38 |
| 22 | 23S1 | 1998 | A | C8-N7 | 6.10 | 1.35 | 1.31 |
| 22 | 23S1 | 2211 | A | N3-C4 | 6.10 | 1.38 | 1.34 |
| 22 | 23S1 | 2660 | A | N3-C4 | 6.10 | 1.38 | 1.34 |
| 22 | 23S1 | 2778 | A | C5-C4 | -6.10 | 1.34 | 1.38 |
| 1 | 16S1 | 1188 | A | C8-N7 | 6.10 | 1.35 | 1.31 |
| 1 | 16S1 | 1311 | A | C5-C4 | -6.10 | 1.34 | 1.38 |
| 22 | 23S1 | 173 | A | C8-N7 | 6.10 | 1.35 | 1.31 |
| 22 | 23S1 | 644 | A | C5-C4 | -6.10 | 1.34 | 1.38 |
| 22 | 23S1 | 1194 | A | C8-N7 | 6.10 | 1.35 | 1.31 |
| 22 | 23S1 | 1689 | A | C5-C4 | -6.10 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 23 | 05S1 | 45 | A | C8-N7 | 6.10 | 1.35 | 1.31 |
| 1 | 16S1 | 309 | A | C5-C4 | -6.10 | 1.34 | 1.38 |
| 22 | 23S1 | 905 | A | C5-C4 | -6.10 | 1.34 | 1.38 |
| 22 | 23S1 | 2602 | A | N3-C4 | 6.10 | 1.38 | 1.34 |
| 1 | 16S1 | 1042 | A | N3-C4 | 6.10 | 1.38 | 1.34 |
| 22 | 23S1 | 2654 | A | C5-C4 | -6.10 | 1.34 | 1.38 |
| 1 | 16S1 | 160 | A | C5-C4 | -6.09 | 1.34 | 1.38 |
| 1 | 16S1 | 878 | A | C5-C4 | -6.09 | 1.34 | 1.38 |
| 1 | 16S1 | 1492 | A | N3-C4 | 6.09 | 1.38 | 1.34 |
| 22 | 23S1 | 590 | A | C5-C4 | -6.09 | 1.34 | 1.38 |
| 22 | 23S1 | 2425 | A | C5-C4 | -6.09 | 1.34 | 1.38 |
| 1 | 16S1 | 784 | A | C8-N7 | 6.09 | 1.35 | 1.31 |
| 22 | 23S1 | 278 | A | N3-C4 | 6.09 | 1.38 | 1.34 |
| 22 | 23S1 | 845 | A | C8-N7 | 6.09 | 1.35 | 1.31 |
| 22 | 23S1 | 2738 | A | C8-N7 | 6.09 | 1.35 | 1.31 |
| 1 | 16S1 | 366 | A | C8-N7 | 6.09 | 1.35 | 1.31 |
| 1 | 16S1 | 1150 | A | C5-C4 | -6.09 | 1.34 | 1.38 |
| 22 | 23S1 | 340 | A | C5-C4 | -6.09 | 1.34 | 1.38 |
| 22 | 23S1 | 1785 | A | C8-N7 | 6.09 | 1.35 | 1.31 |
| 22 | 23S1 | 2776 | A | C5-C4 | -6.09 | 1.34 | 1.38 |
| 22 | 23S1 | 94 | A | C5-C4 | -6.08 | 1.34 | 1.38 |
| 22 | 23S1 | 2322 | A | C8-N7 | 6.08 | 1.35 | 1.31 |
| 1 | 16S1 | 415 | A | N3-C4 | 6.08 | 1.38 | 1.34 |
| 22 | 23S1 | 104 | A | N3-C4 | 6.08 | 1.38 | 1.34 |
| 1 | 16S1 | 1170 | A | N7-C5 | -6.08 | 1.35 | 1.39 |
| 22 | 23S1 | 1275 | A | C8-N7 | 6.08 | 1.35 | 1.31 |
| 22 | 23S1 | 2287 | A | C5-C4 | -6.08 | 1.34 | 1.38 |
| 22 | 23S1 | 2868 | A | C8-N7 | 6.08 | 1.35 | 1.31 |
| 1 | 16S1 | 74 | A | C5-C4 | -6.08 | 1.34 | 1.38 |
| 1 | 16S1 | 167 | A | N3-C4 | 6.08 | 1.38 | 1.34 |
| 1 | 16S1 | 1219 | A | C8-N7 | 6.08 | 1.35 | 1.31 |
| 22 | 23S1 | 936 | A | C8-N7 | 6.08 | 1.35 | 1.31 |
| 22 | 23S1 | 1383 | A | C5-C4 | -6.08 | 1.34 | 1.38 |
| 22 | 23S1 | 1889 | A | C8-N7 | 6.08 | 1.35 | 1.31 |
| 22 | 23S1 | 1927 | A | C8-N7 | 6.08 | 1.35 | 1.31 |
| 22 | 23S1 | 1953 | A | N7-C5 | -6.08 | 1.35 | 1.39 |
| 1 | 16S1 | 1110 | A | C5-C4 | -6.08 | 1.34 | 1.38 |
| 22 | 23S1 | 71 | A | C5-C4 | -6.08 | 1.34 | 1.38 |
| 22 | 23S1 | 614 | A | N3-C4 | 6.08 | 1.38 | 1.34 |
| 22 | 23S1 | 911 | A | C5-C4 | -6.08 | 1.34 | 1.38 |
| 1 | 16S1 | 553 | A | C8-N7 | 6.07 | 1.35 | 1.31 |
| 22 | 23S1 | 1580 | A | C8-N7 | 6.07 | 1.35 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 1634 | A | C5-C4 | -6.07 | 1.34 | 1.38 |
| 22 | 23S1 | 2284 | A | C8-N7 | 6.07 | 1.35 | 1.31 |
| 22 | 23S1 | 1690 | A | C8-N7 | 6.07 | 1.35 | 1.31 |
| 22 | 23S1 | 2534 | A | C8-N7 | 6.07 | 1.35 | 1.31 |
| 1 | 16S1 | 7 | A | C5-C4 | -6.07 | 1.34 | 1.38 |
| 22 | 23S1 | 764 | A | C5-C4 | -6.07 | 1.34 | 1.38 |
| 22 | 23S1 | 152 | A | C8-N7 | 6.07 | 1.35 | 1.31 |
| 22 | 23S1 | 556 | A | C5-C4 | -6.07 | 1.34 | 1.38 |
| 22 | 23S1 | 716 | A | C8-N7 | 6.07 | 1.35 | 1.31 |
| 23 | 05S1 | 101 | A | N3-C4 | 6.07 | 1.38 | 1.34 |
| 1 | 16S1 | 865 | A | C5-C4 | -6.07 | 1.34 | 1.38 |
| 22 | 23S1 | 960 | A | C5-C4 | -6.07 | 1.34 | 1.38 |
| 1 | 16S1 | 621 | A | C5-C4 | -6.06 | 1.34 | 1.38 |
| 22 | 23S1 | 945 | A | C8-N7 | 6.06 | 1.35 | 1.31 |
| 22 | 23S1 | 1632 | A | C8-N7 | 6.06 | 1.35 | 1.31 |
| 23 | 05S1 | 73 | A | C8-N7 | 6.06 | 1.35 | 1.31 |
| 1 | 16S1 | 1319 | A | C5-C4 | -6.06 | 1.34 | 1.38 |
| 22 | 23S1 | 896 | A | N3-C4 | 6.06 | 1.38 | 1.34 |
| 22 | 23S1 | 602 | A | C8-N7 | 6.06 | 1.35 | 1.31 |
| 22 | 23S1 | 2407 | A | C5-C4 | -6.06 | 1.34 | 1.38 |
| 22 | 23S1 | 2705 | A | C5-C4 | -6.06 | 1.34 | 1.38 |
| 1 | 16S1 | 595 | A | C5-C4 | -6.06 | 1.34 | 1.38 |
| 1 | 16S1 | 1261 | A | C5-C4 | -6.06 | 1.34 | 1.38 |
| 1 | 16S1 | 55 | A | C5-C4 | -6.06 | 1.34 | 1.38 |
| 1 | 16S1 | 59 | A | N3-C4 | 6.06 | 1.38 | 1.34 |
| 1 | 16S1 | 282 | A | C5-C4 | -6.06 | 1.34 | 1.38 |
| 22 | 23S1 | 160 | A | C5-C4 | -6.06 | 1.34 | 1.38 |
| 22 | 23S1 | 1039 | A | C5-C4 | -6.06 | 1.34 | 1.38 |
| 22 | 23S1 | 1085 | A | N3-C4 | 6.06 | 1.38 | 1.34 |
| 22 | 23S1 | 1854 | A | C5-C4 | -6.06 | 1.34 | 1.38 |
| 1 | 16S1 | 1067 | A | C8-N7 | 6.06 | 1.35 | 1.31 |
| 22 | 23S1 | 348 | A | N3-C4 | 6.06 | 1.38 | 1.34 |
| 22 | 23S1 | 1853 | A | C8-N7 | 6.06 | 1.35 | 1.31 |
| 1 | 16S1 | 32 | A | C8-N7 | 6.05 | 1.35 | 1.31 |
| 22 | 23S1 | 1928 | A | C5-C4 | -6.05 | 1.34 | 1.38 |
| 1 | 16S1 | 946 | A | C8-N7 | 6.05 | 1.35 | 1.31 |
| 22 | 23S1 | 1780 | A | C5-C4 | -6.05 | 1.34 | 1.38 |
| 22 | 23S1 | 2450 | A | C8-N7 | 6.05 | 1.35 | 1.31 |
| 1 | 16S1 | 600 | A | C5-C4 | -6.05 | 1.34 | 1.38 |
| 1 | 16S1 | 915 | A | C8-N7 | 6.05 | 1.35 | 1.31 |
| 1 | 16S1 | 1306 | A | C8-N7 | 6.05 | 1.35 | 1.31 |
| 22 | 23S1 | 706 | A | C8-N7 | 6.05 | 1.35 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 2893 | A | C8-N7 | 6.05 | 1.35 | 1.31 |
| 22 | 23S1 | 173 | A | C5-C4 | -6.05 | 1.34 | 1.38 |
| 22 | 23S1 | 362 | A | C8-N7 | 6.05 | 1.35 | 1.31 |
| 1 | 16S1 | 790 | A | C8-N7 | 6.05 | 1.35 | 1.31 |
| 22 | 23S1 | 1848 | A | C8-N7 | 6.05 | 1.35 | 1.31 |
| 1 | 16S1 | 914 | A | N3-C4 | 6.04 | 1.38 | 1.34 |
| 1 | 16S1 | 759 | A | C5-C4 | -6.04 | 1.34 | 1.38 |
| 22 | 23S1 | 223 | A | C5-C4 | -6.04 | 1.34 | 1.38 |
| 22 | 23S1 | 1664 | A | C5-C4 | -6.04 | 1.34 | 1.38 |
| 1 | 16S1 | 495 | A | N3-C4 | 6.04 | 1.38 | 1.34 |
| 22 | 23S1 | 1241 | A | C5-C4 | -6.04 | 1.34 | 1.38 |
| 22 | 23S1 | 1598 | A | N3-C4 | 6.04 | 1.38 | 1.34 |
| 22 | 23S1 | 2336 | A | C8-N7 | 6.04 | 1.35 | 1.31 |
| 22 | 23S1 | 402 | A | C5-C4 | -6.04 | 1.34 | 1.38 |
| 22 | 23S1 | 1439 | A | C8-N7 | 6.04 | 1.35 | 1.31 |
| 22 | 23S1 | 73 | A | C5-C4 | -6.04 | 1.34 | 1.38 |
| 22 | 23S1 | 199 | A | C8-N7 | 6.04 | 1.35 | 1.31 |
| 22 | 23S1 | 1713 | A | C5-C4 | -6.04 | 1.34 | 1.38 |
| 22 | 23S1 | 2670 | A | C5-C4 | -6.04 | 1.34 | 1.38 |
| 1 | 16S1 | 397 | A | N3-C4 | 6.04 | 1.38 | 1.34 |
| 22 | 23S1 | 984 | A | N3-C4 | 6.04 | 1.38 | 1.34 |
| 22 | 23S1 | 1780 | A | C8-N7 | 6.04 | 1.35 | 1.31 |
| 22 | 23S1 | 2366 | A | C5-C4 | -6.04 | 1.34 | 1.38 |
| 22 | 23S1 | 2799 | A | C8-N7 | 6.04 | 1.35 | 1.31 |
| 1 | 16S1 | 65 | A | C5-C4 | -6.04 | 1.34 | 1.38 |
| 22 | 23S1 | 131 | A | C5-C4 | -6.04 | 1.34 | 1.38 |
| 1 | 16S1 | 790 | A | C5-C4 | -6.03 | 1.34 | 1.38 |
| 1 | 16S1 | 1288 | A | N3-C4 | 6.03 | 1.38 | 1.34 |
| 22 | 23S1 | 592 | A | C8-N7 | 6.03 | 1.35 | 1.31 |
| 22 | 23S1 | 1147 | A | C5-C4 | -6.03 | 1.34 | 1.38 |
| 22 | 23S1 | 1284 | A | C5-C4 | -6.03 | 1.34 | 1.38 |
| 22 | 23S1 | 1937 | A | C5-C4 | -6.03 | 1.34 | 1.38 |
| 22 | 23S1 | 2886 | A | C8-N7 | 6.03 | 1.35 | 1.31 |
| 1 | 16S1 | 356 | A | C8-N7 | 6.03 | 1.35 | 1.31 |
| 1 | 16S1 | 630 | A | C8-N7 | 6.03 | 1.35 | 1.31 |
| 1 | 16S1 | 1201 | A | N3-C4 | 6.03 | 1.38 | 1.34 |
| 22 | 23S1 | 131 | A | N3-C4 | 6.03 | 1.38 | 1.34 |
| 1 | 16S1 | 977 | A | N3-C4 | 6.03 | 1.38 | 1.34 |
| 1 | 16S1 | 1102 | A | C5-C4 | -6.03 | 1.34 | 1.38 |
| 1 | 16S1 | 1375 | A | C5-C4 | -6.03 | 1.34 | 1.38 |
| 22 | 23S1 | 94 | A | C8-N7 | 6.03 | 1.35 | 1.31 |
| 22 | 23S1 | 918 | A | C5-C4 | -6.03 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 2377 | A | N3-C4 | 6.03 | 1.38 | 1.34 |
| 1 | 16S1 | 174 | A | C8-N7 | 6.03 | 1.35 | 1.31 |
| 1 | 16S1 | 1329 | A | C5-C4 | -6.03 | 1.34 | 1.38 |
| 22 | 23S1 | 104 | A | C8-N7 | 6.03 | 1.35 | 1.31 |
| 1 | 16S1 | 546 | A | C5-C4 | -6.03 | 1.34 | 1.38 |
| 22 | 23S1 | 89 | A | C8-N7 | 6.03 | 1.35 | 1.31 |
| 22 | 23S1 | 1829 | A | C5-C4 | -6.03 | 1.34 | 1.38 |
| 22 | 23S1 | 1872 | A | N3-C4 | 6.03 | 1.38 | 1.34 |
| 22 | 23S1 | 2094 | A | C5-C4 | -6.03 | 1.34 | 1.38 |
| 1 | 16S1 | 199 | A | N3-C4 | 6.02 | 1.38 | 1.34 |
| 22 | 23S1 | 42 | A | C5-C4 | -6.02 | 1.34 | 1.38 |
| 1 | 16S1 | 366 | A | C5-C4 | -6.02 | 1.34 | 1.38 |
| 22 | 23S1 | 149 | A | C8-N7 | 6.02 | 1.35 | 1.31 |
| 22 | 23S1 | 480 | A | C8-N7 | 6.02 | 1.35 | 1.31 |
| 22 | 23S1 | 1214 | A | C8-N7 | 6.02 | 1.35 | 1.31 |
| 1 | 16S1 | 1363 | A | C5-C4 | -6.02 | 1.34 | 1.38 |
| 1 | 16S1 | 181 | A | N3-C4 | 6.02 | 1.38 | 1.34 |
| 22 | 23S1 | 5 | A | C5-C4 | -6.02 | 1.34 | 1.38 |
| 22 | 23S1 | 2765 | A | N3-C4 | 6.02 | 1.38 | 1.34 |
| 1 | 16S1 | 329 | A | C5-C4 | -6.02 | 1.34 | 1.38 |
| 22 | 23S1 | 354 | A | N3-C4 | 6.02 | 1.38 | 1.34 |
| 22 | 23S1 | 1626 | A | C5-C4 | -6.02 | 1.34 | 1.38 |
| 23 | 05S1 | 53 | A | C5-C4 | -6.02 | 1.34 | 1.38 |
| 1 | 16S1 | 320 | A | C8-N7 | 6.01 | 1.35 | 1.31 |
| 22 | 23S1 | 1998 | A | C5-C4 | -6.01 | 1.34 | 1.38 |
| 1 | 16S1 | 675 | A | C8-N7 | 6.01 | 1.35 | 1.31 |
| 22 | 23S1 | 643 | A | C8-N7 | 6.01 | 1.35 | 1.31 |
| 22 | 23S1 | 1029 | A | C5-C4 | -6.01 | 1.34 | 1.38 |
| 22 | 23S1 | 1322 | A | C8-N7 | 6.01 | 1.35 | 1.31 |
| 22 | 23S1 | 1890 | A | C8-N7 | 6.01 | 1.35 | 1.31 |
| 22 | 23S1 | 346 | A | C5-C4 | -6.01 | 1.34 | 1.38 |
| 22 | 23S1 | 1515 | A | C5-C4 | -6.01 | 1.34 | 1.38 |
| 1 | 16S1 | 1188 | A | C5-C4 | -6.01 | 1.34 | 1.38 |
| 1 | 16S1 | 499 | A | N3-C4 | 6.01 | 1.38 | 1.34 |
| 22 | 23S1 | 1029 | A | N3-C4 | 6.01 | 1.38 | 1.34 |
| 22 | 23S1 | 2381 | A | C8-N7 | 6.01 | 1.35 | 1.31 |
| 23 | 05S1 | 99 | A | N3-C4 | 6.01 | 1.38 | 1.34 |
| 1 | 16S1 | 533 | A | N3-C4 | 6.00 | 1.38 | 1.34 |
| 1 | 16S1 | 728 | A | C8-N7 | 6.00 | 1.35 | 1.31 |
| 1 | 16S1 | 1430 | A | C5-C4 | -6.00 | 1.34 | 1.38 |
| 1 | 16S1 | 288 | A | C5-C4 | -6.00 | 1.34 | 1.38 |
| 1 | 16S1 | 559 | A | C8-N7 | 6.00 | 1.35 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 16S1 | 1157 | A | C5-C4 | -6.00 | 1.34 | 1.38 |
| 22 | 23S1 | 299 | A | C8-N7 | 6.00 | 1.35 | 1.31 |
| 22 | 23S1 | 1321 | A | C5-C4 | -6.00 | 1.34 | 1.38 |
| 1 | 16S1 | 8 | A | C8-N7 | 6.00 | 1.35 | 1.31 |
| 1 | 16S1 | 1170 | A | C5-C4 | -6.00 | 1.34 | 1.38 |
| 22 | 23S1 | 131 | A | C8-N7 | 6.00 | 1.35 | 1.31 |
| 22 | 23S1 | 626 | A | N3-C4 | 6.00 | 1.38 | 1.34 |
| 22 | 23S1 | 2883 | A | C8-N7 | 6.00 | 1.35 | 1.31 |
| 55 | PTR1 | 21 | A | N3-C4 | 6.00 | 1.38 | 1.34 |
| 55 | PTR1 | 76 | A | C8-N7 | 6.00 | 1.35 | 1.31 |
| 22 | 23S1 | 13 | A | C8-N7 | 6.00 | 1.35 | 1.31 |
| 22 | 23S1 | 144 | A | C5-C4 | -6.00 | 1.34 | 1.38 |
| 22 | 23S1 | 2453 | A | C8-N7 | 6.00 | 1.35 | 1.31 |
| 22 | 23S1 | 146 | A | C5-C4 | -5.99 | 1.34 | 1.38 |
| 22 | 23S1 | 2284 | A | C5-C4 | -5.99 | 1.34 | 1.38 |
| 22 | 23S1 | 1353 | A | C8-N7 | 5.99 | 1.35 | 1.31 |
| 1 | 16S1 | 371 | A | N3-C4 | 5.99 | 1.38 | 1.34 |
| 1 | 16S1 | 393 | A | N3-C4 | 5.99 | 1.38 | 1.34 |
| 1 | 16S1 | 1081 | A | C5-C4 | -5.99 | 1.34 | 1.38 |
| 22 | 23S1 | 1810 | A | C5-C4 | -5.99 | 1.34 | 1.38 |
| 22 | 23S1 | 2635 | A | C5-C4 | -5.99 | 1.34 | 1.38 |
| 22 | 23S1 | 2899 | A | N3-C4 | 5.99 | 1.38 | 1.34 |
| 22 | 23S1 | 449 | A | C8-N7 | 5.99 | 1.35 | 1.31 |
| 1 | 16S1 | 1197 | A | C8-N7 | 5.99 | 1.35 | 1.31 |
| 22 | 23S1 | 945 | A | C5-C4 | -5.99 | 1.34 | 1.38 |
| 1 | 16S1 | 161 | A | N3-C4 | 5.99 | 1.38 | 1.34 |
| 22 | 23S1 | 126 | A | C5-C4 | -5.99 | 1.34 | 1.38 |
| 22 | 23S1 | 44 | A | N3-C4 | 5.98 | 1.38 | 1.34 |
| 22 | 23S1 | 1569 | A | C8-N7 | 5.98 | 1.35 | 1.31 |
| 23 | 05S1 | 59 | A | N3-C4 | 5.98 | 1.38 | 1.34 |
| 1 | 16S1 | 448 | A | N3-C4 | 5.98 | 1.38 | 1.34 |
| 22 | 23S1 | 1204 | A | C5-C4 | -5.98 | 1.34 | 1.38 |
| 22 | 23S1 | 384 | A | C5-C4 | -5.98 | 1.34 | 1.38 |
| 1 | 16S1 | 274 | A | C5-C4 | -5.98 | 1.34 | 1.38 |
| 1 | 16S1 | 498 | A | C2-N3 | 5.98 | 1.39 | 1.33 |
| 1 | 16S1 | 596 | A | C5-C4 | -5.98 | 1.34 | 1.38 |
| 22 | 23S1 | 909 | A | C5-C4 | -5.98 | 1.34 | 1.38 |
| 22 | 23S1 | 1598 | A | C8-N7 | 5.98 | 1.35 | 1.31 |
| 22 | 23S1 | 1713 | A | C8-N7 | 5.98 | 1.35 | 1.31 |
| 22 | 23S1 | 2094 | A | N3-C4 | 5.98 | 1.38 | 1.34 |
| 22 | 23S1 | 2418 | A | C8-N7 | 5.98 | 1.35 | 1.31 |
| 22 | 23S1 | 1701 | A | C8-N7 | 5.98 | 1.35 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 16S1 | 663 | A | C8-N7 | 5.97 | 1.35 | 1.31 |
| 22 | 23S1 | 182 | A | C8-N7 | 5.97 | 1.35 | 1.31 |
| 23 | 05S1 | 99 | A | C8-N7 | 5.97 | 1.35 | 1.31 |
| 1 | 16S1 | 964 | A | C5-C4 | -5.97 | 1.34 | 1.38 |
| 22 | 23S1 | 330 | A | C8-N7 | 5.97 | 1.35 | 1.31 |
| 22 | 23S1 | 423 | A | C5-C4 | -5.97 | 1.34 | 1.38 |
| 22 | 23S1 | 1246 | A | N3-C4 | 5.97 | 1.38 | 1.34 |
| 22 | 23S1 | 1504 | A | N3-C4 | 5.97 | 1.38 | 1.34 |
| 22 | 23S1 | 2058 | A | C8-N7 | 5.97 | 1.35 | 1.31 |
| 22 | 23S1 | 2873 | A | C5-C4 | -5.97 | 1.34 | 1.38 |
| 22 | 23S1 | 1286 | A | C8-N7 | 5.97 | 1.35 | 1.31 |
| 22 | 23S1 | 1987 | A | C8-N7 | 5.97 | 1.35 | 1.31 |
| 22 | 23S1 | 2273 | A | C5-C4 | -5.97 | 1.34 | 1.38 |
| 1 | 16S1 | 262 | A | C8-N7 | 5.97 | 1.35 | 1.31 |
| 22 | 23S1 | 1545 | A | C5-C4 | -5.97 | 1.34 | 1.38 |
| 22 | 23S1 | 532 | A | N3-C4 | 5.97 | 1.38 | 1.34 |
| 22 | 23S1 | 1871 | A | N3-C4 | 5.97 | 1.38 | 1.34 |
| 1 | 16S1 | 243 | A | C5-C4 | -5.97 | 1.34 | 1.38 |
| 1 | 16S1 | 768 | A | C8-N7 | 5.97 | 1.35 | 1.31 |
| 1 | 16S1 | 792 | A | N3-C4 | 5.97 | 1.38 | 1.34 |
| 22 | 23S1 | 928 | A | C5-C4 | -5.97 | 1.34 | 1.38 |
| 22 | 23S1 | 1327 | A | C8-N7 | 5.97 | 1.35 | 1.31 |
| 1 | 16S1 | 509 | A | C8-N7 | 5.96 | 1.35 | 1.31 |
| 1 | 16S1 | 1368 | A | C5-C4 | -5.96 | 1.34 | 1.38 |
| 22 | 23S1 | 320 | A | C8-N7 | 5.96 | 1.35 | 1.31 |
| 22 | 23S1 | 556 | A | C8-N7 | 5.96 | 1.35 | 1.31 |
| 22 | 23S1 | 2829 | A | N3-C4 | 5.96 | 1.38 | 1.34 |
| 22 | 23S1 | 2430 | A | C8-N7 | 5.96 | 1.35 | 1.31 |
| 22 | 23S1 | 2813 | A | C8-N7 | 5.96 | 1.35 | 1.31 |
| 22 | 23S1 | 6 | A | C5-C4 | -5.96 | 1.34 | 1.38 |
| 1 | 16S1 | 373 | A | C8-N7 | 5.96 | 1.35 | 1.31 |
| 22 | 23S1 | 1889 | A | C5-C4 | -5.96 | 1.34 | 1.38 |
| 1 | 16S1 | 1428 | A | C8-N7 | 5.96 | 1.35 | 1.31 |
| 22 | 23S1 | 793 | A | C5-C4 | -5.96 | 1.34 | 1.38 |
| 22 | 23S1 | 1230 | A | C8-N7 | 5.96 | 1.35 | 1.31 |
| 22 | 23S1 | 1427 | A | C5-C4 | -5.96 | 1.34 | 1.38 |
| 22 | 23S1 | 1548 | A | C5-C4 | -5.96 | 1.34 | 1.38 |
| 1 | 16S1 | 1111 | A | C5-C4 | -5.96 | 1.34 | 1.38 |
| 22 | 23S1 | 1591 | A | C5-C4 | -5.96 | 1.34 | 1.38 |
| 1 | 16S1 | 655 | A | C8-N7 | 5.95 | 1.35 | 1.31 |
| 22 | 23S1 | 973 | A | C8-N7 | 5.95 | 1.35 | 1.31 |
| 55 | PTR1 | 9 | A | N3-C4 | 5.95 | 1.38 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 16S1 | 155 | A | N3-C4 | 5.95 | 1.38 | 1.34 |
| 22 | 23S1 | 1593 | A | N3-C4 | 5.95 | 1.38 | 1.34 |
| 1 | 16S1 | 607 | A | C8-N7 | 5.95 | 1.35 | 1.31 |
| 22 | 23S1 | 599 | A | C8-N7 | 5.95 | 1.35 | 1.31 |
| 22 | 23S1 | 1503 | A | N3-C4 | 5.95 | 1.38 | 1.34 |
| 1 | 16S1 | 327 | A | C8-N7 | 5.94 | 1.35 | 1.31 |
| 22 | 23S1 | 2406 | A | C5-C4 | -5.94 | 1.34 | 1.38 |
| 1 | 16S1 | 303 | A | C8-N7 | 5.94 | 1.35 | 1.31 |
| 22 | 23S1 | 1095 | A | N3-C4 | 5.94 | 1.38 | 1.34 |
| 22 | 23S1 | 1247 | A | C8-N7 | 5.94 | 1.35 | 1.31 |
| 55 | PTR1 | 59 | A | N3-C4 | 5.94 | 1.38 | 1.34 |
| 1 | 16S1 | 139 | A | C5-C4 | -5.94 | 1.34 | 1.38 |
| 1 | 16S1 | 172 | A | N3-C4 | 5.94 | 1.38 | 1.34 |
| 1 | 16S1 | 787 | A | C8-N7 | 5.94 | 1.35 | 1.31 |
| 22 | 23S1 | 2634 | A | C8-N7 | 5.94 | 1.35 | 1.31 |
| 22 | 23S1 | 2879 | A | C5-C4 | -5.94 | 1.34 | 1.38 |
| 1 | 16S1 | 1146 | A | N3-C4 | 5.94 | 1.38 | 1.34 |
| 22 | 23S1 | 447 | A | C8-N7 | 5.93 | 1.35 | 1.31 |
| 22 | 23S1 | 637 | A | N3-C4 | 5.93 | 1.38 | 1.34 |
| 22 | 23S1 | 2062 | A | N3-C4 | 5.93 | 1.38 | 1.34 |
| 22 | 23S1 | 2117 | A | N3-C4 | 5.93 | 1.38 | 1.34 |
| 1 | 16S1 | 182 | A | N3-C4 | 5.93 | 1.38 | 1.34 |
| 22 | 23S1 | 104 | A | C5-C4 | -5.93 | 1.34 | 1.38 |
| 22 | 23S1 | 1246 | A | C8-N7 | 5.93 | 1.35 | 1.31 |
| 22 | 23S1 | 1433 | A | C8-N7 | 5.93 | 1.35 | 1.31 |
| 1 | 16S1 | 300 | A | N3-C4 | 5.93 | 1.38 | 1.34 |
| 22 | 23S1 | 2753 | A | C5-C4 | -5.93 | 1.34 | 1.38 |
| 1 | 16S1 | 878 | A | C8-N7 | 5.93 | 1.35 | 1.31 |
| 1 | 16S1 | 393 | A | C5-C4 | -5.93 | 1.34 | 1.38 |
| 22 | 23S1 | 362 | A | C5-C4 | -5.93 | 1.34 | 1.38 |
| 22 | 23S1 | 538 | A | C5-C4 | -5.93 | 1.34 | 1.38 |
| 1 | 16S1 | 1362 | A | C8-N7 | 5.92 | 1.35 | 1.31 |
| 22 | 23S1 | 251 | A | C5-C4 | -5.92 | 1.34 | 1.38 |
| 22 | 23S1 | 722 | A | C8-N7 | 5.92 | 1.35 | 1.31 |
| 22 | 23S1 | 1596 | A | C5-C4 | -5.92 | 1.34 | 1.38 |
| 22 | 23S1 | 2169 | A | N3-C4 | 5.92 | 1.38 | 1.34 |
| 1 | 16S1 | 1480 | A | C5-C4 | -5.92 | 1.34 | 1.38 |
| 1 | 16S1 | 1493 | A | N3-C4 | 5.92 | 1.38 | 1.34 |
| 1 | 16S1 | 533 | A | C8-N7 | 5.92 | 1.35 | 1.31 |
| 1 | 16S1 | 983 | A | C8-N7 | 5.92 | 1.35 | 1.31 |
| 1 | 16S1 | 119 | A | C5-C4 | -5.92 | 1.34 | 1.38 |
| 22 | 23S1 | 821 | A | C8-N7 | 5.92 | 1.35 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 1477 | A | C5-C4 | -5.92 | 1.34 | 1.38 |
| 22 | 23S1 | 2461 | A | C8-N7 | 5.92 | 1.35 | 1.31 |
| 22 | 23S1 | 2725 | A | C8-N7 | 5.92 | 1.35 | 1.31 |
| 22 | 23S1 | 1274 | A | C5-C4 | -5.92 | 1.34 | 1.38 |
| 1 | 16S1 | 1339 | A | C5-C4 | -5.91 | 1.34 | 1.38 |
| 22 | 23S1 | 374 | A | C8-N7 | 5.91 | 1.35 | 1.31 |
| 22 | 23S1 | 279 | A | N3-C4 | 5.91 | 1.38 | 1.34 |
| 22 | 23S1 | 1717 | A | C8-N7 | 5.91 | 1.35 | 1.31 |
| 22 | 23S1 | 1757 | A | C8-N7 | 5.91 | 1.35 | 1.31 |
| 1 | 16S1 | 1271 | A | C5-C4 | -5.91 | 1.34 | 1.38 |
| 22 | 23S1 | 2314 | A | C5-C4 | -5.91 | 1.34 | 1.38 |
| 22 | 23S1 | 2748 | A | C5-C4 | -5.91 | 1.34 | 1.38 |
| 55 | PTR1 | 14 | A | N3-C4 | 5.91 | 1.38 | 1.34 |
| 1 | 16S1 | 274 | A | N3-C4 | 5.91 | 1.38 | 1.34 |
| 22 | 23S1 | 1169 | A | C5-C4 | -5.91 | 1.34 | 1.38 |
| 22 | 23S1 | 1143 | A | C5-C4 | -5.90 | 1.34 | 1.38 |
| 22 | 23S1 | 1572 | A | C5-C4 | -5.90 | 1.34 | 1.38 |
| 22 | 23S1 | 2899 | A | C8-N7 | 5.90 | 1.35 | 1.31 |
| 23 | 05S1 | 59 | A | C2-N3 | 5.90 | 1.38 | 1.33 |
| 1 | 16S1 | 1324 | A | C5-C4 | -5.90 | 1.34 | 1.38 |
| 22 | 23S1 | 125 | A | C5-C4 | -5.90 | 1.34 | 1.38 |
| 1 | 16S1 | 1357 | A | C5-C4 | -5.90 | 1.34 | 1.38 |
| 1 | 16S1 | 53 | A | C8-N7 | 5.90 | 1.35 | 1.31 |
| 1 | 16S1 | 167 | A | C5-C4 | -5.90 | 1.34 | 1.38 |
| 1 | 16S1 | 430 | A | C5-C4 | -5.90 | 1.34 | 1.38 |
| 1 | 16S1 | 1004 | A | C5-C4 | -5.90 | 1.34 | 1.38 |
| 1 | 16S1 | 1225 | A | N3-C4 | 5.90 | 1.38 | 1.34 |
| 1 | 16S1 | 1269 | A | C8-N7 | 5.90 | 1.35 | 1.31 |
| 22 | 23S1 | 1392 | A | C8-N7 | 5.90 | 1.35 | 1.31 |
| 22 | 23S1 | 2764 | A | C8-N7 | 5.90 | 1.35 | 1.31 |
| 1 | 16S1 | 182 | A | C5-C4 | -5.90 | 1.34 | 1.38 |
| 1 | 16S1 | 655 | A | N3-C4 | 5.90 | 1.38 | 1.34 |
| 22 | 23S1 | 920 | A | C8-N7 | 5.90 | 1.35 | 1.31 |
| 22 | 23S1 | 2776 | A | C8-N7 | 5.90 | 1.35 | 1.31 |
| 1 | 16S1 | 2 | A | C5-C4 | -5.89 | 1.34 | 1.38 |
| 1 | 16S1 | 1155 | A | C5-C4 | -5.89 | 1.34 | 1.38 |
| 1 | 16S1 | 1340 | A | C5-C4 | -5.89 | 1.34 | 1.38 |
| 22 | 23S1 | 661 | A | C8-N7 | 5.89 | 1.35 | 1.31 |
| 22 | 23S1 | 1566 | A | C8-N7 | 5.89 | 1.35 | 1.31 |
| 22 | 23S1 | 2270 | A | C8-N7 | 5.89 | 1.35 | 1.31 |
| 1 | 16S1 | 642 | A | C5-C4 | -5.89 | 1.34 | 1.38 |
| 1 | 16S1 | 482 | A | N3-C4 | 5.89 | 1.38 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 16S1 | 1318 | A | N3-C4 | 5.89 | 1.38 | 1.34 |
| 22 | 23S1 | 217 | A | C8-N7 | 5.89 | 1.35 | 1.31 |
| 1 | 16S1 | 900 | A | C8-N7 | 5.89 | 1.35 | 1.31 |
| 22 | 23S1 | 1745 | A | N3-C4 | 5.89 | 1.38 | 1.34 |
| 1 | 16S1 | 452 | A | C5-C4 | -5.89 | 1.34 | 1.38 |
| 1 | 16S1 | 532 | A | N3-C4 | 5.89 | 1.38 | 1.34 |
| 1 | 16S1 | 681 | A | N3-C4 | 5.89 | 1.38 | 1.34 |
| 1 | 16S1 | 432 | A | N3-C4 | 5.89 | 1.38 | 1.34 |
| 1 | 16S1 | 1229 | A | C5-C4 | -5.89 | 1.34 | 1.38 |
| 22 | 23S1 | 391 | A | C8-N7 | 5.89 | 1.35 | 1.31 |
| 22 | 23S1 | 2340 | A | C5-C4 | -5.89 | 1.34 | 1.38 |
| 22 | 23S1 | 2411 | A | C8-N7 | 5.89 | 1.35 | 1.31 |
| 22 | 23S1 | 2547 | A | C8-N7 | 5.89 | 1.35 | 1.31 |
| 1 | 16S1 | 1360 | A | C5-C4 | -5.88 | 1.34 | 1.38 |
| 22 | 23S1 | 927 | A | N3-C4 | 5.88 | 1.38 | 1.34 |
| 22 | 23S1 | 1328 | A | C8-N7 | 5.88 | 1.35 | 1.31 |
| 22 | 23S1 | 1347 | A | C8-N7 | 5.88 | 1.35 | 1.31 |
| 22 | 23S1 | 2369 | A | C5-C4 | -5.88 | 1.34 | 1.38 |
| 1 | 16S1 | 704 | A | C5-C4 | -5.88 | 1.34 | 1.38 |
| 22 | 23S1 | 2051 | A | N7-C5 | -5.88 | 1.35 | 1.39 |
| 22 | 23S1 | 503 | A | C8-N7 | 5.88 | 1.35 | 1.31 |
| 1 | 16S1 | 1252 | A | C5-C4 | -5.88 | 1.34 | 1.38 |
| 22 | 23S1 | 1549 | A | C8-N7 | 5.88 | 1.35 | 1.31 |
| 22 | 23S1 | 1608 | A | C5-C4 | -5.88 | 1.34 | 1.38 |
| 1 | 16S1 | 143 | A | N3-C4 | 5.88 | 1.38 | 1.34 |
| 1 | 16S1 | 412 | A | C5-C4 | -5.88 | 1.34 | 1.38 |
| 1 | 16S1 | 635 | A | C5-C4 | -5.88 | 1.34 | 1.38 |
| 22 | 23S1 | 1722 | A | N3-C4 | 5.88 | 1.38 | 1.34 |
| 22 | 23S1 | 2778 | A | C8-N7 | 5.88 | 1.35 | 1.31 |
| 22 | 23S1 | 2860 | A | C8-N7 | 5.88 | 1.35 | 1.31 |
| 22 | 23S1 | 928 | A | N3-C4 | 5.88 | 1.38 | 1.34 |
| 1 | 16S1 | 706 | A | C8-N7 | 5.87 | 1.35 | 1.31 |
| 22 | 23S1 | 415 | A | C5-C4 | -5.87 | 1.34 | 1.38 |
| 22 | 23S1 | 1039 | A | N3-C4 | 5.87 | 1.38 | 1.34 |
| 22 | 23S1 | 1098 | A | C8-N7 | 5.87 | 1.35 | 1.31 |
| 22 | 23S1 | 1755 | A | C8-N7 | 5.87 | 1.35 | 1.31 |
| 1 | 16S1 | 129 | A | C5-C4 | -5.87 | 1.34 | 1.38 |
| 22 | 23S1 | 2733 | A | N3-C4 | 5.87 | 1.38 | 1.34 |
| 1 | 16S1 | 695 | A | C8-N7 | 5.87 | 1.35 | 1.31 |
| 1 | 16S1 | 1256 | A | C5-C4 | -5.87 | 1.34 | 1.38 |
| 1 | 16S1 | 1346 | A | C5-C4 | -5.87 | 1.34 | 1.38 |
| 1 | 16S1 | 270 | A | C5-C4 | -5.87 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 103 | A | C5-C4 | -5.87 | 1.34 | 1.38 |
| 22 | 23S1 | 432 | A | C8-N7 | 5.87 | 1.35 | 1.31 |
| 22 | 23S1 | 1403 | A | C8-N7 | 5.87 | 1.35 | 1.31 |
| 1 | 16S1 | 579 | A | C5-C4 | -5.86 | 1.34 | 1.38 |
| 22 | 23S1 | 111 | A | C5-C4 | -5.86 | 1.34 | 1.38 |
| 22 | 23S1 | 789 | A | C8-N7 | 5.86 | 1.35 | 1.31 |
| 22 | 23S1 | 2887 | A | C8-N7 | 5.86 | 1.35 | 1.31 |
| 22 | 23S1 | 38 | A | C5-C4 | -5.86 | 1.34 | 1.38 |
| 22 | 23S1 | 368 | A | C5-C4 | -5.86 | 1.34 | 1.38 |
| 23 | 05S1 | 94 | A | C8-N7 | 5.86 | 1.35 | 1.31 |
| 1 | 16S1 | 44 | A | C5-C4 | -5.86 | 1.34 | 1.38 |
| 1 | 16S1 | 621 | A | C8-N7 | 5.86 | 1.35 | 1.31 |
| 22 | 23S1 | 83 | A | N3-C4 | 5.86 | 1.38 | 1.34 |
| 22 | 23S1 | 348 | A | C5-C4 | -5.86 | 1.34 | 1.38 |
| 22 | 23S1 | 2665 | A | C8-N7 | 5.86 | 1.35 | 1.31 |
| 1 | 16S1 | 32 | A | C5-C4 | -5.86 | 1.34 | 1.38 |
| 1 | 16S1 | 676 | A | C5-C4 | -5.86 | 1.34 | 1.38 |
| 22 | 23S1 | 204 | A | C8-N7 | 5.86 | 1.35 | 1.31 |
| 23 | 05S1 | 57 | A | N3-C4 | 5.86 | 1.38 | 1.34 |
| 1 | 16S1 | 706 | A | C5-C4 | -5.86 | 1.34 | 1.38 |
| 22 | 23S1 | 439 | A | N3-C4 | 5.86 | 1.38 | 1.34 |
| 22 | 23S1 | 602 | A | N3-C4 | 5.86 | 1.38 | 1.34 |
| 22 | 23S1 | 1342 | A | C8-N7 | 5.86 | 1.35 | 1.31 |
| 22 | 23S1 | 2309 | A | N3-C4 | 5.86 | 1.38 | 1.34 |
| 1 | 16S1 | 523 | A | C5-C4 | -5.85 | 1.34 | 1.38 |
| 1 | 16S1 | 977 | A | C8-N7 | 5.85 | 1.35 | 1.31 |
| 22 | 23S1 | 2886 | A | C5-C4 | -5.85 | 1.34 | 1.38 |
| 1 | 16S1 | 452 | A | N3-C4 | 5.85 | 1.38 | 1.34 |
| 22 | 23S1 | 95 | A | C5-C4 | -5.85 | 1.34 | 1.38 |
| 22 | 23S1 | 2738 | A | C5-C4 | -5.85 | 1.34 | 1.38 |
| 55 | PTR1 | 73 | A | N3-C4 | 5.85 | 1.38 | 1.34 |
| 22 | 23S1 | 454 | A | C8-N7 | 5.85 | 1.35 | 1.31 |
| 22 | 23S1 | 609 | A | C8-N7 | 5.85 | 1.35 | 1.31 |
| 22 | 23S1 | 172 | A | N3-C4 | 5.85 | 1.38 | 1.34 |
| 22 | 23S1 | 344 | A | C5-C4 | -5.85 | 1.34 | 1.38 |
| 22 | 23S1 | 1477 | A | N3-C4 | 5.85 | 1.38 | 1.34 |
| 1 | 16S1 | 640 | A | C5-C4 | -5.84 | 1.34 | 1.38 |
| 1 | 16S1 | 938 | A | C8-N7 | 5.84 | 1.35 | 1.31 |
| 22 | 23S1 | 973 | A | C5-C4 | -5.84 | 1.34 | 1.38 |
| 55 | PTR1 | 38 | A | C8-N7 | 5.84 | 1.35 | 1.31 |
| 1 | 16S1 | 3 | A | C5-C4 | -5.84 | 1.34 | 1.38 |
| 22 | 23S1 | 38 | A | C8-N7 | 5.84 | 1.35 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 504 | A | N9-C4 | -5.84 | 1.34 | 1.37 |
| 22 | 23S1 | 514 | A | C8-N7 | 5.84 | 1.35 | 1.31 |
| 22 | 23S1 | 1155 | A | C8-N7 | 5.84 | 1.35 | 1.31 |
| 22 | 23S1 | 1505 | A | N3-C4 | 5.84 | 1.38 | 1.34 |
| 22 | 23S1 | 2433 | A | N7-C5 | -5.84 | 1.35 | 1.39 |
| 22 | 23S1 | 2439 | A | C8-N7 | 5.84 | 1.35 | 1.31 |
| 1 | 16S1 | 1204 | A | C5-C4 | -5.84 | 1.34 | 1.38 |
| 22 | 23S1 | 1048 | A | N3-C4 | 5.84 | 1.38 | 1.34 |
| 22 | 23S1 | 2412 | A | C5-C4 | -5.84 | 1.34 | 1.38 |
| 1 | 16S1 | 1236 | A | C5-C4 | -5.84 | 1.34 | 1.38 |
| 22 | 23S1 | 742 | A | C8-N7 | 5.84 | 1.35 | 1.31 |
| 22 | 23S1 | 933 | A | C8-N7 | 5.84 | 1.35 | 1.31 |
| 22 | 23S1 | 2513 | A | C8-N7 | 5.84 | 1.35 | 1.31 |
| 22 | 23S1 | 2564 | A | C8-N7 | 5.83 | 1.35 | 1.31 |
| 1 | 16S1 | 573 | A | C8-N7 | 5.83 | 1.35 | 1.31 |
| 22 | 23S1 | 590 | A | C8-N7 | 5.83 | 1.35 | 1.31 |
| 22 | 23S1 | 1008 | A | C5-C4 | -5.83 | 1.34 | 1.38 |
| 22 | 23S1 | 1610 | A | C5-C4 | -5.83 | 1.34 | 1.38 |
| 22 | 23S1 | 2377 | A | C5-C4 | -5.83 | 1.34 | 1.38 |
| 1 | 16S1 | 909 | A | C5-C4 | -5.83 | 1.34 | 1.38 |
| 1 | 16S1 | 51 | A | C8-N7 | 5.83 | 1.35 | 1.31 |
| 1 | 16S1 | 364 | A | C8-N7 | 5.83 | 1.35 | 1.31 |
| 1 | 16S1 | 974 | A | C5-C4 | -5.83 | 1.34 | 1.38 |
| 1 | 16S1 | 1433 | A | C8-N7 | 5.83 | 1.35 | 1.31 |
| 22 | 23S1 | 223 | A | C8-N7 | 5.83 | 1.35 | 1.31 |
| 22 | 23S1 | 344 | A | N3-C4 | 5.83 | 1.38 | 1.34 |
| 22 | 23S1 | 572 | A | C5-C4 | -5.83 | 1.34 | 1.38 |
| 22 | 23S1 | 1142 | A | C8-N7 | 5.83 | 1.35 | 1.31 |
| 22 | 23S1 | 1570 | A | C8-N7 | 5.83 | 1.35 | 1.31 |
| 22 | 23S1 | 1739 | A | C5-C4 | -5.83 | 1.34 | 1.38 |
| 1 | 16S1 | 263 | A | N3-C4 | 5.83 | 1.38 | 1.34 |
| 22 | 23S1 | 845 | A | C5-C4 | -5.83 | 1.34 | 1.38 |
| 22 | 23S1 | 2531 | A | N3-C4 | 5.83 | 1.38 | 1.34 |
| 1 | 16S1 | 1111 | A | N3-C4 | 5.82 | 1.38 | 1.34 |
| 1 | 16S1 | 1374 | A | C8-N7 | 5.82 | 1.35 | 1.31 |
| 1 | 16S1 | 1476 | A | C8-N7 | 5.82 | 1.35 | 1.31 |
| 22 | 23S1 | 1502 | A | N3-C4 | 5.82 | 1.38 | 1.34 |
| 1 | 16S1 | 694 | A | C8-N7 | 5.82 | 1.35 | 1.31 |
| 22 | 23S1 | 479 | A | C8-N7 | 5.82 | 1.35 | 1.31 |
| 22 | 23S1 | 457 | A | C8-N7 | 5.82 | 1.35 | 1.31 |
| 22 | 23S1 | 1272 | A | C8-N7 | 5.82 | 1.35 | 1.31 |
| 22 | 23S1 | 1528 | A | N3-C4 | 5.82 | 1.38 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 16S1 | 825 | A | C8-N7 | 5.82 | 1.35 | 1.31 |
| 22 | 23S1 | 1274 | A | C8-N7 | 5.82 | 1.35 | 1.31 |
| 22 | 23S1 | 2298 | A | C8-N7 | 5.82 | 1.35 | 1.31 |
| 1 | 16S1 | 373 | A | N3-C4 | 5.82 | 1.38 | 1.34 |
| 22 | 23S1 | 330 | A | C5-C4 | -5.82 | 1.34 | 1.38 |
| 55 | PTR1 | 26 | A | N3-C4 | 5.82 | 1.38 | 1.34 |
| 1 | 16S1 | 673 | A | N3-C4 | 5.82 | 1.38 | 1.34 |
| 1 | 16S1 | 1014 | A | C5-C4 | -5.82 | 1.34 | 1.38 |
| 22 | 23S1 | 1050 | A | C5-C4 | -5.82 | 1.34 | 1.38 |
| 22 | 23S1 | 1877 | A | C5-C4 | -5.82 | 1.34 | 1.38 |
| 22 | 23S1 | 2482 | A | C8-N7 | 5.82 | 1.35 | 1.31 |
| 22 | 23S1 | 2766 | A | C5-C4 | -5.82 | 1.34 | 1.38 |
| 22 | 23S1 | 1872 | A | C2-N3 | 5.81 | 1.38 | 1.33 |
| 1 | 16S1 | 270 | A | N3-C4 | 5.81 | 1.38 | 1.34 |
| 1 | 16S1 | 371 | A | C5-C4 | -5.81 | 1.34 | 1.38 |
| 1 | 16S1 | 996 | A | N3-C4 | 5.81 | 1.38 | 1.34 |
| 22 | 23S1 | 1285 | A | C8-N7 | 5.81 | 1.35 | 1.31 |
| 55 | PTR1 | 14 | A | C8-N7 | 5.81 | 1.35 | 1.31 |
| 22 | 23S1 | 2468 | A | C8-N7 | 5.81 | 1.35 | 1.31 |
| 1 | 16S1 | 441 | A | C8-N7 | 5.81 | 1.35 | 1.31 |
| 1 | 16S1 | 908 | A | C8-N7 | 5.81 | 1.35 | 1.31 |
| 1 | 16S1 | 1499 | A | N3-C4 | 5.81 | 1.38 | 1.34 |
| 22 | 23S1 | 165 | A | N3-C4 | 5.81 | 1.38 | 1.34 |
| 22 | 23S1 | 1936 | A | C5-C4 | -5.81 | 1.34 | 1.38 |
| 1 | 16S1 | 329 | A | C8-N7 | 5.81 | 1.35 | 1.31 |
| 22 | 23S1 | 899 | A | N3-C4 | 5.80 | 1.38 | 1.34 |
| 1 | 16S1 | 448 | A | C5-C4 | -5.80 | 1.34 | 1.38 |
| 1 | 16S1 | 1271 | A | N3-C4 | 5.80 | 1.38 | 1.34 |
| 1 | 16S1 | 482 | A | C5-C4 | -5.80 | 1.34 | 1.38 |
| 1 | 16S1 | 1110 | A | C8-N7 | 5.80 | 1.35 | 1.31 |
| 22 | 23S1 | 482 | A | C5-C4 | -5.80 | 1.34 | 1.38 |
| 22 | 23S1 | 849 | A | C8-N7 | 5.80 | 1.35 | 1.31 |
| 22 | 23S1 | 2287 | A | N3-C4 | 5.80 | 1.38 | 1.34 |
| 22 | 23S1 | 2851 | A | C8-N7 | 5.80 | 1.35 | 1.31 |
| 22 | 23S1 | 1142 | A | C5-C4 | -5.80 | 1.34 | 1.38 |
| 22 | 23S1 | 1549 | A | C5-C4 | -5.80 | 1.34 | 1.38 |
| 1 | 16S1 | 1350 | A | C5-C4 | -5.80 | 1.34 | 1.38 |
| 22 | 23S1 | 172 | A | C5-C4 | -5.80 | 1.34 | 1.38 |
| 22 | 23S1 | 1580 | A | C5-C4 | -5.79 | 1.34 | 1.38 |
| 1 | 16S1 | 975 | A | C8-N7 | 5.79 | 1.35 | 1.31 |
| 1 | 16S1 | 1219 | A | C5-C4 | -5.79 | 1.34 | 1.38 |
| 22 | 23S1 | 118 | A | C8-N7 | 5.79 | 1.35 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 439 | A | C5-C4 | -5.79 | 1.34 | 1.38 |
| 23 | 05S1 | 29 | A | N3-C4 | 5.79 | 1.38 | 1.34 |
| 1 | 16S1 | 687 | A | C8-N7 | 5.79 | 1.35 | 1.31 |
| 1 | 16S1 | 1081 | A | C8-N7 | 5.79 | 1.35 | 1.31 |
| 1 | 16S1 | 1152 | A | C5-C4 | -5.79 | 1.34 | 1.38 |
| 1 | 16S1 | 1318 | A | C8-N7 | 5.79 | 1.35 | 1.31 |
| 22 | 23S1 | 272 | A | N3-C4 | 5.79 | 1.38 | 1.34 |
| 22 | 23S1 | 309 | A | N3-C4 | 5.79 | 1.38 | 1.34 |
| 22 | 23S1 | 981 | A | C8-N7 | 5.79 | 1.35 | 1.31 |
| 22 | 23S1 | 1009 | A | C8-N7 | 5.79 | 1.35 | 1.31 |
| 1 | 16S1 | 718 | A | N3-C4 | 5.79 | 1.38 | 1.34 |
| 22 | 23S1 | 1679 | A | C5-C4 | -5.79 | 1.34 | 1.38 |
| 1 | 16S1 | 451 | A | C8-N7 | 5.79 | 1.35 | 1.31 |
| 22 | 23S1 | 430 | A | C5-C4 | -5.79 | 1.34 | 1.38 |
| 22 | 23S1 | 668 | A | C8-N7 | 5.79 | 1.35 | 1.31 |
| 22 | 23S1 | 1877 | A | N3-C4 | 5.79 | 1.38 | 1.34 |
| 1 | 16S1 | 949 | A | C8-N7 | 5.79 | 1.35 | 1.31 |
| 1 | 16S1 | 994 | A | N3-C4 | 5.79 | 1.38 | 1.34 |
| 22 | 23S1 | 2432 | A | C8-N7 | 5.79 | 1.35 | 1.31 |
| 22 | 23S1 | 764 | A | C8-N7 | 5.79 | 1.35 | 1.31 |
| 22 | 23S1 | 1583 | A | N3-C4 | 5.79 | 1.38 | 1.34 |
| 1 | 16S1 | 460 | A | C5-C4 | -5.78 | 1.34 | 1.38 |
| 22 | 23S1 | 1503 | A | C5-C4 | -5.78 | 1.34 | 1.38 |
| 22 | 23S1 | 1553 | A | C5-C4 | -5.78 | 1.34 | 1.38 |
| 23 | 05S1 | 52 | A | C5-C4 | -5.78 | 1.34 | 1.38 |
| 1 | 16S1 | 33 | A | C8-N7 | 5.78 | 1.35 | 1.31 |
| 22 | 23S1 | 1829 | A | C8-N7 | 5.78 | 1.35 | 1.31 |
| 22 | 23S1 | 1919 | A | C5-C4 | -5.78 | 1.34 | 1.38 |
| 1 | 16S1 | 190 | A | N3-C4 | 5.78 | 1.38 | 1.34 |
| 1 | 16S1 | 655 | A | C5-C4 | -5.78 | 1.34 | 1.38 |
| 22 | 23S1 | 631 | A | C8-N7 | 5.78 | 1.35 | 1.31 |
| 22 | 23S1 | 1395 | A | C5-C4 | -5.78 | 1.34 | 1.38 |
| 22 | 23S1 | 1744 | A | C5-C4 | -5.78 | 1.34 | 1.38 |
| 22 | 23S1 | 2205 | A | C5-C4 | -5.78 | 1.34 | 1.38 |
| 22 | 23S1 | 2518 | A | N3-C4 | 5.78 | 1.38 | 1.34 |
| 22 | 23S1 | 1847 | A | N3-C4 | 5.78 | 1.38 | 1.34 |
| 22 | 23S1 | 1899 | A | N7-C5 | -5.78 | 1.35 | 1.39 |
| 22 | 23S1 | 2749 | A | C5-C4 | -5.78 | 1.34 | 1.38 |
| 1 | 16S1 | 197 | A | C5-C4 | -5.78 | 1.34 | 1.38 |
| 22 | 23S1 | 825 | A | C8-N7 | 5.78 | 1.35 | 1.31 |
| 1 | 16S1 | 782 | A | C8-N7 | 5.78 | 1.35 | 1.31 |
| 1 | 16S1 | 918 | A | C8-N7 | 5.78 | 1.35 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 515 | A | C8-N7 | 5.78 | 1.35 | 1.31 |
| 22 | 23S1 | 644 | A | N3-C4 | 5.78 | 1.38 | 1.34 |
| 22 | 23S1 | 676 | A | C8-N7 | 5.78 | 1.35 | 1.31 |
| 22 | 23S1 | 1260 | A | C8-N7 | 5.78 | 1.35 | 1.31 |
| 1 | 16S1 | 155 | A | C5-C4 | -5.77 | 1.34 | 1.38 |
| 22 | 23S1 | 643 | A | C5-C4 | -5.77 | 1.34 | 1.38 |
| 22 | 23S1 | 1848 | A | C5-C4 | -5.77 | 1.34 | 1.38 |
| 23 | 05S1 | 58 | A | N3-C4 | 5.77 | 1.38 | 1.34 |
| 1 | 16S1 | 435 | A | C5-C4 | -5.77 | 1.34 | 1.38 |
| 1 | 16S1 | 673 | A | C8-N7 | 5.77 | 1.35 | 1.31 |
| 22 | 23S1 | 256 | A | C8-N7 | 5.77 | 1.35 | 1.31 |
| 22 | 23S1 | 352 | A | C5-C4 | -5.77 | 1.34 | 1.38 |
| 22 | 23S1 | 2814 | A | C8-N7 | 5.77 | 1.35 | 1.31 |
| 22 | 23S1 | 689 | A | C8-N7 | 5.77 | 1.35 | 1.31 |
| 1 | 16S1 | 607 | A | C5-C4 | -5.77 | 1.34 | 1.38 |
| 22 | 23S1 | 368 | A | N3-C4 | 5.77 | 1.38 | 1.34 |
| 22 | 23S1 | 2336 | A | C5-C4 | -5.77 | 1.34 | 1.38 |
| 22 | 23S1 | 52 | A | C5-C4 | -5.77 | 1.34 | 1.38 |
| 22 | 23S1 | 342 | A | N3-C4 | 5.76 | 1.38 | 1.34 |
| 1 | 16S1 | 792 | A | C8-N7 | 5.76 | 1.35 | 1.31 |
| 1 | 16S1 | 66 | A | C5-C4 | -5.76 | 1.34 | 1.38 |
| 22 | 23S1 | 2378 | A | C5-C4 | -5.76 | 1.34 | 1.38 |
| 23 | 05S1 | 99 | A | C5-C4 | -5.76 | 1.34 | 1.38 |
| 23 | 05S1 | 101 | A | C2-N3 | 5.76 | 1.38 | 1.33 |
| 1 | 16S1 | 663 | A | N3-C4 | 5.76 | 1.38 | 1.34 |
| 22 | 23S1 | 1739 | A | C8-N7 | 5.76 | 1.35 | 1.31 |
| 1 | 16S1 | 959 | A | C5-C4 | -5.75 | 1.34 | 1.38 |
| 22 | 23S1 | 294 | A | N3-C4 | 5.75 | 1.38 | 1.34 |
| 22 | 23S1 | 2266 | A | C5-C4 | -5.75 | 1.34 | 1.38 |
| 22 | 23S1 | 2386 | A | C8-N7 | 5.75 | 1.35 | 1.31 |
| 1 | 16S1 | 1398 | A | C5-C4 | -5.75 | 1.34 | 1.38 |
| 22 | 23S1 | 2042 | A | C8-N7 | 5.75 | 1.35 | 1.31 |
| 22 | 23S1 | 2199 | A | C8-N7 | 5.75 | 1.35 | 1.31 |
| 1 | 16S1 | 1044 | A | N3-C4 | 5.75 | 1.38 | 1.34 |
| 1 | 16S1 | 263 | A | C8-N7 | 5.75 | 1.35 | 1.31 |
| 1 | 16S1 | 321 | A | C8-N7 | 5.75 | 1.35 | 1.31 |
| 1 | 16S1 | 493 | A | C5-C4 | -5.75 | 1.34 | 1.38 |
| 22 | 23S1 | 125 | A | N3-C4 | 5.75 | 1.38 | 1.34 |
| 22 | 23S1 | 127 | A | C8-N7 | 5.75 | 1.35 | 1.31 |
| 22 | 23S1 | 1453 | A | N3-C4 | 5.75 | 1.38 | 1.34 |
| 1 | 16S1 | 968 | A | C8-N7 | 5.75 | 1.35 | 1.31 |
| 1 | 16S1 | 983 | A | C5-C4 | -5.75 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 16S1 | 1252 | A | C8-N7 | 5.75 | 1.35 | 1.31 |
| 1 | 16S1 | 1285 | A | C5-C4 | -5.75 | 1.34 | 1.38 |
| 22 | 23S1 | 480 | A | C5-C4 | -5.75 | 1.34 | 1.38 |
| 22 | 23S1 | 2005 | A | C8-N7 | 5.75 | 1.35 | 1.31 |
| 1 | 16S1 | 560 | A | C8-N7 | 5.74 | 1.35 | 1.31 |
| 22 | 23S1 | 1876 | A | C5-C4 | -5.74 | 1.34 | 1.38 |
| 1 | 16S1 | 493 | A | N3-C4 | 5.74 | 1.38 | 1.34 |
| 1 | 16S1 | 572 | A | C8-N7 | 5.74 | 1.35 | 1.31 |
| 1 | 16S1 | 1229 | A | N3-C4 | 5.74 | 1.38 | 1.34 |
| 22 | 23S1 | 1698 | A | C8-N7 | 5.74 | 1.35 | 1.31 |
| 1 | 16S1 | 1225 | A | C5-C4 | -5.74 | 1.34 | 1.38 |
| 22 | 23S1 | 1008 | A | C8-N7 | 5.74 | 1.35 | 1.31 |
| 22 | 23S1 | 2750 | A | C5-C4 | -5.74 | 1.34 | 1.38 |
| 22 | 23S1 | 2835 | A | N3-C4 | 5.74 | 1.38 | 1.34 |
| 22 | 23S1 | 1815 | A | C8-N7 | 5.73 | 1.35 | 1.31 |
| 22 | 23S1 | 2534 | A | C5-C4 | -5.73 | 1.34 | 1.38 |
| 22 | 23S1 | 346 | A | N3-C4 | 5.73 | 1.38 | 1.34 |
| 22 | 23S1 | 1387 | A | C5-C4 | -5.73 | 1.34 | 1.38 |
| 55 | PTR1 | 76 | A | N3-C4 | 5.73 | 1.38 | 1.34 |
| 1 | 16S1 | 1157 | A | N3-C4 | 5.73 | 1.38 | 1.34 |
| 22 | 23S1 | 1668 | A | C8-N7 | 5.73 | 1.35 | 1.31 |
| 23 | 05S1 | 119 | A | C5-C4 | -5.73 | 1.34 | 1.38 |
| 1 | 16S1 | 59 | A | C5-C4 | -5.73 | 1.34 | 1.38 |
| 1 | 16S1 | 373 | A | C5-C4 | -5.73 | 1.34 | 1.38 |
| 1 | 16S1 | 1394 | A | C8-N7 | 5.73 | 1.35 | 1.31 |
| 22 | 23S1 | 479 | A | N3-C4 | 5.73 | 1.38 | 1.34 |
| 22 | 23S1 | 2758 | A | C5-C4 | -5.73 | 1.34 | 1.38 |
| 22 | 23S1 | 2327 | A | C8-N7 | 5.73 | 1.35 | 1.31 |
| 22 | 23S1 | 2654 | A | C8-N7 | 5.73 | 1.35 | 1.31 |
| 1 | 16S1 | 1102 | A | C8-N7 | 5.73 | 1.35 | 1.31 |
| 22 | 23S1 | 89 | A | N3-C4 | 5.73 | 1.38 | 1.34 |
| 1 | 16S1 | 313 | A | C8-N7 | 5.72 | 1.35 | 1.31 |
| 1 | 16S1 | 408 | A | N3-C4 | 5.72 | 1.38 | 1.34 |
| 22 | 23S1 | 345 | A | N3-C4 | 5.72 | 1.38 | 1.34 |
| 22 | 23S1 | 933 | A | N3-C4 | 5.72 | 1.38 | 1.34 |
| 22 | 23S1 | 2058 | A | C5-C4 | -5.72 | 1.34 | 1.38 |
| 1 | 16S1 | 344 | A | N3-C4 | 5.72 | 1.38 | 1.34 |
| 22 | 23S1 | 2893 | A | C5-C4 | -5.72 | 1.34 | 1.38 |
| 1 | 16S1 | 630 | A | C5-C4 | -5.72 | 1.34 | 1.38 |
| 1 | 16S1 | 747 | A | C5-C4 | -5.72 | 1.34 | 1.38 |
| 1 | 16S1 | 1046 | A | C5-C4 | -5.72 | 1.34 | 1.38 |
| 22 | 23S1 | 241 | A | C8-N7 | 5.72 | 1.35 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 756 | A | C8-N7 | 5.72 | 1.35 | 1.31 |
| 22 | 23S1 | 2411 | A | C5-C4 | -5.72 | 1.34 | 1.38 |
| 1 | 16S1 | 681 | A | C5-C4 | -5.72 | 1.34 | 1.38 |
| 1 | 16S1 | 807 | A | C8-N7 | 5.72 | 1.35 | 1.31 |
| 22 | 23S1 | 1641 | A | C5-C4 | -5.72 | 1.34 | 1.38 |
| 22 | 23S1 | 1998 | A | N3-C4 | 5.72 | 1.38 | 1.34 |
| 1 | 16S1 | 461 | A | C5-C4 | -5.71 | 1.34 | 1.38 |
| 22 | 23S1 | 727 | A | N3-C4 | 5.71 | 1.38 | 1.34 |
| 22 | 23S1 | 83 | A | C5-C4 | -5.71 | 1.34 | 1.38 |
| 1 | 16S1 | 196 | A | C5-C4 | -5.71 | 1.34 | 1.38 |
| 1 | 16S1 | 753 | A | N3-C4 | 5.71 | 1.38 | 1.34 |
| 1 | 16S1 | 1167 | A | N3-C4 | 5.71 | 1.38 | 1.34 |
| 22 | 23S1 | 155 | A | N3-C4 | 5.71 | 1.38 | 1.34 |
| 22 | 23S1 | 928 | A | C8-N7 | 5.71 | 1.35 | 1.31 |
| 22 | 23S1 | 2059 | A | C5-C4 | -5.71 | 1.34 | 1.38 |
| 1 | 16S1 | 435 | A | N3-C4 | 5.71 | 1.38 | 1.34 |
| 22 | 23S1 | 44 | A | C5-C4 | -5.71 | 1.34 | 1.38 |
| 22 | 23S1 | 492 | A | N7-C5 | -5.71 | 1.35 | 1.39 |
| 22 | 23S1 | 1528 | A | C5-C4 | -5.71 | 1.34 | 1.38 |
| 22 | 23S1 | 2478 | A | N3-C4 | 5.71 | 1.38 | 1.34 |
| 1 | 16S1 | 663 | A | C5-C4 | -5.71 | 1.34 | 1.38 |
| 22 | 23S1 | 925 | A | C8-N7 | 5.71 | 1.35 | 1.31 |
| 1 | 16S1 | 499 | A | C8-N7 | 5.71 | 1.35 | 1.31 |
| 22 | 23S1 | 877 | A | N3-C4 | 5.71 | 1.38 | 1.34 |
| 22 | 23S1 | 2090 | A | C8-N7 | 5.70 | 1.35 | 1.31 |
| 1 | 16S1 | 579 | A | C8-N7 | 5.70 | 1.35 | 1.31 |
| 22 | 23S1 | 126 | A | C8-N7 | 5.70 | 1.35 | 1.31 |
| 1 | 16S1 | 131 | A | C5-C4 | -5.70 | 1.34 | 1.38 |
| 1 | 16S1 | 1044 | A | C5-C4 | -5.70 | 1.34 | 1.38 |
| 1 | 16S1 | 1146 | A | C5-C4 | -5.70 | 1.34 | 1.38 |
| 22 | 23S1 | 1854 | A | N7-C5 | -5.70 | 1.35 | 1.39 |
| 1 | 16S1 | 649 | A | C5-C4 | -5.70 | 1.34 | 1.38 |
| 1 | 16S1 | 906 | A | C8-N7 | 5.70 | 1.35 | 1.31 |
| 1 | 16S1 | 1508 | A | C5-C4 | -5.70 | 1.34 | 1.38 |
| 22 | 23S1 | 1393 | A | C5-C4 | -5.70 | 1.34 | 1.38 |
| 22 | 23S1 | 2095 | A | C5-C4 | -5.70 | 1.34 | 1.38 |
| 22 | 23S1 | 2764 | A | N3-C4 | 5.70 | 1.38 | 1.34 |
| 22 | 23S1 | 1713 | A | N3-C4 | 5.70 | 1.38 | 1.34 |
| 1 | 16S1 | 648 | A | C5-C4 | -5.70 | 1.34 | 1.38 |
| 22 | 23S1 | 207 | A | C8-N7 | 5.70 | 1.35 | 1.31 |
| 22 | 23S1 | 415 | A | N3-C4 | 5.70 | 1.38 | 1.34 |
| 1 | 16S1 | 65 | A | N3-C4 | 5.69 | 1.38 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 16S1 | 441 | A | C5-C4 | -5.69 | 1.34 | 1.38 |
| 1 | 16S1 | 892 | A | C8-N7 | 5.69 | 1.35 | 1.31 |
| 22 | 23S1 | 1866 | A | C5-C4 | -5.69 | 1.34 | 1.38 |
| 1 | 16S1 | 1346 | A | N3-C4 | 5.69 | 1.38 | 1.34 |
| 55 | PTR1 | 69 | A | N3-C4 | 5.69 | 1.38 | 1.34 |
| 1 | 16S1 | 1012 | A | N3-C4 | 5.69 | 1.38 | 1.34 |
| 1 | 16S1 | 1446 | A | C5-C4 | -5.69 | 1.34 | 1.38 |
| 22 | 23S1 | 101 | A | C8-N7 | 5.69 | 1.35 | 1.31 |
| 22 | 23S1 | 1126 | A | C8-N7 | 5.69 | 1.35 | 1.31 |
| 1 | 16S1 | 749 | A | C5-C4 | -5.69 | 1.34 | 1.38 |
| 22 | 23S1 | 1912 | A | C8-N7 | 5.69 | 1.35 | 1.31 |
| 22 | 23S1 | 2757 | A | N3-C4 | 5.69 | 1.38 | 1.34 |
| 1 | 16S1 | 1169 | A | C5-C4 | -5.68 | 1.34 | 1.38 |
| 22 | 23S1 | 73 | A | C8-N7 | 5.68 | 1.35 | 1.31 |
| 22 | 23S1 | 1598 | A | C5-C4 | -5.68 | 1.34 | 1.38 |
| 1 | 16S1 | 325 | A | C5-C4 | -5.68 | 1.34 | 1.38 |
| 1 | 16S1 | 1319 | A | N3-C4 | 5.68 | 1.38 | 1.34 |
| 22 | 23S1 | 182 | A | C5-C4 | -5.68 | 1.34 | 1.38 |
| 22 | 23S1 | 503 | A | N3-C4 | 5.68 | 1.38 | 1.34 |
| 22 | 23S1 | 1912 | A | N3-C4 | 5.68 | 1.38 | 1.34 |
| 1 | 16S1 | 253 | A | C5-C4 | -5.68 | 1.34 | 1.38 |
| 1 | 16S1 | 1377 | A | C5-C4 | -5.68 | 1.34 | 1.38 |
| 22 | 23S1 | 715 | A | C5-C4 | -5.68 | 1.34 | 1.38 |
| 22 | 23S1 | 2530 | A | N3-C4 | 5.68 | 1.38 | 1.34 |
| 1 | 16S1 | 1246 | A | C5-C4 | -5.68 | 1.34 | 1.38 |
| 22 | 23S1 | 716 | A | N3-C4 | 5.68 | 1.38 | 1.34 |
| 22 | 23S1 | 1608 | A | C8-N7 | 5.68 | 1.35 | 1.31 |
| 22 | 23S1 | 42 | A | N3-C4 | 5.68 | 1.38 | 1.34 |
| 22 | 23S1 | 2070 | A | C8-N7 | 5.68 | 1.35 | 1.31 |
| 55 | PTR1 | 58 | A | C5-C4 | -5.68 | 1.34 | 1.38 |
| 1 | 16S1 | 344 | A | C5-C4 | -5.68 | 1.34 | 1.38 |
| 1 | 16S1 | 382 | A | N3-C4 | 5.68 | 1.38 | 1.34 |
| 1 | 16S1 | 547 | A | C5-C4 | -5.68 | 1.34 | 1.38 |
| 1 | 16S1 | 715 | A | C8-N7 | 5.68 | 1.35 | 1.31 |
| 22 | 23S1 | 983 | A | C8-N7 | 5.68 | 1.35 | 1.31 |
| 22 | 23S1 | 1739 | A | N3-C4 | 5.68 | 1.38 | 1.34 |
| 22 | 23S1 | 2314 | A | N3-C4 | 5.68 | 1.38 | 1.34 |
| 22 | 23S1 | 2317 | A | C5-C4 | -5.68 | 1.34 | 1.38 |
| 22 | 23S1 | 2598 | A | N7-C5 | -5.68 | 1.35 | 1.39 |
| 1 | 16S1 | 7 | A | N3-C4 | 5.67 | 1.38 | 1.34 |
| 1 | 16S1 | 109 | A | C8-N7 | 5.67 | 1.35 | 1.31 |
| 1 | 16S1 | 228 | A | N3-C4 | 5.67 | 1.38 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 16S1 | 1288 | A | C8-N7 | 5.67 | 1.35 | 1.31 |
| 22 | 23S1 | 244 | A | N3-C4 | 5.67 | 1.38 | 1.34 |
| 22 | 23S1 | 988 | A | C8-N7 | 5.67 | 1.35 | 1.31 |
| 22 | 23S1 | 1805 | A | C8-N7 | 5.67 | 1.35 | 1.31 |
| 1 | 16S1 | 195 | A | C5-C4 | -5.67 | 1.34 | 1.38 |
| 22 | 23S1 | 528 | A | N3-C4 | 5.67 | 1.38 | 1.34 |
| 22 | 23S1 | 1433 | A | C5-C4 | -5.67 | 1.34 | 1.38 |
| 1 | 16S1 | 498 | A | C5-C4 | -5.67 | 1.34 | 1.38 |
| 1 | 16S1 | 609 | A | C5-C4 | -5.67 | 1.34 | 1.38 |
| 1 | 16S1 | 1167 | A | C5-C4 | -5.67 | 1.34 | 1.38 |
| 22 | 23S1 | 1133 | A | C8-N7 | 5.67 | 1.35 | 1.31 |
| 22 | 23S1 | 2352 | A | C5-C4 | -5.67 | 1.34 | 1.38 |
| 1 | 16S1 | 161 | A | C8-N7 | 5.67 | 1.35 | 1.31 |
| 1 | 16S1 | 1289 | A | C5-C4 | -5.67 | 1.34 | 1.38 |
| 1 | 16S1 | 595 | A | N3-C4 | 5.67 | 1.38 | 1.34 |
| 22 | 23S1 | 2287 | A | C8-N7 | 5.67 | 1.35 | 1.31 |
| 1 | 16S1 | 262 | A | N3-C4 | 5.67 | 1.38 | 1.34 |
| 1 | 16S1 | 432 | A | C5-C4 | -5.67 | 1.34 | 1.38 |
| 1 | 16S1 | 1188 | A | N3-C4 | 5.67 | 1.38 | 1.34 |
| 1 | 16S1 | 1289 | A | N3-C4 | 5.67 | 1.38 | 1.34 |
| 1 | 16S1 | 1306 | A | N3-C4 | 5.67 | 1.38 | 1.34 |
| 1 | 16S1 | 1311 | A | N3-C4 | 5.67 | 1.38 | 1.34 |
| 22 | 23S1 | 63 | A | N3-C4 | 5.67 | 1.38 | 1.34 |
| 22 | 23S1 | 443 | A | C8-N7 | 5.67 | 1.35 | 1.31 |
| 1 | 16S1 | 195 | A | N3-C4 | 5.67 | 1.38 | 1.34 |
| 22 | 23S1 | 2565 | A | N7-C5 | -5.67 | 1.35 | 1.39 |
| 1 | 16S1 | 1016 | A | C5-C4 | -5.66 | 1.34 | 1.38 |
| 1 | 16S1 | 1357 | A | C8-N7 | 5.66 | 1.35 | 1.31 |
| 22 | 23S1 | 1630 | A | N3-C4 | 5.66 | 1.38 | 1.34 |
| 22 | 23S1 | 2873 | A | C8-N7 | 5.66 | 1.35 | 1.31 |
| 22 | 23S1 | 111 | A | N3-C4 | 5.66 | 1.38 | 1.34 |
| 22 | 23S1 | 2821 | A | C8-N7 | 5.66 | 1.35 | 1.31 |
| 1 | 16S1 | 1456 | A | C5-C4 | -5.66 | 1.34 | 1.38 |
| 22 | 23S1 | 1552 | A | C8-N7 | 5.66 | 1.35 | 1.31 |
| 1 | 16S1 | 1151 | A | N3-C4 | 5.66 | 1.38 | 1.34 |
| 22 | 23S1 | 753 | A | C8-N7 | 5.66 | 1.35 | 1.31 |
| 22 | 23S1 | 2274 | A | C5-C4 | -5.66 | 1.34 | 1.38 |
| 22 | 23S1 | 764 | A | N3-C4 | 5.66 | 1.38 | 1.34 |
| 22 | 23S1 | 1494 | A | N3-C4 | 5.66 | 1.38 | 1.34 |
| 1 | 16S1 | 559 | A | C5-C4 | -5.66 | 1.34 | 1.38 |
| 22 | 23S1 | 196 | A | N3-C4 | 5.66 | 1.38 | 1.34 |
| 22 | 23S1 | 1495 | A | C5-C4 | -5.66 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 2142 | A | C5-C4 | -5.66 | 1.34 | 1.38 |
| 22 | 23S1 | 2273 | A | C8-N7 | 5.66 | 1.35 | 1.31 |
| 1 | 16S1 | 189 | A | N3-C4 | 5.65 | 1.38 | 1.34 |
| 22 | 23S1 | 1144 | A | C8-N7 | 5.65 | 1.35 | 1.31 |
| 22 | 23S1 | 1952 | A | C8-N7 | 5.65 | 1.35 | 1.31 |
| 1 | 16S1 | 72 | A | C5-C4 | -5.65 | 1.34 | 1.38 |
| 1 | 16S1 | 152 | A | C5-C4 | -5.65 | 1.34 | 1.38 |
| 22 | 23S1 | 64 | A | C5-C4 | -5.65 | 1.34 | 1.38 |
| 22 | 23S1 | 627 | A | C8-N7 | 5.65 | 1.35 | 1.31 |
| 22 | 23S1 | 910 | A | C8-N7 | 5.65 | 1.35 | 1.31 |
| 22 | 23S1 | 1367 | A | C8-N7 | 5.65 | 1.35 | 1.31 |
| 22 | 23S1 | 1705 | A | N3-C4 | 5.65 | 1.38 | 1.34 |
| 1 | 16S1 | 1269 | A | C5-C4 | -5.65 | 1.34 | 1.38 |
| 22 | 23S1 | 71 | A | N3-C4 | 5.65 | 1.38 | 1.34 |
| 22 | 23S1 | 1111 | A | N3-C4 | 5.65 | 1.38 | 1.34 |
| 1 | 16S1 | 923 | A | N7-C5 | -5.65 | 1.35 | 1.39 |
| 1 | 16S1 | 1269 | A | N3-C4 | 5.65 | 1.38 | 1.34 |
| 22 | 23S1 | 2792 | A | C5-C4 | -5.65 | 1.34 | 1.38 |
| 22 | 23S1 | 191 | A | N7-C5 | -5.64 | 1.35 | 1.39 |
| 22 | 23S1 | 216 | A | N3-C4 | 5.64 | 1.38 | 1.34 |
| 22 | 23S1 | 1165 | A | C8-N7 | 5.64 | 1.35 | 1.31 |
| 22 | 23S1 | 2654 | A | N3-C4 | 5.64 | 1.38 | 1.34 |
| 23 | 05S1 | 66 | A | C5-C4 | -5.64 | 1.34 | 1.38 |
| 1 | 16S1 | 696 | A | N3-C4 | 5.64 | 1.38 | 1.34 |
| 22 | 23S1 | 793 | A | C8-N7 | 5.64 | 1.35 | 1.31 |
| 22 | 23S1 | 1553 | A | C8-N7 | 5.64 | 1.35 | 1.31 |
| 22 | 23S1 | 2826 | A | N3-C4 | 5.64 | 1.38 | 1.34 |
| 1 | 16S1 | 55 | A | C8-N7 | 5.64 | 1.35 | 1.31 |
| 23 | 05S1 | 101 | A | C5-C4 | -5.64 | 1.34 | 1.38 |
| 1 | 16S1 | 547 | A | N3-C4 | 5.64 | 1.38 | 1.34 |
| 22 | 23S1 | 176 | A | N3-C4 | 5.64 | 1.38 | 1.34 |
| 1 | 16S1 | 1239 | A | C5-C4 | -5.64 | 1.34 | 1.38 |
| 1 | 16S1 | 320 | A | N3-C4 | 5.64 | 1.38 | 1.34 |
| 22 | 23S1 | 1029 | A | N7-C5 | -5.64 | 1.35 | 1.39 |
| 1 | 16S1 | 374 | A | N3-C4 | 5.63 | 1.38 | 1.34 |
| 22 | 23S1 | 1808 | A | C5-C4 | -5.63 | 1.34 | 1.38 |
| 22 | 23S1 | 2809 | A | C5-C4 | -5.63 | 1.34 | 1.38 |
| 22 | 23S1 | 471 | A | N3-C4 | 5.63 | 1.38 | 1.34 |
| 22 | 23S1 | 1147 | A | N3-C4 | 5.63 | 1.38 | 1.34 |
| 22 | 23S1 | 1794 | A | C8-N7 | 5.63 | 1.35 | 1.31 |
| 1 | 16S1 | 1111 | A | C8-N7 | 5.63 | 1.35 | 1.31 |
| 1 | 16S1 | 1176 | A | C5-C4 | -5.63 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 226 | A | C8-N7 | 5.63 | 1.35 | 1.31 |
| 22 | 23S1 | 453 | A | C8-N7 | 5.63 | 1.35 | 1.31 |
| 1 | 16S1 | 635 | A | N3-C4 | 5.62 | 1.38 | 1.34 |
| 22 | 23S1 | 2241 | A | C8-N7 | 5.62 | 1.35 | 1.31 |
| 1 | 16S1 | 71 | A | C5-C4 | -5.62 | 1.34 | 1.38 |
| 1 | 16S1 | 1239 | A | N3-C4 | 5.62 | 1.38 | 1.34 |
| 22 | 23S1 | 28 | A | C8-N7 | 5.62 | 1.35 | 1.31 |
| 22 | 23S1 | 1553 | A | N3-C4 | 5.62 | 1.38 | 1.34 |
| 1 | 16S1 | 1324 | A | C8-N7 | 5.62 | 1.35 | 1.31 |
| 22 | 23S1 | 1470 | A | C8-N7 | 5.62 | 1.35 | 1.31 |
| 22 | 23S1 | 1801 | A | C5-C4 | -5.62 | 1.34 | 1.38 |
| 22 | 23S1 | 161 | A | C5-C4 | -5.62 | 1.34 | 1.38 |
| 22 | 23S1 | 1308 | A | C8-N7 | 5.62 | 1.35 | 1.31 |
| 22 | 23S1 | 2434 | A | C8-N7 | 5.62 | 1.35 | 1.31 |
| 1 | 16S1 | 802 | A | C8-N7 | 5.62 | 1.35 | 1.31 |
| 1 | 16S1 | 1014 | A | C8-N7 | 5.62 | 1.35 | 1.31 |
| 1 | 16S1 | 179 | A | N3-C4 | 5.61 | 1.38 | 1.34 |
| 22 | 23S1 | 142 | A | C8-N7 | 5.61 | 1.35 | 1.31 |
| 22 | 23S1 | 749 | A | C8-N7 | 5.61 | 1.35 | 1.31 |
| 1 | 16S1 | 1093 | A | C8-N7 | 5.61 | 1.35 | 1.31 |
| 1 | 16S1 | 1531 | A | N3-C4 | 5.61 | 1.38 | 1.34 |
| 22 | 23S1 | 218 | A | C8-N7 | 5.61 | 1.35 | 1.31 |
| 22 | 23S1 | 1366 | A | C8-N7 | 5.61 | 1.35 | 1.31 |
| 1 | 16S1 | 465 | A | C5-C4 | -5.61 | 1.34 | 1.38 |
| 1 | 16S1 | 1339 | A | C8-N7 | 5.61 | 1.35 | 1.31 |
| 22 | 23S1 | 2757 | A | C5-C4 | -5.61 | 1.34 | 1.38 |
| 1 | 16S1 | 546 | A | N3-C4 | 5.61 | 1.38 | 1.34 |
| 1 | 16S1 | 716 | A | C8-N7 | 5.61 | 1.35 | 1.31 |
| 1 | 16S1 | 1447 | A | C5-C4 | -5.61 | 1.34 | 1.38 |
| 22 | 23S1 | 13 | A | C5-C4 | -5.61 | 1.34 | 1.38 |
| 22 | 23S1 | 1307 | A | C8-N7 | 5.61 | 1.35 | 1.31 |
| 22 | 23S1 | 2665 | A | C5-C4 | -5.61 | 1.34 | 1.38 |
| 23 | 05S1 | 78 | A | C8-N7 | 5.61 | 1.35 | 1.31 |
| 1 | 16S1 | 609 | A | N3-C4 | 5.60 | 1.38 | 1.34 |
| 1 | 16S1 | 236 | A | C5-C4 | -5.60 | 1.34 | 1.38 |
| 1 | 16S1 | 1055 | A | C8-N7 | 5.60 | 1.35 | 1.31 |
| 22 | 23S1 | 716 | A | C5-C4 | -5.60 | 1.34 | 1.38 |
| 22 | 23S1 | 1365 | A | C5-C4 | -5.60 | 1.34 | 1.38 |
| 22 | 23S1 | 1387 | A | N3-C4 | 5.60 | 1.38 | 1.34 |
| 1 | 16S1 | 77 | A | C2-N3 | 5.60 | 1.38 | 1.33 |
| 1 | 16S1 | 374 | A | C5-C4 | -5.60 | 1.34 | 1.38 |
| 1 | 16S1 | 878 | A | N3-C4 | 5.60 | 1.38 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 347 | A | C5-C4 | -5.60 | 1.34 | 1.38 |
| 22 | 23S1 | 1635 | A | N3-C4 | 5.60 | 1.38 | 1.34 |
| 22 | 23S1 | 2705 | A | C8-N7 | 5.60 | 1.35 | 1.31 |
| 1 | 16S1 | 306 | A | N3-C4 | 5.60 | 1.38 | 1.34 |
| 1 | 16S1 | 466 | A | N3-C4 | 5.60 | 1.38 | 1.34 |
| 22 | 23S1 | 1494 | A | C5-C4 | -5.60 | 1.34 | 1.38 |
| 22 | 23S1 | 1626 | A | C8-N7 | 5.60 | 1.35 | 1.31 |
| 22 | 23S1 | 2682 | A | N3-C4 | 5.60 | 1.38 | 1.34 |
| 22 | 23S1 | 2700 | A | C8-N7 | 5.60 | 1.35 | 1.31 |
| 1 | 16S1 | 706 | A | N3-C4 | 5.60 | 1.38 | 1.34 |
| 1 | 16S1 | 872 | A | C5-C4 | -5.60 | 1.34 | 1.38 |
| 22 | 23S1 | 1508 | A | N3-C4 | 5.59 | 1.38 | 1.34 |
| 22 | 23S1 | 2388 | A | C8-N7 | 5.59 | 1.35 | 1.31 |
| 22 | 23S1 | 2820 | A | C5-C4 | -5.59 | 1.34 | 1.38 |
| 1 | 16S1 | 1227 | A | N3-C4 | 5.59 | 1.38 | 1.34 |
| 22 | 23S1 | 1469 | A | C8-N7 | 5.59 | 1.35 | 1.31 |
| 22 | 23S1 | 2278 | A | C8-N7 | 5.59 | 1.35 | 1.31 |
| 22 | 23S1 | 2749 | A | N3-C4 | 5.59 | 1.38 | 1.34 |
| 22 | 23S1 | 432 | A | N3-C4 | 5.59 | 1.38 | 1.34 |
| 22 | 23S1 | 2810 | A | C5-C4 | -5.59 | 1.34 | 1.38 |
| 1 | 16S1 | 356 | A | N3-C4 | 5.59 | 1.38 | 1.34 |
| 22 | 23S1 | 1786 | A | C8-N7 | 5.59 | 1.35 | 1.31 |
| 22 | 23S1 | 2059 | A | C8-N7 | 5.59 | 1.35 | 1.31 |
| 22 | 23S1 | 721 | A | N3-C4 | 5.59 | 1.38 | 1.34 |
| 1 | 16S1 | 695 | A | C5-C4 | -5.58 | 1.34 | 1.38 |
| 22 | 23S1 | 603 | A | N3-C4 | 5.58 | 1.38 | 1.34 |
| 1 | 16S1 | 451 | A | N3-C4 | 5.58 | 1.38 | 1.34 |
| 22 | 23S1 | 231 | A | N3-C4 | 5.58 | 1.38 | 1.34 |
| 22 | 23S1 | 1938 | A | C8-N7 | 5.58 | 1.35 | 1.31 |
| 1 | 16S1 | 199 | A | C5-C4 | -5.58 | 1.34 | 1.38 |
| 22 | 23S1 | 538 | A | N3-C4 | 5.58 | 1.38 | 1.34 |
| 22 | 23S1 | 1640 | A | C5-C4 | -5.58 | 1.34 | 1.38 |
| 1 | 16S1 | 190 | A | N7-C5 | -5.58 | 1.35 | 1.39 |
| 1 | 16S1 | 1201 | A | C2-N3 | 5.58 | 1.38 | 1.33 |
| 22 | 23S1 | 49 | A | C8-N7 | 5.58 | 1.35 | 1.31 |
| 22 | 23S1 | 819 | A | N7-C5 | -5.58 | 1.35 | 1.39 |
| 22 | 23S1 | 1551 | A | N3-C4 | 5.58 | 1.38 | 1.34 |
| 22 | 23S1 | 1722 | A | C8-N7 | 5.58 | 1.35 | 1.31 |
| 22 | 23S1 | 1918 | A | C5-C4 | -5.58 | 1.34 | 1.38 |
| 22 | 23S1 | 2298 | A | N3-C4 | 5.58 | 1.38 | 1.34 |
| 1 | 16S1 | 1275 | A | N3-C4 | 5.58 | 1.38 | 1.34 |
| 22 | 23S1 | 2614 | A | C5-C4 | -5.58 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 55 | PTR1 | 42 | A | C5-C4 | -5.58 | 1.34 | 1.38 |
| 22 | 23S1 | 501 | A | C5-C4 | -5.57 | 1.34 | 1.38 |
| 22 | 23S1 | 53 | A | C8-N7 | 5.57 | 1.35 | 1.31 |
| 22 | 23S1 | 2015 | A | N3-C4 | 5.57 | 1.38 | 1.34 |
| 22 | 23S1 | 2451 | A | C5-C4 | -5.57 | 1.34 | 1.38 |
| 22 | 23S1 | 2757 | A | C8-N7 | 5.57 | 1.35 | 1.31 |
| 1 | 16S1 | 608 | A | N3-C4 | 5.57 | 1.38 | 1.34 |
| 1 | 16S1 | 781 | A | C8-N7 | 5.57 | 1.35 | 1.31 |
| 22 | 23S1 | 1027 | A | C8-N7 | 5.57 | 1.35 | 1.31 |
| 22 | 23S1 | 1265 | A | C8-N7 | 5.57 | 1.35 | 1.31 |
| 22 | 23S1 | 2288 | A | N3-C4 | 5.57 | 1.38 | 1.34 |
| 22 | 23S1 | 2900 | A | C5-C4 | -5.57 | 1.34 | 1.38 |
| 22 | 23S1 | 643 | A | N3-C4 | 5.57 | 1.38 | 1.34 |
| 1 | 16S1 | 415 | A | C5-C4 | -5.57 | 1.34 | 1.38 |
| 1 | 16S1 | 1329 | A | N3-C4 | 5.57 | 1.38 | 1.34 |
| 55 | PTR1 | 51 | A | C5-C4 | -5.57 | 1.34 | 1.38 |
| 1 | 16S1 | 382 | A | C5-C4 | -5.57 | 1.34 | 1.38 |
| 22 | 23S1 | 2309 | A | C5-C4 | -5.56 | 1.34 | 1.38 |
| 22 | 23S1 | 345 | A | C5-C4 | -5.56 | 1.34 | 1.38 |
| 22 | 23S1 | 1000 | A | C8-N7 | 5.56 | 1.35 | 1.31 |
| 22 | 23S1 | 1321 | A | N3-C4 | 5.56 | 1.38 | 1.34 |
| 22 | 23S1 | 1641 | A | C8-N7 | 5.56 | 1.35 | 1.31 |
| 22 | 23S1 | 1757 | A | N3-C4 | 5.56 | 1.38 | 1.34 |
| 22 | 23S1 | 244 | A | C8-N7 | 5.56 | 1.35 | 1.31 |
| 1 | 16S1 | 1274 | A | C5-C4 | -5.56 | 1.34 | 1.38 |
| 22 | 23S1 | 340 | A | N3-C4 | 5.56 | 1.38 | 1.34 |
| 22 | 23S1 | 470 | A | C8-N7 | 5.56 | 1.35 | 1.31 |
| 22 | 23S1 | 863 | A | C8-N7 | 5.56 | 1.35 | 1.31 |
| 22 | 23S1 | 1735 | A | N3-C4 | 5.56 | 1.38 | 1.34 |
| 22 | 23S1 | 2281 | A | C8-N7 | 5.56 | 1.35 | 1.31 |
| 1 | 16S1 | 1500 | A | N3-C4 | 5.55 | 1.38 | 1.34 |
| 22 | 23S1 | 63 | A | C5-C4 | -5.55 | 1.34 | 1.38 |
| 22 | 23S1 | 2679 | A | C8-N7 | 5.55 | 1.35 | 1.31 |
| 1 | 16S1 | 913 | A | N3-C4 | 5.55 | 1.38 | 1.34 |
| 22 | 23S1 | 666 | A | C8-N7 | 5.55 | 1.35 | 1.31 |
| 1 | 16S1 | 1169 | A | N3-C4 | 5.55 | 1.38 | 1.34 |
| 22 | 23S1 | 507 | A | N3-C4 | 5.55 | 1.38 | 1.34 |
| 22 | 23S1 | 1088 | A | C2-N3 | 5.55 | 1.38 | 1.33 |
| 22 | 23S1 | 1678 | A | C8-N7 | 5.55 | 1.35 | 1.31 |
| 55 | PTR1 | 73 | A | C5-C4 | -5.55 | 1.34 | 1.38 |
| 22 | 23S1 | 300 | A | C8-N7 | 5.55 | 1.35 | 1.31 |
| 1 | 16S1 | 1257 | A | C5-C4 | -5.55 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 16S1 | 1508 | A | N3-C4 | 5.55 | 1.38 | 1.34 |
| 1 | 16S1 | 1014 | A | N3-C4 | 5.55 | 1.38 | 1.34 |
| 55 | PTR1 | 59 | A | C5-C4 | -5.54 | 1.34 | 1.38 |
| 1 | 16S1 | 246 | A | C8-N7 | 5.54 | 1.35 | 1.31 |
| 22 | 23S1 | 1244 | A | C8-N7 | 5.54 | 1.35 | 1.31 |
| 22 | 23S1 | 1635 | A | C8-N7 | 5.54 | 1.35 | 1.31 |
| 22 | 23S1 | 1652 | A | C8-N7 | 5.54 | 1.35 | 1.31 |
| 22 | 23S1 | 2199 | A | N3-C4 | 5.54 | 1.38 | 1.34 |
| 22 | 23S1 | 2352 | A | C8-N7 | 5.54 | 1.35 | 1.31 |
| 1 | 16S1 | 129 | A | N3-C4 | 5.54 | 1.38 | 1.34 |
| 1 | 16S1 | 718 | A | C5-C4 | -5.54 | 1.34 | 1.38 |
| 1 | 16S1 | 1092 | A | C5-C4 | -5.54 | 1.34 | 1.38 |
| 22 | 23S1 | 342 | A | C5-C4 | -5.54 | 1.34 | 1.38 |
| 22 | 23S1 | 362 | A | C2-N3 | 5.54 | 1.38 | 1.33 |
| 22 | 23S1 | 412 | A | C8-N7 | 5.54 | 1.35 | 1.31 |
| 1 | 16S1 | 1374 | A | N3-C4 | 5.54 | 1.38 | 1.34 |
| 22 | 23S1 | 94 | A | N3-C4 | 5.54 | 1.38 | 1.34 |
| 22 | 23S1 | 429 | A | C5-C4 | -5.54 | 1.34 | 1.38 |
| 22 | 23S1 | 505 | A | N3-C4 | 5.54 | 1.38 | 1.34 |
| 22 | 23S1 | 941 | A | C8-N7 | 5.54 | 1.35 | 1.31 |
| 23 | 05S1 | 58 | A | C5-C4 | -5.54 | 1.34 | 1.38 |
| 22 | 23S1 | 2247 | A | C8-N7 | 5.54 | 1.35 | 1.31 |
| 22 | 23S1 | 1744 | A | N3-C4 | 5.54 | 1.38 | 1.34 |
| 22 | 23S1 | 2266 | A | C8-N7 | 5.54 | 1.35 | 1.31 |
| 22 | 23S1 | 320 | A | N3-C4 | 5.53 | 1.38 | 1.34 |
| 22 | 23S1 | 1453 | A | C5-C4 | -5.53 | 1.34 | 1.38 |
| 22 | 23S1 | 1913 | A | N3-C4 | 5.53 | 1.38 | 1.34 |
| 22 | 23S1 | 2154 | A | C2-N3 | 5.53 | 1.38 | 1.33 |
| 23 | 05S1 | 59 | A | C5-C4 | -5.53 | 1.34 | 1.38 |
| 1 | 16S1 | 130 | A | C8-N7 | 5.53 | 1.35 | 1.31 |
| 1 | 16S1 | 1274 | A | N3-C4 | 5.53 | 1.38 | 1.34 |
| 22 | 23S1 | 1284 | A | N3-C4 | 5.53 | 1.38 | 1.34 |
| 22 | 23S1 | 384 | A | C8-N7 | 5.53 | 1.35 | 1.31 |
| 1 | 16S1 | 130 | A | N3-C4 | 5.53 | 1.38 | 1.34 |
| 1 | 16S1 | 228 | A | C5-C4 | -5.53 | 1.34 | 1.38 |
| 22 | 23S1 | 2171 | A | C5-C4 | -5.53 | 1.34 | 1.38 |
| 22 | 23S1 | 428 | A | C8-N7 | 5.53 | 1.35 | 1.31 |
| 22 | 23S1 | 1759 | A | C8-N7 | 5.53 | 1.35 | 1.31 |
| 22 | 23S1 | 2346 | A | C8-N7 | 5.53 | 1.35 | 1.31 |
| 1 | 16S1 | 139 | A | N3-C4 | 5.52 | 1.38 | 1.34 |
| 1 | 16S1 | 1179 | A | C5-C4 | -5.52 | 1.34 | 1.38 |
| 22 | 23S1 | 1286 | A | N3-C4 | 5.52 | 1.38 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 1302 | A | C8-N7 | 5.52 | 1.35 | 1.31 |
| 22 | 23S1 | 1571 | A | N7-C5 | -5.52 | 1.35 | 1.39 |
| 22 | 23S1 | 2893 | A | N3-C4 | 5.52 | 1.38 | 1.34 |
| 1 | 16S1 | 414 | A | C5-C4 | -5.52 | 1.34 | 1.38 |
| 1 | 16S1 | 649 | A | N3-C4 | 5.52 | 1.38 | 1.34 |
| 1 | 16S1 | 1362 | A | N3-C4 | 5.52 | 1.38 | 1.34 |
| 22 | 23S1 | 181 | A | C5-C4 | -5.52 | 1.34 | 1.38 |
| 22 | 23S1 | 222 | A | N3-C4 | 5.52 | 1.38 | 1.34 |
| 22 | 23S1 | 730 | A | N3-C4 | 5.52 | 1.38 | 1.34 |
| 1 | 16S1 | 101 | A | N3-C4 | 5.52 | 1.38 | 1.34 |
| 1 | 16S1 | 746 | A | N3-C4 | 5.52 | 1.38 | 1.34 |
| 22 | 23S1 | 505 | A | C8-N7 | 5.52 | 1.35 | 1.31 |
| 22 | 23S1 | 513 | A | N3-C4 | 5.52 | 1.38 | 1.34 |
| 22 | 23S1 | 1885 | A | N3-C4 | 5.52 | 1.38 | 1.34 |
| 55 | PTR1 | 23 | A | C5-C4 | -5.52 | 1.34 | 1.38 |
| 1 | 16S1 | 596 | A | N3-C4 | 5.52 | 1.38 | 1.34 |
| 22 | 23S1 | 2080 | A | C8-N7 | 5.51 | 1.35 | 1.31 |
| 1 | 16S1 | 1152 | A | N3-C4 | 5.51 | 1.38 | 1.34 |
| 22 | 23S1 | 677 | A | N3-C4 | 5.51 | 1.38 | 1.34 |
| 1 | 16S1 | 600 | A | N3-C4 | 5.51 | 1.38 | 1.34 |
| 22 | 23S1 | 401 | A | C8-N7 | 5.51 | 1.35 | 1.31 |
| 22 | 23S1 | 2476 | A | C8-N7 | 5.51 | 1.35 | 1.31 |
| 22 | 23S1 | 2900 | A | N3-C4 | 5.51 | 1.38 | 1.34 |
| 23 | 05S1 | 78 | A | N3-C4 | 5.51 | 1.38 | 1.34 |
| 1 | 16S1 | 539 | A | C5-C4 | -5.51 | 1.34 | 1.38 |
| 22 | 23S1 | 502 | A | N3-C4 | 5.51 | 1.38 | 1.34 |
| 22 | 23S1 | 632 | A | C8-N7 | 5.51 | 1.35 | 1.31 |
| 22 | 23S1 | 1821 | A | C8-N7 | 5.51 | 1.35 | 1.31 |
| 1 | 16S1 | 116 | A | C8-N7 | 5.51 | 1.35 | 1.31 |
| 1 | 16S1 | 253 | A | N3-C4 | 5.51 | 1.38 | 1.34 |
| 1 | 16S1 | 1499 | A | C8-N7 | 5.50 | 1.35 | 1.31 |
| 22 | 23S1 | 483 | A | N3-C4 | 5.50 | 1.38 | 1.34 |
| 22 | 23S1 | 2872 | A | C5-C4 | -5.50 | 1.34 | 1.38 |
| 1 | 16S1 | 977 | A | C5-C4 | -5.50 | 1.34 | 1.38 |
| 22 | 23S1 | 1393 | A | C8-N7 | 5.50 | 1.35 | 1.31 |
| 1 | 16S1 | 563 | A | N3-C4 | 5.50 | 1.38 | 1.34 |
| 1 | 16S1 | 1285 | A | N3-C4 | 5.50 | 1.38 | 1.34 |
| 22 | 23S1 | 917 | A | C8-N7 | 5.50 | 1.35 | 1.31 |
| 22 | 23S1 | 1572 | A | C8-N7 | 5.50 | 1.35 | 1.31 |
| 22 | 23S1 | 272 | A | C5-C4 | -5.50 | 1.34 | 1.38 |
| 1 | 16S1 | 533 | A | C2-N3 | 5.50 | 1.38 | 1.33 |
| 22 | 23S1 | 996 | A | C8-N7 | 5.50 | 1.35 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 1755 | A | N3-C4 | 5.50 | 1.38 | 1.34 |
| 22 | 23S1 | 2335 | A | C8-N7 | 5.50 | 1.35 | 1.31 |
| 1 | 16S1 | 389 | A | C5-C4 | -5.49 | 1.34 | 1.38 |
| 1 | 16S1 | 949 | A | N3-C4 | 5.49 | 1.38 | 1.34 |
| 1 | 16S1 | 1046 | A | N3-C4 | 5.49 | 1.38 | 1.34 |
| 1 | 16S1 | 1145 | A | N3-C4 | 5.49 | 1.38 | 1.34 |
| 22 | 23S1 | 309 | A | C8-N7 | 5.49 | 1.35 | 1.31 |
| 22 | 23S1 | 1143 | A | N3-C4 | 5.49 | 1.38 | 1.34 |
| 22 | 23S1 | 1254 | A | C8-N7 | 5.49 | 1.35 | 1.31 |
| 22 | 23S1 | 905 | A | N3-C4 | 5.49 | 1.38 | 1.34 |
| 1 | 16S1 | 143 | A | C5-C4 | -5.49 | 1.34 | 1.38 |
| 1 | 16S1 | 640 | A | N3-C4 | 5.49 | 1.38 | 1.34 |
| 22 | 23S1 | 14 | A | C8-N7 | 5.49 | 1.35 | 1.31 |
| 22 | 23S1 | 2009 | A | C8-N7 | 5.49 | 1.35 | 1.31 |
| 22 | 23S1 | 2589 | A | N3-C4 | 5.49 | 1.38 | 1.34 |
| 22 | 23S1 | 1470 | A | N3-C4 | 5.49 | 1.38 | 1.34 |
| 22 | 23S1 | 2665 | A | N3-C4 | 5.49 | 1.38 | 1.34 |
| 22 | 23S1 | 2733 | A | C5-C4 | -5.49 | 1.34 | 1.38 |
| 1 | 16S1 | 1179 | A | N3-C4 | 5.49 | 1.38 | 1.34 |
| 22 | 23S1 | 2266 | A | N3-C4 | 5.49 | 1.38 | 1.34 |
| 1 | 16S1 | 1248 | A | N3-C4 | 5.49 | 1.38 | 1.34 |
| 22 | 23S1 | 603 | A | C5-C4 | -5.49 | 1.34 | 1.38 |
| 22 | 23S1 | 705 | A | N3-C4 | 5.49 | 1.38 | 1.34 |
| 1 | 16S1 | 630 | A | N3-C4 | 5.48 | 1.38 | 1.34 |
| 1 | 16S1 | 746 | A | C5-C4 | -5.48 | 1.34 | 1.38 |
| 1 | 16S1 | 1248 | A | C5-C4 | -5.48 | 1.34 | 1.38 |
| 22 | 23S1 | 415 | A | C8-N7 | 5.48 | 1.35 | 1.31 |
| 1 | 16S1 | 702 | A | C5-C4 | -5.48 | 1.34 | 1.38 |
| 1 | 16S1 | 873 | A | N7-C5 | -5.48 | 1.35 | 1.39 |
| 22 | 23S1 | 149 | A | N3-C4 | 5.48 | 1.38 | 1.34 |
| 22 | 23S1 | 1098 | A | C2-N3 | 5.48 | 1.38 | 1.33 |
| 22 | 23S1 | 2037 | A | N3-C4 | 5.48 | 1.38 | 1.34 |
| 22 | 23S1 | 2225 | A | C8-N7 | 5.48 | 1.35 | 1.31 |
| 22 | 23S1 | 2531 | A | C5-C4 | -5.48 | 1.34 | 1.38 |
| 22 | 23S1 | 1791 | A | N7-C5 | -5.48 | 1.35 | 1.39 |
| 22 | 23S1 | 1808 | A | N3-C4 | 5.48 | 1.38 | 1.34 |
| 1 | 16S1 | 1503 | A | C8-N7 | 5.48 | 1.35 | 1.31 |
| 1 | 16S1 | 101 | A | C5-C4 | -5.48 | 1.34 | 1.38 |
| 1 | 16S1 | 162 | A | C5-C4 | -5.48 | 1.34 | 1.38 |
| 1 | 16S1 | 919 | A | C8-N7 | 5.48 | 1.35 | 1.31 |
| 22 | 23S1 | 478 | A | C8-N7 | 5.48 | 1.35 | 1.31 |
| 22 | 23S1 | 1241 | A | N3-C4 | 5.48 | 1.38 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 16S1 | 50 | A | C5-C4 | -5.48 | 1.34 | 1.38 |
| 1 | 16S1 | 327 | A | N3-C4 | 5.48 | 1.38 | 1.34 |
| 22 | 23S1 | 1265 | A | N3-C4 | 5.48 | 1.38 | 1.34 |
| 22 | 23S1 | 1654 | A | C8-N7 | 5.48 | 1.35 | 1.31 |
| 1 | 16S1 | 1246 | A | N3-C4 | 5.47 | 1.38 | 1.34 |
| 22 | 23S1 | 975 | A | C8-N7 | 5.47 | 1.35 | 1.31 |
| 22 | 23S1 | 2077 | A | N7-C5 | -5.47 | 1.35 | 1.39 |
| 22 | 23S1 | 322 | A | N3-C4 | 5.47 | 1.38 | 1.34 |
| 22 | 23S1 | 1655 | A | C8-N7 | 5.47 | 1.35 | 1.31 |
| 22 | 23S1 | 2317 | A | N3-C4 | 5.47 | 1.38 | 1.34 |
| 22 | 23S1 | 2516 | A | C8-N7 | 5.47 | 1.35 | 1.31 |
| 22 | 23S1 | 149 | A | C5-C4 | -5.47 | 1.34 | 1.38 |
| 22 | 23S1 | 1241 | A | C8-N7 | 5.47 | 1.35 | 1.31 |
| 1 | 16S1 | 19 | A | C8-N7 | 5.47 | 1.35 | 1.31 |
| 22 | 23S1 | 739 | A | C8-N7 | 5.47 | 1.35 | 1.31 |
| 22 | 23S1 | 1276 | A | C8-N7 | 5.47 | 1.35 | 1.31 |
| 22 | 23S1 | 2432 | A | N3-C4 | 5.47 | 1.38 | 1.34 |
| 1 | 16S1 | 181 | A | C5-C4 | -5.47 | 1.34 | 1.38 |
| 22 | 23S1 | 2020 | A | C8-N7 | 5.47 | 1.35 | 1.31 |
| 23 | 05S1 | 73 | A | C5-C4 | -5.47 | 1.34 | 1.38 |
| 1 | 16S1 | 495 | A | C5-C4 | -5.47 | 1.34 | 1.38 |
| 22 | 23S1 | 575 | A | C8-N7 | 5.47 | 1.35 | 1.31 |
| 1 | 16S1 | 687 | A | N3-C4 | 5.46 | 1.38 | 1.34 |
| 1 | 16S1 | 909 | A | N3-C4 | 5.46 | 1.38 | 1.34 |
| 22 | 23S1 | 626 | A | C5-C4 | -5.46 | 1.34 | 1.38 |
| 22 | 23S1 | 2518 | A | C8-N7 | 5.46 | 1.35 | 1.31 |
| 1 | 16S1 | 629 | A | N3-C4 | 5.46 | 1.38 | 1.34 |
| 22 | 23S1 | 2662 | A | N3-C4 | 5.46 | 1.38 | 1.34 |
| 22 | 23S1 | 2758 | A | N3-C4 | 5.46 | 1.38 | 1.34 |
| 1 | 16S1 | 1318 | A | C5-C4 | -5.46 | 1.34 | 1.38 |
| 22 | 23S1 | 279 | A | C5-C4 | -5.46 | 1.34 | 1.38 |
| 22 | 23S1 | 616 | A | N3-C4 | 5.46 | 1.38 | 1.34 |
| 22 | 23S1 | 2369 | A | C8-N7 | 5.46 | 1.35 | 1.31 |
| 22 | 23S1 | 207 | A | N3-C4 | 5.46 | 1.38 | 1.34 |
| 22 | 23S1 | 979 | A | C8-N7 | 5.46 | 1.35 | 1.31 |
| 22 | 23S1 | 1336 | A | N3-C4 | 5.46 | 1.38 | 1.34 |
| 22 | 23S1 | 1342 | A | N3-C4 | 5.46 | 1.38 | 1.34 |
| 55 | PTR1 | 69 | A | C5-C4 | -5.46 | 1.34 | 1.38 |
| 1 | 16S1 | 60 | A | N3-C4 | 5.46 | 1.38 | 1.34 |
| 1 | 16S1 | 487 | A | N3-C4 | 5.46 | 1.38 | 1.34 |
| 1 | 16S1 | 996 | A | C5-C4 | -5.46 | 1.34 | 1.38 |
| 22 | 23S1 | 614 | A | C5-C4 | -5.46 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 2826 | A | C8-N7 | 5.46 | 1.35 | 1.31 |
| 1 | 16S1 | 223 | A | C5-C4 | -5.46 | 1.34 | 1.38 |
| 1 | 16S1 | 383 | A | C2-N3 | 5.46 | 1.38 | 1.33 |
| 22 | 23S1 | 56 | A | C8-N7 | 5.46 | 1.35 | 1.31 |
| 22 | 23S1 | 1301 | A | N3-C4 | 5.46 | 1.38 | 1.34 |
| 22 | 23S1 | 2660 | A | C5-C4 | -5.46 | 1.34 | 1.38 |
| 22 | 23S1 | 800 | A | C8-N7 | 5.46 | 1.35 | 1.31 |
| 22 | 23S1 | 1655 | A | N3-C4 | 5.46 | 1.38 | 1.34 |
| 1 | 16S1 | 648 | A | N3-C4 | 5.45 | 1.38 | 1.34 |
| 1 | 16S1 | 964 | A | N3-C4 | 5.45 | 1.38 | 1.34 |
| 22 | 23S1 | 199 | A | N7-C5 | -5.45 | 1.35 | 1.39 |
| 22 | 23S1 | 2059 | A | N3-C4 | 5.45 | 1.38 | 1.34 |
| 22 | 23S1 | 2412 | A | N3-C4 | 5.45 | 1.38 | 1.34 |
| 22 | 23S1 | 2682 | A | C8-N7 | 5.45 | 1.35 | 1.31 |
| 22 | 23S1 | 64 | A | N3-C4 | 5.45 | 1.38 | 1.34 |
| 22 | 23S1 | 1746 | A | C5-C4 | -5.45 | 1.34 | 1.38 |
| 22 | 23S1 | 2058 | A | N3-C4 | 5.45 | 1.38 | 1.34 |
| 1 | 16S1 | 161 | A | C5-C4 | -5.45 | 1.34 | 1.38 |
| 22 | 23S1 | 1151 | A | N3-C4 | 5.45 | 1.38 | 1.34 |
| 22 | 23S1 | 2205 | A | N3-C4 | 5.45 | 1.38 | 1.34 |
| 22 | 23S1 | 311 | A | N3-C4 | 5.45 | 1.38 | 1.34 |
| 1 | 16S1 | 510 | A | N3-C4 | 5.44 | 1.38 | 1.34 |
| 22 | 23S1 | 1008 | A | N3-C4 | 5.44 | 1.38 | 1.34 |
| 1 | 16S1 | 162 | A | N3-C4 | 5.44 | 1.38 | 1.34 |
| 1 | 16S1 | 712 | A | C5-C4 | -5.44 | 1.34 | 1.38 |
| 22 | 23S1 | 324 | A | N3-C4 | 5.44 | 1.38 | 1.34 |
| 22 | 23S1 | 2335 | A | N3-C4 | 5.44 | 1.38 | 1.34 |
| 1 | 16S1 | 190 | A | C2-N3 | 5.44 | 1.38 | 1.33 |
| 1 | 16S1 | 44 | A | N3-C4 | 5.44 | 1.38 | 1.34 |
| 1 | 16S1 | 487 | A | C5-C4 | -5.44 | 1.34 | 1.38 |
| 1 | 16S1 | 1000 | A | C2-N3 | 5.44 | 1.38 | 1.33 |
| 22 | 23S1 | 217 | A | N3-C4 | 5.43 | 1.38 | 1.34 |
| 22 | 23S1 | 675 | A | C8-N7 | 5.43 | 1.35 | 1.31 |
| 22 | 23S1 | 2378 | A | N3-C4 | 5.43 | 1.38 | 1.34 |
| 55 | PTR1 | 3 | A | C5-C4 | -5.43 | 1.34 | 1.38 |
| 1 | 16S1 | 1396 | A | C8-N7 | 5.43 | 1.35 | 1.31 |
| 22 | 23S1 | 718 | A | C5-C4 | -5.43 | 1.34 | 1.38 |
| 22 | 23S1 | 1579 | A | N3-C4 | 5.43 | 1.38 | 1.34 |
| 22 | 23S1 | 2088 | A | C8-N7 | 5.43 | 1.35 | 1.31 |
| 22 | 23S1 | 2726 | A | N3-C4 | 5.43 | 1.38 | 1.34 |
| 1 | 16S1 | 609 | A | C8-N7 | 5.43 | 1.35 | 1.31 |
| 22 | 23S1 | 1204 | A | N3-C4 | 5.43 | 1.38 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 16S1 | 51 | A | N7-C5 | -5.43 | 1.35 | 1.39 |
| 22 | 23S1 | 2886 | A | N3-C4 | 5.43 | 1.38 | 1.34 |
| 1 | 16S1 | 629 | A | C5-C4 | -5.43 | 1.34 | 1.38 |
| 22 | 23S1 | 492 | A | N3-C4 | 5.43 | 1.38 | 1.34 |
| 1 | 16S1 | 60 | A | C5-C4 | -5.43 | 1.34 | 1.38 |
| 1 | 16S1 | 162 | A | C2-N3 | 5.43 | 1.38 | 1.33 |
| 22 | 23S1 | 227 | A | C8-N7 | 5.43 | 1.35 | 1.31 |
| 22 | 23S1 | 2097 | A | C5-C4 | -5.43 | 1.34 | 1.38 |
| 22 | 23S1 | 2406 | A | N3-C4 | 5.43 | 1.38 | 1.34 |
| 22 | 23S1 | 1637 | A | C8-N7 | 5.42 | 1.35 | 1.31 |
| 22 | 23S1 | 2534 | A | N3-C4 | 5.42 | 1.38 | 1.34 |
| 1 | 16S1 | 1275 | A | C5-C4 | -5.42 | 1.34 | 1.38 |
| 1 | 16S1 | 223 | A | N3-C4 | 5.42 | 1.38 | 1.34 |
| 22 | 23S1 | 941 | A | N3-C4 | 5.42 | 1.38 | 1.34 |
| 22 | 23S1 | 1603 | A | N3-C4 | 5.42 | 1.38 | 1.34 |
| 22 | 23S1 | 1762 | A | C8-N7 | 5.42 | 1.35 | 1.31 |
| 1 | 16S1 | 712 | A | N3-C4 | 5.42 | 1.38 | 1.34 |
| 22 | 23S1 | 918 | A | C8-N7 | 5.42 | 1.35 | 1.31 |
| 1 | 16S1 | 553 | A | N3-C4 | 5.42 | 1.38 | 1.34 |
| 22 | 23S1 | 727 | A | C8-N7 | 5.42 | 1.35 | 1.31 |
| 22 | 23S1 | 1679 | A | C8-N7 | 5.42 | 1.35 | 1.31 |
| 22 | 23S1 | 1754 | A | C8-N7 | 5.42 | 1.35 | 1.31 |
| 1 | 16S1 | 336 | A | C8-N7 | 5.42 | 1.35 | 1.31 |
| 1 | 16S1 | 1036 | A | N3-C4 | 5.42 | 1.38 | 1.34 |
| 22 | 23S1 | 661 | A | N3-C4 | 5.42 | 1.38 | 1.34 |
| 22 | 23S1 | 265 | A | N3-C4 | 5.42 | 1.38 | 1.34 |
| 1 | 16S1 | 959 | A | C8-N7 | 5.41 | 1.35 | 1.31 |
| 1 | 16S1 | 1019 | A | C5-C4 | -5.41 | 1.34 | 1.38 |
| 22 | 23S1 | 1544 | A | C5-C4 | -5.41 | 1.34 | 1.38 |
| 22 | 23S1 | 2435 | A | N3-C4 | 5.41 | 1.38 | 1.34 |
| 22 | 23S1 | 126 | A | N3-C4 | 5.41 | 1.38 | 1.34 |
| 1 | 16S1 | 172 | A | C5-C4 | -5.41 | 1.34 | 1.38 |
| 1 | 16S1 | 1155 | A | N3-C4 | 5.41 | 1.38 | 1.34 |
| 22 | 23S1 | 782 | A | C8-N7 | 5.41 | 1.35 | 1.31 |
| 22 | 23S1 | 1021 | A | N3-C4 | 5.41 | 1.38 | 1.34 |
| 22 | 23S1 | 1634 | A | N3-C4 | 5.41 | 1.38 | 1.34 |
| 22 | 23S1 | 347 | A | N3-C4 | 5.41 | 1.38 | 1.34 |
| 22 | 23S1 | 402 | A | C8-N7 | 5.41 | 1.35 | 1.31 |
| 22 | 23S1 | 2412 | A | C8-N7 | 5.41 | 1.35 | 1.31 |
| 22 | 23S1 | 74 | A | C5-C4 | -5.41 | 1.34 | 1.38 |
| 22 | 23S1 | 2882 | A | N3-C4 | 5.41 | 1.38 | 1.34 |
| 23 | 05S1 | 50 | A | N3-C4 | 5.41 | 1.38 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 820 | A | N7-C5 | -5.40 | 1.36 | 1.39 |
| 22 | 23S1 | 1854 | A | N3-C4 | 5.40 | 1.38 | 1.34 |
| 22 | 23S1 | 2003 | A | C8-N7 | 5.40 | 1.35 | 1.31 |
| 1 | 16S1 | 1363 | A | N3-C4 | 5.40 | 1.38 | 1.34 |
| 22 | 23S1 | 352 | A | N3-C4 | 5.40 | 1.38 | 1.34 |
| 22 | 23S1 | 2376 | A | N3-C4 | 5.40 | 1.38 | 1.34 |
| 1 | 16S1 | 523 | A | N3-C4 | 5.40 | 1.38 | 1.34 |
| 22 | 23S1 | 861 | A | C8-N7 | 5.40 | 1.35 | 1.31 |
| 22 | 23S1 | 38 | A | N3-C4 | 5.40 | 1.38 | 1.34 |
| 1 | 16S1 | 300 | A | C5-C4 | -5.39 | 1.34 | 1.38 |
| 22 | 23S1 | 1129 | A | C8-N7 | 5.39 | 1.35 | 1.31 |
| 22 | 23S1 | 1802 | A | N7-C5 | -5.39 | 1.36 | 1.39 |
| 22 | 23S1 | 1858 | A | N3-C4 | 5.39 | 1.38 | 1.34 |
| 22 | 23S1 | 1916 | A | N3-C4 | 5.39 | 1.38 | 1.34 |
| 22 | 23S1 | 2381 | A | N3-C4 | 5.39 | 1.38 | 1.34 |
| 1 | 16S1 | 171 | A | N3-C4 | 5.39 | 1.38 | 1.34 |
| 1 | 16S1 | 574 | A | C8-N7 | 5.39 | 1.35 | 1.31 |
| 22 | 23S1 | 1247 | A | N3-C4 | 5.39 | 1.38 | 1.34 |
| 22 | 23S1 | 1420 | A | C5-C4 | -5.39 | 1.34 | 1.38 |
| 22 | 23S1 | 1705 | A | C8-N7 | 5.39 | 1.35 | 1.31 |
| 1 | 16S1 | 55 | A | N3-C4 | 5.39 | 1.38 | 1.34 |
| 1 | 16S1 | 1375 | A | N3-C4 | 5.39 | 1.38 | 1.34 |
| 22 | 23S1 | 472 | A | C8-N7 | 5.39 | 1.35 | 1.31 |
| 1 | 16S1 | 642 | A | C8-N7 | 5.39 | 1.35 | 1.31 |
| 1 | 16S1 | 451 | A | C5-C4 | -5.39 | 1.34 | 1.38 |
| 1 | 16S1 | 502 | A | C8-N7 | 5.39 | 1.35 | 1.31 |
| 1 | 16S1 | 749 | A | N3-C4 | 5.39 | 1.38 | 1.34 |
| 1 | 16S1 | 964 | A | C8-N7 | 5.39 | 1.35 | 1.31 |
| 22 | 23S1 | 504 | A | N3-C4 | 5.39 | 1.38 | 1.34 |
| 22 | 23S1 | 1169 | A | N3-C4 | 5.39 | 1.38 | 1.34 |
| 22 | 23S1 | 2868 | A | C5-C4 | -5.39 | 1.34 | 1.38 |
| 1 | 16S1 | 309 | A | N3-C4 | 5.38 | 1.38 | 1.34 |
| 22 | 23S1 | 127 | A | N3-C4 | 5.38 | 1.38 | 1.34 |
| 22 | 23S1 | 1213 | A | N7-C5 | -5.38 | 1.36 | 1.39 |
| 22 | 23S1 | 2352 | A | N3-C4 | 5.38 | 1.38 | 1.34 |
| 22 | 23S1 | 2560 | A | C8-N7 | 5.38 | 1.35 | 1.31 |
| 22 | 23S1 | 1784 | A | C8-N7 | 5.38 | 1.35 | 1.31 |
| 1 | 16S1 | 197 | A | N3-C4 | 5.38 | 1.38 | 1.34 |
| 22 | 23S1 | 1151 | A | C8-N7 | 5.38 | 1.35 | 1.31 |
| 23 | 05S1 | 15 | A | N3-C4 | 5.38 | 1.38 | 1.34 |
| 22 | 23S1 | 980 | A | C8-N7 | 5.38 | 1.35 | 1.31 |
| 22 | 23S1 | 142 | A | N9-C8 | -5.38 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 16S1 | 767 | A | C8-N7 | 5.38 | 1.35 | 1.31 |
| 22 | 23S1 | 2435 | A | C8-N7 | 5.38 | 1.35 | 1.31 |
| 1 | 16S1 | 338 | A | C8-N7 | 5.38 | 1.35 | 1.31 |
| 22 | 23S1 | 1175 | A | C2-N3 | 5.37 | 1.38 | 1.33 |
| 22 | 23S1 | 1580 | A | N3-C4 | 5.37 | 1.38 | 1.34 |
| 22 | 23S1 | 2426 | A | N3-C4 | 5.37 | 1.38 | 1.34 |
| 1 | 16S1 | 747 | A | N3-C4 | 5.37 | 1.38 | 1.34 |
| 1 | 16S1 | 819 | A | N3-C4 | 5.37 | 1.38 | 1.34 |
| 22 | 23S1 | 563 | A | C8-N7 | 5.37 | 1.35 | 1.31 |
| 55 | PTR1 | 26 | A | C5-C4 | -5.37 | 1.34 | 1.38 |
| 1 | 16S1 | 1176 | A | N3-C4 | 5.37 | 1.38 | 1.34 |
| 22 | 23S1 | 466 | A | N7-C5 | -5.37 | 1.36 | 1.39 |
| 22 | 23S1 | 1508 | A | C5-C4 | -5.37 | 1.34 | 1.38 |
| 1 | 16S1 | 1375 | A | C8-N7 | 5.37 | 1.35 | 1.31 |
| 22 | 23S1 | 182 | A | N3-C4 | 5.37 | 1.38 | 1.34 |
| 22 | 23S1 | 972 | A | N7-C5 | -5.37 | 1.36 | 1.39 |
| 22 | 23S1 | 1189 | A | N3-C4 | 5.37 | 1.38 | 1.34 |
| 1 | 16S1 | 414 | A | N3-C4 | 5.37 | 1.38 | 1.34 |
| 1 | 16S1 | 456 | A | N3-C4 | 5.37 | 1.38 | 1.34 |
| 1 | 16S1 | 873 | A | N3-C4 | 5.37 | 1.38 | 1.34 |
| 22 | 23S1 | 2134 | A | C2-N3 | 5.37 | 1.38 | 1.33 |
| 22 | 23S1 | 2721 | A | C8-N7 | 5.37 | 1.35 | 1.31 |
| 1 | 16S1 | 608 | A | C8-N7 | 5.36 | 1.35 | 1.31 |
| 22 | 23S1 | 734 | A | C8-N7 | 5.36 | 1.35 | 1.31 |
| 22 | 23S1 | 1987 | A | N3-C4 | 5.36 | 1.38 | 1.34 |
| 1 | 16S1 | 288 | A | N3-C4 | 5.36 | 1.38 | 1.34 |
| 1 | 16S1 | 1465 | A | N3-C4 | 5.36 | 1.38 | 1.34 |
| 22 | 23S1 | 402 | A | N3-C4 | 5.36 | 1.38 | 1.34 |
| 1 | 16S1 | 1357 | A | N3-C4 | 5.36 | 1.38 | 1.34 |
| 22 | 23S1 | 332 | A | N3-C4 | 5.36 | 1.38 | 1.34 |
| 22 | 23S1 | 2142 | A | C2-N3 | 5.36 | 1.38 | 1.33 |
| 1 | 16S1 | 363 | A | N3-C4 | 5.36 | 1.38 | 1.34 |
| 22 | 23S1 | 1780 | A | N3-C4 | 5.36 | 1.38 | 1.34 |
| 1 | 16S1 | 1408 | A | N3-C4 | 5.36 | 1.38 | 1.34 |
| 22 | 23S1 | 670 | A | C8-N7 | 5.36 | 1.35 | 1.31 |
| 22 | 23S1 | 1802 | A | N3-C4 | 5.36 | 1.38 | 1.34 |
| 22 | 23S1 | 2003 | A | N3-C4 | 5.36 | 1.38 | 1.34 |
| 1 | 16S1 | 53 | A | N3-C4 | 5.35 | 1.38 | 1.34 |
| 22 | 23S1 | 1301 | A | C8-N7 | 5.35 | 1.35 | 1.31 |
| 22 | 23S1 | 1899 | A | N3-C4 | 5.35 | 1.38 | 1.34 |
| 22 | 23S1 | 1918 | A | N3-C4 | 5.35 | 1.38 | 1.34 |
| 23 | 05S1 | 53 | A | N3-C4 | 5.35 | 1.38 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 16S1 | 815 | A | N7-C5 | -5.35 | 1.36 | 1.39 |
| 22 | 23S1 | 482 | A | N3-C4 | 5.35 | 1.38 | 1.34 |
| 55 | PTR1 | 34 | I | C2-N3 | 5.35 | 1.46 | 1.35 |
| 22 | 23S1 | 1021 | A | C8-N7 | 5.35 | 1.35 | 1.31 |
| 22 | 23S1 | 1749 | A | N3-C4 | 5.35 | 1.38 | 1.34 |
| 22 | 23S1 | 849 | A | N3-C4 | 5.35 | 1.38 | 1.34 |
| 22 | 23S1 | 613 | A | C2-N3 | 5.34 | 1.38 | 1.33 |
| 22 | 23S1 | 2227 | A | C8-N7 | 5.34 | 1.35 | 1.31 |
| 22 | 23S1 | 1669 | A | C5-C4 | -5.34 | 1.35 | 1.38 |
| 1 | 16S1 | 533 | A | C5-C4 | -5.34 | 1.35 | 1.38 |
| 22 | 23S1 | 460 | A | C8-N7 | 5.34 | 1.35 | 1.31 |
| 22 | 23S1 | 783 | A | C5-C4 | -5.34 | 1.35 | 1.38 |
| 22 | 23S1 | 1103 | A | C5-C4 | -5.34 | 1.35 | 1.38 |
| 22 | 23S1 | 1268 | A | C8-N7 | 5.34 | 1.35 | 1.31 |
| 22 | 23S1 | 2031 | A | C8-N7 | 5.34 | 1.35 | 1.31 |
| 22 | 23S1 | 2513 | A | N3-C4 | 5.34 | 1.38 | 1.34 |
| 1 | 16S1 | 1441 | A | C2-N3 | 5.34 | 1.38 | 1.33 |
| 22 | 23S1 | 900 | A | C5-C4 | -5.34 | 1.35 | 1.38 |
| 22 | 23S1 | 2459 | A | C8-N7 | 5.34 | 1.35 | 1.31 |
| 1 | 16S1 | 1236 | A | N3-C4 | 5.34 | 1.38 | 1.34 |
| 1 | 16S1 | 1377 | A | N3-C4 | 5.34 | 1.38 | 1.34 |
| 22 | 23S1 | 1532 | A | C5-C4 | -5.34 | 1.35 | 1.38 |
| 22 | 23S1 | 1928 | A | N7-C5 | -5.34 | 1.36 | 1.39 |
| 22 | 23S1 | 2108 | A | C2-N3 | 5.34 | 1.38 | 1.33 |
| 23 | 05S1 | 45 | A | N3-C4 | 5.34 | 1.38 | 1.34 |
| 22 | 23S1 | 422 | A | N3-C4 | 5.33 | 1.38 | 1.34 |
| 22 | 23S1 | 1001 | A | C8-N7 | 5.33 | 1.35 | 1.31 |
| 22 | 23S1 | 2560 | A | N3-C4 | 5.33 | 1.38 | 1.34 |
| 1 | 16S1 | 1534 | A | C2-N3 | 5.33 | 1.38 | 1.33 |
| 22 | 23S1 | 501 | A | N3-C4 | 5.33 | 1.38 | 1.34 |
| 22 | 23S1 | 792 | A | C8-N7 | 5.33 | 1.35 | 1.31 |
| 22 | 23S1 | 911 | A | N3-C4 | 5.33 | 1.38 | 1.34 |
| 22 | 23S1 | 1054 | A | C5-C4 | -5.33 | 1.35 | 1.38 |
| 22 | 23S1 | 1090 | A | N3-C4 | 5.33 | 1.38 | 1.34 |
| 22 | 23S1 | 1900 | A | C8-N7 | 5.33 | 1.35 | 1.31 |
| 1 | 16S1 | 907 | A | N3-C4 | 5.33 | 1.38 | 1.34 |
| 1 | 16S1 | 1502 | A | C8-N7 | 5.33 | 1.35 | 1.31 |
| 22 | 23S1 | 917 | A | N3-C4 | 5.33 | 1.38 | 1.34 |
| 22 | 23S1 | 1785 | A | N3-C4 | 5.33 | 1.38 | 1.34 |
| 22 | 23S1 | 705 | A | N7-C5 | -5.33 | 1.36 | 1.39 |
| 22 | 23S1 | 820 | A | N3-C4 | 5.33 | 1.38 | 1.34 |
| 22 | 23S1 | 1373 | A | C8-N7 | 5.33 | 1.35 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 16S1 | 1152 | A | C8-N7 | 5.33 | 1.35 | 1.31 |
| 22 | 23S1 | 2823 | A | C8-N7 | 5.33 | 1.35 | 1.31 |
| 1 | 16S1 | 1042 | A | C5-C4 | -5.33 | 1.35 | 1.38 |
| 22 | 23S1 | 457 | A | N3-C4 | 5.33 | 1.38 | 1.34 |
| 22 | 23S1 | 1327 | A | N3-C4 | 5.33 | 1.38 | 1.34 |
| 23 | 05S1 | 57 | A | C5-C4 | -5.33 | 1.35 | 1.38 |
| 1 | 16S1 | 1191 | A | C5-C4 | -5.32 | 1.35 | 1.38 |
| 1 | 16S1 | 116 | A | N3-C4 | 5.32 | 1.38 | 1.34 |
| 22 | 23S1 | 1665 | A | C8-N7 | 5.32 | 1.35 | 1.31 |
| 22 | 23S1 | 1746 | A | N3-C4 | 5.32 | 1.38 | 1.34 |
| 55 | PTR1 | 42 | A | N3-C4 | 5.32 | 1.38 | 1.34 |
| 22 | 23S1 | 447 | A | N3-C4 | 5.32 | 1.38 | 1.34 |
| 22 | 23S1 | 1913 | A | C5-C4 | -5.32 | 1.35 | 1.38 |
| 1 | 16S1 | 974 | A | N3-C4 | 5.32 | 1.38 | 1.34 |
| 22 | 23S1 | 1253 | A | N3-C4 | 5.32 | 1.38 | 1.34 |
| 1 | 16S1 | 1468 | A | N3-C4 | 5.32 | 1.38 | 1.34 |
| 22 | 23S1 | 718 | A | N3-C4 | 5.32 | 1.38 | 1.34 |
| 22 | 23S1 | 996 | A | N3-C4 | 5.32 | 1.38 | 1.34 |
| 22 | 23S1 | 1801 | A | C8-N7 | 5.32 | 1.35 | 1.31 |
| 22 | 23S1 | 1969 | A | N3-C4 | 5.32 | 1.38 | 1.34 |
| 1 | 16S1 | 560 | A | N3-C4 | 5.32 | 1.38 | 1.34 |
| 22 | 23S1 | 2879 | A | C8-N7 | 5.32 | 1.35 | 1.31 |
| 22 | 23S1 | 2340 | A | N3-C4 | 5.31 | 1.38 | 1.34 |
| 22 | 23S1 | 1916 | A | C5-C4 | -5.31 | 1.35 | 1.38 |
| 22 | 23S1 | 1085 | A | C2-N3 | 5.31 | 1.38 | 1.33 |
| 1 | 16S1 | 1508 | A | C8-N7 | 5.31 | 1.35 | 1.31 |
| 22 | 23S1 | 219 | A | N3-C4 | 5.31 | 1.38 | 1.34 |
| 22 | 23S1 | 2198 | A | N3-C4 | 5.31 | 1.38 | 1.34 |
| 22 | 23S1 | 218 | A | N3-C4 | 5.31 | 1.38 | 1.34 |
| 22 | 23S1 | 1548 | A | N3-C4 | 5.31 | 1.38 | 1.34 |
| 23 | 05S1 | 109 | A | N3-C4 | 5.31 | 1.38 | 1.34 |
| 22 | 23S1 | 422 | A | C8-N7 | 5.30 | 1.35 | 1.31 |
| 22 | 23S1 | 478 | A | N3-C4 | 5.30 | 1.38 | 1.34 |
| 22 | 23S1 | 2711 | A | C8-N7 | 5.30 | 1.35 | 1.31 |
| 1 | 16S1 | 2 | A | N3-C4 | 5.30 | 1.38 | 1.34 |
| 1 | 16S1 | 901 | A | N3-C4 | 5.30 | 1.38 | 1.34 |
| 1 | 16S1 | 1503 | A | N3-C4 | 5.30 | 1.38 | 1.34 |
| 22 | 23S1 | 91 | A | C5-C4 | -5.30 | 1.35 | 1.38 |
| 22 | 23S1 | 156 | A | C5-C4 | -5.30 | 1.35 | 1.38 |
| 22 | 23S1 | 1545 | A | N3-C4 | 5.30 | 1.38 | 1.34 |
| 22 | 23S1 | 1773 | A | N3-C4 | 5.30 | 1.38 | 1.34 |
| 22 | 23S1 | 1819 | A | C8-N7 | 5.30 | 1.35 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 2407 | A | C8-N7 | 5.30 | 1.35 | 1.31 |
| 22 | 23S1 | 74 | A | N3-C4 | 5.30 | 1.38 | 1.34 |
| 1 | 16S1 | 768 | A | N3-C4 | 5.30 | 1.38 | 1.34 |
| 22 | 23S1 | 1810 | A | N3-C4 | 5.30 | 1.38 | 1.34 |
| 1 | 16S1 | 831 | A | N3-C4 | 5.29 | 1.38 | 1.34 |
| 22 | 23S1 | 1287 | A | C8-N7 | 5.29 | 1.35 | 1.31 |
| 22 | 23S1 | 1969 | A | C8-N7 | 5.29 | 1.35 | 1.31 |
| 55 | PTR1 | 14 | A | C5-C4 | -5.29 | 1.35 | 1.38 |
| 1 | 16S1 | 349 | A | N3-C4 | 5.29 | 1.38 | 1.34 |
| 1 | 16S1 | 781 | A | N3-C4 | 5.29 | 1.38 | 1.34 |
| 22 | 23S1 | 354 | A | C5-C4 | -5.29 | 1.35 | 1.38 |
| 22 | 23S1 | 756 | A | N3-C4 | 5.29 | 1.38 | 1.34 |
| 22 | 23S1 | 1276 | A | N3-C4 | 5.29 | 1.38 | 1.34 |
| 22 | 23S1 | 1759 | A | N3-C4 | 5.29 | 1.38 | 1.34 |
| 55 | PTR1 | 58 | A | N3-C4 | 5.29 | 1.38 | 1.34 |
| 1 | 16S1 | 1507 | A | C8-N7 | 5.29 | 1.35 | 1.31 |
| 22 | 23S1 | 1809 | A | C8-N7 | 5.29 | 1.35 | 1.31 |
| 22 | 23S1 | 49 | A | N3-C4 | 5.29 | 1.38 | 1.34 |
| 22 | 23S1 | 563 | A | N7-C5 | -5.29 | 1.36 | 1.39 |
| 22 | 23S1 | 608 | A | C8-N7 | 5.29 | 1.35 | 1.31 |
| 22 | 23S1 | 2856 | A | N3-C4 | 5.29 | 1.38 | 1.34 |
| 1 | 16S1 | 98 | A | N3-C4 | 5.28 | 1.38 | 1.34 |
| 22 | 23S1 | 789 | A | N3-C4 | 5.28 | 1.38 | 1.34 |
| 22 | 23S1 | 1040 | A | N3-C4 | 5.28 | 1.38 | 1.34 |
| 22 | 23S1 | 1111 | A | C5-C4 | -5.28 | 1.35 | 1.38 |
| 22 | 23S1 | 1515 | A | N3-C4 | 5.28 | 1.38 | 1.34 |
| 1 | 16S1 | 456 | A | C5-C4 | -5.28 | 1.35 | 1.38 |
| 22 | 23S1 | 532 | A | C8-N7 | 5.28 | 1.35 | 1.31 |
| 22 | 23S1 | 1572 | A | N3-C4 | 5.28 | 1.38 | 1.34 |
| 22 | 23S1 | 2054 | A | N3-C4 | 5.28 | 1.38 | 1.34 |
| 22 | 23S1 | 2119 | A | C5-C4 | -5.28 | 1.35 | 1.38 |
| 22 | 23S1 | 1384 | A | N3-C4 | 5.28 | 1.38 | 1.34 |
| 22 | 23S1 | 1689 | A | N3-C4 | 5.28 | 1.38 | 1.34 |
| 1 | 16S1 | 468 | A | C5-C4 | -5.28 | 1.35 | 1.38 |
| 22 | 23S1 | 2700 | A | N3-C4 | 5.28 | 1.38 | 1.34 |
| 22 | 23S1 | 2241 | A | N3-C4 | 5.27 | 1.38 | 1.34 |
| 22 | 23S1 | 947 | A | N3-C4 | 5.27 | 1.38 | 1.34 |
| 22 | 23S1 | 1347 | A | N3-C4 | 5.27 | 1.38 | 1.34 |
| 22 | 23S1 | 1794 | A | N3-C4 | 5.27 | 1.38 | 1.34 |
| 1 | 16S1 | 98 | A | C2-N3 | 5.27 | 1.38 | 1.33 |
| 1 | 16S1 | 790 | A | N3-C4 | 5.27 | 1.38 | 1.34 |
| 22 | 23S1 | 959 | A | C8-N7 | 5.27 | 1.35 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 1866 | A | N3-C4 | 5.27 | 1.38 | 1.34 |
| 22 | 23S1 | 2052 | A | C8-N7 | 5.27 | 1.35 | 1.31 |
| 1 | 16S1 | 1130 | A | N3-C4 | 5.26 | 1.38 | 1.34 |
| 22 | 23S1 | 1028 | A | C8-N7 | 5.26 | 1.35 | 1.31 |
| 22 | 23S1 | 1032 | A | N3-C4 | 5.26 | 1.38 | 1.34 |
| 22 | 23S1 | 1872 | A | C8-N7 | 5.26 | 1.35 | 1.31 |
| 22 | 23S1 | 2748 | A | N3-C4 | 5.26 | 1.38 | 1.34 |
| 23 | 05S1 | 101 | A | C8-N7 | 5.26 | 1.35 | 1.31 |
| 1 | 16S1 | 383 | A | C5-C4 | -5.26 | 1.35 | 1.38 |
| 1 | 16S1 | 914 | A | C8-N7 | 5.26 | 1.35 | 1.31 |
| 1 | 16S1 | 192 | A | C5-C4 | -5.26 | 1.35 | 1.38 |
| 22 | 23S1 | 633 | A | C8-N7 | 5.26 | 1.35 | 1.31 |
| 22 | 23S1 | 1583 | A | C5-C4 | -5.26 | 1.35 | 1.38 |
| 22 | 23S1 | 1590 | A | C5-C4 | -5.26 | 1.35 | 1.38 |
| 1 | 16S1 | 8 | A | N3-C4 | 5.26 | 1.38 | 1.34 |
| 1 | 16S1 | 460 | A | C2-N3 | 5.26 | 1.38 | 1.33 |
| 1 | 16S1 | 968 | A | N3-C4 | 5.26 | 1.38 | 1.34 |
| 22 | 23S1 | 196 | A | C8-N7 | 5.26 | 1.35 | 1.31 |
| 1 | 16S1 | 174 | A | N3-C4 | 5.25 | 1.38 | 1.34 |
| 1 | 16S1 | 889 | A | N3-C4 | 5.25 | 1.38 | 1.34 |
| 1 | 16S1 | 1219 | A | N3-C4 | 5.25 | 1.38 | 1.34 |
| 1 | 16S1 | 78 | A | C5-C4 | -5.25 | 1.35 | 1.38 |
| 1 | 16S1 | 1500 | A | C8-N7 | 5.25 | 1.35 | 1.31 |
| 22 | 23S1 | 1669 | A | C8-N7 | 5.25 | 1.35 | 1.31 |
| 22 | 23S1 | 1689 | A | C8-N7 | 5.25 | 1.35 | 1.31 |
| 22 | 23S1 | 2781 | A | N7-C5 | -5.25 | 1.36 | 1.39 |
| 22 | 23S1 | 1876 | A | N3-C4 | 5.25 | 1.38 | 1.34 |
| 1 | 16S1 | 1254 | A | C5-C4 | -5.25 | 1.35 | 1.38 |
| 22 | 23S1 | 750 | A | C8-N7 | 5.25 | 1.35 | 1.31 |
| 22 | 23S1 | 793 | A | N3-C4 | 5.25 | 1.38 | 1.34 |
| 22 | 23S1 | 2868 | A | N3-C4 | 5.25 | 1.38 | 1.34 |
| 22 | 23S1 | 2725 | A | N3-C4 | 5.25 | 1.38 | 1.34 |
| 1 | 16S1 | 994 | A | C5-C4 | -5.25 | 1.35 | 1.38 |
| 22 | 23S1 | 1640 | A | N3-C4 | 5.25 | 1.38 | 1.34 |
| 22 | 23S1 | 574 | A | C8-N7 | 5.24 | 1.35 | 1.31 |
| 1 | 16S1 | 408 | A | C5-C4 | -5.24 | 1.35 | 1.38 |
| 22 | 23S1 | 430 | A | N3-C4 | 5.24 | 1.38 | 1.34 |
| 22 | 23S1 | 2711 | A | N3-C4 | 5.24 | 1.38 | 1.34 |
| 22 | 23S1 | 52 | A | C8-N7 | 5.24 | 1.35 | 1.31 |
| 22 | 23S1 | 255 | A | N3-C4 | 5.23 | 1.38 | 1.34 |
| 1 | 16S1 | 80 | A | C2-N3 | 5.23 | 1.38 | 1.33 |
| 22 | 23S1 | 53 | A | N3-C4 | 5.23 | 1.38 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 1735 | A | C5-C4 | -5.23 | 1.35 | 1.38 |
| 1 | 16S1 | 478 | A | C2-N3 | 5.23 | 1.38 | 1.33 |
| 1 | 16S1 | 1413 | A | N3-C4 | 5.23 | 1.38 | 1.34 |
| 22 | 23S1 | 2792 | A | N3-C4 | 5.23 | 1.38 | 1.34 |
| 22 | 23S1 | 2837 | A | N3-C4 | 5.23 | 1.38 | 1.34 |
| 22 | 23S1 | 443 | A | N3-C4 | 5.23 | 1.38 | 1.34 |
| 22 | 23S1 | 1419 | A | N3-C4 | 5.23 | 1.38 | 1.34 |
| 22 | 23S1 | 2879 | A | N3-C4 | 5.23 | 1.38 | 1.34 |
| 1 | 16S1 | 430 | A | N3-C4 | 5.23 | 1.38 | 1.34 |
| 22 | 23S1 | 1439 | A | N3-C4 | 5.23 | 1.38 | 1.34 |
| 22 | 23S1 | 1936 | A | N3-C4 | 5.23 | 1.38 | 1.34 |
| 22 | 23S1 | 2274 | A | N7-C5 | -5.23 | 1.36 | 1.39 |
| 22 | 23S1 | 460 | A | N3-C4 | 5.22 | 1.38 | 1.34 |
| 22 | 23S1 | 1745 | A | C5-C4 | -5.22 | 1.35 | 1.38 |
| 22 | 23S1 | 2297 | A | N3-C4 | 5.22 | 1.38 | 1.34 |
| 1 | 16S1 | 1227 | A | C2-N3 | 5.22 | 1.38 | 1.33 |
| 22 | 23S1 | 1966 | A | C8-N7 | 5.22 | 1.35 | 1.31 |
| 22 | 23S1 | 2433 | A | C8-N7 | 5.22 | 1.35 | 1.31 |
| 23 | 05S1 | 34 | A | N3-C4 | 5.22 | 1.38 | 1.34 |
| 1 | 16S1 | 563 | A | C8-N7 | 5.22 | 1.35 | 1.31 |
| 1 | 16S1 | 978 | A | N3-C4 | 5.22 | 1.38 | 1.34 |
| 1 | 16S1 | 1339 | A | N3-C4 | 5.22 | 1.38 | 1.34 |
| 22 | 23S1 | 118 | A | N3-C4 | 5.22 | 1.38 | 1.34 |
| 1 | 16S1 | 1170 | A | N3-C4 | 5.21 | 1.38 | 1.34 |
| 22 | 23S1 | 522 | A | C8-N7 | 5.21 | 1.35 | 1.31 |
| 1 | 16S1 | 1324 | A | N3-C4 | 5.21 | 1.38 | 1.34 |
| 1 | 16S1 | 907 | A | C8-N7 | 5.21 | 1.35 | 1.31 |
| 1 | 16S1 | 1368 | A | N3-C4 | 5.21 | 1.38 | 1.34 |
| 22 | 23S1 | 103 | A | N3-C4 | 5.21 | 1.38 | 1.34 |
| 22 | 23S1 | 556 | A | N3-C4 | 5.21 | 1.38 | 1.34 |
| 22 | 23S1 | 878 | A | C5-C4 | -5.21 | 1.35 | 1.38 |
| 22 | 23S1 | 1048 | A | C5-C4 | -5.21 | 1.35 | 1.38 |
| 22 | 23S1 | 1226 | A | N3-C4 | 5.21 | 1.38 | 1.34 |
| 22 | 23S1 | 2211 | A | C5-C4 | -5.21 | 1.35 | 1.38 |
| 22 | 23S1 | 2799 | A | C5-C4 | -5.21 | 1.35 | 1.38 |
| 1 | 16S1 | 179 | A | C5-C4 | -5.20 | 1.35 | 1.38 |
| 1 | 16S1 | 807 | A | N3-C4 | 5.20 | 1.38 | 1.34 |
| 1 | 16S1 | 1150 | A | N3-C4 | 5.20 | 1.38 | 1.34 |
| 22 | 23S1 | 1593 | A | C5-C4 | -5.20 | 1.35 | 1.38 |
| 22 | 23S1 | 1677 | A | C8-N7 | 5.20 | 1.35 | 1.31 |
| 22 | 23S1 | 2426 | A | C8-N7 | 5.20 | 1.35 | 1.31 |
| 22 | 23S1 | 734 | A | N3-C4 | 5.20 | 1.38 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 16S1 | 1349 | A | N3-C4 | 5.20 | 1.38 | 1.34 |
| 22 | 23S1 | 2080 | A | N3-C4 | 5.20 | 1.38 | 1.34 |
| 22 | 23S1 | 2171 | A | C2-N3 | 5.20 | 1.38 | 1.33 |
| 23 | 05S1 | 29 | A | C5-C4 | -5.20 | 1.35 | 1.38 |
| 1 | 16S1 | 33 | A | N3-C4 | 5.20 | 1.38 | 1.34 |
| 1 | 16S1 | 1492 | A | C5-C4 | -5.20 | 1.35 | 1.38 |
| 22 | 23S1 | 532 | A | N7-C5 | -5.20 | 1.36 | 1.39 |
| 22 | 23S1 | 829 | A | N3-C4 | 5.20 | 1.38 | 1.34 |
| 22 | 23S1 | 1014 | A | N3-C4 | 5.19 | 1.38 | 1.34 |
| 1 | 16S1 | 814 | A | N3-C4 | 5.19 | 1.38 | 1.34 |
| 22 | 23S1 | 1789 | A | N3-C4 | 5.19 | 1.38 | 1.34 |
| 1 | 16S1 | 715 | A | N3-C4 | 5.19 | 1.38 | 1.34 |
| 1 | 16S1 | 814 | A | C8-N7 | 5.19 | 1.35 | 1.31 |
| 1 | 16S1 | 1216 | A | C5-C4 | -5.19 | 1.35 | 1.38 |
| 1 | 16S1 | 1261 | A | N3-C4 | 5.19 | 1.38 | 1.34 |
| 22 | 23S1 | 449 | A | N3-C4 | 5.19 | 1.38 | 1.34 |
| 22 | 23S1 | 715 | A | N3-C4 | 5.19 | 1.38 | 1.34 |
| 22 | 23S1 | 802 | A | C8-N7 | 5.19 | 1.35 | 1.31 |
| 22 | 23S1 | 2070 | A | N3-C4 | 5.19 | 1.38 | 1.34 |
| 1 | 16S1 | 559 | A | N3-C4 | 5.19 | 1.38 | 1.34 |
| 1 | 16S1 | 865 | A | N7-C5 | -5.19 | 1.36 | 1.39 |
| 22 | 23S1 | 526 | A | N3-C4 | 5.19 | 1.38 | 1.34 |
| 22 | 23S1 | 1919 | A | C8-N7 | 5.19 | 1.35 | 1.31 |
| 22 | 23S1 | 2268 | A | N3-C4 | 5.19 | 1.38 | 1.34 |
| 22 | 23S1 | 2541 | A | C8-N7 | 5.19 | 1.35 | 1.31 |
| 22 | 23S1 | 21 | A | N3-C4 | 5.19 | 1.38 | 1.34 |
| 22 | 23S1 | 1889 | A | N3-C4 | 5.19 | 1.38 | 1.34 |
| 22 | 23S1 | 2887 | A | N3-C4 | 5.19 | 1.38 | 1.34 |
| 22 | 23S1 | 173 | A | N3-C4 | 5.18 | 1.38 | 1.34 |
| 55 | PTR1 | 14 | A | C2-N3 | 5.18 | 1.38 | 1.33 |
| 1 | 16S1 | 338 | A | N3-C4 | 5.18 | 1.38 | 1.34 |
| 22 | 23S1 | 19 | A | C8-N7 | 5.18 | 1.35 | 1.31 |
| 22 | 23S1 | 146 | A | N3-C4 | 5.18 | 1.38 | 1.34 |
| 22 | 23S1 | 825 | A | N3-C4 | 5.18 | 1.38 | 1.34 |
| 22 | 23S1 | 979 | A | N3-C4 | 5.18 | 1.38 | 1.34 |
| 22 | 23S1 | 1027 | A | N3-C4 | 5.18 | 1.38 | 1.34 |
| 22 | 23S1 | 2632 | A | N3-C4 | 5.18 | 1.38 | 1.34 |
| 22 | 23S1 | 2734 | A | N3-C4 | 5.18 | 1.38 | 1.34 |
| 1 | 16S1 | 825 | A | N3-C4 | 5.18 | 1.38 | 1.34 |
| 23 | 05S1 | 119 | A | C2-N3 | 5.18 | 1.38 | 1.33 |
| 1 | 16S1 | 120 | A | N3-C4 | 5.18 | 1.38 | 1.34 |
| 1 | 16S1 | 397 | A | C8-N7 | 5.18 | 1.35 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 199 | A | N3-C4 | 5.18 | 1.38 | 1.34 |
| 22 | 23S1 | 2268 | A | C8-N7 | 5.18 | 1.35 | 1.31 |
| 1 | 16S1 | 496 | A | C5-C4 | -5.17 | 1.35 | 1.38 |
| 1 | 16S1 | 583 | A | N3-C4 | 5.17 | 1.38 | 1.34 |
| 22 | 23S1 | 866 | A | N3-C4 | 5.17 | 1.38 | 1.34 |
| 22 | 23S1 | 1090 | A | C5-C4 | -5.17 | 1.35 | 1.38 |
| 22 | 23S1 | 2060 | A | N3-C4 | 5.17 | 1.38 | 1.34 |
| 22 | 23S1 | 2425 | A | C8-N7 | 5.17 | 1.35 | 1.31 |
| 22 | 23S1 | 1000 | A | N7-C5 | -5.17 | 1.36 | 1.39 |
| 22 | 23S1 | 1773 | A | C8-N7 | 5.17 | 1.35 | 1.31 |
| 1 | 16S1 | 303 | A | N3-C4 | 5.17 | 1.38 | 1.34 |
| 1 | 16S1 | 1055 | A | N3-C4 | 5.17 | 1.38 | 1.34 |
| 22 | 23S1 | 2411 | A | N3-C4 | 5.17 | 1.38 | 1.34 |
| 1 | 16S1 | 535 | A | N3-C4 | 5.17 | 1.38 | 1.34 |
| 22 | 23S1 | 844 | A | N3-C4 | 5.17 | 1.38 | 1.34 |
| 22 | 23S1 | 1936 | A | C8-N7 | 5.17 | 1.35 | 1.31 |
| 22 | 23S1 | 2675 | A | N3-C4 | 5.17 | 1.38 | 1.34 |
| 1 | 16S1 | 1418 | A | N3-C4 | 5.17 | 1.38 | 1.34 |
| 22 | 23S1 | 1383 | A | N3-C4 | 5.17 | 1.38 | 1.34 |
| 22 | 23S1 | 1586 | A | C5-C4 | -5.17 | 1.35 | 1.38 |
| 1 | 16S1 | 1256 | A | N3-C4 | 5.17 | 1.38 | 1.34 |
| 22 | 23S1 | 1676 | A | N7-C5 | -5.17 | 1.36 | 1.39 |
| 22 | 23S1 | 255 | A | N7-C5 | -5.16 | 1.36 | 1.39 |
| 22 | 23S1 | 330 | A | N3-C4 | 5.16 | 1.38 | 1.34 |
| 22 | 23S1 | 574 | A | N3-C4 | 5.16 | 1.38 | 1.34 |
| 22 | 23S1 | 608 | A | N3-C4 | 5.16 | 1.38 | 1.34 |
| 22 | 23S1 | 1505 | A | C5-C4 | -5.16 | 1.35 | 1.38 |
| 22 | 23S1 | 1977 | A | N3-C4 | 5.16 | 1.38 | 1.34 |
| 22 | 23S1 | 2169 | A | C2-N3 | 5.16 | 1.38 | 1.33 |
| 55 | PTR1 | 51 | A | N3-C4 | 5.16 | 1.38 | 1.34 |
| 1 | 16S1 | 1080 | A | C8-N7 | 5.16 | 1.35 | 1.31 |
| 22 | 23S1 | 990 | A | C8-N7 | 5.16 | 1.35 | 1.31 |
| 1 | 16S1 | 1022 | A | C2-N3 | 5.16 | 1.38 | 1.33 |
| 22 | 23S1 | 621 | A | N3-C4 | 5.16 | 1.38 | 1.34 |
| 22 | 23S1 | 1050 | A | C2-N3 | 5.16 | 1.38 | 1.33 |
| 22 | 23S1 | 1509 | A | C5-C4 | -5.16 | 1.35 | 1.38 |
| 1 | 16S1 | 459 | A | C5-C4 | -5.16 | 1.35 | 1.38 |
| 22 | 23S1 | 655 | A | N3-C4 | 5.16 | 1.38 | 1.34 |
| 22 | 23S1 | 1001 | A | N7-C5 | -5.16 | 1.36 | 1.39 |
| 22 | 23S1 | 2451 | A | N3-C4 | 5.16 | 1.38 | 1.34 |
| 1 | 16S1 | 78 | A | C2-N3 | 5.16 | 1.38 | 1.33 |
| 1 | 16S1 | 71 | A | N3-C4 | 5.15 | 1.38 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 16S1 | 411 | A | N3-C4 | 5.15 | 1.38 | 1.34 |
| 22 | 23S1 | 1528 | A | N7-C5 | -5.15 | 1.36 | 1.39 |
| 1 | 16S1 | 1171 | A | C5-C4 | -5.15 | 1.35 | 1.38 |
| 22 | 23S1 | 471 | A | C8-N7 | 5.15 | 1.35 | 1.31 |
| 22 | 23S1 | 693 | A | C8-N7 | 5.15 | 1.35 | 1.31 |
| 22 | 23S1 | 960 | A | N3-C4 | 5.15 | 1.38 | 1.34 |
| 22 | 23S1 | 1603 | A | C8-N7 | 5.15 | 1.35 | 1.31 |
| 22 | 23S1 | 1936 | A | N7-C5 | -5.15 | 1.36 | 1.39 |
| 23 | 05S1 | 115 | A | N3-C4 | 5.15 | 1.38 | 1.34 |
| 1 | 16S1 | 520 | A | C5-C4 | -5.15 | 1.35 | 1.38 |
| 22 | 23S1 | 2278 | A | N3-C4 | 5.15 | 1.38 | 1.34 |
| 1 | 16S1 | 1299 | A | C5-C4 | -5.15 | 1.35 | 1.38 |
| 22 | 23S1 | 1089 | A | C2-N3 | 5.15 | 1.38 | 1.33 |
| 22 | 23S1 | 1509 | A | N3-C4 | 5.15 | 1.38 | 1.34 |
| 22 | 23S1 | 2476 | A | N3-C4 | 5.15 | 1.38 | 1.34 |
| 31 | L131 | 108 | MET | C-N | -5.15 | 1.22 | 1.34 |
| 1 | 16S1 | 1428 | A | N3-C4 | 5.14 | 1.38 | 1.34 |
| 22 | 23S1 | 233 | A | N3-C4 | 5.14 | 1.38 | 1.34 |
| 22 | 23S1 | 2227 | A | N3-C4 | 5.14 | 1.38 | 1.34 |
| 22 | 23S1 | 2284 | A | N3-C4 | 5.14 | 1.38 | 1.34 |
| 22 | 23S1 | 2706 | A | N3-C4 | 5.14 | 1.38 | 1.34 |
| 22 | 23S1 | 2778 | A | N3-C4 | 5.14 | 1.38 | 1.34 |
| 22 | 23S1 | 2662 | A | N7-C5 | -5.14 | 1.36 | 1.39 |
| 1 | 16S1 | 19 | A | N3-C4 | 5.14 | 1.38 | 1.34 |
| 1 | 16S1 | 579 | A | N3-C4 | 5.14 | 1.38 | 1.34 |
| 22 | 23S1 | 2634 | A | N3-C4 | 5.14 | 1.38 | 1.34 |
| 1 | 16S1 | 189 | A | C2-N3 | 5.14 | 1.38 | 1.33 |
| 1 | 16S1 | 642 | A | N3-C4 | 5.14 | 1.38 | 1.34 |
| 22 | 23S1 | 975 | A | N3-C4 | 5.14 | 1.38 | 1.34 |
| 1 | 16S1 | 199 | A | C2-N3 | 5.13 | 1.38 | 1.33 |
| 1 | 16S1 | 1171 | A | C2-N3 | 5.13 | 1.38 | 1.33 |
| 22 | 23S1 | 197 | A | N3-C4 | 5.13 | 1.38 | 1.34 |
| 55 | PTR1 | 38 | A | N3-C4 | 5.13 | 1.38 | 1.34 |
| 1 | 16S1 | 364 | A | N3-C4 | 5.13 | 1.38 | 1.34 |
| 1 | 16S1 | 1483 | A | N7-C5 | -5.13 | 1.36 | 1.39 |
| 22 | 23S1 | 477 | A | C8-N7 | 5.13 | 1.35 | 1.31 |
| 22 | 23S1 | 677 | A | C8-N7 | 5.13 | 1.35 | 1.31 |
| 22 | 23S1 | 2082 | A | C8-N7 | 5.13 | 1.35 | 1.31 |
| 22 | 23S1 | 2191 | A | C2-N3 | 5.13 | 1.38 | 1.33 |
| 22 | 23S1 | 2386 | A | N3-C4 | 5.13 | 1.38 | 1.34 |
| 22 | 23S1 | 2461 | A | N3-C4 | 5.13 | 1.38 | 1.34 |
| 22 | 23S1 | 146 | A | C2-N3 | 5.13 | 1.38 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 16S1 | 978 | A | C5-C4 | -5.13 | 1.35 | 1.38 |
| 1 | 16S1 | 1340 | A | N3-C4 | 5.13 | 1.38 | 1.34 |
| 1 | 16S1 | 1456 | A | N3-C4 | 5.13 | 1.38 | 1.34 |
| 22 | 23S1 | 936 | A | N3-C4 | 5.13 | 1.38 | 1.34 |
| 22 | 23S1 | 2336 | A | N3-C4 | 5.13 | 1.38 | 1.34 |
| 22 | 23S1 | 2670 | A | N3-C4 | 5.13 | 1.38 | 1.34 |
| 22 | 23S1 | 2740 | A | N3-C4 | 5.13 | 1.38 | 1.34 |
| 1 | 16S1 | 702 | A | N3-C4 | 5.12 | 1.38 | 1.34 |
| 22 | 23S1 | 167 | A | N3-C4 | 5.12 | 1.38 | 1.34 |
| 1 | 16S1 | 1213 | A | C5-C4 | -5.12 | 1.35 | 1.38 |
| 22 | 23S1 | 592 | A | N3-C4 | 5.12 | 1.38 | 1.34 |
| 22 | 23S1 | 2013 | A | N7-C5 | -5.12 | 1.36 | 1.39 |
| 1 | 16S1 | 1021 | A | C5-C4 | -5.12 | 1.35 | 1.38 |
| 22 | 23S1 | 528 | A | C8-N7 | 5.12 | 1.35 | 1.31 |
| 1 | 16S1 | 780 | A | N7-C5 | -5.12 | 1.36 | 1.39 |
| 1 | 16S1 | 325 | A | N3-C4 | 5.12 | 1.38 | 1.34 |
| 22 | 23S1 | 990 | A | N3-C4 | 5.12 | 1.38 | 1.34 |
| 22 | 23S1 | 1717 | A | N3-C4 | 5.12 | 1.38 | 1.34 |
| 22 | 23S1 | 2776 | A | N3-C4 | 5.12 | 1.38 | 1.34 |
| 22 | 23S1 | 190 | A | N7-C5 | -5.12 | 1.36 | 1.39 |
| 22 | 23S1 | 1054 | A | C2-N3 | 5.12 | 1.38 | 1.33 |
| 22 | 23S1 | 1262 | A | C8-N7 | 5.12 | 1.35 | 1.31 |
| 22 | 23S1 | 1287 | A | N3-C4 | 5.12 | 1.38 | 1.34 |
| 22 | 23S1 | 1385 | A | N3-C4 | 5.12 | 1.38 | 1.34 |
| 22 | 23S1 | 2135 | A | C2-N3 | 5.12 | 1.38 | 1.33 |
| 1 | 16S1 | 498 | A | N1-C2 | 5.11 | 1.39 | 1.34 |
| 22 | 23S1 | 56 | A | N3-C4 | 5.11 | 1.38 | 1.34 |
| 22 | 23S1 | 384 | A | N3-C4 | 5.11 | 1.38 | 1.34 |
| 22 | 23S1 | 699 | A | C8-N7 | 5.11 | 1.35 | 1.31 |
| 22 | 23S1 | 1872 | A | N7-C5 | -5.11 | 1.36 | 1.39 |
| 22 | 23S1 | 1156 | A | C8-N7 | 5.11 | 1.35 | 1.31 |
| 1 | 16S1 | 892 | A | N3-C4 | 5.11 | 1.38 | 1.34 |
| 22 | 23S1 | 1641 | A | N3-C4 | 5.11 | 1.38 | 1.34 |
| 22 | 23S1 | 1701 | A | N3-C4 | 5.11 | 1.38 | 1.34 |
| 22 | 23S1 | 2274 | A | N3-C4 | 5.11 | 1.38 | 1.34 |
| 23 | 05S1 | 94 | A | N3-C4 | 5.11 | 1.38 | 1.34 |
| 1 | 16S1 | 510 | A | C8-N7 | 5.11 | 1.35 | 1.31 |
| 1 | 16S1 | 607 | A | N3-C4 | 5.11 | 1.38 | 1.34 |
| 1 | 16S1 | 1280 | A | N3-C4 | 5.11 | 1.38 | 1.34 |
| 22 | 23S1 | 1772 | A | C8-N7 | 5.11 | 1.35 | 1.31 |
| 22 | 23S1 | 1069 | A | C5-C4 | -5.11 | 1.35 | 1.38 |
| 22 | 23S1 | 1073 | A | C5-C4 | -5.11 | 1.35 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 16S1 | 72 | A | C2-N3 | 5.10 | 1.38 | 1.33 |
| 1 | 16S1 | 704 | A | N3-C4 | 5.10 | 1.38 | 1.34 |
| 22 | 23S1 | 152 | A | N3-C4 | 5.10 | 1.38 | 1.34 |
| 22 | 23S1 | 693 | A | N3-C4 | 5.10 | 1.38 | 1.34 |
| 22 | 23S1 | 1420 | A | C2-N3 | 5.10 | 1.38 | 1.33 |
| 22 | 23S1 | 2657 | A | N3-C4 | 5.10 | 1.38 | 1.34 |
| 1 | 16S1 | 250 | A | C5-C4 | -5.10 | 1.35 | 1.38 |
| 22 | 23S1 | 256 | A | N3-C4 | 5.10 | 1.38 | 1.34 |
| 1 | 16S1 | 1082 | A | N3-C4 | 5.10 | 1.38 | 1.34 |
| 22 | 23S1 | 1596 | A | N3-C4 | 5.10 | 1.38 | 1.34 |
| 22 | 23S1 | 1610 | A | N3-C4 | 5.10 | 1.38 | 1.34 |
| 22 | 23S1 | 2158 | A | C2-N3 | 5.10 | 1.38 | 1.33 |
| 1 | 16S1 | 1216 | A | N3-C4 | 5.10 | 1.38 | 1.34 |
| 1 | 16S1 | 695 | A | N3-C4 | 5.09 | 1.38 | 1.34 |
| 22 | 23S1 | 190 | A | C8-N7 | 5.09 | 1.35 | 1.31 |
| 22 | 23S1 | 2662 | A | C8-N7 | 5.09 | 1.35 | 1.31 |
| 1 | 16S1 | 109 | A | N3-C4 | 5.09 | 1.38 | 1.34 |
| 1 | 16S1 | 621 | A | N3-C4 | 5.09 | 1.38 | 1.34 |
| 22 | 23S1 | 1591 | A | C2-N3 | 5.09 | 1.38 | 1.33 |
| 22 | 23S1 | 1597 | A | N3-C4 | 5.09 | 1.38 | 1.34 |
| 22 | 23S1 | 2225 | A | N3-C4 | 5.09 | 1.38 | 1.34 |
| 22 | 23S1 | 2675 | A | C8-N7 | 5.09 | 1.35 | 1.31 |
| 1 | 16S1 | 282 | A | N3-C4 | 5.09 | 1.38 | 1.34 |
| 1 | 16S1 | 119 | A | N3-C4 | 5.09 | 1.38 | 1.34 |
| 22 | 23S1 | 735 | A | C8-N7 | 5.09 | 1.35 | 1.31 |
| 22 | 23S1 | 1569 | A | N3-C4 | 5.09 | 1.38 | 1.34 |
| 22 | 23S1 | 1522 | A | N3-C4 | 5.08 | 1.38 | 1.34 |
| 22 | 23S1 | 2799 | A | C2-N3 | 5.08 | 1.38 | 1.33 |
| 1 | 16S1 | 353 | A | N3-C4 | 5.08 | 1.37 | 1.34 |
| 1 | 16S1 | 729 | A | C8-N7 | 5.08 | 1.35 | 1.31 |
| 1 | 16S1 | 1130 | A | C5-C4 | -5.08 | 1.35 | 1.38 |
| 22 | 23S1 | 10 | A | N3-C4 | 5.08 | 1.37 | 1.34 |
| 22 | 23S1 | 1127 | A | N7-C5 | -5.08 | 1.36 | 1.39 |
| 22 | 23S1 | 2119 | A | C2-N3 | 5.08 | 1.38 | 1.33 |
| 22 | 23S1 | 2635 | A | N3-C4 | 5.08 | 1.37 | 1.34 |
| 22 | 23S1 | 2753 | A | N3-C4 | 5.08 | 1.38 | 1.34 |
| 55 | PTR1 | 23 | A | C2-N3 | 5.08 | 1.38 | 1.33 |
| 1 | 16S1 | 1016 | A | N3-C4 | 5.08 | 1.37 | 1.34 |
| 1 | 16S1 | 98 | A | C5-C4 | -5.08 | 1.35 | 1.38 |
| 1 | 16S1 | 539 | A | N3-C4 | 5.08 | 1.37 | 1.34 |
| 22 | 23S1 | 819 | A | N3-C4 | 5.08 | 1.37 | 1.34 |
| 22 | 23S1 | 1354 | A | C8-N7 | 5.08 | 1.35 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 2077 | A | C8-N7 | 5.08 | 1.35 | 1.31 |
| 1 | 16S1 | 746 | A | C2-N3 | 5.08 | 1.38 | 1.33 |
| 1 | 16S1 | 864 | A | N7-C5 | -5.08 | 1.36 | 1.39 |
| 1 | 16S1 | 1507 | A | N3-C4 | 5.08 | 1.37 | 1.34 |
| 22 | 23S1 | 300 | A | N3-C4 | 5.08 | 1.37 | 1.34 |
| 22 | 23S1 | 2267 | A | N3-C4 | 5.08 | 1.37 | 1.34 |
| 22 | 23S1 | 2471 | A | N3-C4 | 5.08 | 1.37 | 1.34 |
| 22 | 23S1 | 2873 | A | N7-C5 | -5.08 | 1.36 | 1.39 |
| 23 | 05S1 | 59 | A | N1-C2 | 5.08 | 1.39 | 1.34 |
| 1 | 16S1 | 152 | A | N3-C4 | 5.07 | 1.37 | 1.34 |
| 22 | 23S1 | 788 | A | C8-N7 | 5.07 | 1.35 | 1.31 |
| 22 | 23S1 | 863 | A | N3-C4 | 5.07 | 1.37 | 1.34 |
| 22 | 23S1 | 918 | A | N3-C4 | 5.07 | 1.37 | 1.34 |
| 22 | 23S1 | 984 | A | N7-C5 | -5.07 | 1.36 | 1.39 |
| 22 | 23S1 | 1080 | A | C5-C4 | -5.07 | 1.35 | 1.38 |
| 22 | 23S1 | 1264 | A | C8-N7 | 5.07 | 1.35 | 1.31 |
| 22 | 23S1 | 1586 | A | C2-N3 | 5.07 | 1.38 | 1.33 |
| 22 | 23S1 | 197 | A | C8-N7 | 5.07 | 1.35 | 1.31 |
| 22 | 23S1 | 1155 | A | N3-C4 | 5.07 | 1.37 | 1.34 |
| 22 | 23S1 | 255 | A | C8-N7 | 5.07 | 1.35 | 1.31 |
| 1 | 16S1 | 969 | A | N3-C4 | 5.07 | 1.37 | 1.34 |
| 22 | 23S1 | 632 | A | N3-C4 | 5.07 | 1.37 | 1.34 |
| 22 | 23S1 | 2031 | A | N3-C4 | 5.07 | 1.37 | 1.34 |
| 1 | 16S1 | 1227 | A | N1-C2 | 5.07 | 1.39 | 1.34 |
| 22 | 23S1 | 1127 | A | C8-N7 | 5.07 | 1.35 | 1.31 |
| 1 | 16S1 | 1229 | A | C2-N3 | 5.07 | 1.38 | 1.33 |
| 22 | 23S1 | 1010 | A | C8-N7 | 5.07 | 1.35 | 1.31 |
| 22 | 23S1 | 1070 | A | C2-N3 | 5.07 | 1.38 | 1.33 |
| 1 | 16S1 | 66 | A | N3-C4 | 5.06 | 1.37 | 1.34 |
| 22 | 23S1 | 2358 | A | C8-N7 | 5.06 | 1.35 | 1.31 |
| 1 | 16S1 | 16 | A | N3-C4 | 5.06 | 1.37 | 1.34 |
| 22 | 23S1 | 1133 | A | N3-C4 | 5.06 | 1.37 | 1.34 |
| 23 | 05S1 | 108 | A | N3-C4 | 5.06 | 1.37 | 1.34 |
| 1 | 16S1 | 26 | A | N3-C4 | 5.06 | 1.37 | 1.34 |
| 22 | 23S1 | 1490 | A | C5-C4 | -5.06 | 1.35 | 1.38 |
| 1 | 16S1 | 819 | A | C8-N7 | 5.06 | 1.35 | 1.31 |
| 1 | 16S1 | 1000 | A | C5-C4 | -5.06 | 1.35 | 1.38 |
| 22 | 23S1 | 1155 | A | N7-C5 | -5.06 | 1.36 | 1.39 |
| 55 | PTR1 | 9 | A | C5-C4 | -5.06 | 1.35 | 1.38 |
| 22 | 23S1 | 282 | A | C2-N3 | 5.05 | 1.38 | 1.33 |
| 22 | 23S1 | 2741 | A | C8-N7 | 5.05 | 1.35 | 1.31 |
| 22 | 23S1 | 572 | A | C8-N7 | 5.05 | 1.35 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 2614 | A | N3-C4 | 5.05 | 1.37 | 1.34 |
| 22 | 23S1 | 1637 | A | N3-C4 | 5.05 | 1.37 | 1.34 |
| 22 | 23S1 | 2352 | A | N7-C5 | -5.05 | 1.36 | 1.39 |
| 55 | PTR1 | 21 | A | C5-C4 | -5.05 | 1.35 | 1.38 |
| 1 | 16S1 | 431 | A | N3-C4 | 5.05 | 1.37 | 1.34 |
| 22 | 23S1 | 1528 | A | C2-N3 | 5.05 | 1.38 | 1.33 |
| 22 | 23S1 | 2281 | A | N3-C4 | 5.05 | 1.37 | 1.34 |
| 1 | 16S1 | 298 | A | N3-C4 | 5.05 | 1.37 | 1.34 |
| 22 | 23S1 | 227 | A | N3-C4 | 5.05 | 1.37 | 1.34 |
| 22 | 23S1 | 1668 | A | N7-C5 | -5.05 | 1.36 | 1.39 |
| 22 | 23S1 | 1700 | A | N3-C4 | 5.05 | 1.37 | 1.34 |
| 22 | 23S1 | 2439 | A | N3-C4 | 5.05 | 1.37 | 1.34 |
| 22 | 23S1 | 2765 | A | N7-C5 | -5.04 | 1.36 | 1.39 |
| 22 | 23S1 | 1073 | A | C2-N3 | 5.04 | 1.38 | 1.33 |
| 22 | 23S1 | 1077 | A | C5-C4 | -5.04 | 1.35 | 1.38 |
| 22 | 23S1 | 1549 | A | N3-C4 | 5.04 | 1.37 | 1.34 |
| 22 | 23S1 | 1803 | A | N7-C5 | -5.04 | 1.36 | 1.39 |
| 1 | 16S1 | 766 | A | N3-C4 | 5.04 | 1.37 | 1.34 |
| 1 | 16S1 | 782 | A | N3-C4 | 5.04 | 1.37 | 1.34 |
| 22 | 23S1 | 470 | A | N3-C4 | 5.04 | 1.37 | 1.34 |
| 22 | 23S1 | 644 | A | C8-N7 | 5.04 | 1.35 | 1.31 |
| 22 | 23S1 | 983 | A | N7-C5 | -5.04 | 1.36 | 1.39 |
| 22 | 23S1 | 1241 | A | C2-N3 | 5.04 | 1.38 | 1.33 |
| 22 | 23S1 | 1237 | A | N3-C4 | 5.04 | 1.37 | 1.34 |
| 1 | 16S1 | 759 | A | N3-C4 | 5.04 | 1.37 | 1.34 |
| 1 | 16S1 | 1163 | A | C2-N3 | 5.04 | 1.38 | 1.33 |
| 22 | 23S1 | 221 | A | N3-C4 | 5.04 | 1.37 | 1.34 |
| 22 | 23S1 | 900 | A | C2-N3 | 5.04 | 1.38 | 1.33 |
| 22 | 23S1 | 1593 | A | C2-N3 | 5.04 | 1.38 | 1.33 |
| 22 | 23S1 | 2037 | A | C8-N7 | 5.04 | 1.35 | 1.31 |
| 1 | 16S1 | 906 | A | N3-C4 | 5.03 | 1.37 | 1.34 |
| 1 | 16S1 | 1170 | A | C2-N3 | 5.03 | 1.38 | 1.33 |
| 22 | 23S1 | 1134 | A | N3-C4 | 5.03 | 1.37 | 1.34 |
| 22 | 23S1 | 1528 | A | C8-N7 | 5.03 | 1.35 | 1.31 |
| 22 | 23S1 | 1143 | A | C8-N7 | 5.03 | 1.35 | 1.31 |
| 1 | 16S1 | 1431 | A | N3-C4 | 5.03 | 1.37 | 1.34 |
| 22 | 23S1 | 572 | A | N7-C5 | -5.03 | 1.36 | 1.39 |
| 22 | 23S1 | 1403 | A | N3-C4 | 5.03 | 1.37 | 1.34 |
| 22 | 23S1 | 2392 | A | C8-N7 | 5.03 | 1.35 | 1.31 |
| 22 | 23S1 | 2097 | A | C2-N3 | 5.03 | 1.38 | 1.33 |
| 22 | 23S1 | 1230 | A | N3-C4 | 5.02 | 1.37 | 1.34 |
| 1 | 16S1 | 149 | A | C5-C4 | -5.02 | 1.35 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 1722 | A | C2-N3 | 5.02 | 1.38 | 1.33 |
| 22 | 23S1 | 13 | A | N3-C4 | 5.02 | 1.37 | 1.34 |
| 22 | 23S1 | 2792 | A | C2-N3 | 5.02 | 1.38 | 1.33 |
| 22 | 23S1 | 2823 | A | N3-C4 | 5.02 | 1.37 | 1.34 |
| 1 | 16S1 | 246 | A | N3-C4 | 5.02 | 1.37 | 1.34 |
| 22 | 23S1 | 1010 | A | N3-C4 | 5.02 | 1.37 | 1.34 |
| 22 | 23S1 | 1156 | A | N3-C4 | 5.02 | 1.37 | 1.34 |
| 1 | 16S1 | 236 | A | N3-C4 | 5.02 | 1.37 | 1.34 |
| 1 | 16S1 | 270 | A | C2-N3 | 5.02 | 1.38 | 1.33 |
| 22 | 23S1 | 310 | A | N3-C4 | 5.01 | 1.37 | 1.34 |
| 22 | 23S1 | 404 | A | N3-C4 | 5.01 | 1.37 | 1.34 |
| 22 | 23S1 | 1142 | A | N3-C4 | 5.01 | 1.37 | 1.34 |
| 22 | 23S1 | 1722 | A | C5-C4 | -5.01 | 1.35 | 1.38 |
| 22 | 23S1 | 983 | A | N3-C4 | 5.01 | 1.37 | 1.34 |
| 22 | 23S1 | 1735 | A | C2-N3 | 5.01 | 1.38 | 1.33 |
| 55 | PTR1 | 14 | A | N7-C5 | -5.01 | 1.36 | 1.39 |
| 1 | 16S1 | 205 | A | C2-N3 | 5.01 | 1.38 | 1.33 |
| 1 | 16S1 | 845 | A | C2-N3 | 5.01 | 1.38 | 1.33 |
| 22 | 23S1 | 101 | A | C5-C4 | -5.01 | 1.35 | 1.38 |
| 22 | 23S1 | 1009 | A | N3-C4 | 5.01 | 1.37 | 1.34 |
| 1 | 16S1 | 1410 | A | N3-C4 | 5.01 | 1.37 | 1.34 |
| 22 | 23S1 | 1871 | A | C2-N3 | 5.01 | 1.38 | 1.33 |
| 22 | 23S1 | 2850 | A | N3-C4 | 5.01 | 1.37 | 1.34 |
| 22 | 23S1 | 1084 | A | C2-N3 | 5.01 | 1.38 | 1.33 |
| 22 | 23S1 | 1275 | A | N3-C4 | 5.01 | 1.37 | 1.34 |
| 22 | 23S1 | 1700 | A | C8-N7 | 5.01 | 1.35 | 1.31 |
| 22 | 23S1 | 2565 | A | C8-N7 | 5.01 | 1.35 | 1.31 |
| 1 | 16S1 | 1394 | A | N3-C4 | 5.00 | 1.37 | 1.34 |
| 22 | 23S1 | 1080 | A | C2-N3 | 5.00 | 1.38 | 1.33 |
| 22 | 23S1 | 1711 | A | N3-C4 | 5.00 | 1.37 | 1.34 |
| 1 | 16S1 | 1333 | A | N3-C4 | 5.00 | 1.37 | 1.34 |
| 22 | 23S1 | 52 | A | N7-C5 | -5.00 | 1.36 | 1.39 |
| 22 | 23S1 | 203 | A | N7-C5 | -5.00 | 1.36 | 1.39 |
| 22 | 23S1 | 2126 | A | C2-N3 | 5.00 | 1.38 | 1.33 |

All (13371) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 2872 | A | N1-C6-N6 | -26.65 | 102.61 | 118.60 |
| 22 | 23S1 | 504 | A | N1-C2-N3 | -25.85 | 116.38 | 129.30 |
| 22 | 23S1 | 1434 | A | N1-C6-N6 | -24.57 | 103.86 | 118.60 |
| 22 | 23S1 | 1937 | A | N1-C6-N6 | -23.75 | 104.35 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 1004 | A | C2-N3-C4 | 23.60 | 122.40 | 110.60 |
| 1 | 16S1 | 554 | A | N1-C6-N6 | -23.60 | 104.44 | 118.60 |
| 1 | 16S1 | 431 | A | N1-C6-N6 | -23.42 | 104.55 | 118.60 |
| 1 | 16S1 | 520 | A | N1-C6-N6 | -23.25 | 104.65 | 118.60 |
| 22 | 23S1 | 845 | A | C2-N3-C4 | 23.19 | 122.19 | 110.60 |
| 22 | 23S1 | 1515 | A | N1-C6-N6 | -22.79 | 104.92 | 118.60 |
| 1 | 16S1 | 704 | A | N1-C6-N6 | -22.70 | 104.98 | 118.60 |
| 22 | 23S1 | 783 | A | C2-N3-C4 | 22.67 | 121.93 | 110.60 |
| 22 | 23S1 | 1544 | A | C2-N3-C4 | 22.58 | 121.89 | 110.60 |
| 1 | 16S1 | 1213 | A | N1-C6-N6 | -22.55 | 105.07 | 118.60 |
| 1 | 16S1 | 2 | A | C2-N3-C4 | 22.52 | 121.86 | 110.60 |
| 1 | 16S1 | 465 | A | C2-N3-C4 | 22.50 | 121.85 | 110.60 |
| 22 | 23S1 | 1021 | A | C2-N3-C4 | 22.47 | 121.84 | 110.60 |
| 1 | 16S1 | 151 | A | N1-C6-N6 | -22.45 | 105.13 | 118.60 |
| 22 | 23S1 | 10 | A | N1-C6-N6 | -22.40 | 105.16 | 118.60 |
| 1 | 16S1 | 716 | A | C2-N3-C4 | 22.35 | 121.78 | 110.60 |
| 22 | 23S1 | 1809 | A | C2-N3-C4 | 22.34 | 121.77 | 110.60 |
| 22 | 23S1 | 2566 | A | N1-C2-N3 | -22.33 | 118.14 | 129.30 |
| 1 | 16S1 | 389 | A | C2-N3-C4 | 22.26 | 121.73 | 110.60 |
| 1 | 16S1 | 498 | A | N1-C6-N6 | -22.12 | 105.33 | 118.60 |
| 1 | 16S1 | 914 | A | N1-C2-N3 | -22.07 | 118.27 | 129.30 |
| 22 | 23S1 | 1392 | A | C2-N3-C4 | 22.05 | 121.63 | 110.60 |
| 22 | 23S1 | 2173 | A | C2-N3-C4 | 22.03 | 121.61 | 110.60 |
| 1 | 16S1 | 913 | A | N1-C2-N3 | -22.02 | 118.29 | 129.30 |
| 1 | 16S1 | 1225 | A | C2-N3-C4 | 22.01 | 121.61 | 110.60 |
| 22 | 23S1 | 1020 | A | N1-C2-N3 | -21.95 | 118.32 | 129.30 |
| 22 | 23S1 | 2451 | A | N1-C6-N6 | -21.95 | 105.43 | 118.60 |
| 22 | 23S1 | 514 | A | C2-N3-C4 | 21.95 | 121.58 | 110.60 |
| 22 | 23S1 | 983 | A | N1-C2-N3 | -21.88 | 118.36 | 129.30 |
| 1 | 16S1 | 977 | A | C2-N3-C4 | 21.84 | 121.52 | 110.60 |
| 1 | 16S1 | 1500 | A | N1-C2-N3 | -21.83 | 118.38 | 129.30 |
| 22 | 23S1 | 2101 | A | N1-C6-N6 | -21.81 | 105.51 | 118.60 |
| 22 | 23S1 | 2765 | A | C2-N3-C4 | 21.78 | 121.49 | 110.60 |
| 22 | 23S1 | 195 | A | N1-C6-N6 | -21.78 | 105.53 | 118.60 |
| 1 | 16S1 | 498 | A | C2-N3-C4 | 21.75 | 121.48 | 110.60 |
| 1 | 16S1 | 621 | A | C2-N3-C4 | 21.73 | 121.47 | 110.60 |
| 22 | 23S1 | 752 | A | N1-C6-N6 | -21.72 | 105.57 | 118.60 |
| 22 | 23S1 | 1597 | A | N1-C6-N6 | -21.72 | 105.57 | 118.60 |
| 22 | 23S1 | 299 | A | C2-N3-C4 | 21.66 | 121.43 | 110.60 |
| 22 | 23S1 | 933 | A | C2-N3-C4 | 21.63 | 121.42 | 110.60 |
| 1 | 16S1 | 728 | A | C2-N3-C4 | 21.61 | 121.41 | 110.60 |
| 1 | 16S1 | 151 | A | C2-N3-C4 | 21.60 | 121.40 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 1004 | A | N1-C6-N6 | -21.59 | 105.64 | 118.60 |
| 22 | 23S1 | 1395 | A | N1-C6-N6 | -21.57 | 105.66 | 118.60 |
| 1 | 16S1 | 496 | A | N1-C2-N3 | -21.54 | 118.53 | 129.30 |
| 22 | 23S1 | 221 | A | N1-C2-N3 | -21.54 | 118.53 | 129.30 |
| 22 | 23S1 | 2311 | A | C2-N3-C4 | 21.51 | 121.35 | 110.60 |
| 1 | 16S1 | 983 | A | C2-N3-C4 | 21.50 | 121.35 | 110.60 |
| 22 | 23S1 | 1668 | A | N1-C6-N6 | -21.48 | 105.71 | 118.60 |
| 1 | 16S1 | 1225 | A | N1-C6-N6 | -21.46 | 105.72 | 118.60 |
| 22 | 23S1 | 1669 | A | C2-N3-C4 | 21.46 | 121.33 | 110.60 |
| 22 | 23S1 | 2311 | A | N1-C2-N3 | -21.46 | 118.57 | 129.30 |
| 22 | 23S1 | 1353 | A | N1-C6-N6 | -21.45 | 105.73 | 118.60 |
| 22 | 23S1 | 196 | A | C2-N3-C4 | 21.44 | 121.32 | 110.60 |
| 22 | 23S1 | 1755 | A | N1-C6-N6 | -21.43 | 105.74 | 118.60 |
| 1 | 16S1 | 563 | A | C2-N3-C4 | 21.43 | 121.31 | 110.60 |
| 22 | 23S1 | 1328 | A | N1-C6-N6 | -21.41 | 105.75 | 118.60 |
| 22 | 23S1 | 910 | A | N1-C6-N6 | -21.40 | 105.76 | 118.60 |
| 22 | 23S1 | 1359 | A | N1-C6-N6 | -21.40 | 105.76 | 118.60 |
| 1 | 16S1 | 716 | A | N1-C2-N3 | -21.34 | 118.63 | 129.30 |
| 22 | 23S1 | 1086 | A | C2-N3-C4 | 21.34 | 121.27 | 110.60 |
| 22 | 23S1 | 1204 | A | N1-C6-N6 | -21.34 | 105.80 | 118.60 |
| 23 | 05S1 | 59 | A | C2-N3-C4 | 21.33 | 121.27 | 110.60 |
| 1 | 16S1 | 728 | A | N1-C6-N6 | -21.32 | 105.81 | 118.60 |
| 22 | 23S1 | 1009 | A | C2-N3-C4 | 21.32 | 121.26 | 110.60 |
| 1 | 16S1 | 622 | A | N1-C6-N6 | -21.30 | 105.82 | 118.60 |
| 1 | 16S1 | 397 | A | C2-N3-C4 | 21.29 | 121.24 | 110.60 |
| 1 | 16S1 | 1363 | A | C2-N3-C4 | 21.29 | 121.24 | 110.60 |
| 22 | 23S1 | 1353 | A | C2-N3-C4 | 21.29 | 121.24 | 110.60 |
| 22 | 23S1 | 449 | A | C2-N3-C4 | 21.28 | 121.24 | 110.60 |
| 1 | 16S1 | 389 | A | N1-C6-N6 | -21.27 | 105.84 | 118.60 |
| 1 | 16S1 | 1145 | A | N1-C6-N6 | -21.25 | 105.85 | 118.60 |
| 22 | 23S1 | 278 | A | C2-N3-C4 | 21.25 | 121.22 | 110.60 |
| 22 | 23S1 | 160 | A | C2-N3-C4 | 21.22 | 121.21 | 110.60 |
| 22 | 23S1 | 794 | A | C2-N3-C4 | 21.22 | 121.21 | 110.60 |
| 22 | 23S1 | 1175 | A | C2-N3-C4 | 21.22 | 121.21 | 110.60 |
| 22 | 23S1 | 1490 | A | C2-N3-C4 | 21.21 | 121.21 | 110.60 |
| 1 | 16S1 | 1499 | A | C2-N3-C4 | 21.21 | 121.20 | 110.60 |
| 22 | 23S1 | 160 | A | N1-C6-N6 | -21.21 | 105.88 | 118.60 |
| 22 | 23S1 | 1028 | A | C2-N3-C4 | 21.20 | 121.20 | 110.60 |
| 22 | 23S1 | 84 | A | N1-C2-N3 | -21.18 | 118.71 | 129.30 |
| 1 | 16S1 | 1201 | A | C2-N3-C4 | 21.16 | 121.18 | 110.60 |
| 22 | 23S1 | 2572 | A | N1-C2-N3 | -21.14 | 118.73 | 129.30 |
| 22 | 23S1 | 2572 | A | N1-C6-N6 | -21.13 | 105.92 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 514 | A | N1-C2-N3 | -21.12 | 118.74 | 129.30 |
| 22 | 23S1 | 119 | A | N1-C6-N6 | -21.12 | 105.93 | 118.60 |
| 22 | 23S1 | 892 | A | C2-N3-C4 | 21.11 | 121.16 | 110.60 |
| 22 | 23S1 | 643 | A | N1-C2-N3 | -21.10 | 118.75 | 129.30 |
| 22 | 23S1 | 2657 | A | N1-C2-N3 | -21.10 | 118.75 | 129.30 |
| 1 | 16S1 | 1499 | A | N1-C2-N3 | -21.09 | 118.75 | 129.30 |
| 22 | 23S1 | 2311 | A | N1-C6-N6 | -21.09 | 105.95 | 118.60 |
| 22 | 23S1 | 2564 | A | N1-C2-N3 | -21.09 | 118.76 | 129.30 |
| 22 | 23S1 | 529 | A | N1-C6-N6 | -21.08 | 105.95 | 118.60 |
| 22 | 23S1 | 1784 | A | N1-C2-N3 | -21.08 | 118.76 | 129.30 |
| 22 | 23S1 | 1427 | A | N1-C6-N6 | -21.07 | 105.96 | 118.60 |
| 22 | 23S1 | 2273 | A | C2-N3-C4 | 21.07 | 121.14 | 110.60 |
| 1 | 16S1 | 152 | A | N1-C6-N6 | -21.05 | 105.97 | 118.60 |
| 22 | 23S1 | 1853 | A | N1-C2-N3 | -21.04 | 118.78 | 129.30 |
| 22 | 23S1 | 2740 | A | C2-N3-C4 | 21.02 | 121.11 | 110.60 |
| 22 | 23S1 | 195 | A | N1-C2-N3 | -21.01 | 118.79 | 129.30 |
| 22 | 23S1 | 1000 | A | C2-N3-C4 | 21.00 | 121.10 | 110.60 |
| 22 | 23S1 | 532 | A | C2-N3-C4 | 21.00 | 121.10 | 110.60 |
| 22 | 23S1 | 563 | A | C2-N3-C4 | 21.00 | 121.10 | 110.60 |
| 23 | 05S1 | 29 | A | N1-C6-N6 | -21.00 | 106.00 | 118.60 |
| 22 | 23S1 | 1308 | A | N1-C6-N6 | -21.00 | 106.00 | 118.60 |
| 22 | 23S1 | 2060 | A | N1-C2-N3 | -21.00 | 118.80 | 129.30 |
| 1 | 16S1 | 412 | A | N1-C2-N3 | -20.99 | 118.80 | 129.30 |
| 22 | 23S1 | 2212 | A | N1-C2-N3 | -20.98 | 118.81 | 129.30 |
| 22 | 23S1 | 2726 | A | N1-C6-N6 | -20.97 | 106.02 | 118.60 |
| 22 | 23S1 | 2173 | A | N1-C6-N6 | -20.97 | 106.02 | 118.60 |
| 22 | 23S1 | 299 | A | N1-C2-N3 | -20.95 | 118.82 | 129.30 |
| 1 | 16S1 | 1446 | A | C2-N3-C4 | 20.95 | 121.07 | 110.60 |
| 22 | 23S1 | 825 | A | C2-N3-C4 | 20.94 | 121.07 | 110.60 |
| 22 | 23S1 | 821 | A | N1-C6-N6 | -20.93 | 106.04 | 118.60 |
| 22 | 23S1 | 127 | A | N1-C2-N3 | -20.93 | 118.83 | 129.30 |
| 1 | 16S1 | 496 | A | C2-N3-C4 | 20.93 | 121.06 | 110.60 |
| 22 | 23S1 | 2212 | A | C2-N3-C4 | 20.90 | 121.05 | 110.60 |
| 1 | 16S1 | 978 | A | N1-C6-N6 | -20.89 | 106.07 | 118.60 |
| 22 | 23S1 | 2566 | A | N1-C6-N6 | -20.88 | 106.07 | 118.60 |
| 22 | 23S1 | 2872 | A | N1-C2-N3 | -20.88 | 118.86 | 129.30 |
| 22 | 23S1 | 2766 | A | C2-N3-C4 | 20.88 | 121.04 | 110.60 |
| 1 | 16S1 | 622 | A | N1-C2-N3 | -20.88 | 118.86 | 129.30 |
| 22 | 23S1 | 910 | A | C2-N3-C4 | 20.87 | 121.03 | 110.60 |
| 22 | 23S1 | 2114 | A | C2-N3-C4 | 20.87 | 121.03 | 110.60 |
| 22 | 23S1 | 739 | A | C2-N3-C4 | 20.87 | 121.03 | 110.60 |
| 22 | 23S1 | 1275 | A | N1-C2-N3 | -20.86 | 118.87 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 833 | A | C2-N3-C4 | 20.86 | 121.03 | 110.60 |
| 1 | 16S1 | 573 | A | C2-N3-C4 | 20.84 | 121.02 | 110.60 |
| 22 | 23S1 | 1966 | A | C2-N3-C4 | 20.84 | 121.02 | 110.60 |
| 22 | 23S1 | 1419 | A | N1-C2-N3 | -20.84 | 118.88 | 129.30 |
| 1 | 16S1 | 1101 | A | N1-C6-N6 | -20.83 | 106.10 | 118.60 |
| 22 | 23S1 | 241 | A | N1-C2-N3 | -20.83 | 118.88 | 129.30 |
| 22 | 23S1 | 1952 | A | C2-N3-C4 | 20.82 | 121.01 | 110.60 |
| 22 | 23S1 | 1378 | A | N1-C6-N6 | -20.80 | 106.12 | 118.60 |
| 22 | 23S1 | 1655 | A | C2-N3-C4 | 20.79 | 120.99 | 110.60 |
| 22 | 23S1 | 1214 | A | N1-C2-N3 | -20.77 | 118.91 | 129.30 |
| 22 | 23S1 | 2267 | A | C2-N3-C4 | 20.77 | 120.98 | 110.60 |
| 22 | 23S1 | 1304 | A | N1-C6-N6 | -20.76 | 106.14 | 118.60 |
| 1 | 16S1 | 116 | A | N1-C2-N3 | -20.76 | 118.92 | 129.30 |
| 1 | 16S1 | 583 | A | N1-C6-N6 | -20.76 | 106.15 | 118.60 |
| 1 | 16S1 | 607 | A | N1-C2-N3 | -20.76 | 118.92 | 129.30 |
| 22 | 23S1 | 196 | A | N1-C6-N6 | -20.76 | 106.15 | 118.60 |
| 22 | 23S1 | 761 | A | C2-N3-C4 | 20.75 | 120.98 | 110.60 |
| 22 | 23S1 | 761 | A | N1-C6-N6 | -20.75 | 106.15 | 118.60 |
| 22 | 23S1 | 2542 | A | N1-C6-N6 | -20.75 | 106.15 | 118.60 |
| 1 | 16S1 | 572 | A | N1-C2-N3 | -20.73 | 118.93 | 129.30 |
| 22 | 23S1 | 219 | A | C2-N3-C4 | 20.73 | 120.97 | 110.60 |
| 22 | 23S1 | 2823 | A | N1-C2-N3 | -20.73 | 118.94 | 129.30 |
| 22 | 23S1 | 802 | A | C2-N3-C4 | 20.72 | 120.96 | 110.60 |
| 22 | 23S1 | 981 | A | N1-C6-N6 | -20.72 | 106.17 | 118.60 |
| 22 | 23S1 | 1287 | A | N1-C2-N3 | -20.70 | 118.95 | 129.30 |
| 22 | 23S1 | 1919 | A | N1-C2-N3 | -20.70 | 118.95 | 129.30 |
| 1 | 16S1 | 872 | A | C2-N3-C4 | 20.70 | 120.95 | 110.60 |
| 1 | 16S1 | 900 | A | N1-C6-N6 | -20.70 | 106.18 | 118.60 |
| 22 | 23S1 | 800 | A | N1-C6-N6 | -20.70 | 106.18 | 118.60 |
| 1 | 16S1 | 179 | A | N1-C6-N6 | -20.70 | 106.18 | 118.60 |
| 22 | 23S1 | 973 | A | N1-C2-N3 | -20.69 | 118.96 | 129.30 |
| 22 | 23S1 | 1544 | A | N1-C2-N3 | -20.68 | 118.96 | 129.30 |
| 1 | 16S1 | 1145 | A | N1-C2-N3 | -20.68 | 118.96 | 129.30 |
| 1 | 16S1 | 1299 | A | C2-N3-C4 | 20.66 | 120.93 | 110.60 |
| 22 | 23S1 | 644 | A | C2-N3-C4 | 20.66 | 120.93 | 110.60 |
| 1 | 16S1 | 414 | A | N1-C6-N6 | -20.65 | 106.21 | 118.60 |
| 1 | 16S1 | 16 | A | N1-C2-N3 | -20.64 | 118.98 | 129.30 |
| 23 | 05S1 | 73 | A | C2-N3-C4 | 20.63 | 120.92 | 110.60 |
| 22 | 23S1 | 1952 | A | N1-C2-N3 | -20.63 | 118.98 | 129.30 |
| 22 | 23S1 | 1652 | A | N1-C6-N6 | -20.63 | 106.22 | 118.60 |
| 22 | 23S1 | 1759 | A | C2-N3-C4 | 20.63 | 120.92 | 110.60 |
| 55 | PTR1 | 76 | A | N1-C2-N3 | -20.63 | 118.99 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1551 | A | C2-N3-C4 | 20.62 | 120.91 | 110.60 |
| 1 | 16S1 | 1333 | A | N1-C6-N6 | -20.62 | 106.23 | 118.60 |
| 22 | 23S1 | 84 | A | N1-C6-N6 | -20.62 | 106.23 | 118.60 |
| 22 | 23S1 | 1214 | A | C2-N3-C4 | 20.62 | 120.91 | 110.60 |
| 22 | 23S1 | 1668 | A | C2-N3-C4 | 20.62 | 120.91 | 110.60 |
| 22 | 23S1 | 190 | A | C2-N3-C4 | 20.61 | 120.91 | 110.60 |
| 22 | 23S1 | 654 | A | C2-N3-C4 | 20.61 | 120.90 | 110.60 |
| 22 | 23S1 | 980 | A | N1-C2-N3 | -20.60 | 119.00 | 129.30 |
| 22 | 23S1 | 2614 | A | C2-N3-C4 | 20.60 | 120.90 | 110.60 |
| 22 | 23S1 | 980 | A | C2-N3-C4 | 20.59 | 120.90 | 110.60 |
| 1 | 16S1 | 1067 | A | N1-C2-N3 | -20.59 | 119.00 | 129.30 |
| 22 | 23S1 | 1147 | A | N1-C6-N6 | -20.58 | 106.25 | 118.60 |
| 23 | 05S1 | 99 | A | C2-N3-C4 | 20.57 | 120.89 | 110.60 |
| 22 | 23S1 | 1032 | A | N1-C6-N6 | -20.57 | 106.26 | 118.60 |
| 22 | 23S1 | 783 | A | N1-C6-N6 | -20.55 | 106.27 | 118.60 |
| 1 | 16S1 | 16 | A | N1-C6-N6 | -20.55 | 106.27 | 118.60 |
| 22 | 23S1 | 1754 | A | N1-C2-N3 | -20.55 | 119.03 | 129.30 |
| 22 | 23S1 | 2450 | A | N1-C2-N3 | -20.55 | 119.03 | 129.30 |
| 1 | 16S1 | 478 | A | C2-N3-C4 | 20.54 | 120.87 | 110.60 |
| 22 | 23S1 | 207 | A | N1-C2-N3 | -20.54 | 119.03 | 129.30 |
| 22 | 23S1 | 861 | A | C2-N3-C4 | 20.54 | 120.87 | 110.60 |
| 1 | 16S1 | 493 | A | N1-C2-N3 | -20.54 | 119.03 | 129.30 |
| 23 | 05S1 | 29 | A | C2-N3-C4 | 20.54 | 120.87 | 110.60 |
| 1 | 16S1 | 431 | A | N1-C2-N3 | -20.53 | 119.03 | 129.30 |
| 22 | 23S1 | 1254 | A | N1-C2-N3 | -20.53 | 119.04 | 129.30 |
| 1 | 16S1 | 1004 | A | N1-C2-N3 | -20.52 | 119.04 | 129.30 |
| 1 | 16S1 | 665 | A | N1-C6-N6 | -20.52 | 106.29 | 118.60 |
| 22 | 23S1 | 563 | A | N1-C2-N3 | -20.52 | 119.04 | 129.30 |
| 22 | 23S1 | 1655 | A | N1-C2-N3 | -20.52 | 119.04 | 129.30 |
| 22 | 23S1 | 2031 | A | C2-N3-C4 | 20.52 | 120.86 | 110.60 |
| 1 | 16S1 | 533 | A | C2-N3-C4 | 20.50 | 120.85 | 110.60 |
| 22 | 23S1 | 1632 | A | C2-N3-C4 | 20.50 | 120.85 | 110.60 |
| 22 | 23S1 | 984 | A | C2-N3-C4 | 20.50 | 120.85 | 110.60 |
| 22 | 23S1 | 118 | A | N1-C2-N3 | -20.49 | 119.05 | 129.30 |
| 22 | 23S1 | 1640 | A | N1-C6-N6 | -20.49 | 106.30 | 118.60 |
| 1 | 16S1 | 412 | A | N1-C6-N6 | -20.49 | 106.30 | 118.60 |
| 1 | 16S1 | 768 | A | C2-N3-C4 | 20.49 | 120.84 | 110.60 |
| 22 | 23S1 | 2826 | A | N1-C2-N3 | -20.48 | 119.06 | 129.30 |
| 22 | 23S1 | 631 | A | C2-N3-C4 | 20.48 | 120.84 | 110.60 |
| 1 | 16S1 | 1360 | A | N1-C6-N6 | -20.47 | 106.32 | 118.60 |
| 22 | 23S1 | 764 | A | N1-C2-N3 | -20.46 | 119.07 | 129.30 |
| 1 | 16S1 | 889 | A | N1-C6-N6 | -20.46 | 106.32 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 322 | A | N1-C2-N3 | -20.46 | 119.07 | 129.30 |
| 1 | 16S1 | 704 | A | N1-C2-N3 | -20.45 | 119.07 | 129.30 |
| 22 | 23S1 | 1544 | A | N1-C6-N6 | -20.45 | 106.33 | 118.60 |
| 22 | 23S1 | 1630 | A | N1-C6-N6 | -20.45 | 106.33 | 118.60 |
| 22 | 23S1 | 1785 | A | N1-C6-N6 | -20.45 | 106.33 | 118.60 |
| 22 | 23S1 | 981 | A | N1-C2-N3 | -20.44 | 119.08 | 129.30 |
| 1 | 16S1 | 520 | A | C2-N3-C4 | 20.44 | 120.82 | 110.60 |
| 22 | 23S1 | 1927 | A | N1-C6-N6 | -20.41 | 106.35 | 118.60 |
| 1 | 16S1 | 768 | A | N1-C2-N3 | -20.41 | 119.09 | 129.30 |
| 22 | 23S1 | 1927 | A | C2-N3-C4 | 20.41 | 120.80 | 110.60 |
| 1 | 16S1 | 171 | A | C2-N3-C4 | 20.41 | 120.80 | 110.60 |
| 22 | 23S1 | 972 | A | C2-N3-C4 | 20.41 | 120.80 | 110.60 |
| 22 | 23S1 | 74 | A | C2-N3-C4 | 20.39 | 120.79 | 110.60 |
| 22 | 23S1 | 863 | A | C2-N3-C4 | 20.39 | 120.80 | 110.60 |
| 22 | 23S1 | 1000 | A | N1-C2-N3 | -20.39 | 119.11 | 129.30 |
| 22 | 23S1 | 101 | A | C2-N3-C4 | 20.38 | 120.79 | 110.60 |
| 1 | 16S1 | 583 | A | N1-C2-N3 | -20.38 | 119.11 | 129.30 |
| 22 | 23S1 | 2740 | A | N1-C2-N3 | -20.38 | 119.11 | 129.30 |
| 22 | 23S1 | 1286 | A | N1-C2-N3 | -20.38 | 119.11 | 129.30 |
| 22 | 23S1 | 1809 | A | N1-C2-N3 | -20.38 | 119.11 | 129.30 |
| 22 | 23S1 | 2837 | A | N1-C2-N3 | -20.38 | 119.11 | 129.30 |
| 22 | 23S1 | 1966 | A | N1-C2-N3 | -20.37 | 119.11 | 129.30 |
| 22 | 23S1 | 2033 | A | N1-C6-N6 | -20.37 | 106.38 | 118.60 |
| 22 | 23S1 | 1253 | A | N1-C2-N3 | -20.36 | 119.12 | 129.30 |
| 1 | 16S1 | 270 | A | C2-N3-C4 | 20.36 | 120.78 | 110.60 |
| 22 | 23S1 | 443 | A | N1-C6-N6 | -20.36 | 106.39 | 118.60 |
| 22 | 23S1 | 1569 | A | N1-C2-N3 | -20.36 | 119.12 | 129.30 |
| 1 | 16S1 | 44 | A | N1-C6-N6 | -20.36 | 106.39 | 118.60 |
| 1 | 16S1 | 465 | A | N1-C2-N3 | -20.35 | 119.12 | 129.30 |
| 22 | 23S1 | 330 | A | C2-N3-C4 | 20.35 | 120.78 | 110.60 |
| 1 | 16S1 | 130 | A | C2-N3-C4 | 20.35 | 120.78 | 110.60 |
| 1 | 16S1 | 116 | A | C2-N3-C4 | 20.35 | 120.77 | 110.60 |
| 22 | 23S1 | 2572 | A | C2-N3-C4 | 20.35 | 120.77 | 110.60 |
| 1 | 16S1 | 1333 | A | C2-N3-C4 | 20.34 | 120.77 | 110.60 |
| 22 | 23S1 | 454 | A | N1-C6-N6 | -20.34 | 106.39 | 118.60 |
| 22 | 23S1 | 1570 | A | N1-C6-N6 | -20.34 | 106.39 | 118.60 |
| 22 | 23S1 | 1780 | A | N1-C2-N3 | -20.34 | 119.13 | 129.30 |
| 22 | 23S1 | 38 | A | N1-C6-N6 | -20.34 | 106.40 | 118.60 |
| 22 | 23S1 | 804 | A | N1-C6-N6 | -20.34 | 106.40 | 118.60 |
| 22 | 23S1 | 515 | A | N1-C6-N6 | -20.33 | 106.40 | 118.60 |
| 22 | 23S1 | 1347 | A | N1-C6-N6 | -20.33 | 106.40 | 118.60 |
| 1 | 16S1 | 1238 | A | C2-N3-C4 | 20.33 | 120.76 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 1408 | A | N1-C2-N3 | -20.33 | 119.14 | 129.30 |
| 22 | 23S1 | 1566 | A | N1-C2-N3 | -20.33 | 119.14 | 129.30 |
| 22 | 23S1 | 1749 | A | C2-N3-C4 | 20.33 | 120.76 | 110.60 |
| 22 | 23S1 | 2809 | A | C2-N3-C4 | 20.32 | 120.76 | 110.60 |
| 22 | 23S1 | 2418 | A | C2-N3-C4 | 20.32 | 120.76 | 110.60 |
| 22 | 23S1 | 802 | A | N1-C2-N3 | -20.32 | 119.14 | 129.30 |
| 22 | 23S1 | 1301 | A | C2-N3-C4 | 20.32 | 120.76 | 110.60 |
| 22 | 23S1 | 38 | A | C2-N3-C4 | 20.32 | 120.76 | 110.60 |
| 22 | 23S1 | 693 | A | C2-N3-C4 | 20.31 | 120.76 | 110.60 |
| 1 | 16S1 | 958 | A | C2-N3-C4 | 20.31 | 120.75 | 110.60 |
| 1 | 16S1 | 975 | A | N1-C2-N3 | -20.31 | 119.15 | 129.30 |
| 22 | 23S1 | 1794 | A | C2-N3-C4 | 20.30 | 120.75 | 110.60 |
| 22 | 23S1 | 457 | A | N1-C2-N3 | -20.30 | 119.15 | 129.30 |
| 22 | 23S1 | 675 | A | C2-N3-C4 | 20.30 | 120.75 | 110.60 |
| 22 | 23S1 | 2031 | A | N1-C2-N3 | -20.29 | 119.16 | 129.30 |
| 22 | 23S1 | 2297 | A | N1-C6-N6 | -20.29 | 106.43 | 118.60 |
| 22 | 23S1 | 73 | A | N1-C2-N3 | -20.28 | 119.16 | 129.30 |
| 22 | 23S1 | 2062 | A | C2-N3-C4 | 20.27 | 120.74 | 110.60 |
| 22 | 23S1 | 2883 | A | N1-C2-N3 | -20.27 | 119.16 | 129.30 |
| 1 | 16S1 | 195 | A | N1-C2-N3 | -20.27 | 119.16 | 129.30 |
| 22 | 23S1 | 849 | A | C2-N3-C4 | 20.27 | 120.73 | 110.60 |
| 22 | 23S1 | 2513 | A | N1-C6-N6 | -20.27 | 106.44 | 118.60 |
| 1 | 16S1 | 814 | A | C2-N3-C4 | 20.27 | 120.73 | 110.60 |
| 1 | 16S1 | 815 | A | C2-N3-C4 | 20.27 | 120.73 | 110.60 |
| 22 | 23S1 | 10 | A | N1-C2-N3 | -20.27 | 119.17 | 129.30 |
| 22 | 23S1 | 2823 | A | C2-N3-C4 | 20.27 | 120.73 | 110.60 |
| 22 | 23S1 | 861 | A | N1-C2-N3 | -20.27 | 119.17 | 129.30 |
| 1 | 16S1 | 171 | A | N1-C2-N3 | -20.26 | 119.17 | 129.30 |
| 22 | 23S1 | 2274 | A | N1-C2-N3 | -20.26 | 119.17 | 129.30 |
| 22 | 23S1 | 2632 | A | N1-C6-N6 | -20.26 | 106.44 | 118.60 |
| 1 | 16S1 | 938 | A | C2-N3-C4 | 20.26 | 120.73 | 110.60 |
| 22 | 23S1 | 821 | A | N1-C2-N3 | -20.25 | 119.17 | 129.30 |
| 22 | 23S1 | 2564 | A | N1-C6-N6 | -20.25 | 106.45 | 118.60 |
| 22 | 23S1 | 2388 | A | N1-C6-N6 | -20.25 | 106.45 | 118.60 |
| 1 | 16S1 | 872 | A | N1-C6-N6 | -20.24 | 106.45 | 118.60 |
| 22 | 23S1 | 749 | A | N1-C6-N6 | -20.24 | 106.45 | 118.60 |
| 1 | 16S1 | 718 | A | C2-N3-C4 | 20.24 | 120.72 | 110.60 |
| 22 | 23S1 | 507 | A | N1-C2-N3 | -20.24 | 119.18 | 129.30 |
| 1 | 16S1 | 81 | A | N1-C6-N6 | -20.24 | 106.46 | 118.60 |
| 22 | 23S1 | 1522 | A | C2-N3-C4 | 20.24 | 120.72 | 110.60 |
| 1 | 16S1 | 1398 | A | N1-C6-N6 | -20.23 | 106.46 | 118.60 |
| 1 | 16S1 | 313 | A | C2-N3-C4 | 20.23 | 120.72 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 270 | A | N1-C2-N3 | -20.23 | 119.19 | 129.30 |
| 22 | 23S1 | 1342 | A | N1-C2-N3 | -20.23 | 119.19 | 129.30 |
| 1 | 16S1 | 262 | A | N1-C2-N3 | -20.23 | 119.19 | 129.30 |
| 22 | 23S1 | 2823 | A | N1-C6-N6 | -20.23 | 106.46 | 118.60 |
| 22 | 23S1 | 526 | A | N1-C6-N6 | -20.23 | 106.47 | 118.60 |
| 22 | 23S1 | 750 | A | N1-C2-N3 | -20.23 | 119.19 | 129.30 |
| 22 | 23S1 | 1676 | A | N1-C2-N3 | -20.23 | 119.19 | 129.30 |
| 1 | 16S1 | 1101 | A | N1-C2-N3 | -20.22 | 119.19 | 129.30 |
| 22 | 23S1 | 2051 | A | C2-N3-C4 | 20.22 | 120.71 | 110.60 |
| 1 | 16S1 | 574 | A | N1-C6-N6 | -20.22 | 106.47 | 118.60 |
| 22 | 23S1 | 2675 | A | N1-C2-N3 | -20.22 | 119.19 | 129.30 |
| 22 | 23S1 | 2589 | A | N1-C2-N3 | -20.22 | 119.19 | 129.30 |
| 1 | 16S1 | 364 | A | N1-C6-N6 | -20.21 | 106.47 | 118.60 |
| 22 | 23S1 | 761 | A | N1-C2-N3 | -20.21 | 119.19 | 129.30 |
| 22 | 23S1 | 1009 | A | N1-C2-N3 | -20.21 | 119.19 | 129.30 |
| 1 | 16S1 | 1092 | A | N1-C6-N6 | -20.21 | 106.47 | 118.60 |
| 1 | 16S1 | 1499 | A | N1-C6-N6 | -20.21 | 106.48 | 118.60 |
| 22 | 23S1 | 382 | A | N1-C6-N6 | -20.21 | 106.47 | 118.60 |
| 22 | 23S1 | 927 | A | N1-C6-N6 | -20.21 | 106.47 | 118.60 |
| 1 | 16S1 | 59 | A | C2-N3-C4 | 20.21 | 120.70 | 110.60 |
| 1 | 16S1 | 151 | A | N1-C2-N3 | -20.20 | 119.20 | 129.30 |
| 22 | 23S1 | 845 | A | N1-C2-N3 | -20.20 | 119.20 | 129.30 |
| 22 | 23S1 | 207 | A | C2-N3-C4 | 20.20 | 120.70 | 110.60 |
| 22 | 23S1 | 742 | A | C2-N3-C4 | 20.20 | 120.70 | 110.60 |
| 22 | 23S1 | 804 | A | C2-N3-C4 | 20.20 | 120.70 | 110.60 |
| 22 | 23S1 | 2518 | A | C2-N3-C4 | 20.20 | 120.70 | 110.60 |
| 1 | 16S1 | 2 | A | N1-C6-N6 | -20.20 | 106.48 | 118.60 |
| 22 | 23S1 | 14 | A | N1-C6-N6 | -20.20 | 106.48 | 118.60 |
| 22 | 23S1 | 1144 | A | C2-N3-C4 | 20.19 | 120.70 | 110.60 |
| 22 | 23S1 | 2386 | A | C2-N3-C4 | 20.19 | 120.70 | 110.60 |
| 1 | 16S1 | 900 | A | C2-N3-C4 | 20.19 | 120.70 | 110.60 |
| 1 | 16S1 | 964 | A | C2-N3-C4 | 20.19 | 120.69 | 110.60 |
| 1 | 16S1 | 768 | A | N1-C6-N6 | -20.19 | 106.49 | 118.60 |
| 22 | 23S1 | 161 | A | N1-C6-N6 | -20.18 | 106.49 | 118.60 |
| 22 | 23S1 | 219 | A | N1-C2-N3 | -20.18 | 119.21 | 129.30 |
| 22 | 23S1 | 1028 | A | N1-C2-N3 | -20.18 | 119.21 | 129.30 |
| 22 | 23S1 | 449 | A | N1-C6-N6 | -20.18 | 106.49 | 118.60 |
| 22 | 23S1 | 497 | A | N1-C6-N6 | -20.18 | 106.49 | 118.60 |
| 22 | 23S1 | 2513 | A | C2-N3-C4 | 20.18 | 120.69 | 110.60 |
| 22 | 23S1 | 371 | A | N1-C6-N6 | -20.17 | 106.50 | 118.60 |
| 22 | 23S1 | 621 | A | N1-C2-N3 | -20.17 | 119.21 | 129.30 |
| 1 | 16S1 | 98 | A | C2-N3-C4 | 20.17 | 120.69 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 825 | A | N1-C6-N6 | -20.17 | 106.50 | 118.60 |
| 22 | 23S1 | 346 | A | N1-C6-N6 | -20.17 | 106.50 | 118.60 |
| 22 | 23S1 | 2241 | A | C2-N3-C4 | 20.17 | 120.68 | 110.60 |
| 1 | 16S1 | 1179 | A | N1-C6-N6 | -20.17 | 106.50 | 118.60 |
| 22 | 23S1 | 89 | A | N1-C2-N3 | -20.16 | 119.22 | 129.30 |
| 1 | 16S1 | 873 | A | N1-C2-N3 | -20.16 | 119.22 | 129.30 |
| 22 | 23S1 | 1655 | A | N1-C6-N6 | -20.16 | 106.51 | 118.60 |
| 22 | 23S1 | 479 | A | N1-C2-N3 | -20.15 | 119.22 | 129.30 |
| 22 | 23S1 | 2117 | A | N1-C2-N3 | -20.15 | 119.22 | 129.30 |
| 22 | 23S1 | 1522 | A | N1-C6-N6 | -20.15 | 106.51 | 118.60 |
| 22 | 23S1 | 2632 | A | C2-N3-C4 | 20.14 | 120.67 | 110.60 |
| 1 | 16S1 | 815 | A | N1-C2-N3 | -20.14 | 119.23 | 129.30 |
| 1 | 16S1 | 1346 | A | N1-C6-N6 | -20.14 | 106.52 | 118.60 |
| 22 | 23S1 | 750 | A | C2-N3-C4 | 20.14 | 120.67 | 110.60 |
| 22 | 23S1 | 1253 | A | N1-C6-N6 | -20.14 | 106.52 | 118.60 |
| 22 | 23S1 | 1515 | A | N1-C2-N3 | -20.14 | 119.23 | 129.30 |
| 22 | 23S1 | 160 | A | N1-C2-N3 | -20.14 | 119.23 | 129.30 |
| 1 | 16S1 | 495 | A | N1-C2-N3 | -20.14 | 119.23 | 129.30 |
| 1 | 16S1 | 802 | A | N1-C2-N3 | -20.14 | 119.23 | 129.30 |
| 22 | 23S1 | 2753 | A | N1-C6-N6 | -20.13 | 106.52 | 118.60 |
| 1 | 16S1 | 1280 | A | N1-C2-N3 | -20.13 | 119.23 | 129.30 |
| 22 | 23S1 | 1246 | A | N1-C6-N6 | -20.13 | 106.52 | 118.60 |
| 1 | 16S1 | 509 | A | C2-N3-C4 | 20.13 | 120.67 | 110.60 |
| 22 | 23S1 | 2453 | A | C2-N3-C4 | 20.13 | 120.66 | 110.60 |
| 1 | 16S1 | 60 | A | N1-C6-N6 | -20.12 | 106.53 | 118.60 |
| 22 | 23S1 | 917 | A | C2-N3-C4 | 20.12 | 120.66 | 110.60 |
| 22 | 23S1 | 13 | A | N1-C6-N6 | -20.12 | 106.53 | 118.60 |
| 22 | 23S1 | 1327 | A | N1-C2-N3 | -20.12 | 119.24 | 129.30 |
| 22 | 23S1 | 502 | A | N1-C6-N6 | -20.12 | 106.53 | 118.60 |
| 22 | 23S1 | 1701 | A | N1-C6-N6 | -20.12 | 106.53 | 118.60 |
| 22 | 23S1 | 1265 | A | C2-N3-C4 | 20.11 | 120.66 | 110.60 |
| 22 | 23S1 | 2227 | A | N1-C6-N6 | -20.11 | 106.53 | 118.60 |
| 22 | 23S1 | 1535 | A | N1-C6-N6 | -20.11 | 106.54 | 118.60 |
| 22 | 23S1 | 2682 | A | N1-C2-N3 | -20.11 | 119.25 | 129.30 |
| 22 | 23S1 | 2388 | A | N1-C2-N3 | -20.10 | 119.25 | 129.30 |
| 1 | 16S1 | 572 | A | N1-C6-N6 | -20.09 | 106.55 | 118.60 |
| 22 | 23S1 | 1010 | A | N1-C2-N3 | -20.09 | 119.26 | 129.30 |
| 22 | 23S1 | 528 | A | C2-N3-C4 | 20.09 | 120.64 | 110.60 |
| 1 | 16S1 | 1447 | A | N1-C6-N6 | -20.09 | 106.55 | 118.60 |
| 22 | 23S1 | 833 | A | N1-C2-N3 | -20.08 | 119.26 | 129.30 |
| 23 | 05S1 | 101 | A | C2-N3-C4 | 20.08 | 120.64 | 110.60 |
| 22 | 23S1 | 2766 | A | N1-C2-N3 | -20.08 | 119.26 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 559 | A | N1-C2-N3 | -20.07 | 119.26 | 129.30 |
| 22 | 23S1 | 2453 | A | N1-C6-N6 | -20.07 | 106.56 | 118.60 |
| 22 | 23S1 | 1977 | A | N1-C2-N3 | -20.07 | 119.26 | 129.30 |
| 22 | 23S1 | 1088 | A | C2-N3-C4 | 20.07 | 120.64 | 110.60 |
| 22 | 23S1 | 1392 | A | N1-C6-N6 | -20.07 | 106.56 | 118.60 |
| 1 | 16S1 | 72 | A | N1-C2-N3 | -20.07 | 119.27 | 129.30 |
| 22 | 23S1 | 613 | A | C2-N3-C4 | 20.07 | 120.63 | 110.60 |
| 22 | 23S1 | 2635 | A | N1-C6-N6 | -20.07 | 106.56 | 118.60 |
| 1 | 16S1 | 787 | A | N1-C2-N3 | -20.06 | 119.27 | 129.30 |
| 22 | 23S1 | 675 | A | N1-C2-N3 | -20.06 | 119.27 | 129.30 |
| 22 | 23S1 | 975 | A | N1-C2-N3 | -20.06 | 119.27 | 129.30 |
| 1 | 16S1 | 72 | A | C2-N3-C4 | 20.06 | 120.63 | 110.60 |
| 22 | 23S1 | 1265 | A | N1-C6-N6 | -20.06 | 106.56 | 118.60 |
| 22 | 23S1 | 144 | A | C2-N3-C4 | 20.06 | 120.63 | 110.60 |
| 1 | 16S1 | 223 | A | C2-N3-C4 | 20.05 | 120.63 | 110.60 |
| 22 | 23S1 | 655 | A | N1-C2-N3 | -20.05 | 119.27 | 129.30 |
| 22 | 23S1 | 2266 | A | C2-N3-C4 | 20.05 | 120.63 | 110.60 |
| 22 | 23S1 | 1762 | A | C2-N3-C4 | 20.05 | 120.63 | 110.60 |
| 22 | 23S1 | 2706 | A | C2-N3-C4 | 20.05 | 120.62 | 110.60 |
| 22 | 23S1 | 2183 | A | N1-C6-N6 | -20.05 | 106.57 | 118.60 |
| 1 | 16S1 | 777 | A | N1-C2-N3 | -20.05 | 119.28 | 129.30 |
| 22 | 23S1 | 789 | A | N1-C2-N3 | -20.05 | 119.28 | 129.30 |
| 22 | 23S1 | 2158 | A | N1-C2-N3 | -20.05 | 119.28 | 129.30 |
| 1 | 16S1 | 574 | A | N1-C2-N3 | -20.04 | 119.28 | 129.30 |
| 1 | 16S1 | 1502 | A | N1-C2-N3 | -20.04 | 119.28 | 129.30 |
| 1 | 16S1 | 915 | A | N1-C6-N6 | -20.04 | 106.58 | 118.60 |
| 22 | 23S1 | 782 | A | C2-N3-C4 | 20.04 | 120.62 | 110.60 |
| 22 | 23S1 | 1952 | A | N1-C6-N6 | -20.04 | 106.58 | 118.60 |
| 22 | 23S1 | 800 | A | N1-C2-N3 | -20.04 | 119.28 | 129.30 |
| 1 | 16S1 | 915 | A | N1-C2-N3 | -20.03 | 119.28 | 129.30 |
| 22 | 23S1 | 528 | A | N1-C2-N3 | -20.03 | 119.28 | 129.30 |
| 22 | 23S1 | 2273 | A | N1-C2-N3 | -20.03 | 119.28 | 129.30 |
| 22 | 23S1 | 1155 | A | N1-C2-N3 | -20.03 | 119.28 | 129.30 |
| 22 | 23S1 | 1918 | A | N1-C6-N6 | -20.03 | 106.58 | 118.60 |
| 22 | 23S1 | 265 | A | N1-C2-N3 | -20.03 | 119.29 | 129.30 |
| 22 | 23S1 | 2037 | A | N1-C2-N3 | -20.03 | 119.29 | 129.30 |
| 22 | 23S1 | 1901 | A | N1-C6-N6 | -20.02 | 106.59 | 118.60 |
| 1 | 16S1 | 1250 | A | N1-C2-N3 | -20.01 | 119.29 | 129.30 |
| 22 | 23S1 | 637 | A | N1-C2-N3 | -20.01 | 119.29 | 129.30 |
| 22 | 23S1 | 1630 | A | N1-C2-N3 | -20.01 | 119.29 | 129.30 |
| 22 | 23S1 | 2013 | A | C2-N3-C4 | 20.01 | 120.61 | 110.60 |
| 22 | 23S1 | 764 | A | C2-N3-C4 | 20.01 | 120.61 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 973 | A | N1-C6-N6 | -20.01 | 106.59 | 118.60 |
| 22 | 23S1 | 1610 | A | N1-C2-N3 | -20.01 | 119.30 | 129.30 |
| 22 | 23S1 | 1569 | A | N1-C6-N6 | -20.01 | 106.60 | 118.60 |
| 22 | 23S1 | 2013 | A | N1-C2-N3 | -20.01 | 119.30 | 129.30 |
| 22 | 23S1 | 104 | A | C2-N3-C4 | 20.01 | 120.60 | 110.60 |
| 22 | 23S1 | 2461 | A | C2-N3-C4 | 20.01 | 120.60 | 110.60 |
| 1 | 16S1 | 1117 | A | N1-C2-N3 | -20.00 | 119.30 | 129.30 |
| 22 | 23S1 | 631 | A | N1-C6-N6 | -20.00 | 106.60 | 118.60 |
| 22 | 23S1 | 2327 | A | C2-N3-C4 | 20.00 | 120.60 | 110.60 |
| 22 | 23S1 | 984 | A | N1-C6-N6 | -20.00 | 106.60 | 118.60 |
| 22 | 23S1 | 1477 | A | N1-C2-N3 | -20.00 | 119.30 | 129.30 |
| 23 | 05S1 | 99 | A | N1-C2-N3 | -20.00 | 119.30 | 129.30 |
| 1 | 16S1 | 687 | A | N1-C2-N3 | -20.00 | 119.30 | 129.30 |
| 1 | 16S1 | 715 | A | N1-C2-N3 | -20.00 | 119.30 | 129.30 |
| 55 | PTR1 | 51 | A | N1-C6-N6 | -20.00 | 106.60 | 118.60 |
| 22 | 23S1 | 677 | A | C2-N3-C4 | 19.99 | 120.60 | 110.60 |
| 22 | 23S1 | 502 | A | N1-C2-N3 | -19.99 | 119.30 | 129.30 |
| 22 | 23S1 | 1522 | A | N1-C2-N3 | -19.99 | 119.30 | 129.30 |
| 22 | 23S1 | 706 | A | N1-C6-N6 | -19.99 | 106.61 | 118.60 |
| 22 | 23S1 | 1937 | A | C2-N3-C4 | 19.99 | 120.59 | 110.60 |
| 22 | 23S1 | 1086 | A | N1-C2-N3 | -19.98 | 119.31 | 129.30 |
| 22 | 23S1 | 2418 | A | N1-C6-N6 | -19.98 | 106.61 | 118.60 |
| 22 | 23S1 | 661 | A | C2-N3-C4 | 19.98 | 120.59 | 110.60 |
| 22 | 23S1 | 2758 | A | N1-C6-N6 | -19.98 | 106.61 | 118.60 |
| 22 | 23S1 | 526 | A | N1-C2-N3 | -19.98 | 119.31 | 129.30 |
| 22 | 23S1 | 1787 | A | C2-N3-C4 | 19.98 | 120.59 | 110.60 |
| 22 | 23S1 | 1274 | A | N1-C6-N6 | -19.97 | 106.62 | 118.60 |
| 22 | 23S1 | 2587 | A | N1-C2-N3 | -19.97 | 119.31 | 129.30 |
| 22 | 23S1 | 1214 | A | N1-C6-N6 | -19.96 | 106.62 | 118.60 |
| 22 | 23S1 | 2826 | A | C2-N3-C4 | 19.96 | 120.58 | 110.60 |
| 22 | 23S1 | 1189 | A | C2-N3-C4 | 19.96 | 120.58 | 110.60 |
| 22 | 23S1 | 1901 | A | C2-N3-C4 | 19.96 | 120.58 | 110.60 |
| 1 | 16S1 | 665 | A | N1-C2-N3 | -19.96 | 119.32 | 129.30 |
| 22 | 23S1 | 244 | A | C2-N3-C4 | 19.96 | 120.58 | 110.60 |
| 22 | 23S1 | 947 | A | C2-N3-C4 | 19.96 | 120.58 | 110.60 |
| 22 | 23S1 | 1634 | A | N1-C6-N6 | -19.96 | 106.62 | 118.60 |
| 22 | 23S1 | 21 | A | C2-N3-C4 | 19.96 | 120.58 | 110.60 |
| 22 | 23S1 | 878 | A | N1-C6-N6 | -19.96 | 106.63 | 118.60 |
| 1 | 16S1 | 109 | A | N1-C2-N3 | -19.96 | 119.32 | 129.30 |
| 22 | 23S1 | 5 | A | C2-N3-C4 | 19.95 | 120.58 | 110.60 |
| 22 | 23S1 | 1853 | A | C2-N3-C4 | 19.95 | 120.57 | 110.60 |
| 22 | 23S1 | 1262 | A | N1-C6-N6 | -19.95 | 106.63 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 2564 | A | C2-N3-C4 | 19.94 | 120.57 | 110.60 |
| 22 | 23S1 | 2738 | A | N1-C2-N3 | -19.94 | 119.33 | 129.30 |
| 22 | 23S1 | 1552 | A | C2-N3-C4 | 19.94 | 120.57 | 110.60 |
| 22 | 23S1 | 1762 | A | N1-C6-N6 | -19.94 | 106.64 | 118.60 |
| 22 | 23S1 | 1829 | A | N1-C6-N6 | -19.94 | 106.64 | 118.60 |
| 22 | 23S1 | 1665 | A | C2-N3-C4 | 19.93 | 120.57 | 110.60 |
| 1 | 16S1 | 130 | A | N1-C2-N3 | -19.93 | 119.34 | 129.30 |
| 22 | 23S1 | 309 | A | C2-N3-C4 | 19.93 | 120.56 | 110.60 |
| 22 | 23S1 | 1393 | A | N1-C2-N3 | -19.92 | 119.34 | 129.30 |
| 22 | 23S1 | 1668 | A | N1-C2-N3 | -19.92 | 119.34 | 129.30 |
| 22 | 23S1 | 1494 | A | N1-C2-N3 | -19.92 | 119.34 | 129.30 |
| 22 | 23S1 | 71 | A | C2-N3-C4 | 19.91 | 120.56 | 110.60 |
| 22 | 23S1 | 1226 | A | N1-C2-N3 | -19.91 | 119.34 | 129.30 |
| 1 | 16S1 | 573 | A | N1-C2-N3 | -19.91 | 119.35 | 129.30 |
| 1 | 16S1 | 1251 | A | N1-C2-N3 | -19.91 | 119.35 | 129.30 |
| 22 | 23S1 | 402 | A | N1-C2-N3 | -19.91 | 119.35 | 129.30 |
| 1 | 16S1 | 393 | A | C2-N3-C4 | 19.90 | 120.55 | 110.60 |
| 22 | 23S1 | 226 | A | N1-C2-N3 | -19.90 | 119.35 | 129.30 |
| 22 | 23S1 | 1354 | A | N1-C2-N3 | -19.90 | 119.35 | 129.30 |
| 1 | 16S1 | 327 | A | N1-C2-N3 | -19.90 | 119.35 | 129.30 |
| 1 | 16S1 | 1239 | A | N1-C6-N6 | -19.90 | 106.66 | 118.60 |
| 22 | 23S1 | 294 | A | N1-C2-N3 | -19.90 | 119.35 | 129.30 |
| 1 | 16S1 | 918 | A | C2-N3-C4 | 19.90 | 120.55 | 110.60 |
| 22 | 23S1 | 2835 | A | N1-C2-N3 | -19.90 | 119.35 | 129.30 |
| 1 | 16S1 | 197 | A | N1-C2-N3 | -19.89 | 119.35 | 129.30 |
| 22 | 23S1 | 1654 | A | N1-C6-N6 | -19.89 | 106.66 | 118.60 |
| 22 | 23S1 | 2882 | A | N1-C2-N3 | -19.89 | 119.35 | 129.30 |
| 22 | 23S1 | 2198 | A | N1-C2-N3 | -19.89 | 119.35 | 129.30 |
| 22 | 23S1 | 2434 | A | N1-C6-N6 | -19.89 | 106.67 | 118.60 |
| 1 | 16S1 | 172 | A | N1-C2-N3 | -19.89 | 119.36 | 129.30 |
| 22 | 23S1 | 1039 | A | N1-C2-N3 | -19.89 | 119.36 | 129.30 |
| 22 | 23S1 | 1321 | A | C2-N3-C4 | 19.89 | 120.54 | 110.60 |
| 22 | 23S1 | 2497 | A | C2-N3-C4 | 19.88 | 120.54 | 110.60 |
| 1 | 16S1 | 766 | A | N1-C2-N3 | -19.88 | 119.36 | 129.30 |
| 22 | 23S1 | 1858 | A | C2-N3-C4 | 19.88 | 120.54 | 110.60 |
| 1 | 16S1 | 2 | A | N1-C2-N3 | -19.88 | 119.36 | 129.30 |
| 22 | 23S1 | 972 | A | N1-C2-N3 | -19.88 | 119.36 | 129.30 |
| 22 | 23S1 | 689 | A | C2-N3-C4 | 19.87 | 120.54 | 110.60 |
| 22 | 23S1 | 936 | A | C2-N3-C4 | 19.87 | 120.54 | 110.60 |
| 1 | 16S1 | 807 | A | C2-N3-C4 | 19.87 | 120.53 | 110.60 |
| 22 | 23S1 | 497 | A | N1-C2-N3 | -19.87 | 119.36 | 129.30 |
| 1 | 16S1 | 1151 | A | C2-N3-C4 | 19.87 | 120.53 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1155 | A | N1-C6-N6 | -19.87 | 106.68 | 118.60 |
| 22 | 23S1 | 1890 | A | N1-C2-N3 | -19.87 | 119.37 | 129.30 |
| 22 | 23S1 | 2700 | A | C2-N3-C4 | 19.87 | 120.53 | 110.60 |
| 1 | 16S1 | 468 | A | C2-N3-C4 | 19.87 | 120.53 | 110.60 |
| 22 | 23S1 | 1583 | A | N1-C6-N6 | -19.87 | 106.68 | 118.60 |
| 22 | 23S1 | 2476 | A | C2-N3-C4 | 19.87 | 120.53 | 110.60 |
| 22 | 23S1 | 514 | A | N1-C6-N6 | -19.86 | 106.68 | 118.60 |
| 22 | 23S1 | 2037 | A | C2-N3-C4 | 19.86 | 120.53 | 110.60 |
| 1 | 16S1 | 547 | A | N1-C2-N3 | -19.86 | 119.37 | 129.30 |
| 22 | 23S1 | 2450 | A | N1-C6-N6 | -19.86 | 106.68 | 118.60 |
| 22 | 23S1 | 2837 | A | C2-N3-C4 | 19.86 | 120.53 | 110.60 |
| 22 | 23S1 | 925 | A | C2-N3-C4 | 19.86 | 120.53 | 110.60 |
| 22 | 23S1 | 2590 | A | N1-C2-N3 | -19.86 | 119.37 | 129.30 |
| 1 | 16S1 | 777 | A | C2-N3-C4 | 19.86 | 120.53 | 110.60 |
| 1 | 16S1 | 1480 | A | N1-C6-N6 | -19.86 | 106.69 | 118.60 |
| 22 | 23S1 | 195 | A | C2-N3-C4 | 19.86 | 120.53 | 110.60 |
| 22 | 23S1 | 330 | A | N1-C6-N6 | -19.86 | 106.69 | 118.60 |
| 22 | 23S1 | 792 | A | N1-C6-N6 | -19.86 | 106.69 | 118.60 |
| 22 | 23S1 | 1246 | A | C2-N3-C4 | 19.86 | 120.53 | 110.60 |
| 22 | 23S1 | 2054 | A | C2-N3-C4 | 19.86 | 120.53 | 110.60 |
| 22 | 23S1 | 2288 | A | N1-C2-N3 | -19.86 | 119.37 | 129.30 |
| 22 | 23S1 | 53 | A | N1-C2-N3 | -19.85 | 119.37 | 129.30 |
| 22 | 23S1 | 1129 | A | N1-C2-N3 | -19.85 | 119.37 | 129.30 |
| 22 | 23S1 | 1749 | A | N1-C2-N3 | -19.85 | 119.37 | 129.30 |
| 22 | 23S1 | 1786 | A | C2-N3-C4 | 19.85 | 120.53 | 110.60 |
| 1 | 16S1 | 1329 | A | N1-C6-N6 | -19.85 | 106.69 | 118.60 |
| 22 | 23S1 | 1165 | A | N1-C2-N3 | -19.84 | 119.38 | 129.30 |
| 1 | 16S1 | 1374 | A | C2-N3-C4 | 19.84 | 120.52 | 110.60 |
| 1 | 16S1 | 1289 | A | N1-C2-N3 | -19.84 | 119.38 | 129.30 |
| 22 | 23S1 | 1247 | A | C2-N3-C4 | 19.84 | 120.52 | 110.60 |
| 22 | 23S1 | 752 | A | C2-N3-C4 | 19.84 | 120.52 | 110.60 |
| 22 | 23S1 | 1302 | A | N1-C2-N3 | -19.84 | 119.38 | 129.30 |
| 22 | 23S1 | 631 | A | N1-C2-N3 | -19.84 | 119.38 | 129.30 |
| 1 | 16S1 | 607 | A | N1-C6-N6 | -19.84 | 106.70 | 118.60 |
| 1 | 16S1 | 1329 | A | C2-N3-C4 | 19.84 | 120.52 | 110.60 |
| 22 | 23S1 | 849 | A | N1-C6-N6 | -19.84 | 106.70 | 118.60 |
| 22 | 23S1 | 2813 | A | N1-C6-N6 | -19.83 | 106.70 | 118.60 |
| 22 | 23S1 | 1286 | A | C2-N3-C4 | 19.83 | 120.52 | 110.60 |
| 22 | 23S1 | 1754 | A | N1-C6-N6 | -19.83 | 106.70 | 118.60 |
| 1 | 16S1 | 816 | A | N1-C2-N3 | -19.83 | 119.39 | 129.30 |
| 22 | 23S1 | 910 | A | N1-C2-N3 | -19.83 | 119.39 | 129.30 |
| 1 | 16S1 | 794 | A | N1-C6-N6 | -19.83 | 106.70 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1677 | A | N1-C2-N3 | -19.83 | 119.39 | 129.30 |
| 22 | 23S1 | 1789 | A | N1-C2-N3 | -19.82 | 119.39 | 129.30 |
| 22 | 23S1 | 2284 | A | C2-N3-C4 | 19.82 | 120.51 | 110.60 |
| 22 | 23S1 | 2435 | A | N1-C6-N6 | -19.82 | 106.70 | 118.60 |
| 22 | 23S1 | 2476 | A | N1-C2-N3 | -19.82 | 119.39 | 129.30 |
| 23 | 05S1 | 53 | A | N1-C2-N3 | -19.82 | 119.39 | 129.30 |
| 1 | 16S1 | 923 | A | C2-N3-C4 | 19.82 | 120.51 | 110.60 |
| 22 | 23S1 | 2560 | A | C2-N3-C4 | 19.82 | 120.51 | 110.60 |
| 22 | 23S1 | 983 | A | C2-N3-C4 | 19.82 | 120.51 | 110.60 |
| 22 | 23S1 | 1126 | A | N1-C6-N6 | -19.82 | 106.71 | 118.60 |
| 1 | 16S1 | 199 | A | C2-N3-C4 | 19.82 | 120.51 | 110.60 |
| 1 | 16S1 | 1082 | A | C2-N3-C4 | 19.82 | 120.51 | 110.60 |
| 22 | 23S1 | 216 | A | N1-C6-N6 | -19.82 | 106.71 | 118.60 |
| 22 | 23S1 | 973 | A | C2-N3-C4 | 19.82 | 120.51 | 110.60 |
| 23 | 05S1 | 50 | A | C2-N3-C4 | 19.82 | 120.51 | 110.60 |
| 22 | 23S1 | 1427 | A | N1-C2-N3 | -19.81 | 119.39 | 129.30 |
| 22 | 23S1 | 1786 | A | N1-C6-N6 | -19.81 | 106.71 | 118.60 |
| 22 | 23S1 | 959 | A | C2-N3-C4 | 19.81 | 120.51 | 110.60 |
| 22 | 23S1 | 1032 | A | N1-C2-N3 | -19.81 | 119.39 | 129.30 |
| 22 | 23S1 | 918 | A | N1-C2-N3 | -19.81 | 119.40 | 129.30 |
| 22 | 23S1 | 2821 | A | N1-C2-N3 | -19.81 | 119.39 | 129.30 |
| 22 | 23S1 | 1805 | A | C2-N3-C4 | 19.81 | 120.50 | 110.60 |
| 1 | 16S1 | 313 | A | N1-C6-N6 | -19.81 | 106.72 | 118.60 |
| 22 | 23S1 | 119 | A | N1-C2-N3 | -19.81 | 119.40 | 129.30 |
| 22 | 23S1 | 470 | A | C2-N3-C4 | 19.81 | 120.50 | 110.60 |
| 22 | 23S1 | 480 | A | C2-N3-C4 | 19.81 | 120.50 | 110.60 |
| 22 | 23S1 | 1998 | A | C2-N3-C4 | 19.81 | 120.50 | 110.60 |
| 22 | 23S1 | 2451 | A | C2-N3-C4 | 19.80 | 120.50 | 110.60 |
| 22 | 23S1 | 1387 | A | C2-N3-C4 | 19.80 | 120.50 | 110.60 |
| 22 | 23S1 | 1637 | A | N1-C6-N6 | -19.80 | 106.72 | 118.60 |
| 22 | 23S1 | 1285 | A | N1-C6-N6 | -19.80 | 106.72 | 118.60 |
| 1 | 16S1 | 1196 | A | C2-N3-C4 | 19.80 | 120.50 | 110.60 |
| 22 | 23S1 | 933 | A | N1-C2-N3 | -19.79 | 119.40 | 129.30 |
| 1 | 16S1 | 414 | A | C2-N3-C4 | 19.79 | 120.50 | 110.60 |
| 22 | 23S1 | 1347 | A | C2-N3-C4 | 19.79 | 120.50 | 110.60 |
| 1 | 16S1 | 1101 | A | C2-N3-C4 | 19.79 | 120.50 | 110.60 |
| 22 | 23S1 | 582 | A | C2-N3-C4 | 19.79 | 120.49 | 110.60 |
| 22 | 23S1 | 1829 | A | C2-N3-C4 | 19.79 | 120.49 | 110.60 |
| 1 | 16S1 | 1044 | A | C2-N3-C4 | 19.79 | 120.49 | 110.60 |
| 1 | 16S1 | 282 | A | N1-C6-N6 | -19.79 | 106.73 | 118.60 |
| 22 | 23S1 | 1439 | A | N1-C2-N3 | -19.79 | 119.41 | 129.30 |
| 22 | 23S1 | 1616 | A | N1-C2-N3 | -19.78 | 119.41 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 332 | A | N1-C6-N6 | -19.78 | 106.73 | 118.60 |
| 1 | 16S1 | 583 | A | C2-N3-C4 | 19.78 | 120.49 | 110.60 |
| 1 | 16S1 | 994 | A | C2-N3-C4 | 19.78 | 120.49 | 110.60 |
| 22 | 23S1 | 1744 | A | N1-C6-N6 | -19.78 | 106.73 | 118.60 |
| 22 | 23S1 | 1919 | A | N1-C6-N6 | -19.78 | 106.73 | 118.60 |
| 1 | 16S1 | 1311 | A | C2-N3-C4 | 19.78 | 120.49 | 110.60 |
| 1 | 16S1 | 563 | A | N1-C2-N3 | -19.78 | 119.41 | 129.30 |
| 1 | 16S1 | 171 | A | N1-C6-N6 | -19.77 | 106.73 | 118.60 |
| 1 | 16S1 | 702 | A | N1-C2-N3 | -19.77 | 119.41 | 129.30 |
| 22 | 23S1 | 165 | A | N1-C6-N6 | -19.77 | 106.73 | 118.60 |
| 1 | 16S1 | 149 | A | N1-C6-N6 | -19.77 | 106.74 | 118.60 |
| 22 | 23S1 | 1189 | A | N1-C2-N3 | -19.77 | 119.42 | 129.30 |
| 22 | 23S1 | 1470 | A | N1-C2-N3 | -19.77 | 119.42 | 129.30 |
| 22 | 23S1 | 2632 | A | N1-C2-N3 | -19.77 | 119.42 | 129.30 |
| 22 | 23S1 | 1000 | A | N1-C6-N6 | -19.77 | 106.74 | 118.60 |
| 22 | 23S1 | 909 | A | C2-N3-C4 | 19.76 | 120.48 | 110.60 |
| 1 | 16S1 | 937 | A | C2-N3-C4 | 19.76 | 120.48 | 110.60 |
| 1 | 16S1 | 1251 | A | C2-N3-C4 | 19.76 | 120.48 | 110.60 |
| 22 | 23S1 | 1757 | A | N1-C6-N6 | -19.76 | 106.74 | 118.60 |
| 22 | 23S1 | 616 | A | N1-C2-N3 | -19.76 | 119.42 | 129.30 |
| 23 | 05S1 | 73 | A | N1-C2-N3 | -19.76 | 119.42 | 129.30 |
| 1 | 16S1 | 1476 | A | N1-C6-N6 | -19.75 | 106.75 | 118.60 |
| 22 | 23S1 | 1085 | A | C2-N3-C4 | 19.75 | 120.48 | 110.60 |
| 22 | 23S1 | 1570 | A | N1-C2-N3 | -19.75 | 119.42 | 129.30 |
| 22 | 23S1 | 2590 | A | N1-C6-N6 | -19.75 | 106.75 | 118.60 |
| 22 | 23S1 | 2147 | A | N1-C2-N3 | -19.75 | 119.42 | 129.30 |
| 1 | 16S1 | 1046 | A | N1-C6-N6 | -19.75 | 106.75 | 118.60 |
| 22 | 23S1 | 1129 | A | N1-C6-N6 | -19.75 | 106.75 | 118.60 |
| 22 | 23S1 | 2407 | A | C2-N3-C4 | 19.75 | 120.48 | 110.60 |
| 22 | 23S1 | 1392 | A | N1-C2-N3 | -19.75 | 119.42 | 129.30 |
| 23 | 05S1 | 99 | A | N1-C6-N6 | -19.75 | 106.75 | 118.60 |
| 22 | 23S1 | 661 | A | N1-C2-N3 | -19.75 | 119.43 | 129.30 |
| 22 | 23S1 | 1515 | A | C2-N3-C4 | 19.75 | 120.47 | 110.60 |
| 22 | 23S1 | 1654 | A | C2-N3-C4 | 19.75 | 120.47 | 110.60 |
| 22 | 23S1 | 216 | A | C2-N3-C4 | 19.75 | 120.47 | 110.60 |
| 22 | 23S1 | 1780 | A | C2-N3-C4 | 19.75 | 120.47 | 110.60 |
| 22 | 23S1 | 2725 | A | C2-N3-C4 | 19.74 | 120.47 | 110.60 |
| 22 | 23S1 | 792 | A | C2-N3-C4 | 19.74 | 120.47 | 110.60 |
| 22 | 23S1 | 1789 | A | C2-N3-C4 | 19.74 | 120.47 | 110.60 |
| 22 | 23S1 | 1785 | A | N1-C2-N3 | -19.74 | 119.43 | 129.30 |
| 22 | 23S1 | 2173 | A | N1-C2-N3 | -19.74 | 119.43 | 129.30 |
| 1 | 16S1 | 781 | A | N1-C2-N3 | -19.74 | 119.43 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 586 | A | N1-C2-N3 | -19.74 | 119.43 | 129.30 |
| 22 | 23S1 | 637 | A | N1-C6-N6 | -19.74 | 106.76 | 118.60 |
| 22 | 23S1 | 2418 | A | N1-C2-N3 | -19.74 | 119.43 | 129.30 |
| 22 | 23S1 | 2860 | A | N1-C2-N3 | -19.73 | 119.43 | 129.30 |
| 22 | 23S1 | 1744 | A | C2-N3-C4 | 19.73 | 120.47 | 110.60 |
| 1 | 16S1 | 155 | A | C2-N3-C4 | 19.73 | 120.47 | 110.60 |
| 22 | 23S1 | 825 | A | N1-C2-N3 | -19.73 | 119.44 | 129.30 |
| 1 | 16S1 | 1360 | A | C2-N3-C4 | 19.73 | 120.47 | 110.60 |
| 1 | 16S1 | 1468 | A | C2-N3-C4 | 19.73 | 120.46 | 110.60 |
| 23 | 05S1 | 108 | A | N1-C2-N3 | -19.73 | 119.44 | 129.30 |
| 1 | 16S1 | 784 | A | C2-N3-C4 | 19.73 | 120.46 | 110.60 |
| 22 | 23S1 | 1354 | A | C2-N3-C4 | 19.73 | 120.46 | 110.60 |
| 1 | 16S1 | 1428 | A | N1-C6-N6 | -19.73 | 106.77 | 118.60 |
| 22 | 23S1 | 1757 | A | N1-C2-N3 | -19.73 | 119.44 | 129.30 |
| 1 | 16S1 | 80 | A | C2-N3-C4 | 19.72 | 120.46 | 110.60 |
| 22 | 23S1 | 608 | A | C2-N3-C4 | 19.72 | 120.46 | 110.60 |
| 22 | 23S1 | 1194 | A | N1-C6-N6 | -19.72 | 106.77 | 118.60 |
| 22 | 23S1 | 2005 | A | N1-C2-N3 | -19.72 | 119.44 | 129.30 |
| 22 | 23S1 | 28 | A | N1-C2-N3 | -19.72 | 119.44 | 129.30 |
| 22 | 23S1 | 507 | A | N1-C6-N6 | -19.72 | 106.77 | 118.60 |
| 22 | 23S1 | 675 | A | N1-C6-N6 | -19.72 | 106.77 | 118.60 |
| 22 | 23S1 | 1254 | A | C2-N3-C4 | 19.72 | 120.46 | 110.60 |
| 1 | 16S1 | 1408 | A | N1-C6-N6 | -19.72 | 106.77 | 118.60 |
| 1 | 16S1 | 747 | A | C2-N3-C4 | 19.72 | 120.46 | 110.60 |
| 1 | 16S1 | 1287 | A | N1-C2-N3 | -19.71 | 119.44 | 129.30 |
| 1 | 16S1 | 1363 | A | N1-C6-N6 | -19.71 | 106.77 | 118.60 |
| 22 | 23S1 | 2726 | A | N1-C2-N3 | -19.71 | 119.44 | 129.30 |
| 1 | 16S1 | 408 | A | C2-N3-C4 | 19.71 | 120.45 | 110.60 |
| 1 | 16S1 | 1431 | A | N1-C2-N3 | -19.71 | 119.45 | 129.30 |
| 23 | 05S1 | 119 | A | C2-N3-C4 | 19.71 | 120.45 | 110.60 |
| 1 | 16S1 | 460 | A | C2-N3-C4 | 19.71 | 120.45 | 110.60 |
| 22 | 23S1 | 1419 | A | N1-C6-N6 | -19.70 | 106.78 | 118.60 |
| 55 | PTR1 | 21 | A | N1-C2-N3 | -19.70 | 119.45 | 129.30 |
| 1 | 16S1 | 1476 | A | C2-N3-C4 | 19.70 | 120.45 | 110.60 |
| 22 | 23S1 | 676 | A | N1-C6-N6 | -19.70 | 106.78 | 118.60 |
| 22 | 23S1 | 2741 | A | N1-C2-N3 | -19.70 | 119.45 | 129.30 |
| 22 | 23S1 | 2386 | A | N1-C2-N3 | -19.70 | 119.45 | 129.30 |
| 23 | 05S1 | 78 | A | N1-C2-N3 | -19.70 | 119.45 | 129.30 |
| 55 | PTR1 | 58 | A | N1-C6-N6 | -19.70 | 106.78 | 118.60 |
| 1 | 16S1 | 766 | A | N1-C6-N6 | -19.70 | 106.78 | 118.60 |
| 22 | 23S1 | 432 | A | C2-N3-C4 | 19.70 | 120.45 | 110.60 |
| 22 | 23S1 | 1439 | A | N1-C6-N6 | -19.70 | 106.78 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1759 | A | N1-C2-N3 | -19.70 | 119.45 | 129.30 |
| 22 | 23S1 | 2376 | A | C2-N3-C4 | 19.70 | 120.45 | 110.60 |
| 1 | 16S1 | 860 | A | N1-C6-N6 | -19.70 | 106.78 | 118.60 |
| 22 | 23S1 | 529 | A | C2-N3-C4 | 19.69 | 120.45 | 110.60 |
| 22 | 23S1 | 384 | A | N1-C2-N3 | -19.69 | 119.45 | 129.30 |
| 22 | 23S1 | 892 | A | N1-C6-N6 | -19.69 | 106.78 | 118.60 |
| 22 | 23S1 | 146 | A | C2-N3-C4 | 19.69 | 120.44 | 110.60 |
| 22 | 23S1 | 1155 | A | C2-N3-C4 | 19.69 | 120.44 | 110.60 |
| 22 | 23S1 | 1427 | A | C2-N3-C4 | 19.69 | 120.44 | 110.60 |
| 1 | 16S1 | 363 | A | N1-C2-N3 | -19.68 | 119.46 | 129.30 |
| 1 | 16S1 | 1239 | A | N1-C2-N3 | -19.68 | 119.46 | 129.30 |
| 22 | 23S1 | 219 | A | N1-C6-N6 | -19.68 | 106.79 | 118.60 |
| 22 | 23S1 | 792 | A | N1-C2-N3 | -19.68 | 119.46 | 129.30 |
| 22 | 23S1 | 1032 | A | C2-N3-C4 | 19.68 | 120.44 | 110.60 |
| 22 | 23S1 | 1809 | A | N1-C6-N6 | -19.68 | 106.79 | 118.60 |
| 22 | 23S1 | 2835 | A | C2-N3-C4 | 19.68 | 120.44 | 110.60 |
| 1 | 16S1 | 129 | A | N1-C2-N3 | -19.68 | 119.46 | 129.30 |
| 1 | 16S1 | 1346 | A | N1-C2-N3 | -19.68 | 119.46 | 129.30 |
| 22 | 23S1 | 19 | A | C2-N3-C4 | 19.68 | 120.44 | 110.60 |
| 22 | 23S1 | 2821 | A | C2-N3-C4 | 19.68 | 120.44 | 110.60 |
| 22 | 23S1 | 432 | A | N1-C2-N3 | -19.68 | 119.46 | 129.30 |
| 22 | 23S1 | 1746 | A | N1-C6-N6 | -19.68 | 106.79 | 118.60 |
| 1 | 16S1 | 306 | A | C2-N3-C4 | 19.68 | 120.44 | 110.60 |
| 22 | 23S1 | 941 | A | C2-N3-C4 | 19.68 | 120.44 | 110.60 |
| 22 | 23S1 | 155 | A | C2-N3-C4 | 19.68 | 120.44 | 110.60 |
| 1 | 16S1 | 814 | A | N1-C6-N6 | -19.67 | 106.80 | 118.60 |
| 22 | 23S1 | 532 | A | N1-C6-N6 | -19.67 | 106.80 | 118.60 |
| 22 | 23S1 | 1630 | A | C2-N3-C4 | 19.67 | 120.44 | 110.60 |
| 22 | 23S1 | 2090 | A | C2-N3-C4 | 19.67 | 120.44 | 110.60 |
| 1 | 16S1 | 197 | A | N1-C6-N6 | -19.67 | 106.80 | 118.60 |
| 22 | 23S1 | 1021 | A | N1-C2-N3 | -19.67 | 119.47 | 129.30 |
| 22 | 23S1 | 204 | A | N1-C6-N6 | -19.67 | 106.80 | 118.60 |
| 22 | 23S1 | 1570 | A | C2-N3-C4 | 19.67 | 120.43 | 110.60 |
| 22 | 23S1 | 751 | A | N1-C2-N3 | -19.66 | 119.47 | 129.30 |
| 22 | 23S1 | 1525 | A | N1-C6-N6 | -19.66 | 106.80 | 118.60 |
| 1 | 16S1 | 964 | A | N1-C2-N3 | -19.66 | 119.47 | 129.30 |
| 22 | 23S1 | 204 | A | N1-C2-N3 | -19.66 | 119.47 | 129.30 |
| 23 | 05S1 | 46 | A | N1-C6-N6 | -19.66 | 106.80 | 118.60 |
| 22 | 23S1 | 756 | A | C2-N3-C4 | 19.66 | 120.43 | 110.60 |
| 22 | 23S1 | 819 | A | C2-N3-C4 | 19.66 | 120.43 | 110.60 |
| 22 | 23S1 | 2199 | A | C2-N3-C4 | 19.66 | 120.43 | 110.60 |
| 1 | 16S1 | 19 | A | C2-N3-C4 | 19.66 | 120.43 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 816 | A | C2-N3-C4 | 19.66 | 120.43 | 110.60 |
| 1 | 16S1 | 1465 | A | C2-N3-C4 | 19.66 | 120.43 | 110.60 |
| 1 | 16S1 | 1434 | A | N1-C2-N3 | -19.66 | 119.47 | 129.30 |
| 22 | 23S1 | 614 | A | N1-C6-N6 | -19.66 | 106.81 | 118.60 |
| 23 | 05S1 | 57 | A | N1-C2-N3 | -19.66 | 119.47 | 129.30 |
| 1 | 16S1 | 1340 | A | N1-C6-N6 | -19.65 | 106.81 | 118.60 |
| 22 | 23S1 | 1938 | A | N1-C2-N3 | -19.65 | 119.47 | 129.30 |
| 55 | PTR1 | 42 | A | C2-N3-C4 | 19.65 | 120.43 | 110.60 |
| 22 | 23S1 | 1265 | A | N1-C2-N3 | -19.65 | 119.47 | 129.30 |
| 22 | 23S1 | 104 | A | N1-C2-N3 | -19.65 | 119.47 | 129.30 |
| 1 | 16S1 | 560 | A | C2-N3-C4 | 19.65 | 120.42 | 110.60 |
| 1 | 16S1 | 1429 | A | N1-C6-N6 | -19.65 | 106.81 | 118.60 |
| 22 | 23S1 | 10 | A | C2-N3-C4 | 19.65 | 120.42 | 110.60 |
| 22 | 23S1 | 1262 | A | C2-N3-C4 | 19.65 | 120.42 | 110.60 |
| 22 | 23S1 | 2727 | A | C2-N3-C4 | 19.64 | 120.42 | 110.60 |
| 22 | 23S1 | 439 | A | C2-N3-C4 | 19.64 | 120.42 | 110.60 |
| 22 | 23S1 | 1858 | A | N1-C6-N6 | -19.64 | 106.81 | 118.60 |
| 22 | 23S1 | 1932 | A | N1-C2-N3 | -19.64 | 119.48 | 129.30 |
| 22 | 23S1 | 14 | A | N1-C2-N3 | -19.64 | 119.48 | 129.30 |
| 23 | 05S1 | 101 | A | N1-C6-N6 | -19.64 | 106.82 | 118.60 |
| 1 | 16S1 | 8 | A | N1-C2-N3 | -19.64 | 119.48 | 129.30 |
| 22 | 23S1 | 529 | A | N1-C2-N3 | -19.64 | 119.48 | 129.30 |
| 1 | 16S1 | 621 | A | N1-C6-N6 | -19.63 | 106.82 | 118.60 |
| 1 | 16S1 | 560 | A | N1-C6-N6 | -19.63 | 106.82 | 118.60 |
| 1 | 16S1 | 900 | A | N1-C2-N3 | -19.63 | 119.48 | 129.30 |
| 22 | 23S1 | 262 | A | N1-C6-N6 | -19.63 | 106.82 | 118.60 |
| 22 | 23S1 | 1987 | A | N1-C2-N3 | -19.63 | 119.48 | 129.30 |
| 1 | 16S1 | 262 | A | C2-N3-C4 | 19.63 | 120.42 | 110.60 |
| 1 | 16S1 | 1204 | A | N1-C6-N6 | -19.63 | 106.82 | 118.60 |
| 22 | 23S1 | 2426 | A | N1-C2-N3 | -19.63 | 119.48 | 129.30 |
| 22 | 23S1 | 2670 | A | C2-N3-C4 | 19.63 | 120.42 | 110.60 |
| 22 | 23S1 | 2899 | A | N1-C2-N3 | -19.63 | 119.48 | 129.30 |
| 1 | 16S1 | 502 | A | C2-N3-C4 | 19.63 | 120.41 | 110.60 |
| 1 | 16S1 | 1333 | A | N1-C2-N3 | -19.63 | 119.49 | 129.30 |
| 1 | 16S1 | 288 | A | N1-C6-N6 | -19.62 | 106.83 | 118.60 |
| 1 | 16S1 | 792 | A | N1-C2-N3 | -19.62 | 119.49 | 129.30 |
| 1 | 16S1 | 889 | A | N1-C2-N3 | -19.62 | 119.49 | 129.30 |
| 1 | 16S1 | 1413 | A | N1-C6-N6 | -19.62 | 106.83 | 118.60 |
| 22 | 23S1 | 131 | A | C2-N3-C4 | 19.62 | 120.41 | 110.60 |
| 22 | 23S1 | 941 | A | N1-C2-N3 | -19.62 | 119.49 | 129.30 |
| 55 | PTR1 | 59 | A | N1-C2-N3 | -19.62 | 119.49 | 129.30 |
| 1 | 16S1 | 1410 | A | C2-N3-C4 | 19.62 | 120.41 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1194 | A | C2-N3-C4 | 19.62 | 120.41 | 110.60 |
| 1 | 16S1 | 167 | A | C2-N3-C4 | 19.62 | 120.41 | 110.60 |
| 1 | 16S1 | 182 | A | N1-C2-N3 | -19.62 | 119.49 | 129.30 |
| 1 | 16S1 | 263 | A | C2-N3-C4 | 19.62 | 120.41 | 110.60 |
| 22 | 23S1 | 320 | A | C2-N3-C4 | 19.62 | 120.41 | 110.60 |
| 22 | 23S1 | 1230 | A | C2-N3-C4 | 19.62 | 120.41 | 110.60 |
| 22 | 23S1 | 783 | A | N1-C2-N3 | -19.61 | 119.49 | 129.30 |
| 22 | 23S1 | 1383 | A | N1-C2-N3 | -19.61 | 119.49 | 129.30 |
| 1 | 16S1 | 1446 | A | N1-C2-N3 | -19.61 | 119.49 | 129.30 |
| 22 | 23S1 | 1987 | A | C2-N3-C4 | 19.61 | 120.41 | 110.60 |
| 22 | 23S1 | 2835 | A | N1-C6-N6 | -19.61 | 106.83 | 118.60 |
| 1 | 16S1 | 119 | A | N1-C2-N3 | -19.61 | 119.50 | 129.30 |
| 1 | 16S1 | 728 | A | N1-C2-N3 | -19.61 | 119.50 | 129.30 |
| 22 | 23S1 | 1147 | A | C2-N3-C4 | 19.61 | 120.40 | 110.60 |
| 1 | 16S1 | 167 | A | N1-C2-N3 | -19.60 | 119.50 | 129.30 |
| 22 | 23S1 | 1502 | A | N1-C6-N6 | -19.60 | 106.84 | 118.60 |
| 22 | 23S1 | 2033 | A | N1-C2-N3 | -19.60 | 119.50 | 129.30 |
| 1 | 16S1 | 977 | A | N1-C2-N3 | -19.60 | 119.50 | 129.30 |
| 22 | 23S1 | 905 | A | N1-C6-N6 | -19.60 | 106.84 | 118.60 |
| 1 | 16S1 | 468 | A | N1-C6-N6 | -19.60 | 106.84 | 118.60 |
| 1 | 16S1 | 918 | A | N1-C6-N6 | -19.60 | 106.84 | 118.60 |
| 1 | 16S1 | 1067 | A | N1-C6-N6 | -19.60 | 106.84 | 118.60 |
| 1 | 16S1 | 1238 | A | N1-C6-N6 | -19.60 | 106.84 | 118.60 |
| 22 | 23S1 | 320 | A | N1-C2-N3 | -19.60 | 119.50 | 129.30 |
| 22 | 23S1 | 753 | A | C2-N3-C4 | 19.60 | 120.40 | 110.60 |
| 22 | 23S1 | 804 | A | N1-C2-N3 | -19.60 | 119.50 | 129.30 |
| 22 | 23S1 | 2052 | A | C2-N3-C4 | 19.60 | 120.40 | 110.60 |
| 22 | 23S1 | 668 | A | N1-C6-N6 | -19.59 | 106.84 | 118.60 |
| 22 | 23S1 | 1264 | A | N1-C2-N3 | -19.59 | 119.50 | 129.30 |
| 22 | 23S1 | 2639 | A | N1-C2-N3 | -19.59 | 119.50 | 129.30 |
| 22 | 23S1 | 217 | A | N1-C2-N3 | -19.59 | 119.50 | 129.30 |
| 22 | 23S1 | 621 | A | N1-C6-N6 | -19.59 | 106.84 | 118.60 |
| 1 | 16S1 | 969 | A | N1-C2-N3 | -19.59 | 119.50 | 129.30 |
| 1 | 16S1 | 371 | A | C2-N3-C4 | 19.59 | 120.39 | 110.60 |
| 1 | 16S1 | 1250 | A | C2-N3-C4 | 19.59 | 120.39 | 110.60 |
| 1 | 16S1 | 1280 | A | N1-C6-N6 | -19.59 | 106.85 | 118.60 |
| 22 | 23S1 | 1889 | A | N1-C2-N3 | -19.59 | 119.51 | 129.30 |
| 22 | 23S1 | 2033 | A | C2-N3-C4 | 19.59 | 120.39 | 110.60 |
| 1 | 16S1 | 1275 | A | C2-N3-C4 | 19.59 | 120.39 | 110.60 |
| 22 | 23S1 | 1900 | A | N1-C2-N3 | -19.59 | 119.51 | 129.30 |
| 22 | 23S1 | 1175 | A | N1-C2-N3 | -19.58 | 119.51 | 129.30 |
| 22 | 23S1 | 1819 | A | C2-N3-C4 | 19.58 | 120.39 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 2660 | A | C2-N3-C4 | 19.58 | 120.39 | 110.60 |
| 22 | 23S1 | 2851 | A | N1-C2-N3 | -19.58 | 119.51 | 129.30 |
| 22 | 23S1 | 347 | A | C2-N3-C4 | 19.58 | 120.39 | 110.60 |
| 22 | 23S1 | 2327 | A | N1-C6-N6 | -19.58 | 106.85 | 118.60 |
| 22 | 23S1 | 2478 | A | C2-N3-C4 | 19.58 | 120.39 | 110.60 |
| 1 | 16S1 | 969 | A | N1-C6-N6 | -19.58 | 106.85 | 118.60 |
| 22 | 23S1 | 2134 | A | N1-C6-N6 | -19.58 | 106.85 | 118.60 |
| 1 | 16S1 | 892 | A | C2-N3-C4 | 19.58 | 120.39 | 110.60 |
| 22 | 23S1 | 1434 | A | N1-C2-N3 | -19.58 | 119.51 | 129.30 |
| 22 | 23S1 | 1889 | A | C2-N3-C4 | 19.58 | 120.39 | 110.60 |
| 1 | 16S1 | 1110 | A | N1-C2-N3 | -19.57 | 119.51 | 129.30 |
| 22 | 23S1 | 742 | A | N1-C2-N3 | -19.57 | 119.51 | 129.30 |
| 22 | 23S1 | 983 | A | N1-C6-N6 | -19.57 | 106.86 | 118.60 |
| 22 | 23S1 | 1551 | A | N1-C2-N3 | -19.57 | 119.51 | 129.30 |
| 22 | 23S1 | 2031 | A | N1-C6-N6 | -19.57 | 106.86 | 118.60 |
| 22 | 23S1 | 2478 | A | N1-C2-N3 | -19.57 | 119.51 | 129.30 |
| 1 | 16S1 | 781 | A | C2-N3-C4 | 19.57 | 120.39 | 110.60 |
| 1 | 16S1 | 1500 | A | C2-N3-C4 | 19.57 | 120.39 | 110.60 |
| 22 | 23S1 | 216 | A | N1-C2-N3 | -19.57 | 119.51 | 129.30 |
| 1 | 16S1 | 309 | A | N1-C6-N6 | -19.57 | 106.86 | 118.60 |
| 22 | 23S1 | 233 | A | C2-N3-C4 | 19.57 | 120.39 | 110.60 |
| 1 | 16S1 | 655 | A | C2-N3-C4 | 19.57 | 120.38 | 110.60 |
| 22 | 23S1 | 1009 | A | N1-C6-N6 | -19.57 | 106.86 | 118.60 |
| 22 | 23S1 | 103 | A | N1-C6-N6 | -19.56 | 106.86 | 118.60 |
| 22 | 23S1 | 1853 | A | N1-C6-N6 | -19.56 | 106.86 | 118.60 |
| 22 | 23S1 | 2761 | A | C2-N3-C4 | 19.56 | 120.38 | 110.60 |
| 22 | 23S1 | 2829 | A | N1-C2-N3 | -19.56 | 119.52 | 129.30 |
| 55 | PTR1 | 23 | A | C2-N3-C4 | 19.56 | 120.38 | 110.60 |
| 1 | 16S1 | 26 | A | C2-N3-C4 | 19.56 | 120.38 | 110.60 |
| 22 | 23S1 | 42 | A | N1-C2-N3 | -19.56 | 119.52 | 129.30 |
| 22 | 23S1 | 126 | A | N1-C6-N6 | -19.56 | 106.86 | 118.60 |
| 22 | 23S1 | 739 | A | N1-C2-N3 | -19.56 | 119.52 | 129.30 |
| 22 | 23S1 | 2184 | A | C2-N3-C4 | 19.56 | 120.38 | 110.60 |
| 22 | 23S1 | 2764 | A | N1-C2-N3 | -19.56 | 119.52 | 129.30 |
| 22 | 23S1 | 2019 | A | N1-C6-N6 | -19.56 | 106.86 | 118.60 |
| 1 | 16S1 | 743 | A | C2-N3-C4 | 19.56 | 120.38 | 110.60 |
| 22 | 23S1 | 176 | A | C2-N3-C4 | 19.55 | 120.38 | 110.60 |
| 1 | 16S1 | 983 | A | N1-C2-N3 | -19.55 | 119.52 | 129.30 |
| 22 | 23S1 | 1701 | A | C2-N3-C4 | 19.55 | 120.38 | 110.60 |
| 22 | 23S1 | 2381 | A | N1-C2-N3 | -19.55 | 119.52 | 129.30 |
| 22 | 23S1 | 2675 | A | C2-N3-C4 | 19.55 | 120.38 | 110.60 |
| 1 | 16S1 | 55 | A | C2-N3-C4 | 19.55 | 120.38 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 119 | A | N1-C6-N6 | -19.55 | 106.87 | 118.60 |
| 1 | 16S1 | 802 | A | N1-C6-N6 | -19.55 | 106.87 | 118.60 |
| 22 | 23S1 | 471 | A | N1-C2-N3 | -19.55 | 119.53 | 129.30 |
| 22 | 23S1 | 125 | A | N1-C2-N3 | -19.55 | 119.53 | 129.30 |
| 22 | 23S1 | 309 | A | N1-C2-N3 | -19.55 | 119.53 | 129.30 |
| 22 | 23S1 | 626 | A | N1-C2-N3 | -19.55 | 119.53 | 129.30 |
| 22 | 23S1 | 2080 | A | C2-N3-C4 | 19.55 | 120.37 | 110.60 |
| 22 | 23S1 | 936 | A | N1-C2-N3 | -19.55 | 119.53 | 129.30 |
| 23 | 05S1 | 59 | A | N1-C6-N6 | -19.54 | 106.87 | 118.60 |
| 1 | 16S1 | 172 | A | N1-C6-N6 | -19.54 | 106.87 | 118.60 |
| 1 | 16S1 | 320 | A | N1-C6-N6 | -19.54 | 106.87 | 118.60 |
| 22 | 23S1 | 928 | A | C2-N3-C4 | 19.54 | 120.37 | 110.60 |
| 1 | 16S1 | 1299 | A | N1-C6-N6 | -19.54 | 106.88 | 118.60 |
| 22 | 23S1 | 2009 | A | N1-C6-N6 | -19.54 | 106.88 | 118.60 |
| 22 | 23S1 | 2757 | A | N1-C2-N3 | -19.54 | 119.53 | 129.30 |
| 22 | 23S1 | 2314 | A | C2-N3-C4 | 19.54 | 120.37 | 110.60 |
| 1 | 16S1 | 1146 | A | N1-C6-N6 | -19.54 | 106.88 | 118.60 |
| 1 | 16S1 | 1374 | A | N1-C2-N3 | -19.54 | 119.53 | 129.30 |
| 22 | 23S1 | 1815 | A | N1-C6-N6 | -19.54 | 106.88 | 118.60 |
| 1 | 16S1 | 539 | A | C2-N3-C4 | 19.53 | 120.37 | 110.60 |
| 22 | 23S1 | 1001 | A | N1-C2-N3 | -19.53 | 119.53 | 129.30 |
| 22 | 23S1 | 1304 | A | C2-N3-C4 | 19.53 | 120.37 | 110.60 |
| 1 | 16S1 | 1019 | A | N1-C2-N3 | -19.53 | 119.53 | 129.30 |
| 22 | 23S1 | 2872 | A | C2-N3-C4 | 19.53 | 120.37 | 110.60 |
| 22 | 23S1 | 454 | A | C2-N3-C4 | 19.53 | 120.36 | 110.60 |
| 22 | 23S1 | 454 | A | N1-C2-N3 | -19.53 | 119.53 | 129.30 |
| 22 | 23S1 | 1284 | A | N1-C2-N3 | -19.53 | 119.53 | 129.30 |
| 22 | 23S1 | 2566 | A | C2-N3-C4 | 19.53 | 120.36 | 110.60 |
| 23 | 05S1 | 45 | A | C2-N3-C4 | 19.53 | 120.36 | 110.60 |
| 1 | 16S1 | 1196 | A | N1-C2-N3 | -19.53 | 119.54 | 129.30 |
| 1 | 16S1 | 1332 | A | N1-C6-N6 | -19.53 | 106.88 | 118.60 |
| 22 | 23S1 | 1084 | A | N1-C6-N6 | -19.53 | 106.88 | 118.60 |
| 22 | 23S1 | 1213 | A | C2-N3-C4 | 19.53 | 120.36 | 110.60 |
| 22 | 23S1 | 1353 | A | N1-C2-N3 | -19.53 | 119.54 | 129.30 |
| 22 | 23S1 | 2005 | A | N1-C6-N6 | -19.53 | 106.89 | 118.60 |
| 22 | 23S1 | 911 | A | N1-C2-N3 | -19.52 | 119.54 | 129.30 |
| 22 | 23S1 | 1960 | A | C2-N3-C4 | 19.52 | 120.36 | 110.60 |
| 1 | 16S1 | 482 | A | C2-N3-C4 | 19.52 | 120.36 | 110.60 |
| 1 | 16S1 | 759 | A | N1-C2-N3 | -19.52 | 119.54 | 129.30 |
| 1 | 16S1 | 1394 | A | N1-C2-N3 | -19.52 | 119.54 | 129.30 |
| 1 | 16S1 | 696 | A | N1-C2-N3 | -19.52 | 119.54 | 129.30 |
| 1 | 16S1 | 648 | A | C2-N3-C4 | 19.52 | 120.36 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1151 | A | C2-N3-C4 | 19.52 | 120.36 | 110.60 |
| 22 | 23S1 | 2247 | A | C2-N3-C4 | 19.52 | 120.36 | 110.60 |
| 22 | 23S1 | 909 | A | N1-C6-N6 | -19.52 | 106.89 | 118.60 |
| 22 | 23S1 | 2851 | A | N1-C6-N6 | -19.52 | 106.89 | 118.60 |
| 1 | 16S1 | 704 | A | C2-N3-C4 | 19.51 | 120.36 | 110.60 |
| 1 | 16S1 | 1155 | A | C2-N3-C4 | 19.51 | 120.36 | 110.60 |
| 22 | 23S1 | 947 | A | N1-C2-N3 | -19.51 | 119.54 | 129.30 |
| 22 | 23S1 | 1287 | A | C2-N3-C4 | 19.51 | 120.36 | 110.60 |
| 1 | 16S1 | 461 | A | N1-C2-N3 | -19.51 | 119.55 | 129.30 |
| 22 | 23S1 | 1156 | A | N1-C2-N3 | -19.51 | 119.55 | 129.30 |
| 22 | 23S1 | 1552 | A | N1-C2-N3 | -19.51 | 119.55 | 129.30 |
| 22 | 23S1 | 2726 | A | C2-N3-C4 | 19.51 | 120.36 | 110.60 |
| 22 | 23S1 | 126 | A | N1-C2-N3 | -19.51 | 119.55 | 129.30 |
| 23 | 05S1 | 58 | A | C2-N3-C4 | 19.51 | 120.35 | 110.60 |
| 1 | 16S1 | 306 | A | N1-C2-N3 | -19.51 | 119.55 | 129.30 |
| 22 | 23S1 | 2547 | A | N1-C6-N6 | -19.51 | 106.89 | 118.60 |
| 1 | 16S1 | 695 | A | C2-N3-C4 | 19.51 | 120.35 | 110.60 |
| 22 | 23S1 | 1586 | A | C2-N3-C4 | 19.51 | 120.35 | 110.60 |
| 1 | 16S1 | 825 | A | N1-C2-N3 | -19.50 | 119.55 | 129.30 |
| 1 | 16S1 | 1250 | A | N1-C6-N6 | -19.50 | 106.90 | 118.60 |
| 22 | 23S1 | 172 | A | C2-N3-C4 | 19.50 | 120.35 | 110.60 |
| 22 | 23S1 | 1142 | A | C2-N3-C4 | 19.50 | 120.35 | 110.60 |
| 22 | 23S1 | 2577 | A | N1-C6-N6 | -19.50 | 106.90 | 118.60 |
| 22 | 23S1 | 1504 | A | N1-C2-N3 | -19.50 | 119.55 | 129.30 |
| 22 | 23S1 | 1583 | A | N1-C2-N3 | -19.50 | 119.55 | 129.30 |
| 22 | 23S1 | 1634 | A | N1-C2-N3 | -19.50 | 119.55 | 129.30 |
| 1 | 16S1 | 298 | A | N1-C2-N3 | -19.50 | 119.55 | 129.30 |
| 1 | 16S1 | 794 | A | C2-N3-C4 | 19.50 | 120.35 | 110.60 |
| 22 | 23S1 | 980 | A | N1-C6-N6 | -19.50 | 106.90 | 118.60 |
| 22 | 23S1 | 1366 | A | N1-C2-N3 | -19.50 | 119.55 | 129.30 |
| 1 | 16S1 | 353 | A | N1-C2-N3 | -19.49 | 119.55 | 129.30 |
| 22 | 23S1 | 74 | A | N1-C6-N6 | -19.49 | 106.90 | 118.60 |
| 22 | 23S1 | 2733 | A | N1-C6-N6 | -19.49 | 106.90 | 118.60 |
| 1 | 16S1 | 787 | A | C2-N3-C4 | 19.49 | 120.35 | 110.60 |
| 1 | 16S1 | 1229 | A | C2-N3-C4 | 19.49 | 120.35 | 110.60 |
| 22 | 23S1 | 866 | A | N1-C2-N3 | -19.49 | 119.55 | 129.30 |
| 22 | 23S1 | 1254 | A | N1-C6-N6 | -19.49 | 106.90 | 118.60 |
| 1 | 16S1 | 26 | A | N1-C2-N3 | -19.49 | 119.55 | 129.30 |
| 1 | 16S1 | 228 | A | N1-C2-N3 | -19.49 | 119.56 | 129.30 |
| 1 | 16S1 | 1288 | A | N1-C2-N3 | -19.49 | 119.55 | 129.30 |
| 22 | 23S1 | 447 | A | N1-C2-N3 | -19.49 | 119.56 | 129.30 |
| 22 | 23S1 | 572 | A | C2-N3-C4 | 19.49 | 120.34 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1054 | A | C2-N3-C4 | 19.49 | 120.34 | 110.60 |
| 22 | 23S1 | 2336 | A | N1-C2-N3 | -19.49 | 119.56 | 129.30 |
| 22 | 23S1 | 2358 | A | N1-C6-N6 | -19.49 | 106.91 | 118.60 |
| 22 | 23S1 | 788 | A | N1-C2-N3 | -19.49 | 119.56 | 129.30 |
| 22 | 23S1 | 1244 | A | C2-N3-C4 | 19.49 | 120.34 | 110.60 |
| 1 | 16S1 | 10 | A | C2-N3-C4 | 19.48 | 120.34 | 110.60 |
| 1 | 16S1 | 1368 | A | C2-N3-C4 | 19.48 | 120.34 | 110.60 |
| 22 | 23S1 | 599 | A | N1-C2-N3 | -19.48 | 119.56 | 129.30 |
| 22 | 23S1 | 1579 | A | N1-C2-N3 | -19.48 | 119.56 | 129.30 |
| 22 | 23S1 | 2003 | A | C2-N3-C4 | 19.48 | 120.34 | 110.60 |
| 22 | 23S1 | 2758 | A | N1-C2-N3 | -19.48 | 119.56 | 129.30 |
| 22 | 23S1 | 478 | A | C2-N3-C4 | 19.48 | 120.34 | 110.60 |
| 1 | 16S1 | 1111 | A | N1-C2-N3 | -19.48 | 119.56 | 129.30 |
| 1 | 16S1 | 1197 | A | C2-N3-C4 | 19.48 | 120.34 | 110.60 |
| 22 | 23S1 | 190 | A | N1-C2-N3 | -19.48 | 119.56 | 129.30 |
| 22 | 23S1 | 1469 | A | C2-N3-C4 | 19.48 | 120.34 | 110.60 |
| 22 | 23S1 | 2199 | A | N1-C2-N3 | -19.48 | 119.56 | 129.30 |
| 22 | 23S1 | 820 | A | C2-N3-C4 | 19.48 | 120.34 | 110.60 |
| 22 | 23S1 | 1508 | A | N1-C2-N3 | -19.48 | 119.56 | 129.30 |
| 22 | 23S1 | 2119 | A | N1-C6-N6 | -19.48 | 106.91 | 118.60 |
| 1 | 16S1 | 559 | A | C2-N3-C4 | 19.48 | 120.34 | 110.60 |
| 22 | 23S1 | 1654 | A | N1-C2-N3 | -19.48 | 119.56 | 129.30 |
| 22 | 23S1 | 2700 | A | N1-C2-N3 | -19.48 | 119.56 | 129.30 |
| 1 | 16S1 | 325 | A | C2-N3-C4 | 19.48 | 120.34 | 110.60 |
| 1 | 16S1 | 1150 | A | N1-C6-N6 | -19.48 | 106.91 | 118.60 |
| 22 | 23S1 | 666 | A | N1-C2-N3 | -19.48 | 119.56 | 129.30 |
| 22 | 23S1 | 1496 | A | N1-C2-N3 | -19.48 | 119.56 | 129.30 |
| 22 | 23S1 | 2169 | A | C2-N3-C4 | 19.48 | 120.34 | 110.60 |
| 1 | 16S1 | 456 | A | N1-C2-N3 | -19.47 | 119.56 | 129.30 |
| 1 | 16S1 | 814 | A | N1-C2-N3 | -19.47 | 119.56 | 129.30 |
| 22 | 23S1 | 1927 | A | N1-C2-N3 | -19.47 | 119.56 | 129.30 |
| 1 | 16S1 | 718 | A | N1-C2-N3 | -19.47 | 119.56 | 129.30 |
| 22 | 23S1 | 556 | A | C2-N3-C4 | 19.47 | 120.34 | 110.60 |
| 22 | 23S1 | 1021 | A | N1-C6-N6 | -19.47 | 106.92 | 118.60 |
| 22 | 23S1 | 1566 | A | C2-N3-C4 | 19.47 | 120.34 | 110.60 |
| 22 | 23S1 | 2826 | A | N1-C6-N6 | -19.47 | 106.92 | 118.60 |
| 1 | 16S1 | 243 | A | N1-C2-N3 | -19.47 | 119.57 | 129.30 |
| 22 | 23S1 | 2014 | A | N1-C2-N3 | -19.47 | 119.56 | 129.30 |
| 22 | 23S1 | 2800 | A | N1-C2-N3 | -19.47 | 119.57 | 129.30 |
| 1 | 16S1 | 152 | A | N1-C2-N3 | -19.47 | 119.57 | 129.30 |
| 22 | 23S1 | 300 | A | C2-N3-C4 | 19.47 | 120.33 | 110.60 |
| 1 | 16S1 | 270 | A | N1-C2-N3 | -19.46 | 119.57 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 1311 | A | N1-C6-N6 | -19.46 | 106.92 | 118.60 |
| 1 | 16S1 | 349 | A | N1-C2-N3 | -19.46 | 119.57 | 129.30 |
| 22 | 23S1 | 655 | A | C2-N3-C4 | 19.46 | 120.33 | 110.60 |
| 22 | 23S1 | 1204 | A | N1-C2-N3 | -19.46 | 119.57 | 129.30 |
| 22 | 23S1 | 1871 | A | C2-N3-C4 | 19.46 | 120.33 | 110.60 |
| 22 | 23S1 | 2589 | A | C2-N3-C4 | 19.46 | 120.33 | 110.60 |
| 22 | 23S1 | 2765 | A | N1-C2-N3 | -19.46 | 119.57 | 129.30 |
| 22 | 23S1 | 2287 | A | C2-N3-C4 | 19.46 | 120.33 | 110.60 |
| 1 | 16S1 | 3 | A | N1-C2-N3 | -19.46 | 119.57 | 129.30 |
| 22 | 23S1 | 226 | A | N1-C6-N6 | -19.46 | 106.93 | 118.60 |
| 22 | 23S1 | 1085 | A | N1-C6-N6 | -19.46 | 106.93 | 118.60 |
| 22 | 23S1 | 2377 | A | N1-C2-N3 | -19.46 | 119.57 | 129.30 |
| 22 | 23S1 | 1384 | A | N1-C2-N3 | -19.45 | 119.57 | 129.30 |
| 1 | 16S1 | 977 | A | N1-C6-N6 | -19.45 | 106.93 | 118.60 |
| 22 | 23S1 | 1069 | A | N1-C2-N3 | -19.45 | 119.57 | 129.30 |
| 55 | PTR1 | 58 | A | C2-N3-C4 | 19.45 | 120.33 | 110.60 |
| 55 | PTR1 | 38 | A | C2-N3-C4 | 19.45 | 120.33 | 110.60 |
| 1 | 16S1 | 1287 | A | C2-N3-C4 | 19.45 | 120.33 | 110.60 |
| 1 | 16S1 | 621 | A | N1-C2-N3 | -19.45 | 119.58 | 129.30 |
| 22 | 23S1 | 89 | A | C2-N3-C4 | 19.45 | 120.32 | 110.60 |
| 22 | 23S1 | 2266 | A | N1-C6-N6 | -19.45 | 106.93 | 118.60 |
| 22 | 23S1 | 391 | A | C2-N3-C4 | 19.45 | 120.32 | 110.60 |
| 22 | 23S1 | 2776 | A | N1-C2-N3 | -19.45 | 119.58 | 129.30 |
| 22 | 23S1 | 278 | A | N1-C6-N6 | -19.45 | 106.93 | 118.60 |
| 22 | 23S1 | 203 | A | N1-C2-N3 | -19.44 | 119.58 | 129.30 |
| 22 | 23S1 | 943 | A | N1-C2-N3 | -19.44 | 119.58 | 129.30 |
| 55 | PTR1 | 38 | A | N1-C2-N3 | -19.44 | 119.58 | 129.30 |
| 22 | 23S1 | 2541 | A | N1-C6-N6 | -19.44 | 106.94 | 118.60 |
| 1 | 16S1 | 716 | A | N1-C6-N6 | -19.44 | 106.94 | 118.60 |
| 1 | 16S1 | 1287 | A | N1-C6-N6 | -19.44 | 106.94 | 118.60 |
| 1 | 16S1 | 1340 | A | N1-C2-N3 | -19.44 | 119.58 | 129.30 |
| 22 | 23S1 | 743 | A | C2-N3-C4 | 19.44 | 120.32 | 110.60 |
| 22 | 23S1 | 2381 | A | C2-N3-C4 | 19.44 | 120.32 | 110.60 |
| 1 | 16S1 | 246 | A | N1-C2-N3 | -19.44 | 119.58 | 129.30 |
| 22 | 23S1 | 279 | A | N1-C6-N6 | -19.44 | 106.94 | 118.60 |
| 22 | 23S1 | 384 | A | C2-N3-C4 | 19.44 | 120.32 | 110.60 |
| 22 | 23S1 | 2565 | A | N1-C2-N3 | -19.44 | 119.58 | 129.30 |
| 22 | 23S1 | 1603 | A | C2-N3-C4 | 19.44 | 120.32 | 110.60 |
| 22 | 23S1 | 2101 | A | C2-N3-C4 | 19.43 | 120.32 | 110.60 |
| 22 | 23S1 | 2225 | A | C2-N3-C4 | 19.43 | 120.32 | 110.60 |
| 22 | 23S1 | 2497 | A | N1-C6-N6 | -19.43 | 106.94 | 118.60 |
| 22 | 23S1 | 2679 | A | C2-N3-C4 | 19.43 | 120.32 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 553 | A | C2-N3-C4 | 19.43 | 120.31 | 110.60 |
| 22 | 23S1 | 294 | A | N1-C6-N6 | -19.43 | 106.94 | 118.60 |
| 22 | 23S1 | 311 | A | C2-N3-C4 | 19.43 | 120.32 | 110.60 |
| 22 | 23S1 | 1525 | A | C2-N3-C4 | 19.43 | 120.31 | 110.60 |
| 22 | 23S1 | 501 | A | N1-C6-N6 | -19.43 | 106.94 | 118.60 |
| 1 | 16S1 | 1080 | A | N1-C2-N3 | -19.43 | 119.59 | 129.30 |
| 22 | 23S1 | 2761 | A | N1-C6-N6 | -19.42 | 106.95 | 118.60 |
| 22 | 23S1 | 764 | A | N1-C6-N6 | -19.42 | 106.95 | 118.60 |
| 1 | 16S1 | 712 | A | C2-N3-C4 | 19.42 | 120.31 | 110.60 |
| 22 | 23S1 | 382 | A | C2-N3-C4 | 19.42 | 120.31 | 110.60 |
| 22 | 23S1 | 608 | A | N1-C2-N3 | -19.42 | 119.59 | 129.30 |
| 22 | 23S1 | 1040 | A | N1-C2-N3 | -19.42 | 119.59 | 129.30 |
| 22 | 23S1 | 1759 | A | N1-C6-N6 | -19.42 | 106.95 | 118.60 |
| 22 | 23S1 | 1772 | A | N1-C6-N6 | -19.42 | 106.95 | 118.60 |
| 22 | 23S1 | 2015 | A | N1-C2-N3 | -19.42 | 119.59 | 129.30 |
| 1 | 16S1 | 510 | A | N1-C2-N3 | -19.41 | 119.59 | 129.30 |
| 1 | 16S1 | 1082 | A | N1-C2-N3 | -19.41 | 119.59 | 129.30 |
| 22 | 23S1 | 793 | A | C2-N3-C4 | 19.41 | 120.31 | 110.60 |
| 22 | 23S1 | 1165 | A | C2-N3-C4 | 19.41 | 120.31 | 110.60 |
| 22 | 23S1 | 1635 | A | N1-C2-N3 | -19.41 | 119.59 | 129.30 |
| 1 | 16S1 | 460 | A | N1-C2-N3 | -19.41 | 119.60 | 129.30 |
| 1 | 16S1 | 892 | A | N1-C2-N3 | -19.41 | 119.60 | 129.30 |
| 22 | 23S1 | 53 | A | C2-N3-C4 | 19.41 | 120.30 | 110.60 |
| 1 | 16S1 | 746 | A | N1-C6-N6 | -19.40 | 106.96 | 118.60 |
| 1 | 16S1 | 1350 | A | C2-N3-C4 | 19.40 | 120.30 | 110.60 |
| 22 | 23S1 | 1365 | A | C2-N3-C4 | 19.40 | 120.30 | 110.60 |
| 22 | 23S1 | 1395 | A | N1-C2-N3 | -19.40 | 119.60 | 129.30 |
| 1 | 16S1 | 412 | A | C2-N3-C4 | 19.40 | 120.30 | 110.60 |
| 22 | 23S1 | 1336 | A | C2-N3-C4 | 19.40 | 120.30 | 110.60 |
| 22 | 23S1 | 515 | A | N1-C2-N3 | -19.40 | 119.60 | 129.30 |
| 22 | 23S1 | 1885 | A | N1-C2-N3 | -19.40 | 119.60 | 129.30 |
| 22 | 23S1 | 2809 | A | N1-C2-N3 | -19.40 | 119.60 | 129.30 |
| 22 | 23S1 | 2868 | A | C2-N3-C4 | 19.40 | 120.30 | 110.60 |
| 1 | 16S1 | 1146 | A | C2-N3-C4 | 19.40 | 120.30 | 110.60 |
| 22 | 23S1 | 1276 | A | C2-N3-C4 | 19.40 | 120.30 | 110.60 |
| 23 | 05S1 | 109 | A | N1-C2-N3 | -19.40 | 119.60 | 129.30 |
| 1 | 16S1 | 382 | A | C2-N3-C4 | 19.40 | 120.30 | 110.60 |
| 22 | 23S1 | 1383 | A | C2-N3-C4 | 19.40 | 120.30 | 110.60 |
| 22 | 23S1 | 371 | A | C2-N3-C4 | 19.39 | 120.30 | 110.60 |
| 22 | 23S1 | 1609 | A | N1-C2-N3 | -19.39 | 119.60 | 129.30 |
| 22 | 23S1 | 802 | A | N1-C6-N6 | -19.39 | 106.96 | 118.60 |
| 22 | 23S1 | 1794 | A | N1-C6-N6 | -19.39 | 106.96 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 2734 | A | N1-C2-N3 | -19.39 | 119.60 | 129.30 |
| 1 | 16S1 | 1180 | A | N1-C6-N6 | -19.39 | 106.97 | 118.60 |
| 22 | 23S1 | 342 | A | C2-N3-C4 | 19.39 | 120.30 | 110.60 |
| 22 | 23S1 | 453 | A | N1-C6-N6 | -19.39 | 106.97 | 118.60 |
| 22 | 23S1 | 1067 | A | C2-N3-C4 | 19.39 | 120.30 | 110.60 |
| 22 | 23S1 | 1936 | A | C2-N3-C4 | 19.39 | 120.30 | 110.60 |
| 1 | 16S1 | 478 | A | N1-C2-N3 | -19.39 | 119.61 | 129.30 |
| 22 | 23S1 | 412 | A | C2-N3-C4 | 19.39 | 120.29 | 110.60 |
| 22 | 23S1 | 430 | A | N1-C6-N6 | -19.39 | 106.97 | 118.60 |
| 22 | 23S1 | 1014 | A | C2-N3-C4 | 19.39 | 120.29 | 110.60 |
| 22 | 23S1 | 1808 | A | N1-C2-N3 | -19.39 | 119.61 | 129.30 |
| 1 | 16S1 | 152 | A | C2-N3-C4 | 19.39 | 120.29 | 110.60 |
| 22 | 23S1 | 340 | A | C2-N3-C4 | 19.39 | 120.29 | 110.60 |
| 22 | 23S1 | 1998 | A | N1-C6-N6 | -19.39 | 106.97 | 118.60 |
| 1 | 16S1 | 915 | A | C2-N3-C4 | 19.39 | 120.29 | 110.60 |
| 22 | 23S1 | 2518 | A | N1-C2-N3 | -19.39 | 119.61 | 129.30 |
| 1 | 16S1 | 1225 | A | N1-C2-N3 | -19.38 | 119.61 | 129.30 |
| 22 | 23S1 | 311 | A | N1-C2-N3 | -19.38 | 119.61 | 129.30 |
| 22 | 23S1 | 1551 | A | N1-C6-N6 | -19.38 | 106.97 | 118.60 |
| 22 | 23S1 | 1773 | A | C2-N3-C4 | 19.38 | 120.29 | 110.60 |
| 1 | 16S1 | 595 | A | N1-C2-N3 | -19.38 | 119.61 | 129.30 |
| 22 | 23S1 | 94 | A | N1-C2-N3 | -19.38 | 119.61 | 129.30 |
| 22 | 23S1 | 1321 | A | N1-C2-N3 | -19.38 | 119.61 | 129.30 |
| 22 | 23S1 | 1322 | A | N1-C2-N3 | -19.38 | 119.61 | 129.30 |
| 22 | 23S1 | 2736 | A | N1-C6-N6 | -19.38 | 106.97 | 118.60 |
| 1 | 16S1 | 3 | A | N1-C6-N6 | -19.38 | 106.97 | 118.60 |
| 1 | 16S1 | 59 | A | N1-C2-N3 | -19.38 | 119.61 | 129.30 |
| 1 | 16S1 | 320 | A | C2-N3-C4 | 19.38 | 120.29 | 110.60 |
| 1 | 16S1 | 913 | A | N1-C6-N6 | -19.38 | 106.97 | 118.60 |
| 22 | 23S1 | 1665 | A | N1-C6-N6 | -19.37 | 106.98 | 118.60 |
| 22 | 23S1 | 943 | A | C2-N3-C4 | 19.37 | 120.28 | 110.60 |
| 1 | 16S1 | 1306 | A | N1-C2-N3 | -19.37 | 119.61 | 129.30 |
| 22 | 23S1 | 1470 | A | C2-N3-C4 | 19.37 | 120.28 | 110.60 |
| 22 | 23S1 | 1637 | A | C2-N3-C4 | 19.36 | 120.28 | 110.60 |
| 22 | 23S1 | 2211 | A | N1-C2-N3 | -19.36 | 119.62 | 129.30 |
| 22 | 23S1 | 2541 | A | C2-N3-C4 | 19.36 | 120.28 | 110.60 |
| 22 | 23S1 | 1230 | A | N1-C6-N6 | -19.36 | 106.98 | 118.60 |
| 22 | 23S1 | 2062 | A | N1-C2-N3 | -19.36 | 119.62 | 129.30 |
| 1 | 16S1 | 120 | A | N1-C2-N3 | -19.36 | 119.62 | 129.30 |
| 1 | 16S1 | 747 | A | N1-C2-N3 | -19.36 | 119.62 | 129.30 |
| 1 | 16S1 | 1238 | A | N1-C2-N3 | -19.36 | 119.62 | 129.30 |
| 22 | 23S1 | 503 | A | C2-N3-C4 | 19.36 | 120.28 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 592 | A | N1-C2-N3 | -19.36 | 119.62 | 129.30 |
| 1 | 16S1 | 746 | A | C2-N3-C4 | 19.36 | 120.28 | 110.60 |
| 22 | 23S1 | 502 | A | C2-N3-C4 | 19.36 | 120.28 | 110.60 |
| 22 | 23S1 | 1503 | A | N1-C6-N6 | -19.36 | 106.99 | 118.60 |
| 1 | 16S1 | 559 | A | N1-C6-N6 | -19.36 | 106.99 | 118.60 |
| 22 | 23S1 | 1039 | A | C2-N3-C4 | 19.36 | 120.28 | 110.60 |
| 1 | 16S1 | 356 | A | C2-N3-C4 | 19.35 | 120.28 | 110.60 |
| 22 | 23S1 | 1264 | A | N1-C6-N6 | -19.35 | 106.99 | 118.60 |
| 22 | 23S1 | 1384 | A | N1-C6-N6 | -19.35 | 106.99 | 118.60 |
| 22 | 23S1 | 2376 | A | N1-C2-N3 | -19.35 | 119.62 | 129.30 |
| 22 | 23S1 | 2639 | A | C2-N3-C4 | 19.35 | 120.28 | 110.60 |
| 1 | 16S1 | 162 | A | C2-N3-C4 | 19.35 | 120.28 | 110.60 |
| 1 | 16S1 | 767 | A | N1-C2-N3 | -19.35 | 119.62 | 129.30 |
| 22 | 23S1 | 541 | A | N1-C6-N6 | -19.35 | 106.99 | 118.60 |
| 22 | 23S1 | 223 | A | N1-C2-N3 | -19.35 | 119.62 | 129.30 |
| 22 | 23S1 | 1635 | A | C2-N3-C4 | 19.35 | 120.28 | 110.60 |
| 22 | 23S1 | 2587 | A | C2-N3-C4 | 19.35 | 120.28 | 110.60 |
| 1 | 16S1 | 53 | A | C2-N3-C4 | 19.35 | 120.27 | 110.60 |
| 1 | 16S1 | 228 | A | C2-N3-C4 | 19.35 | 120.27 | 110.60 |
| 22 | 23S1 | 6 | A | C2-N3-C4 | 19.35 | 120.27 | 110.60 |
| 22 | 23S1 | 1503 | A | C2-N3-C4 | 19.35 | 120.27 | 110.60 |
| 22 | 23S1 | 2531 | A | N1-C6-N6 | -19.35 | 106.99 | 118.60 |
| 1 | 16S1 | 315 | A | C2-N3-C4 | 19.35 | 120.27 | 110.60 |
| 1 | 16S1 | 673 | A | C2-N3-C4 | 19.34 | 120.27 | 110.60 |
| 22 | 23S1 | 13 | A | C2-N3-C4 | 19.34 | 120.27 | 110.60 |
| 22 | 23S1 | 222 | A | C2-N3-C4 | 19.34 | 120.27 | 110.60 |
| 22 | 23S1 | 1791 | A | N1-C2-N3 | -19.34 | 119.63 | 129.30 |
| 22 | 23S1 | 2635 | A | C2-N3-C4 | 19.34 | 120.27 | 110.60 |
| 1 | 16S1 | 1219 | A | C2-N3-C4 | 19.34 | 120.27 | 110.60 |
| 22 | 23S1 | 1264 | A | C2-N3-C4 | 19.34 | 120.27 | 110.60 |
| 22 | 23S1 | 430 | A | C2-N3-C4 | 19.34 | 120.27 | 110.60 |
| 22 | 23S1 | 2887 | A | N1-C2-N3 | -19.34 | 119.63 | 129.30 |
| 23 | 05S1 | 108 | A | C2-N3-C4 | 19.34 | 120.27 | 110.60 |
| 1 | 16S1 | 553 | A | N1-C6-N6 | -19.34 | 107.00 | 118.60 |
| 1 | 16S1 | 546 | A | N1-C2-N3 | -19.34 | 119.63 | 129.30 |
| 22 | 23S1 | 513 | A | C2-N3-C4 | 19.34 | 120.27 | 110.60 |
| 22 | 23S1 | 793 | A | N1-C2-N3 | -19.34 | 119.63 | 129.30 |
| 1 | 16S1 | 792 | A | C2-N3-C4 | 19.33 | 120.27 | 110.60 |
| 22 | 23S1 | 1359 | A | N1-C2-N3 | -19.33 | 119.63 | 129.30 |
| 22 | 23S1 | 1403 | A | C2-N3-C4 | 19.33 | 120.27 | 110.60 |
| 23 | 05S1 | 115 | A | N1-C2-N3 | -19.33 | 119.64 | 129.30 |
| 1 | 16S1 | 288 | A | C2-N3-C4 | 19.32 | 120.26 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 332 | A | N1-C2-N3 | -19.32 | 119.64 | 129.30 |
| 22 | 23S1 | 1204 | A | C2-N3-C4 | 19.32 | 120.26 | 110.60 |
| 22 | 23S1 | 1439 | A | C2-N3-C4 | 19.32 | 120.26 | 110.60 |
| 22 | 23S1 | 1593 | A | C2-N3-C4 | 19.32 | 120.26 | 110.60 |
| 22 | 23S1 | 1632 | A | N1-C6-N6 | -19.32 | 107.00 | 118.60 |
| 22 | 23S1 | 322 | A | N1-C6-N6 | -19.32 | 107.01 | 118.60 |
| 22 | 23S1 | 666 | A | C2-N3-C4 | 19.32 | 120.26 | 110.60 |
| 1 | 16S1 | 1434 | A | C2-N3-C4 | 19.32 | 120.26 | 110.60 |
| 22 | 23S1 | 1205 | A | N1-C6-N6 | -19.32 | 107.01 | 118.60 |
| 22 | 23S1 | 422 | A | C2-N3-C4 | 19.32 | 120.26 | 110.60 |
| 22 | 23S1 | 173 | A | C2-N3-C4 | 19.32 | 120.26 | 110.60 |
| 22 | 23S1 | 575 | A | N1-C2-N3 | -19.32 | 119.64 | 129.30 |
| 1 | 16S1 | 160 | A | N1-C2-N3 | -19.31 | 119.64 | 129.30 |
| 1 | 16S1 | 909 | A | N1-C2-N3 | -19.31 | 119.65 | 129.30 |
| 1 | 16S1 | 994 | A | N1-C2-N3 | -19.31 | 119.65 | 129.30 |
| 1 | 16S1 | 1021 | A | N1-C2-N3 | -19.31 | 119.65 | 129.30 |
| 1 | 16S1 | 1413 | A | N1-C2-N3 | -19.31 | 119.65 | 129.30 |
| 22 | 23S1 | 685 | A | C2-N3-C4 | 19.31 | 120.25 | 110.60 |
| 22 | 23S1 | 2052 | A | N1-C2-N3 | -19.31 | 119.65 | 129.30 |
| 22 | 23S1 | 2270 | A | N1-C6-N6 | -19.31 | 107.02 | 118.60 |
| 22 | 23S1 | 2665 | A | N1-C2-N3 | -19.31 | 119.65 | 129.30 |
| 22 | 23S1 | 1603 | A | N1-C2-N3 | -19.30 | 119.65 | 129.30 |
| 22 | 23S1 | 1698 | A | N1-C6-N6 | -19.30 | 107.02 | 118.60 |
| 22 | 23S1 | 126 | A | C2-N3-C4 | 19.30 | 120.25 | 110.60 |
| 22 | 23S1 | 1918 | A | C2-N3-C4 | 19.30 | 120.25 | 110.60 |
| 22 | 23S1 | 2314 | A | N1-C2-N3 | -19.30 | 119.65 | 129.30 |
| 1 | 16S1 | 1396 | A | N1-C2-N3 | -19.30 | 119.65 | 129.30 |
| 22 | 23S1 | 354 | A | N1-C2-N3 | -19.30 | 119.65 | 129.30 |
| 22 | 23S1 | 1268 | A | N1-C2-N3 | -19.30 | 119.65 | 129.30 |
| 1 | 16S1 | 495 | A | C2-N3-C4 | 19.30 | 120.25 | 110.60 |
| 22 | 23S1 | 522 | A | C2-N3-C4 | 19.30 | 120.25 | 110.60 |
| 22 | 23S1 | 749 | A | N1-C2-N3 | -19.30 | 119.65 | 129.30 |
| 1 | 16S1 | 149 | A | N1-C2-N3 | -19.30 | 119.65 | 129.30 |
| 1 | 16S1 | 1503 | A | N1-C2-N3 | -19.30 | 119.65 | 129.30 |
| 22 | 23S1 | 74 | A | N1-C2-N3 | -19.30 | 119.65 | 129.30 |
| 22 | 23S1 | 270 | A | N1-C6-N6 | -19.30 | 107.02 | 118.60 |
| 22 | 23S1 | 722 | A | N1-C2-N3 | -19.30 | 119.65 | 129.30 |
| 22 | 23S1 | 927 | A | C2-N3-C4 | 19.30 | 120.25 | 110.60 |
| 22 | 23S1 | 310 | A | N1-C6-N6 | -19.29 | 107.02 | 118.60 |
| 22 | 23S1 | 2212 | A | N1-C6-N6 | -19.29 | 107.02 | 118.60 |
| 22 | 23S1 | 676 | A | N1-C2-N3 | -19.29 | 119.65 | 129.30 |
| 22 | 23S1 | 2660 | A | N1-C2-N3 | -19.29 | 119.65 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 412 | A | N1-C6-N6 | -19.29 | 107.03 | 118.60 |
| 22 | 23S1 | 1420 | A | N1-C2-N3 | -19.29 | 119.65 | 129.30 |
| 22 | 23S1 | 1548 | A | C2-N3-C4 | 19.29 | 120.25 | 110.60 |
| 1 | 16S1 | 274 | A | N1-C2-N3 | -19.29 | 119.66 | 129.30 |
| 22 | 23S1 | 574 | A | N1-C2-N3 | -19.29 | 119.66 | 129.30 |
| 22 | 23S1 | 2778 | A | C2-N3-C4 | 19.29 | 120.25 | 110.60 |
| 22 | 23S1 | 2163 | A | N1-C2-N3 | -19.29 | 119.66 | 129.30 |
| 1 | 16S1 | 1082 | A | N1-C6-N6 | -19.28 | 107.03 | 118.60 |
| 22 | 23S1 | 167 | A | N1-C2-N3 | -19.28 | 119.66 | 129.30 |
| 22 | 23S1 | 346 | A | C2-N3-C4 | 19.28 | 120.24 | 110.60 |
| 22 | 23S1 | 1067 | A | N1-C2-N3 | -19.28 | 119.66 | 129.30 |
| 22 | 23S1 | 1912 | A | C2-N3-C4 | 19.28 | 120.24 | 110.60 |
| 22 | 23S1 | 423 | A | N1-C6-N6 | -19.28 | 107.03 | 118.60 |
| 22 | 23S1 | 2829 | A | C2-N3-C4 | 19.28 | 120.24 | 110.60 |
| 1 | 16S1 | 1508 | A | C2-N3-C4 | 19.28 | 120.24 | 110.60 |
| 22 | 23S1 | 2432 | A | N1-C2-N3 | -19.28 | 119.66 | 129.30 |
| 22 | 23S1 | 2764 | A | N1-C6-N6 | -19.28 | 107.03 | 118.60 |
| 1 | 16S1 | 553 | A | N1-C2-N3 | -19.28 | 119.66 | 129.30 |
| 1 | 16S1 | 1493 | A | N1-C6-N6 | -19.28 | 107.03 | 118.60 |
| 22 | 23S1 | 181 | A | C2-N3-C4 | 19.28 | 120.24 | 110.60 |
| 22 | 23S1 | 1453 | A | N1-C2-N3 | -19.28 | 119.66 | 129.30 |
| 22 | 23S1 | 1640 | A | C2-N3-C4 | 19.28 | 120.24 | 110.60 |
| 22 | 23S1 | 1307 | A | C2-N3-C4 | 19.28 | 120.24 | 110.60 |
| 22 | 23S1 | 330 | A | N1-C2-N3 | -19.27 | 119.66 | 129.30 |
| 22 | 23S1 | 829 | A | N1-C2-N3 | -19.27 | 119.66 | 129.30 |
| 22 | 23S1 | 1095 | A | N1-C6-N6 | -19.27 | 107.04 | 118.60 |
| 1 | 16S1 | 694 | A | N1-C2-N3 | -19.27 | 119.67 | 129.30 |
| 1 | 16S1 | 1016 | A | N1-C2-N3 | -19.27 | 119.67 | 129.30 |
| 22 | 23S1 | 2602 | A | N1-C6-N6 | -19.27 | 107.04 | 118.60 |
| 1 | 16S1 | 1275 | A | N1-C2-N3 | -19.27 | 119.67 | 129.30 |
| 22 | 23S1 | 429 | A | C2-N3-C4 | 19.27 | 120.23 | 110.60 |
| 22 | 23S1 | 479 | A | C2-N3-C4 | 19.27 | 120.23 | 110.60 |
| 22 | 23S1 | 1434 | A | C2-N3-C4 | 19.27 | 120.23 | 110.60 |
| 22 | 23S1 | 1890 | A | N1-C6-N6 | -19.27 | 107.04 | 118.60 |
| 1 | 16S1 | 718 | A | N1-C6-N6 | -19.27 | 107.04 | 118.60 |
| 22 | 23S1 | 470 | A | N1-C2-N3 | -19.27 | 119.67 | 129.30 |
| 1 | 16S1 | 448 | A | C2-N3-C4 | 19.26 | 120.23 | 110.60 |
| 22 | 23S1 | 1678 | A | N1-C6-N6 | -19.26 | 107.04 | 118.60 |
| 22 | 23S1 | 1757 | A | C2-N3-C4 | 19.26 | 120.23 | 110.60 |
| 1 | 16S1 | 781 | A | N1-C6-N6 | -19.26 | 107.04 | 118.60 |
| 22 | 23S1 | 412 | A | N1-C2-N3 | -19.26 | 119.67 | 129.30 |
| 22 | 23S1 | 1597 | A | C2-N3-C4 | 19.26 | 120.23 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1786 | A | N1-C2-N3 | -19.26 | 119.67 | 129.30 |
| 1 | 16S1 | 539 | A | N1-C2-N3 | -19.26 | 119.67 | 129.30 |
| 22 | 23S1 | 2297 | A | C2-N3-C4 | 19.26 | 120.23 | 110.60 |
| 22 | 23S1 | 354 | A | N1-C6-N6 | -19.26 | 107.05 | 118.60 |
| 22 | 23S1 | 404 | A | N1-C2-N3 | -19.26 | 119.67 | 129.30 |
| 22 | 23S1 | 1366 | A | C2-N3-C4 | 19.26 | 120.23 | 110.60 |
| 22 | 23S1 | 1453 | A | C2-N3-C4 | 19.26 | 120.23 | 110.60 |
| 22 | 23S1 | 1744 | A | N1-C2-N3 | -19.26 | 119.67 | 129.30 |
| 1 | 16S1 | 1035 | A | N1-C6-N6 | -19.25 | 107.05 | 118.60 |
| 22 | 23S1 | 602 | A | C2-N3-C4 | 19.25 | 120.23 | 110.60 |
| 22 | 23S1 | 1609 | A | C2-N3-C4 | 19.25 | 120.23 | 110.60 |
| 22 | 23S1 | 2097 | A | C2-N3-C4 | 19.25 | 120.23 | 110.60 |
| 22 | 23S1 | 2781 | A | N1-C2-N3 | -19.25 | 119.67 | 129.30 |
| 1 | 16S1 | 509 | A | N1-C6-N6 | -19.25 | 107.05 | 118.60 |
| 1 | 16S1 | 1285 | A | N1-C2-N3 | -19.25 | 119.67 | 129.30 |
| 22 | 23S1 | 300 | A | N1-C2-N3 | -19.25 | 119.67 | 129.30 |
| 22 | 23S1 | 244 | A | N1-C2-N3 | -19.25 | 119.67 | 129.30 |
| 22 | 23S1 | 602 | A | N1-C2-N3 | -19.25 | 119.68 | 129.30 |
| 1 | 16S1 | 520 | A | N1-C2-N3 | -19.25 | 119.68 | 129.30 |
| 22 | 23S1 | 2469 | A | N1-C2-N3 | -19.25 | 119.68 | 129.30 |
| 1 | 16S1 | 411 | A | N1-C2-N3 | -19.24 | 119.68 | 129.30 |
| 1 | 16S1 | 560 | A | N1-C2-N3 | -19.24 | 119.68 | 129.30 |
| 1 | 16S1 | 298 | A | C2-N3-C4 | 19.24 | 120.22 | 110.60 |
| 1 | 16S1 | 364 | A | N1-C2-N3 | -19.24 | 119.68 | 129.30 |
| 1 | 16S1 | 1188 | A | N1-C2-N3 | -19.24 | 119.68 | 129.30 |
| 1 | 16S1 | 1357 | A | N1-C2-N3 | -19.24 | 119.68 | 129.30 |
| 22 | 23S1 | 255 | A | C2-N3-C4 | 19.24 | 120.22 | 110.60 |
| 22 | 23S1 | 693 | A | N1-C2-N3 | -19.24 | 119.68 | 129.30 |
| 22 | 23S1 | 371 | A | N1-C2-N3 | -19.24 | 119.68 | 129.30 |
| 22 | 23S1 | 1080 | A | C2-N3-C4 | 19.24 | 120.22 | 110.60 |
| 22 | 23S1 | 2406 | A | N1-C2-N3 | -19.24 | 119.68 | 129.30 |
| 22 | 23S1 | 2471 | A | N1-C6-N6 | -19.24 | 107.06 | 118.60 |
| 22 | 23S1 | 2600 | A | C2-N3-C4 | 19.24 | 120.22 | 110.60 |
| 1 | 16S1 | 179 | A | N1-C2-N3 | -19.24 | 119.68 | 129.30 |
| 1 | 16S1 | 313 | A | N1-C2-N3 | -19.24 | 119.68 | 129.30 |
| 22 | 23S1 | 1937 | A | N1-C2-N3 | -19.24 | 119.68 | 129.30 |
| 1 | 16S1 | 1500 | A | N1-C6-N6 | -19.24 | 107.06 | 118.60 |
| 22 | 23S1 | 217 | A | C2-N3-C4 | 19.24 | 120.22 | 110.60 |
| 22 | 23S1 | 1700 | A | N1-C6-N6 | -19.24 | 107.06 | 118.60 |
| 22 | 23S1 | 2298 | A | N1-C2-N3 | -19.24 | 119.68 | 129.30 |
| 22 | 23S1 | 432 | A | N1-C6-N6 | -19.23 | 107.06 | 118.60 |
| 22 | 23S1 | 1385 | A | N1-C6-N6 | -19.23 | 107.06 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1679 | A | N1-C6-N6 | -19.23 | 107.06 | 118.60 |
| 1 | 16S1 | 1357 | A | C2-N3-C4 | 19.23 | 120.22 | 110.60 |
| 22 | 23S1 | 265 | A | N1-C6-N6 | -19.23 | 107.06 | 118.60 |
| 22 | 23S1 | 1785 | A | C2-N3-C4 | 19.23 | 120.22 | 110.60 |
| 22 | 23S1 | 2070 | A | N1-C6-N6 | -19.23 | 107.06 | 118.60 |
| 22 | 23S1 | 2757 | A | C2-N3-C4 | 19.23 | 120.22 | 110.60 |
| 22 | 23S1 | 706 | A | C2-N3-C4 | 19.23 | 120.22 | 110.60 |
| 22 | 23S1 | 2288 | A | C2-N3-C4 | 19.23 | 120.21 | 110.60 |
| 22 | 23S1 | 820 | A | N1-C2-N3 | -19.23 | 119.69 | 129.30 |
| 22 | 23S1 | 1496 | A | C2-N3-C4 | 19.23 | 120.21 | 110.60 |
| 1 | 16S1 | 546 | A | C2-N3-C4 | 19.22 | 120.21 | 110.60 |
| 1 | 16S1 | 600 | A | C2-N3-C4 | 19.22 | 120.21 | 110.60 |
| 1 | 16S1 | 649 | A | N1-C6-N6 | -19.22 | 107.07 | 118.60 |
| 1 | 16S1 | 1021 | A | C2-N3-C4 | 19.22 | 120.21 | 110.60 |
| 22 | 23S1 | 1260 | A | N1-C6-N6 | -19.22 | 107.07 | 118.60 |
| 1 | 16S1 | 815 | A | N1-C6-N6 | -19.22 | 107.07 | 118.60 |
| 1 | 16S1 | 1102 | A | C2-N3-C4 | 19.22 | 120.21 | 110.60 |
| 1 | 16S1 | 274 | A | C2-N3-C4 | 19.22 | 120.21 | 110.60 |
| 1 | 16S1 | 1430 | A | N1-C6-N6 | -19.21 | 107.07 | 118.60 |
| 22 | 23S1 | 592 | A | C2-N3-C4 | 19.21 | 120.21 | 110.60 |
| 22 | 23S1 | 1098 | A | C2-N3-C4 | 19.21 | 120.21 | 110.60 |
| 22 | 23S1 | 1213 | A | N1-C2-N3 | -19.21 | 119.69 | 129.30 |
| 22 | 23S1 | 1780 | A | N1-C6-N6 | -19.21 | 107.07 | 118.60 |
| 1 | 16S1 | 411 | A | C2-N3-C4 | 19.21 | 120.20 | 110.60 |
| 22 | 23S1 | 1634 | A | C2-N3-C4 | 19.21 | 120.20 | 110.60 |
| 22 | 23S1 | 1960 | A | N1-C6-N6 | -19.21 | 107.07 | 118.60 |
| 23 | 05S1 | 57 | A | C2-N3-C4 | 19.21 | 120.21 | 110.60 |
| 22 | 23S1 | 2516 | A | C2-N3-C4 | 19.21 | 120.20 | 110.60 |
| 22 | 23S1 | 2749 | A | N1-C2-N3 | -19.21 | 119.70 | 129.30 |
| 22 | 23S1 | 668 | A | N1-C2-N3 | -19.20 | 119.70 | 129.30 |
| 22 | 23S1 | 781 | A | N1-C6-N6 | -19.20 | 107.08 | 118.60 |
| 22 | 23S1 | 793 | A | N1-C6-N6 | -19.20 | 107.08 | 118.60 |
| 22 | 23S1 | 1328 | A | C2-N3-C4 | 19.20 | 120.20 | 110.60 |
| 22 | 23S1 | 2448 | A | N1-C6-N6 | -19.20 | 107.08 | 118.60 |
| 55 | PTR1 | 73 | A | N1-C2-N3 | -19.20 | 119.70 | 129.30 |
| 1 | 16S1 | 949 | A | C2-N3-C4 | 19.20 | 120.20 | 110.60 |
| 22 | 23S1 | 460 | A | N1-C2-N3 | -19.20 | 119.70 | 129.30 |
| 22 | 23S1 | 2247 | A | N1-C6-N6 | -19.20 | 107.08 | 118.60 |
| 22 | 23S1 | 2328 | A | C2-N3-C4 | 19.20 | 120.20 | 110.60 |
| 1 | 16S1 | 44 | A | C2-N3-C4 | 19.20 | 120.20 | 110.60 |
| 1 | 16S1 | 1005 | A | C2-N3-C4 | 19.20 | 120.20 | 110.60 |
| 22 | 23S1 | 203 | A | C2-N3-C4 | 19.20 | 120.20 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 2183 | A | C2-N3-C4 | 19.20 | 120.20 | 110.60 |
| 22 | 23S1 | 1301 | A | N1-C2-N3 | -19.20 | 119.70 | 129.30 |
| 22 | 23S1 | 1641 | A | C2-N3-C4 | 19.20 | 120.20 | 110.60 |
| 22 | 23S1 | 1672 | A | N1-C2-N3 | -19.20 | 119.70 | 129.30 |
| 1 | 16S1 | 1000 | A | C2-N3-C4 | 19.20 | 120.20 | 110.60 |
| 22 | 23S1 | 49 | A | C2-N3-C4 | 19.20 | 120.20 | 110.60 |
| 22 | 23S1 | 197 | A | C2-N3-C4 | 19.20 | 120.20 | 110.60 |
| 22 | 23S1 | 1308 | A | C2-N3-C4 | 19.20 | 120.20 | 110.60 |
| 55 | PTR1 | 26 | A | N1-C2-N3 | -19.20 | 119.70 | 129.30 |
| 22 | 23S1 | 270 | A | C2-N3-C4 | 19.20 | 120.20 | 110.60 |
| 22 | 23S1 | 1077 | A | N1-C2-N3 | -19.20 | 119.70 | 129.30 |
| 22 | 23S1 | 1877 | A | C2-N3-C4 | 19.20 | 120.20 | 110.60 |
| 22 | 23S1 | 1569 | A | C2-N3-C4 | 19.19 | 120.20 | 110.60 |
| 22 | 23S1 | 1805 | A | N1-C2-N3 | -19.19 | 119.70 | 129.30 |
| 22 | 23S1 | 2309 | A | N1-C2-N3 | -19.19 | 119.70 | 129.30 |
| 22 | 23S1 | 1008 | A | N1-C2-N3 | -19.19 | 119.70 | 129.30 |
| 22 | 23S1 | 125 | A | C2-N3-C4 | 19.19 | 120.20 | 110.60 |
| 22 | 23S1 | 2062 | A | N1-C6-N6 | -19.19 | 107.08 | 118.60 |
| 22 | 23S1 | 2287 | A | N1-C2-N3 | -19.19 | 119.70 | 129.30 |
| 22 | 23S1 | 2547 | A | C2-N3-C4 | 19.19 | 120.19 | 110.60 |
| 1 | 16S1 | 819 | A | C2-N3-C4 | 19.19 | 120.19 | 110.60 |
| 22 | 23S1 | 1304 | A | N1-C2-N3 | -19.19 | 119.70 | 129.30 |
| 1 | 16S1 | 872 | A | N1-C2-N3 | -19.19 | 119.71 | 129.30 |
| 1 | 16S1 | 969 | A | C2-N3-C4 | 19.19 | 120.19 | 110.60 |
| 22 | 23S1 | 727 | A | N1-C2-N3 | -19.19 | 119.71 | 129.30 |
| 22 | 23S1 | 1268 | A | C2-N3-C4 | 19.19 | 120.19 | 110.60 |
| 1 | 16S1 | 364 | A | C2-N3-C4 | 19.19 | 120.19 | 110.60 |
| 1 | 16S1 | 408 | A | N1-C6-N6 | -19.19 | 107.09 | 118.60 |
| 1 | 16S1 | 602 | A | N1-C6-N6 | -19.19 | 107.09 | 118.60 |
| 22 | 23S1 | 1545 | A | N1-C6-N6 | -19.19 | 107.09 | 118.60 |
| 1 | 16S1 | 282 | A | C2-N3-C4 | 19.18 | 120.19 | 110.60 |
| 1 | 16S1 | 1067 | A | C2-N3-C4 | 19.18 | 120.19 | 110.60 |
| 1 | 16S1 | 1285 | A | N1-C6-N6 | -19.18 | 107.09 | 118.60 |
| 22 | 23S1 | 590 | A | N1-C6-N6 | -19.18 | 107.09 | 118.60 |
| 22 | 23S1 | 1872 | A | C2-N3-C4 | 19.18 | 120.19 | 110.60 |
| 22 | 23S1 | 1772 | A | N1-C2-N3 | -19.18 | 119.71 | 129.30 |
| 1 | 16S1 | 373 | A | C2-N3-C4 | 19.18 | 120.19 | 110.60 |
| 1 | 16S1 | 1046 | A | C2-N3-C4 | 19.18 | 120.19 | 110.60 |
| 22 | 23S1 | 892 | A | N1-C2-N3 | -19.18 | 119.71 | 129.30 |
| 22 | 23S1 | 1142 | A | N1-C6-N6 | -19.18 | 107.09 | 118.60 |
| 22 | 23S1 | 1772 | A | C2-N3-C4 | 19.18 | 120.19 | 110.60 |
| 22 | 23S1 | 1932 | A | N1-C6-N6 | -19.18 | 107.09 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 918 | A | N1-C6-N6 | -19.18 | 107.09 | 118.60 |
| 1 | 16S1 | 60 | A | N1-C2-N3 | -19.18 | 119.71 | 129.30 |
| 1 | 16S1 | 1176 | A | C2-N3-C4 | 19.18 | 120.19 | 110.60 |
| 1 | 16S1 | 1246 | A | C2-N3-C4 | 19.18 | 120.19 | 110.60 |
| 1 | 16S1 | 1465 | A | N1-C6-N6 | -19.18 | 107.09 | 118.60 |
| 22 | 23S1 | 789 | A | C2-N3-C4 | 19.18 | 120.19 | 110.60 |
| 22 | 23S1 | 1784 | A | C2-N3-C4 | 19.18 | 120.19 | 110.60 |
| 1 | 16S1 | 236 | A | C2-N3-C4 | 19.18 | 120.19 | 110.60 |
| 22 | 23S1 | 556 | A | N1-C2-N3 | -19.18 | 119.71 | 129.30 |
| 1 | 16S1 | 640 | A | C2-N3-C4 | 19.18 | 120.19 | 110.60 |
| 1 | 16S1 | 825 | A | C2-N3-C4 | 19.18 | 120.19 | 110.60 |
| 1 | 16S1 | 1441 | A | N1-C2-N3 | -19.18 | 119.71 | 129.30 |
| 22 | 23S1 | 443 | A | N1-C2-N3 | -19.18 | 119.71 | 129.30 |
| 22 | 23S1 | 722 | A | C2-N3-C4 | 19.18 | 120.19 | 110.60 |
| 22 | 23S1 | 1262 | A | N1-C2-N3 | -19.18 | 119.71 | 129.30 |
| 1 | 16S1 | 1130 | A | N1-C6-N6 | -19.17 | 107.10 | 118.60 |
| 22 | 23S1 | 118 | A | C2-N3-C4 | 19.17 | 120.19 | 110.60 |
| 22 | 23S1 | 1165 | A | N1-C6-N6 | -19.17 | 107.10 | 118.60 |
| 1 | 16S1 | 649 | A | C2-N3-C4 | 19.17 | 120.19 | 110.60 |
| 1 | 16S1 | 1145 | A | C2-N3-C4 | 19.17 | 120.19 | 110.60 |
| 22 | 23S1 | 1260 | A | C2-N3-C4 | 19.17 | 120.19 | 110.60 |
| 1 | 16S1 | 306 | A | N1-C6-N6 | -19.17 | 107.10 | 118.60 |
| 22 | 23S1 | 149 | A | C2-N3-C4 | 19.17 | 120.18 | 110.60 |
| 22 | 23S1 | 241 | A | N1-C6-N6 | -19.17 | 107.10 | 118.60 |
| 22 | 23S1 | 2497 | A | N1-C2-N3 | -19.17 | 119.72 | 129.30 |
| 22 | 23S1 | 2614 | A | N1-C6-N6 | -19.17 | 107.10 | 118.60 |
| 22 | 23S1 | 896 | A | N1-C2-N3 | -19.17 | 119.72 | 129.30 |
| 1 | 16S1 | 1213 | A | C2-N3-C4 | 19.16 | 120.18 | 110.60 |
| 22 | 23S1 | 2366 | A | C2-N3-C4 | 19.16 | 120.18 | 110.60 |
| 22 | 23S1 | 2820 | A | N1-C2-N3 | -19.16 | 119.72 | 129.30 |
| 1 | 16S1 | 1306 | A | C2-N3-C4 | 19.16 | 120.18 | 110.60 |
| 22 | 23S1 | 2778 | A | N1-C2-N3 | -19.16 | 119.72 | 129.30 |
| 1 | 16S1 | 487 | A | C2-N3-C4 | 19.16 | 120.18 | 110.60 |
| 1 | 16S1 | 1324 | A | C2-N3-C4 | 19.16 | 120.18 | 110.60 |
| 22 | 23S1 | 42 | A | C2-N3-C4 | 19.16 | 120.18 | 110.60 |
| 22 | 23S1 | 111 | A | C2-N3-C4 | 19.16 | 120.18 | 110.60 |
| 22 | 23S1 | 1057 | A | N1-C2-N3 | -19.16 | 119.72 | 129.30 |
| 22 | 23S1 | 1453 | A | N1-C6-N6 | -19.16 | 107.10 | 118.60 |
| 1 | 16S1 | 1239 | A | C2-N3-C4 | 19.16 | 120.18 | 110.60 |
| 1 | 16S1 | 1318 | A | C2-N3-C4 | 19.16 | 120.18 | 110.60 |
| 1 | 16S1 | 1236 | A | C2-N3-C4 | 19.16 | 120.18 | 110.60 |
| 22 | 23S1 | 1365 | A | N1-C6-N6 | -19.16 | 107.11 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 2322 | A | N1-C6-N6 | -19.16 | 107.11 | 118.60 |
| 22 | 23S1 | 2369 | A | C2-N3-C4 | 19.16 | 120.18 | 110.60 |
| 1 | 16S1 | 452 | A | C2-N3-C4 | 19.16 | 120.18 | 110.60 |
| 1 | 16S1 | 630 | A | C2-N3-C4 | 19.16 | 120.18 | 110.60 |
| 22 | 23S1 | 730 | A | C2-N3-C4 | 19.16 | 120.18 | 110.60 |
| 22 | 23S1 | 1494 | A | N1-C6-N6 | -19.16 | 107.11 | 118.60 |
| 22 | 23S1 | 1791 | A | C2-N3-C4 | 19.16 | 120.18 | 110.60 |
| 22 | 23S1 | 352 | A | N1-C6-N6 | -19.16 | 107.11 | 118.60 |
| 22 | 23S1 | 2019 | A | C2-N3-C4 | 19.16 | 120.18 | 110.60 |
| 22 | 23S1 | 2060 | A | N1-C6-N6 | -19.15 | 107.11 | 118.60 |
| 22 | 23S1 | 2829 | A | N1-C6-N6 | -19.15 | 107.11 | 118.60 |
| 1 | 16S1 | 10 | A | N1-C2-N3 | -19.15 | 119.72 | 129.30 |
| 1 | 16S1 | 119 | A | C2-N3-C4 | 19.15 | 120.18 | 110.60 |
| 1 | 16S1 | 1157 | A | C2-N3-C4 | 19.15 | 120.18 | 110.60 |
| 1 | 16S1 | 1171 | A | C2-N3-C4 | 19.15 | 120.18 | 110.60 |
| 1 | 16S1 | 1368 | A | N1-C6-N6 | -19.15 | 107.11 | 118.60 |
| 22 | 23S1 | 1040 | A | C2-N3-C4 | 19.15 | 120.18 | 110.60 |
| 22 | 23S1 | 2171 | A | N1-C2-N3 | -19.15 | 119.72 | 129.30 |
| 1 | 16S1 | 7 | A | N1-C2-N3 | -19.15 | 119.72 | 129.30 |
| 1 | 16S1 | 906 | A | N1-C2-N3 | -19.15 | 119.73 | 129.30 |
| 1 | 16S1 | 596 | A | N1-C6-N6 | -19.15 | 107.11 | 118.60 |
| 22 | 23S1 | 71 | A | N1-C2-N3 | -19.15 | 119.73 | 129.30 |
| 22 | 23S1 | 2003 | A | N1-C6-N6 | -19.15 | 107.11 | 118.60 |
| 1 | 16S1 | 937 | A | N1-C6-N6 | -19.15 | 107.11 | 118.60 |
| 1 | 16S1 | 782 | A | N1-C6-N6 | -19.14 | 107.11 | 118.60 |
| 1 | 16S1 | 1456 | A | N1-C6-N6 | -19.14 | 107.11 | 118.60 |
| 1 | 16S1 | 371 | A | N1-C6-N6 | -19.14 | 107.11 | 118.60 |
| 1 | 16S1 | 1005 | A | N1-C2-N3 | -19.14 | 119.73 | 129.30 |
| 22 | 23S1 | 324 | A | C2-N3-C4 | 19.14 | 120.17 | 110.60 |
| 55 | PTR1 | 3 | A | N1-C2-N3 | -19.14 | 119.73 | 129.30 |
| 22 | 23S1 | 294 | A | C2-N3-C4 | 19.14 | 120.17 | 110.60 |
| 1 | 16S1 | 663 | A | C2-N3-C4 | 19.14 | 120.17 | 110.60 |
| 1 | 16S1 | 702 | A | N1-C6-N6 | -19.14 | 107.12 | 118.60 |
| 22 | 23S1 | 918 | A | C2-N3-C4 | 19.14 | 120.17 | 110.60 |
| 22 | 23S1 | 1490 | A | N1-C2-N3 | -19.14 | 119.73 | 129.30 |
| 1 | 16S1 | 579 | A | C2-N3-C4 | 19.14 | 120.17 | 110.60 |
| 22 | 23S1 | 1815 | A | N1-C2-N3 | -19.14 | 119.73 | 129.30 |
| 22 | 23S1 | 2005 | A | C2-N3-C4 | 19.14 | 120.17 | 110.60 |
| 22 | 23S1 | 2009 | A | N1-C2-N3 | -19.14 | 119.73 | 129.30 |
| 22 | 23S1 | 152 | A | C2-N3-C4 | 19.13 | 120.17 | 110.60 |
| 22 | 23S1 | 222 | A | N1-C2-N3 | -19.13 | 119.73 | 129.30 |
| 1 | 16S1 | 499 | A | N1-C2-N3 | -19.13 | 119.73 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 23 | 05S1 | 15 | A | N1-C2-N3 | -19.13 | 119.73 | 129.30 |
| 1 | 16S1 | 819 | A | N1-C2-N3 | -19.13 | 119.73 | 129.30 |
| 22 | 23S1 | 199 | A | C2-N3-C4 | 19.13 | 120.17 | 110.60 |
| 22 | 23S1 | 1286 | A | N1-C6-N6 | -19.13 | 107.12 | 118.60 |
| 22 | 23S1 | 2108 | A | N1-C6-N6 | -19.13 | 107.12 | 118.60 |
| 55 | PTR1 | 58 | A | N1-C2-N3 | -19.13 | 119.73 | 129.30 |
| 22 | 23S1 | 2665 | A | C2-N3-C4 | 19.13 | 120.16 | 110.60 |
| 1 | 16S1 | 321 | A | N1-C6-N6 | -19.13 | 107.12 | 118.60 |
| 1 | 16S1 | 338 | A | N1-C2-N3 | -19.13 | 119.74 | 129.30 |
| 1 | 16S1 | 640 | A | N1-C6-N6 | -19.13 | 107.12 | 118.60 |
| 1 | 16S1 | 794 | A | N1-C2-N3 | -19.12 | 119.74 | 129.30 |
| 1 | 16S1 | 1350 | A | N1-C6-N6 | -19.12 | 107.12 | 118.60 |
| 22 | 23S1 | 616 | A | C2-N3-C4 | 19.12 | 120.16 | 110.60 |
| 22 | 23S1 | 941 | A | N1-C6-N6 | -19.12 | 107.12 | 118.60 |
| 1 | 16S1 | 958 | A | N1-C2-N3 | -19.12 | 119.74 | 129.30 |
| 22 | 23S1 | 1701 | A | N1-C2-N3 | -19.12 | 119.74 | 129.30 |
| 22 | 23S1 | 1916 | A | N1-C6-N6 | -19.12 | 107.13 | 118.60 |
| 22 | 23S1 | 632 | A | N1-C2-N3 | -19.12 | 119.74 | 129.30 |
| 22 | 23S1 | 670 | A | C2-N3-C4 | 19.12 | 120.16 | 110.60 |
| 22 | 23S1 | 1535 | A | C2-N3-C4 | 19.12 | 120.16 | 110.60 |
| 22 | 23S1 | 1001 | A | N1-C6-N6 | -19.12 | 107.13 | 118.60 |
| 1 | 16S1 | 363 | A | C2-N3-C4 | 19.12 | 120.16 | 110.60 |
| 1 | 16S1 | 784 | A | N1-C6-N6 | -19.12 | 107.13 | 118.60 |
| 22 | 23S1 | 402 | A | N1-C6-N6 | -19.12 | 107.13 | 118.60 |
| 22 | 23S1 | 735 | A | N1-C2-N3 | -19.12 | 119.74 | 129.30 |
| 22 | 23S1 | 1669 | A | N1-C6-N6 | -19.12 | 107.13 | 118.60 |
| 1 | 16S1 | 344 | A | N1-C2-N3 | -19.11 | 119.74 | 129.30 |
| 22 | 23S1 | 627 | A | C2-N3-C4 | 19.11 | 120.16 | 110.60 |
| 22 | 23S1 | 945 | A | N1-C6-N6 | -19.11 | 107.13 | 118.60 |
| 22 | 23S1 | 1272 | A | N1-C2-N3 | -19.11 | 119.74 | 129.30 |
| 22 | 23S1 | 2270 | A | C2-N3-C4 | 19.11 | 120.16 | 110.60 |
| 23 | 05S1 | 45 | A | N1-C2-N3 | -19.11 | 119.74 | 129.30 |
| 22 | 23S1 | 2070 | A | C2-N3-C4 | 19.11 | 120.16 | 110.60 |
| 22 | 23S1 | 1090 | A | N1-C6-N6 | -19.11 | 107.13 | 118.60 |
| 1 | 16S1 | 482 | A | N1-C2-N3 | -19.11 | 119.75 | 129.30 |
| 22 | 23S1 | 909 | A | N1-C2-N3 | -19.11 | 119.75 | 129.30 |
| 22 | 23S1 | 1395 | A | C2-N3-C4 | 19.11 | 120.16 | 110.60 |
| 22 | 23S1 | 14 | A | C2-N3-C4 | 19.11 | 120.15 | 110.60 |
| 22 | 23S1 | 2147 | A | C2-N3-C4 | 19.11 | 120.15 | 110.60 |
| 22 | 23S1 | 428 | A | C2-N3-C4 | 19.11 | 120.15 | 110.60 |
| 22 | 23S1 | 782 | A | N1-C6-N6 | -19.11 | 107.14 | 118.60 |
| 22 | 23S1 | 1431 | A | C2-N3-C4 | 19.11 | 120.15 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 2333 | A | N1-C2-N3 | -19.11 | 119.75 | 129.30 |
| 1 | 16S1 | 753 | A | C2-N3-C4 | 19.11 | 120.15 | 110.60 |
| 22 | 23S1 | 226 | A | C2-N3-C4 | 19.11 | 120.15 | 110.60 |
| 22 | 23S1 | 1378 | A | N1-C2-N3 | -19.10 | 119.75 | 129.30 |
| 22 | 23S1 | 603 | A | N1-C2-N3 | -19.10 | 119.75 | 129.30 |
| 1 | 16S1 | 33 | A | C2-N3-C4 | 19.10 | 120.15 | 110.60 |
| 1 | 16S1 | 195 | A | C2-N3-C4 | 19.10 | 120.15 | 110.60 |
| 22 | 23S1 | 119 | A | C2-N3-C4 | 19.10 | 120.15 | 110.60 |
| 1 | 16S1 | 65 | A | N1-C2-N3 | -19.09 | 119.75 | 129.30 |
| 1 | 16S1 | 909 | A | C2-N3-C4 | 19.09 | 120.15 | 110.60 |
| 1 | 16S1 | 1150 | A | N1-C2-N3 | -19.09 | 119.75 | 129.30 |
| 1 | 16S1 | 1408 | A | C2-N3-C4 | 19.09 | 120.15 | 110.60 |
| 22 | 23S1 | 959 | A | N1-C2-N3 | -19.09 | 119.75 | 129.30 |
| 22 | 23S1 | 613 | A | N1-C2-N3 | -19.09 | 119.75 | 129.30 |
| 22 | 23S1 | 996 | A | C2-N3-C4 | 19.09 | 120.15 | 110.60 |
| 22 | 23S1 | 1073 | A | C2-N3-C4 | 19.09 | 120.15 | 110.60 |
| 22 | 23S1 | 2530 | A | N1-C2-N3 | -19.09 | 119.75 | 129.30 |
| 1 | 16S1 | 181 | A | C2-N3-C4 | 19.09 | 120.14 | 110.60 |
| 1 | 16S1 | 825 | A | N1-C6-N6 | -19.09 | 107.14 | 118.60 |
| 22 | 23S1 | 2776 | A | N1-C6-N6 | -19.09 | 107.15 | 118.60 |
| 1 | 16S1 | 71 | A | N1-C2-N3 | -19.09 | 119.75 | 129.30 |
| 1 | 16S1 | 1271 | A | N1-C2-N3 | -19.09 | 119.76 | 129.30 |
| 22 | 23S1 | 2170 | A | N1-C6-N6 | -19.09 | 107.15 | 118.60 |
| 1 | 16S1 | 149 | A | C2-N3-C4 | 19.09 | 120.14 | 110.60 |
| 22 | 23S1 | 1717 | A | N1-C2-N3 | -19.09 | 119.76 | 129.30 |
| 22 | 23S1 | 2634 | A | C2-N3-C4 | 19.09 | 120.14 | 110.60 |
| 22 | 23S1 | 2333 | A | C2-N3-C4 | 19.08 | 120.14 | 110.60 |
| 1 | 16S1 | 906 | A | N1-C6-N6 | -19.08 | 107.15 | 118.60 |
| 1 | 16S1 | 1429 | A | C2-N3-C4 | 19.08 | 120.14 | 110.60 |
| 1 | 16S1 | 1502 | A | N1-C6-N6 | -19.08 | 107.15 | 118.60 |
| 1 | 16S1 | 7 | A | N1-C6-N6 | -19.08 | 107.15 | 118.60 |
| 1 | 16S1 | 1377 | A | C2-N3-C4 | 19.08 | 120.14 | 110.60 |
| 22 | 23S1 | 592 | A | N1-C6-N6 | -19.08 | 107.15 | 118.60 |
| 22 | 23S1 | 899 | A | N1-C6-N6 | -19.08 | 107.15 | 118.60 |
| 1 | 16S1 | 777 | A | N1-C6-N6 | -19.08 | 107.15 | 118.60 |
| 22 | 23S1 | 21 | A | N1-C6-N6 | -19.08 | 107.15 | 118.60 |
| 22 | 23S1 | 1057 | A | C2-N3-C4 | 19.08 | 120.14 | 110.60 |
| 1 | 16S1 | 602 | A | C2-N3-C4 | 19.08 | 120.14 | 110.60 |
| 1 | 16S1 | 1433 | A | C2-N3-C4 | 19.08 | 120.14 | 110.60 |
| 22 | 23S1 | 2042 | A | C2-N3-C4 | 19.08 | 120.14 | 110.60 |
| 22 | 23S1 | 1090 | A | C2-N3-C4 | 19.07 | 120.14 | 110.60 |
| 22 | 23S1 | 1978 | A | C2-N3-C4 | 19.07 | 120.14 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 101 | A | C2-N3-C4 | 19.07 | 120.14 | 110.60 |
| 22 | 23S1 | 603 | A | N1-C6-N6 | -19.07 | 107.16 | 118.60 |
| 22 | 23S1 | 1858 | A | N1-C2-N3 | -19.07 | 119.76 | 129.30 |
| 22 | 23S1 | 368 | A | N1-C2-N3 | -19.07 | 119.77 | 129.30 |
| 22 | 23S1 | 2205 | A | N1-C6-N6 | -19.07 | 107.16 | 118.60 |
| 1 | 16S1 | 143 | A | N1-C2-N3 | -19.07 | 119.77 | 129.30 |
| 1 | 16S1 | 1437 | A | N1-C2-N3 | -19.07 | 119.77 | 129.30 |
| 22 | 23S1 | 262 | A | C2-N3-C4 | 19.07 | 120.13 | 110.60 |
| 22 | 23S1 | 1247 | A | N1-C2-N3 | -19.07 | 119.77 | 129.30 |
| 22 | 23S1 | 2810 | A | C2-N3-C4 | 19.07 | 120.14 | 110.60 |
| 55 | PTR1 | 59 | A | N1-C6-N6 | -19.07 | 107.16 | 118.60 |
| 1 | 16S1 | 759 | A | C2-N3-C4 | 19.07 | 120.13 | 110.60 |
| 22 | 23S1 | 927 | A | N1-C2-N3 | -19.07 | 119.77 | 129.30 |
| 1 | 16S1 | 1110 | A | C2-N3-C4 | 19.07 | 120.13 | 110.60 |
| 22 | 23S1 | 2227 | A | C2-N3-C4 | 19.07 | 120.13 | 110.60 |
| 22 | 23S1 | 2298 | A | C2-N3-C4 | 19.07 | 120.13 | 110.60 |
| 1 | 16S1 | 53 | A | N1-C2-N3 | -19.06 | 119.77 | 129.30 |
| 23 | 05S1 | 52 | A | N1-C2-N3 | -19.06 | 119.77 | 129.30 |
| 1 | 16S1 | 441 | A | N1-C2-N3 | -19.06 | 119.77 | 129.30 |
| 22 | 23S1 | 1711 | A | C2-N3-C4 | 19.06 | 120.13 | 110.60 |
| 22 | 23S1 | 2882 | A | C2-N3-C4 | 19.06 | 120.13 | 110.60 |
| 1 | 16S1 | 456 | A | C2-N3-C4 | 19.06 | 120.13 | 110.60 |
| 22 | 23S1 | 103 | A | C2-N3-C4 | 19.06 | 120.13 | 110.60 |
| 1 | 16S1 | 946 | A | C2-N3-C4 | 19.06 | 120.13 | 110.60 |
| 22 | 23S1 | 2095 | A | N1-C6-N6 | -19.06 | 107.17 | 118.60 |
| 1 | 16S1 | 327 | A | C2-N3-C4 | 19.06 | 120.13 | 110.60 |
| 22 | 23S1 | 429 | A | N1-C6-N6 | -19.05 | 107.17 | 118.60 |
| 22 | 23S1 | 1029 | A | N1-C2-N3 | -19.05 | 119.77 | 129.30 |
| 22 | 23S1 | 429 | A | N1-C2-N3 | -19.05 | 119.77 | 129.30 |
| 22 | 23S1 | 599 | A | C2-N3-C4 | 19.05 | 120.13 | 110.60 |
| 22 | 23S1 | 643 | A | C2-N3-C4 | 19.05 | 120.13 | 110.60 |
| 22 | 23S1 | 2183 | A | N1-C2-N3 | -19.05 | 119.77 | 129.30 |
| 1 | 16S1 | 1191 | A | C2-N3-C4 | 19.05 | 120.13 | 110.60 |
| 22 | 23S1 | 563 | A | N1-C6-N6 | -19.05 | 107.17 | 118.60 |
| 22 | 23S1 | 1591 | A | C2-N3-C4 | 19.05 | 120.12 | 110.60 |
| 22 | 23S1 | 28 | A | C2-N3-C4 | 19.05 | 120.12 | 110.60 |
| 22 | 23S1 | 1590 | A | C2-N3-C4 | 19.05 | 120.12 | 110.60 |
| 1 | 16S1 | 1257 | A | N1-C2-N3 | -19.05 | 119.78 | 129.30 |
| 1 | 16S1 | 1428 | A | C2-N3-C4 | 19.05 | 120.12 | 110.60 |
| 22 | 23S1 | 2471 | A | C2-N3-C4 | 19.05 | 120.12 | 110.60 |
| 1 | 16S1 | 892 | A | N1-C6-N6 | -19.05 | 107.17 | 118.60 |
| 1 | 16S1 | 1093 | A | C2-N3-C4 | 19.05 | 120.12 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1241 | A | C2-N3-C4 | 19.05 | 120.12 | 110.60 |
| 22 | 23S1 | 2434 | A | C2-N3-C4 | 19.05 | 120.12 | 110.60 |
| 22 | 23S1 | 844 | A | C2-N3-C4 | 19.04 | 120.12 | 110.60 |
| 22 | 23S1 | 1327 | A | C2-N3-C4 | 19.04 | 120.12 | 110.60 |
| 22 | 23S1 | 2154 | A | C2-N3-C4 | 19.04 | 120.12 | 110.60 |
| 1 | 16S1 | 831 | A | C2-N3-C4 | 19.04 | 120.12 | 110.60 |
| 22 | 23S1 | 685 | A | N1-C6-N6 | -19.04 | 107.17 | 118.60 |
| 1 | 16S1 | 336 | A | N1-C2-N3 | -19.04 | 119.78 | 129.30 |
| 22 | 23S1 | 1129 | A | C2-N3-C4 | 19.04 | 120.12 | 110.60 |
| 22 | 23S1 | 1640 | A | N1-C2-N3 | -19.04 | 119.78 | 129.30 |
| 22 | 23S1 | 2639 | A | N1-C6-N6 | -19.04 | 107.18 | 118.60 |
| 22 | 23S1 | 1755 | A | N1-C2-N3 | -19.04 | 119.78 | 129.30 |
| 23 | 05S1 | 50 | A | N1-C2-N3 | -19.04 | 119.78 | 129.30 |
| 1 | 16S1 | 1413 | A | C2-N3-C4 | 19.04 | 120.12 | 110.60 |
| 22 | 23S1 | 91 | A | N1-C2-N3 | -19.04 | 119.78 | 129.30 |
| 22 | 23S1 | 265 | A | C2-N3-C4 | 19.04 | 120.12 | 110.60 |
| 22 | 23S1 | 547 | A | N1-C2-N3 | -19.04 | 119.78 | 129.30 |
| 22 | 23S1 | 654 | A | N1-C2-N3 | -19.04 | 119.78 | 129.30 |
| 22 | 23S1 | 2459 | A | C2-N3-C4 | 19.04 | 120.12 | 110.60 |
| 22 | 23S1 | 103 | A | N1-C2-N3 | -19.04 | 119.78 | 129.30 |
| 22 | 23S1 | 706 | A | N1-C2-N3 | -19.03 | 119.78 | 129.30 |
| 22 | 23S1 | 1322 | A | N1-C6-N6 | -19.03 | 107.18 | 118.60 |
| 55 | PTR1 | 23 | A | N1-C6-N6 | -19.03 | 107.18 | 118.60 |
| 22 | 23S1 | 670 | A | N1-C2-N3 | -19.03 | 119.78 | 129.30 |
| 22 | 23S1 | 1503 | A | N1-C2-N3 | -19.03 | 119.78 | 129.30 |
| 1 | 16S1 | 1191 | A | N1-C2-N3 | -19.03 | 119.78 | 129.30 |
| 22 | 23S1 | 1932 | A | C2-N3-C4 | 19.03 | 120.11 | 110.60 |
| 1 | 16S1 | 288 | A | N1-C2-N3 | -19.03 | 119.79 | 129.30 |
| 1 | 16S1 | 415 | A | N1-C6-N6 | -19.03 | 107.18 | 118.60 |
| 1 | 16S1 | 574 | A | C2-N3-C4 | 19.03 | 120.11 | 110.60 |
| 22 | 23S1 | 19 | A | N1-C2-N3 | -19.03 | 119.79 | 129.30 |
| 22 | 23S1 | 1237 | A | N1-C2-N3 | -19.03 | 119.79 | 129.30 |
| 22 | 23S1 | 2015 | A | C2-N3-C4 | 19.03 | 120.11 | 110.60 |
| 22 | 23S1 | 227 | A | N1-C2-N3 | -19.03 | 119.79 | 129.30 |
| 22 | 23S1 | 1713 | A | N1-C2-N3 | -19.03 | 119.79 | 129.30 |
| 22 | 23S1 | 478 | A | N1-C2-N3 | -19.02 | 119.79 | 129.30 |
| 22 | 23S1 | 905 | A | N1-C2-N3 | -19.02 | 119.79 | 129.30 |
| 22 | 23S1 | 917 | A | N1-C2-N3 | -19.02 | 119.79 | 129.30 |
| 22 | 23S1 | 1133 | A | N1-C2-N3 | -19.02 | 119.79 | 129.30 |
| 22 | 23S1 | 173 | A | N1-C2-N3 | -19.02 | 119.79 | 129.30 |
| 22 | 23S1 | 1749 | A | N1-C6-N6 | -19.02 | 107.19 | 118.60 |
| 22 | 23S1 | 2513 | A | N1-C2-N3 | -19.02 | 119.79 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 233 | A | N1-C2-N3 | -19.02 | 119.79 | 129.30 |
| 22 | 23S1 | 781 | A | C2-N3-C4 | 19.02 | 120.11 | 110.60 |
| 22 | 23S1 | 176 | A | N1-C2-N3 | -19.02 | 119.79 | 129.30 |
| 22 | 23S1 | 1805 | A | N1-C6-N6 | -19.02 | 107.19 | 118.60 |
| 1 | 16S1 | 129 | A | C2-N3-C4 | 19.02 | 120.11 | 110.60 |
| 1 | 16S1 | 749 | A | N1-C2-N3 | -19.02 | 119.79 | 129.30 |
| 1 | 16S1 | 1410 | A | N1-C6-N6 | -19.02 | 107.19 | 118.60 |
| 22 | 23S1 | 1591 | A | N1-C2-N3 | -19.02 | 119.79 | 129.30 |
| 22 | 23S1 | 2191 | A | C2-N3-C4 | 19.02 | 120.11 | 110.60 |
| 1 | 16S1 | 461 | A | C2-N3-C4 | 19.01 | 120.11 | 110.60 |
| 1 | 16S1 | 1269 | A | C2-N3-C4 | 19.01 | 120.11 | 110.60 |
| 23 | 05S1 | 34 | A | C2-N3-C4 | 19.01 | 120.11 | 110.60 |
| 23 | 05S1 | 94 | A | C2-N3-C4 | 19.01 | 120.11 | 110.60 |
| 1 | 16S1 | 535 | A | N1-C2-N3 | -19.01 | 119.80 | 129.30 |
| 1 | 16S1 | 938 | A | N1-C6-N6 | -19.01 | 107.19 | 118.60 |
| 22 | 23S1 | 975 | A | C2-N3-C4 | 19.01 | 120.11 | 110.60 |
| 22 | 23S1 | 2020 | A | N1-C2-N3 | -19.01 | 119.79 | 129.30 |
| 22 | 23S1 | 5 | A | N1-C2-N3 | -19.01 | 119.80 | 129.30 |
| 1 | 16S1 | 1176 | A | N1-C6-N6 | -19.01 | 107.20 | 118.60 |
| 1 | 16S1 | 1318 | A | N1-C2-N3 | -19.01 | 119.80 | 129.30 |
| 22 | 23S1 | 309 | A | N1-C6-N6 | -19.01 | 107.20 | 118.60 |
| 1 | 16S1 | 1362 | A | C2-N3-C4 | 19.01 | 120.10 | 110.60 |
| 22 | 23S1 | 282 | A | N1-C2-N3 | -19.00 | 119.80 | 129.30 |
| 22 | 23S1 | 1632 | A | N1-C2-N3 | -19.00 | 119.80 | 129.30 |
| 1 | 16S1 | 415 | A | C2-N3-C4 | 19.00 | 120.10 | 110.60 |
| 22 | 23S1 | 532 | A | N1-C2-N3 | -19.00 | 119.80 | 129.30 |
| 22 | 23S1 | 990 | A | N1-C2-N3 | -19.00 | 119.80 | 129.30 |
| 22 | 23S1 | 1144 | A | N1-C2-N3 | -19.00 | 119.80 | 129.30 |
| 1 | 16S1 | 831 | A | N1-C6-N6 | -19.00 | 107.20 | 118.60 |
| 22 | 23S1 | 241 | A | C2-N3-C4 | 19.00 | 120.10 | 110.60 |
| 22 | 23S1 | 1089 | A | C2-N3-C4 | 19.00 | 120.10 | 110.60 |
| 1 | 16S1 | 909 | A | N1-C6-N6 | -19.00 | 107.20 | 118.60 |
| 1 | 16S1 | 1271 | A | C2-N3-C4 | 19.00 | 120.10 | 110.60 |
| 22 | 23S1 | 64 | A | C2-N3-C4 | 19.00 | 120.10 | 110.60 |
| 22 | 23S1 | 1916 | A | C2-N3-C4 | 19.00 | 120.10 | 110.60 |
| 23 | 05S1 | 15 | A | C2-N3-C4 | 19.00 | 120.10 | 110.60 |
| 22 | 23S1 | 1598 | A | C2-N3-C4 | 19.00 | 120.10 | 110.60 |
| 22 | 23S1 | 2711 | A | N1-C2-N3 | -19.00 | 119.80 | 129.30 |
| 22 | 23S1 | 1690 | A | N1-C2-N3 | -19.00 | 119.80 | 129.30 |
| 22 | 23S1 | 621 | A | C2-N3-C4 | 19.00 | 120.10 | 110.60 |
| 22 | 23S1 | 676 | A | C2-N3-C4 | 19.00 | 120.10 | 110.60 |
| 22 | 23S1 | 2267 | A | N1-C6-N6 | -19.00 | 107.20 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 1150 | A | C2-N3-C4 | 18.99 | 120.10 | 110.60 |
| 22 | 23S1 | 905 | A | C2-N3-C4 | 18.99 | 120.10 | 110.60 |
| 22 | 23S1 | 1789 | A | N1-C6-N6 | -18.99 | 107.20 | 118.60 |
| 1 | 16S1 | 845 | A | N1-C6-N6 | -18.99 | 107.20 | 118.60 |
| 22 | 23S1 | 196 | A | N1-C2-N3 | -18.99 | 119.80 | 129.30 |
| 1 | 16S1 | 1349 | A | C2-N3-C4 | 18.99 | 120.09 | 110.60 |
| 22 | 23S1 | 2758 | A | C2-N3-C4 | 18.99 | 120.09 | 110.60 |
| 22 | 23S1 | 144 | A | N1-C2-N3 | -18.99 | 119.81 | 129.30 |
| 22 | 23S1 | 223 | A | N1-C6-N6 | -18.99 | 107.21 | 118.60 |
| 22 | 23S1 | 1247 | A | N1-C6-N6 | -18.99 | 107.21 | 118.60 |
| 22 | 23S1 | 2058 | A | N1-C6-N6 | -18.99 | 107.21 | 118.60 |
| 1 | 16S1 | 1437 | A | C2-N3-C4 | 18.99 | 120.09 | 110.60 |
| 22 | 23S1 | 1205 | A | N1-C2-N3 | -18.99 | 119.81 | 129.30 |
| 22 | 23S1 | 453 | A | C2-N3-C4 | 18.99 | 120.09 | 110.60 |
| 22 | 23S1 | 1885 | A | C2-N3-C4 | 18.99 | 120.09 | 110.60 |
| 22 | 23S1 | 460 | A | C2-N3-C4 | 18.98 | 120.09 | 110.60 |
| 22 | 23S1 | 1420 | A | C2-N3-C4 | 18.98 | 120.09 | 110.60 |
| 22 | 23S1 | 1871 | A | N1-C6-N6 | -18.98 | 107.21 | 118.60 |
| 22 | 23S1 | 2478 | A | N1-C6-N6 | -18.98 | 107.21 | 118.60 |
| 23 | 05S1 | 39 | A | N1-C2-N3 | -18.98 | 119.81 | 129.30 |
| 22 | 23S1 | 2598 | A | N1-C2-N3 | -18.98 | 119.81 | 129.30 |
| 22 | 23S1 | 457 | A | N1-C6-N6 | -18.98 | 107.21 | 118.60 |
| 22 | 23S1 | 877 | A | N1-C6-N6 | -18.98 | 107.21 | 118.60 |
| 22 | 23S1 | 996 | A | N1-C6-N6 | -18.98 | 107.21 | 118.60 |
| 22 | 23S1 | 2682 | A | C2-N3-C4 | 18.98 | 120.09 | 110.60 |
| 22 | 23S1 | 1981 | A | N1-C6-N6 | -18.98 | 107.21 | 118.60 |
| 1 | 16S1 | 309 | A | N1-C2-N3 | -18.98 | 119.81 | 129.30 |
| 1 | 16S1 | 802 | A | C2-N3-C4 | 18.98 | 120.09 | 110.60 |
| 22 | 23S1 | 2014 | A | C2-N3-C4 | 18.98 | 120.09 | 110.60 |
| 1 | 16S1 | 608 | A | C2-N3-C4 | 18.98 | 120.09 | 110.60 |
| 22 | 23S1 | 176 | A | N1-C6-N6 | -18.98 | 107.21 | 118.60 |
| 22 | 23S1 | 310 | A | N1-C2-N3 | -18.98 | 119.81 | 129.30 |
| 1 | 16S1 | 889 | A | C2-N3-C4 | 18.97 | 120.09 | 110.60 |
| 22 | 23S1 | 1070 | A | C2-N3-C4 | 18.97 | 120.09 | 110.60 |
| 1 | 16S1 | 729 | A | C2-N3-C4 | 18.97 | 120.09 | 110.60 |
| 22 | 23S1 | 845 | A | N1-C6-N6 | -18.97 | 107.22 | 118.60 |
| 22 | 23S1 | 2518 | A | N1-C6-N6 | -18.97 | 107.22 | 118.60 |
| 22 | 23S1 | 2734 | A | C2-N3-C4 | 18.97 | 120.09 | 110.60 |
| 22 | 23S1 | 443 | A | C2-N3-C4 | 18.97 | 120.08 | 110.60 |
| 22 | 23S1 | 715 | A | N1-C6-N6 | -18.97 | 107.22 | 118.60 |
| 22 | 23S1 | 2388 | A | C2-N3-C4 | 18.97 | 120.09 | 110.60 |
| 22 | 23S1 | 2725 | A | N1-C2-N3 | -18.97 | 119.81 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 468 | A | N1-C2-N3 | -18.97 | 119.82 | 129.30 |
| 22 | 23S1 | 1253 | A | C2-N3-C4 | 18.97 | 120.08 | 110.60 |
| 22 | 23S1 | 1936 | A | N1-C2-N3 | -18.97 | 119.82 | 129.30 |
| 22 | 23S1 | 2184 | A | N1-C6-N6 | -18.97 | 107.22 | 118.60 |
| 22 | 23S1 | 2274 | A | N1-C6-N6 | -18.97 | 107.22 | 118.60 |
| 1 | 16S1 | 968 | A | N1-C2-N3 | -18.97 | 119.82 | 129.30 |
| 1 | 16S1 | 1163 | A | C2-N3-C4 | 18.97 | 120.08 | 110.60 |
| 1 | 16S1 | 1493 | A | N1-C2-N3 | -18.97 | 119.82 | 129.30 |
| 22 | 23S1 | 340 | A | N1-C2-N3 | -18.97 | 119.82 | 129.30 |
| 22 | 23S1 | 1048 | A | N1-C2-N3 | -18.97 | 119.82 | 129.30 |
| 1 | 16S1 | 459 | A | N1-C2-N3 | -18.97 | 119.82 | 129.30 |
| 1 | 16S1 | 596 | A | C2-N3-C4 | 18.97 | 120.08 | 110.60 |
| 22 | 23S1 | 988 | A | C2-N3-C4 | 18.97 | 120.08 | 110.60 |
| 22 | 23S1 | 1342 | A | N1-C6-N6 | -18.97 | 107.22 | 118.60 |
| 22 | 23S1 | 2335 | A | N1-C2-N3 | -18.97 | 119.82 | 129.30 |
| 22 | 23S1 | 2376 | A | N1-C6-N6 | -18.97 | 107.22 | 118.60 |
| 1 | 16S1 | 109 | A | C2-N3-C4 | 18.96 | 120.08 | 110.60 |
| 22 | 23S1 | 979 | A | N1-C2-N3 | -18.96 | 119.82 | 129.30 |
| 23 | 05S1 | 115 | A | C2-N3-C4 | 18.96 | 120.08 | 110.60 |
| 1 | 16S1 | 19 | A | N1-C2-N3 | -18.96 | 119.82 | 129.30 |
| 1 | 16S1 | 958 | A | N1-C6-N6 | -18.96 | 107.22 | 118.60 |
| 22 | 23S1 | 1090 | A | N1-C2-N3 | -18.96 | 119.82 | 129.30 |
| 1 | 16S1 | 205 | A | C2-N3-C4 | 18.96 | 120.08 | 110.60 |
| 22 | 23S1 | 508 | A | C2-N3-C4 | 18.96 | 120.08 | 110.60 |
| 22 | 23S1 | 1970 | A | N1-C2-N3 | -18.96 | 119.82 | 129.30 |
| 22 | 23S1 | 1847 | A | C2-N3-C4 | 18.96 | 120.08 | 110.60 |
| 22 | 23S1 | 167 | A | C2-N3-C4 | 18.96 | 120.08 | 110.60 |
| 22 | 23S1 | 2205 | A | C2-N3-C4 | 18.96 | 120.08 | 110.60 |
| 22 | 23S1 | 2281 | A | C2-N3-C4 | 18.96 | 120.08 | 110.60 |
| 22 | 23S1 | 415 | A | C2-N3-C4 | 18.95 | 120.08 | 110.60 |
| 22 | 23S1 | 478 | A | N1-C6-N6 | -18.95 | 107.23 | 118.60 |
| 22 | 23S1 | 508 | A | N1-C2-N3 | -18.95 | 119.82 | 129.30 |
| 22 | 23S1 | 2813 | A | N1-C2-N3 | -18.95 | 119.82 | 129.30 |
| 22 | 23S1 | 345 | A | C2-N3-C4 | 18.95 | 120.08 | 110.60 |
| 22 | 23S1 | 844 | A | N1-C2-N3 | -18.95 | 119.82 | 129.30 |
| 22 | 23S1 | 1794 | A | N1-C2-N3 | -18.95 | 119.82 | 129.30 |
| 22 | 23S1 | 2268 | A | N1-C2-N3 | -18.95 | 119.83 | 129.30 |
| 1 | 16S1 | 32 | A | C2-N3-C4 | 18.95 | 120.08 | 110.60 |
| 22 | 23S1 | 156 | A | C2-N3-C4 | 18.95 | 120.07 | 110.60 |
| 1 | 16S1 | 706 | A | C2-N3-C4 | 18.95 | 120.07 | 110.60 |
| 1 | 16S1 | 1167 | A | N1-C2-N3 | -18.95 | 119.83 | 129.30 |
| 22 | 23S1 | 849 | A | N1-C2-N3 | -18.95 | 119.83 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 2163 | A | C2-N3-C4 | 18.95 | 120.07 | 110.60 |
| 55 | PTR1 | 59 | A | C2-N3-C4 | 18.95 | 120.07 | 110.60 |
| 1 | 16S1 | 315 | A | N1-C6-N6 | -18.95 | 107.23 | 118.60 |
| 22 | 23S1 | 2749 | A | C2-N3-C4 | 18.95 | 120.07 | 110.60 |
| 22 | 23S1 | 2893 | A | N1-C2-N3 | -18.95 | 119.83 | 129.30 |
| 1 | 16S1 | 131 | A | N1-C6-N6 | -18.95 | 107.23 | 118.60 |
| 1 | 16S1 | 907 | A | C2-N3-C4 | 18.94 | 120.07 | 110.60 |
| 1 | 16S1 | 1055 | A | N1-C2-N3 | -18.94 | 119.83 | 129.30 |
| 1 | 16S1 | 1213 | A | N1-C2-N3 | -18.94 | 119.83 | 129.30 |
| 1 | 16S1 | 1431 | A | C2-N3-C4 | 18.94 | 120.07 | 110.60 |
| 22 | 23S1 | 1413 | A | C2-N3-C4 | 18.94 | 120.07 | 110.60 |
| 1 | 16S1 | 1269 | A | N1-C2-N3 | -18.94 | 119.83 | 129.30 |
| 22 | 23S1 | 1802 | A | C2-N3-C4 | 18.94 | 120.07 | 110.60 |
| 1 | 16S1 | 1396 | A | C2-N3-C4 | 18.94 | 120.07 | 110.60 |
| 22 | 23S1 | 643 | A | N1-C6-N6 | -18.94 | 107.24 | 118.60 |
| 22 | 23S1 | 1373 | A | C2-N3-C4 | 18.94 | 120.07 | 110.60 |
| 22 | 23S1 | 1413 | A | N1-C2-N3 | -18.94 | 119.83 | 129.30 |
| 55 | PTR1 | 3 | A | C2-N3-C4 | 18.94 | 120.07 | 110.60 |
| 1 | 16S1 | 675 | A | N1-C2-N3 | -18.94 | 119.83 | 129.30 |
| 22 | 23S1 | 466 | A | N1-C2-N3 | -18.94 | 119.83 | 129.30 |
| 22 | 23S1 | 715 | A | C2-N3-C4 | 18.94 | 120.07 | 110.60 |
| 22 | 23S1 | 2042 | A | N1-C2-N3 | -18.94 | 119.83 | 129.30 |
| 1 | 16S1 | 790 | A | N1-C2-N3 | -18.94 | 119.83 | 129.30 |
| 1 | 16S1 | 767 | A | C2-N3-C4 | 18.93 | 120.07 | 110.60 |
| 1 | 16S1 | 780 | A | C2-N3-C4 | 18.93 | 120.07 | 110.60 |
| 1 | 16S1 | 1433 | A | N1-C2-N3 | -18.93 | 119.83 | 129.30 |
| 22 | 23S1 | 21 | A | N1-C2-N3 | -18.93 | 119.83 | 129.30 |
| 22 | 23S1 | 1746 | A | C2-N3-C4 | 18.93 | 120.07 | 110.60 |
| 22 | 23S1 | 734 | A | N1-C6-N6 | -18.93 | 107.24 | 118.60 |
| 22 | 23S1 | 1010 | A | C2-N3-C4 | 18.93 | 120.07 | 110.60 |
| 22 | 23S1 | 1384 | A | C2-N3-C4 | 18.93 | 120.07 | 110.60 |
| 22 | 23S1 | 2879 | A | C2-N3-C4 | 18.93 | 120.06 | 110.60 |
| 1 | 16S1 | 435 | A | C2-N3-C4 | 18.93 | 120.06 | 110.60 |
| 1 | 16S1 | 478 | A | N1-C6-N6 | -18.93 | 107.24 | 118.60 |
| 1 | 16S1 | 1036 | A | N1-C6-N6 | -18.93 | 107.24 | 118.60 |
| 1 | 16S1 | 1110 | A | N1-C6-N6 | -18.93 | 107.24 | 118.60 |
| 22 | 23S1 | 340 | A | N1-C6-N6 | -18.93 | 107.24 | 118.60 |
| 22 | 23S1 | 374 | A | N1-C2-N3 | -18.93 | 119.84 | 129.30 |
| 22 | 23S1 | 1275 | A | N1-C6-N6 | -18.93 | 107.24 | 118.60 |
| 22 | 23S1 | 925 | A | N1-C2-N3 | -18.93 | 119.84 | 129.30 |
| 22 | 23S1 | 1650 | A | N1-C2-N3 | -18.93 | 119.84 | 129.30 |
| 1 | 16S1 | 44 | A | N1-C2-N3 | -18.92 | 119.84 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 179 | A | C2-N3-C4 | 18.92 | 120.06 | 110.60 |
| 1 | 16S1 | 1151 | A | N1-C2-N3 | -18.92 | 119.84 | 129.30 |
| 22 | 23S1 | 1525 | A | N1-C2-N3 | -18.92 | 119.84 | 129.30 |
| 22 | 23S1 | 2097 | A | N1-C2-N3 | -18.92 | 119.84 | 129.30 |
| 1 | 16S1 | 753 | A | N1-C6-N6 | -18.92 | 107.25 | 118.60 |
| 22 | 23S1 | 1490 | A | N1-C6-N6 | -18.92 | 107.25 | 118.60 |
| 22 | 23S1 | 2114 | A | N1-C6-N6 | -18.92 | 107.25 | 118.60 |
| 23 | 05S1 | 39 | A | C2-N3-C4 | 18.92 | 120.06 | 110.60 |
| 1 | 16S1 | 1261 | A | N1-C2-N3 | -18.92 | 119.84 | 129.30 |
| 22 | 23S1 | 1678 | A | N1-C2-N3 | -18.92 | 119.84 | 129.30 |
| 22 | 23S1 | 2163 | A | N1-C6-N6 | -18.92 | 107.25 | 118.60 |
| 22 | 23S1 | 111 | A | N1-C6-N6 | -18.92 | 107.25 | 118.60 |
| 22 | 23S1 | 1593 | A | N1-C2-N3 | -18.92 | 119.84 | 129.30 |
| 22 | 23S1 | 111 | A | N1-C2-N3 | -18.91 | 119.84 | 129.30 |
| 22 | 23S1 | 1069 | A | N1-C6-N6 | -18.91 | 107.25 | 118.60 |
| 22 | 23S1 | 1143 | A | N1-C2-N3 | -18.91 | 119.84 | 129.30 |
| 22 | 23S1 | 2851 | A | C2-N3-C4 | 18.91 | 120.06 | 110.60 |
| 22 | 23S1 | 2241 | A | N1-C2-N3 | -18.91 | 119.84 | 129.30 |
| 1 | 16S1 | 28 | A | C2-N3-C4 | 18.91 | 120.06 | 110.60 |
| 1 | 16S1 | 937 | A | N1-C2-N3 | -18.91 | 119.84 | 129.30 |
| 1 | 16S1 | 325 | A | N1-C2-N3 | -18.91 | 119.84 | 129.30 |
| 1 | 16S1 | 749 | A | C2-N3-C4 | 18.91 | 120.06 | 110.60 |
| 22 | 23S1 | 920 | A | N1-C2-N3 | -18.91 | 119.84 | 129.30 |
| 22 | 23S1 | 1050 | A | C2-N3-C4 | 18.91 | 120.05 | 110.60 |
| 1 | 16S1 | 547 | A | N1-C6-N6 | -18.91 | 107.26 | 118.60 |
| 1 | 16S1 | 1248 | A | N1-C2-N3 | -18.91 | 119.85 | 129.30 |
| 1 | 16S1 | 1329 | A | N1-C2-N3 | -18.91 | 119.85 | 129.30 |
| 1 | 16S1 | 676 | A | N1-C6-N6 | -18.91 | 107.26 | 118.60 |
| 1 | 16S1 | 648 | A | N1-C6-N6 | -18.90 | 107.26 | 118.60 |
| 22 | 23S1 | 2020 | A | N1-C6-N6 | -18.90 | 107.26 | 118.60 |
| 1 | 16S1 | 393 | A | N1-C2-N3 | -18.90 | 119.85 | 129.30 |
| 1 | 16S1 | 665 | A | C2-N3-C4 | 18.90 | 120.05 | 110.60 |
| 22 | 23S1 | 1583 | A | C2-N3-C4 | 18.90 | 120.05 | 110.60 |
| 22 | 23S1 | 2516 | A | N1-C2-N3 | -18.90 | 119.85 | 129.30 |
| 22 | 23S1 | 2886 | A | N1-C2-N3 | -18.90 | 119.85 | 129.30 |
| 22 | 23S1 | 1269 | A | N1-C6-N6 | -18.90 | 107.26 | 118.60 |
| 22 | 23S1 | 2266 | A | N1-C2-N3 | -18.90 | 119.85 | 129.30 |
| 22 | 23S1 | 2090 | A | N1-C2-N3 | -18.90 | 119.85 | 129.30 |
| 22 | 23S1 | 501 | A | C2-N3-C4 | 18.90 | 120.05 | 110.60 |
| 22 | 23S1 | 1553 | A | N1-C2-N3 | -18.90 | 119.85 | 129.30 |
| 22 | 23S1 | 2872 | A | C5-C6-N6 | 18.90 | 138.82 | 123.70 |
| 1 | 16S1 | 1035 | A | N1-C2-N3 | -18.89 | 119.85 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 590 | A | C2-N3-C4 | 18.89 | 120.05 | 110.60 |
| 22 | 23S1 | 2270 | A | N1-C2-N3 | -18.89 | 119.85 | 129.30 |
| 1 | 16S1 | 1289 | A | N1-C6-N6 | -18.89 | 107.26 | 118.60 |
| 1 | 16S1 | 1377 | A | N1-C6-N6 | -18.89 | 107.26 | 118.60 |
| 22 | 23S1 | 1502 | A | C2-N3-C4 | 18.89 | 120.05 | 110.60 |
| 22 | 23S1 | 2184 | A | N1-C2-N3 | -18.89 | 119.85 | 129.30 |
| 55 | PTR1 | 42 | A | N1-C2-N3 | -18.89 | 119.85 | 129.30 |
| 1 | 16S1 | 373 | A | N1-C2-N3 | -18.89 | 119.86 | 129.30 |
| 22 | 23S1 | 1046 | A | C2-N3-C4 | 18.89 | 120.05 | 110.60 |
| 22 | 23S1 | 1705 | A | N1-C2-N3 | -18.89 | 119.85 | 129.30 |
| 1 | 16S1 | 1105 | A | C2-N3-C4 | 18.89 | 120.04 | 110.60 |
| 22 | 23S1 | 199 | A | N1-C6-N6 | -18.89 | 107.27 | 118.60 |
| 22 | 23S1 | 374 | A | C2-N3-C4 | 18.89 | 120.04 | 110.60 |
| 22 | 23S1 | 1069 | A | C2-N3-C4 | 18.89 | 120.04 | 110.60 |
| 22 | 23S1 | 1664 | A | N1-C6-N6 | -18.89 | 107.27 | 118.60 |
| 22 | 23S1 | 1705 | A | C2-N3-C4 | 18.89 | 120.04 | 110.60 |
| 22 | 23S1 | 2381 | A | N1-C6-N6 | -18.89 | 107.27 | 118.60 |
| 1 | 16S1 | 393 | A | N1-C6-N6 | -18.89 | 107.27 | 118.60 |
| 22 | 23S1 | 1103 | A | N1-C2-N3 | -18.89 | 119.86 | 129.30 |
| 22 | 23S1 | 5 | A | N1-C6-N6 | -18.88 | 107.27 | 118.60 |
| 23 | 05S1 | 104 | A | C2-N3-C4 | 18.88 | 120.04 | 110.60 |
| 1 | 16S1 | 946 | A | N1-C6-N6 | -18.88 | 107.27 | 118.60 |
| 22 | 23S1 | 2461 | A | N1-C6-N6 | -18.88 | 107.27 | 118.60 |
| 1 | 16S1 | 167 | A | N1-C6-N6 | -18.88 | 107.27 | 118.60 |
| 1 | 16S1 | 681 | A | C2-N3-C4 | 18.88 | 120.04 | 110.60 |
| 22 | 23S1 | 614 | A | N1-C2-N3 | -18.88 | 119.86 | 129.30 |
| 22 | 23S1 | 1127 | A | N1-C2-N3 | -18.88 | 119.86 | 129.30 |
| 22 | 23S1 | 1596 | A | N1-C6-N6 | -18.88 | 107.27 | 118.60 |
| 1 | 16S1 | 1197 | A | N1-C2-N3 | -18.88 | 119.86 | 129.30 |
| 22 | 23S1 | 352 | A | N1-C2-N3 | -18.88 | 119.86 | 129.30 |
| 1 | 16S1 | 389 | A | N1-C2-N3 | -18.88 | 119.86 | 129.30 |
| 22 | 23S1 | 1385 | A | N1-C2-N3 | -18.88 | 119.86 | 129.30 |
| 22 | 23S1 | 2335 | A | C2-N3-C4 | 18.88 | 120.04 | 110.60 |
| 1 | 16S1 | 1146 | A | N1-C2-N3 | -18.88 | 119.86 | 129.30 |
| 22 | 23S1 | 501 | A | N1-C2-N3 | -18.88 | 119.86 | 129.30 |
| 22 | 23S1 | 2094 | A | C2-N3-C4 | 18.88 | 120.04 | 110.60 |
| 22 | 23S1 | 197 | A | N1-C6-N6 | -18.87 | 107.28 | 118.60 |
| 1 | 16S1 | 1252 | A | C2-N3-C4 | 18.87 | 120.03 | 110.60 |
| 1 | 16S1 | 1492 | A | C2-N3-C4 | 18.87 | 120.03 | 110.60 |
| 22 | 23S1 | 2749 | A | N1-C6-N6 | -18.87 | 107.28 | 118.60 |
| 22 | 23S1 | 614 | A | C2-N3-C4 | 18.87 | 120.03 | 110.60 |
| 1 | 16S1 | 1042 | A | C2-N3-C4 | 18.87 | 120.03 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1244 | A | N1-C2-N3 | -18.87 | 119.87 | 129.30 |
| 22 | 23S1 | 1608 | A | C2-N3-C4 | 18.87 | 120.03 | 110.60 |
| 22 | 23S1 | 1969 | A | N1-C2-N3 | -18.87 | 119.87 | 129.30 |
| 22 | 23S1 | 2051 | A | N1-C2-N3 | -18.87 | 119.87 | 129.30 |
| 22 | 23S1 | 899 | A | C2-N3-C4 | 18.86 | 120.03 | 110.60 |
| 22 | 23S1 | 1046 | A | N1-C2-N3 | -18.86 | 119.87 | 129.30 |
| 22 | 23S1 | 1367 | A | N1-C2-N3 | -18.86 | 119.87 | 129.30 |
| 1 | 16S1 | 432 | A | C2-N3-C4 | 18.86 | 120.03 | 110.60 |
| 22 | 23S1 | 526 | A | C2-N3-C4 | 18.86 | 120.03 | 110.60 |
| 22 | 23S1 | 627 | A | N1-C2-N3 | -18.86 | 119.87 | 129.30 |
| 22 | 23S1 | 1433 | A | N1-C6-N6 | -18.86 | 107.28 | 118.60 |
| 22 | 23S1 | 2191 | A | N1-C2-N3 | -18.86 | 119.87 | 129.30 |
| 1 | 16S1 | 1169 | A | N1-C2-N3 | -18.86 | 119.87 | 129.30 |
| 1 | 16S1 | 1362 | A | N1-C2-N3 | -18.86 | 119.87 | 129.30 |
| 22 | 23S1 | 556 | A | N1-C6-N6 | -18.86 | 107.28 | 118.60 |
| 22 | 23S1 | 2227 | A | N1-C2-N3 | -18.86 | 119.87 | 129.30 |
| 22 | 23S1 | 699 | A | N1-C2-N3 | -18.86 | 119.87 | 129.30 |
| 22 | 23S1 | 1126 | A | C2-N3-C4 | 18.86 | 120.03 | 110.60 |
| 1 | 16S1 | 1368 | A | N1-C2-N3 | -18.86 | 119.87 | 129.30 |
| 22 | 23S1 | 1419 | A | C2-N3-C4 | 18.85 | 120.03 | 110.60 |
| 1 | 16S1 | 759 | A | N1-C6-N6 | -18.85 | 107.29 | 118.60 |
| 22 | 23S1 | 1050 | A | N1-C6-N6 | -18.85 | 107.29 | 118.60 |
| 22 | 23S1 | 2142 | A | C2-N3-C4 | 18.85 | 120.03 | 110.60 |
| 1 | 16S1 | 414 | A | N1-C2-N3 | -18.85 | 119.88 | 129.30 |
| 22 | 23S1 | 345 | A | N1-C2-N3 | -18.85 | 119.87 | 129.30 |
| 22 | 23S1 | 1978 | A | N1-C2-N3 | -18.85 | 119.88 | 129.30 |
| 22 | 23S1 | 2426 | A | C2-N3-C4 | 18.85 | 120.03 | 110.60 |
| 22 | 23S1 | 821 | A | C2-N3-C4 | 18.85 | 120.02 | 110.60 |
| 22 | 23S1 | 492 | A | C2-N3-C4 | 18.85 | 120.02 | 110.60 |
| 22 | 23S1 | 877 | A | C2-N3-C4 | 18.85 | 120.02 | 110.60 |
| 1 | 16S1 | 595 | A | C2-N3-C4 | 18.84 | 120.02 | 110.60 |
| 22 | 23S1 | 345 | A | N1-C6-N6 | -18.84 | 107.29 | 118.60 |
| 22 | 23S1 | 1762 | A | N1-C2-N3 | -18.84 | 119.88 | 129.30 |
| 22 | 23S1 | 2541 | A | N1-C2-N3 | -18.84 | 119.88 | 129.30 |
| 1 | 16S1 | 1180 | A | C2-N3-C4 | 18.84 | 120.02 | 110.60 |
| 22 | 23S1 | 1901 | A | N1-C2-N3 | -18.84 | 119.88 | 129.30 |
| 22 | 23S1 | 2327 | A | N1-C2-N3 | -18.84 | 119.88 | 129.30 |
| 22 | 23S1 | 149 | A | N1-C2-N3 | -18.84 | 119.88 | 129.30 |
| 22 | 23S1 | 172 | A | N1-C2-N3 | -18.84 | 119.88 | 129.30 |
| 22 | 23S1 | 1089 | A | N1-C2-N3 | -18.84 | 119.88 | 129.30 |
| 22 | 23S1 | 1431 | A | N1-C2-N3 | -18.84 | 119.88 | 129.30 |
| 22 | 23S1 | 2211 | A | N1-C6-N6 | -18.84 | 107.30 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1089 | A | N1-C6-N6 | -18.84 | 107.30 | 118.60 |
| 22 | 23S1 | 1509 | A | N1-C6-N6 | -18.84 | 107.30 | 118.60 |
| 1 | 16S1 | 694 | A | C2-N3-C4 | 18.84 | 120.02 | 110.60 |
| 1 | 16S1 | 978 | A | N1-C2-N3 | -18.84 | 119.88 | 129.30 |
| 22 | 23S1 | 2813 | A | C2-N3-C4 | 18.84 | 120.02 | 110.60 |
| 1 | 16S1 | 712 | A | N1-C6-N6 | -18.84 | 107.30 | 118.60 |
| 1 | 16S1 | 1254 | A | C2-N3-C4 | 18.84 | 120.02 | 110.60 |
| 22 | 23S1 | 483 | A | N1-C6-N6 | -18.84 | 107.30 | 118.60 |
| 1 | 16S1 | 28 | A | N1-C6-N6 | -18.83 | 107.30 | 118.60 |
| 22 | 23S1 | 1928 | A | N1-C6-N6 | -18.83 | 107.30 | 118.60 |
| 22 | 23S1 | 2850 | A | N1-C2-N3 | -18.83 | 119.88 | 129.30 |
| 1 | 16S1 | 676 | A | C2-N3-C4 | 18.83 | 120.01 | 110.60 |
| 22 | 23S1 | 199 | A | N1-C2-N3 | -18.83 | 119.89 | 129.30 |
| 22 | 23S1 | 685 | A | N1-C2-N3 | -18.83 | 119.89 | 129.30 |
| 22 | 23S1 | 1378 | A | C2-N3-C4 | 18.83 | 120.02 | 110.60 |
| 1 | 16S1 | 50 | A | N1-C2-N3 | -18.83 | 119.89 | 129.30 |
| 22 | 23S1 | 1626 | A | N1-C2-N3 | -18.83 | 119.89 | 129.30 |
| 22 | 23S1 | 2868 | A | N1-C6-N6 | -18.83 | 107.30 | 118.60 |
| 1 | 16S1 | 374 | A | N1-C2-N3 | -18.82 | 119.89 | 129.30 |
| 22 | 23S1 | 878 | A | N1-C2-N3 | -18.82 | 119.89 | 129.30 |
| 1 | 16S1 | 129 | A | N1-C6-N6 | -18.82 | 107.31 | 118.60 |
| 1 | 16S1 | 784 | A | N1-C2-N3 | -18.82 | 119.89 | 129.30 |
| 22 | 23S1 | 1919 | A | C2-N3-C4 | 18.82 | 120.01 | 110.60 |
| 1 | 16S1 | 1433 | A | N1-C6-N6 | -18.82 | 107.31 | 118.60 |
| 1 | 16S1 | 196 | A | N1-C6-N6 | -18.82 | 107.31 | 118.60 |
| 22 | 23S1 | 800 | A | C2-N3-C4 | 18.82 | 120.01 | 110.60 |
| 22 | 23S1 | 878 | A | C2-N3-C4 | 18.82 | 120.01 | 110.60 |
| 22 | 23S1 | 1755 | A | C2-N3-C4 | 18.82 | 120.01 | 110.60 |
| 22 | 23S1 | 1876 | A | C2-N3-C4 | 18.82 | 120.01 | 110.60 |
| 22 | 23S1 | 1912 | A | N1-C2-N3 | -18.82 | 119.89 | 129.30 |
| 22 | 23S1 | 2013 | A | N1-C6-N6 | -18.82 | 107.31 | 118.60 |
| 22 | 23S1 | 2080 | A | N1-C2-N3 | -18.82 | 119.89 | 129.30 |
| 22 | 23S1 | 2225 | A | N1-C2-N3 | -18.82 | 119.89 | 129.30 |
| 1 | 16S1 | 8 | A | C2-N3-C4 | 18.82 | 120.01 | 110.60 |
| 1 | 16S1 | 865 | A | C2-N3-C4 | 18.82 | 120.01 | 110.60 |
| 1 | 16S1 | 1022 | A | C2-N3-C4 | 18.82 | 120.01 | 110.60 |
| 1 | 16S1 | 533 | A | N1-C6-N6 | -18.82 | 107.31 | 118.60 |
| 1 | 16S1 | 1229 | A | N1-C6-N6 | -18.82 | 107.31 | 118.60 |
| 22 | 23S1 | 541 | A | C2-N3-C4 | 18.82 | 120.01 | 110.60 |
| 1 | 16S1 | 253 | A | N1-C6-N6 | -18.81 | 107.31 | 118.60 |
| 1 | 16S1 | 1035 | A | C2-N3-C4 | 18.81 | 120.01 | 110.60 |
| 22 | 23S1 | 181 | A | N1-C2-N3 | -18.81 | 119.89 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1579 | A | C2-N3-C4 | 18.81 | 120.01 | 110.60 |
| 1 | 16S1 | 448 | A | N1-C2-N3 | -18.81 | 119.89 | 129.30 |
| 22 | 23S1 | 1301 | A | N1-C6-N6 | -18.81 | 107.31 | 118.60 |
| 22 | 23S1 | 2873 | A | C2-N3-C4 | 18.81 | 120.01 | 110.60 |
| 1 | 16S1 | 1447 | A | N1-C2-N3 | -18.81 | 119.89 | 129.30 |
| 22 | 23S1 | 699 | A | C2-N3-C4 | 18.81 | 120.00 | 110.60 |
| 22 | 23S1 | 1347 | A | N1-C2-N3 | -18.81 | 119.89 | 129.30 |
| 22 | 23S1 | 1532 | A | N1-C2-N3 | -18.81 | 119.89 | 129.30 |
| 22 | 23S1 | 2054 | A | N1-C2-N3 | -18.81 | 119.89 | 129.30 |
| 22 | 23S1 | 1590 | A | N1-C2-N3 | -18.81 | 119.90 | 129.30 |
| 22 | 23S1 | 2432 | A | C2-N3-C4 | 18.81 | 120.00 | 110.60 |
| 22 | 23S1 | 2468 | A | C2-N3-C4 | 18.81 | 120.00 | 110.60 |
| 22 | 23S1 | 384 | A | N1-C6-N6 | -18.81 | 107.32 | 118.60 |
| 22 | 23S1 | 1014 | A | N1-C2-N3 | -18.81 | 119.90 | 129.30 |
| 22 | 23S1 | 1652 | A | N1-C2-N3 | -18.80 | 119.90 | 129.30 |
| 23 | 05S1 | 53 | A | N1-C6-N6 | -18.80 | 107.32 | 118.60 |
| 1 | 16S1 | 1398 | A | N1-C2-N3 | -18.80 | 119.90 | 129.30 |
| 1 | 16S1 | 1441 | A | C2-N3-C4 | 18.80 | 120.00 | 110.60 |
| 22 | 23S1 | 1890 | A | C2-N3-C4 | 18.80 | 120.00 | 110.60 |
| 22 | 23S1 | 2764 | A | C2-N3-C4 | 18.80 | 120.00 | 110.60 |
| 1 | 16S1 | 630 | A | N1-C2-N3 | -18.80 | 119.90 | 129.30 |
| 22 | 23S1 | 483 | A | N1-C2-N3 | -18.80 | 119.90 | 129.30 |
| 22 | 23S1 | 508 | A | N1-C6-N6 | -18.80 | 107.32 | 118.60 |
| 22 | 23S1 | 1433 | A | C2-N3-C4 | 18.80 | 120.00 | 110.60 |
| 22 | 23S1 | 204 | A | C2-N3-C4 | 18.80 | 120.00 | 110.60 |
| 22 | 23S1 | 513 | A | N1-C2-N3 | -18.80 | 119.90 | 129.30 |
| 22 | 23S1 | 44 | A | N1-C2-N3 | -18.80 | 119.90 | 129.30 |
| 22 | 23S1 | 739 | A | N1-C6-N6 | -18.80 | 107.32 | 118.60 |
| 22 | 23S1 | 1553 | A | C2-N3-C4 | 18.80 | 120.00 | 110.60 |
| 22 | 23S1 | 2158 | A | C2-N3-C4 | 18.80 | 120.00 | 110.60 |
| 22 | 23S1 | 2352 | A | C2-N3-C4 | 18.80 | 120.00 | 110.60 |
| 22 | 23S1 | 2468 | A | N1-C2-N3 | -18.80 | 119.90 | 129.30 |
| 1 | 16S1 | 819 | A | N1-C6-N6 | -18.79 | 107.32 | 118.60 |
| 22 | 23S1 | 609 | A | C2-N3-C4 | 18.79 | 120.00 | 110.60 |
| 22 | 23S1 | 2750 | A | N1-C6-N6 | -18.79 | 107.32 | 118.60 |
| 23 | 05S1 | 58 | A | N1-C2-N3 | -18.79 | 119.90 | 129.30 |
| 1 | 16S1 | 1319 | A | N1-C2-N3 | -18.79 | 119.90 | 129.30 |
| 22 | 23S1 | 1133 | A | N1-C6-N6 | -18.79 | 107.33 | 118.60 |
| 1 | 16S1 | 174 | A | C2-N3-C4 | 18.79 | 120.00 | 110.60 |
| 1 | 16S1 | 192 | A | C2-N3-C4 | 18.79 | 120.00 | 110.60 |
| 22 | 23S1 | 346 | A | N1-C2-N3 | -18.79 | 119.91 | 129.30 |
| 22 | 23S1 | 2587 | A | N1-C6-N6 | -18.79 | 107.33 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 2009 | A | C2-N3-C4 | 18.79 | 120.00 | 110.60 |
| 1 | 16S1 | 238 | A | N1-C6-N6 | -18.79 | 107.33 | 118.60 |
| 22 | 23S1 | 2119 | A | N1-C2-N3 | -18.79 | 119.91 | 129.30 |
| 22 | 23S1 | 538 | A | N1-C2-N3 | -18.79 | 119.91 | 129.30 |
| 22 | 23S1 | 749 | A | C2-N3-C4 | 18.79 | 119.99 | 110.60 |
| 22 | 23S1 | 1545 | A | N1-C2-N3 | -18.79 | 119.91 | 129.30 |
| 1 | 16S1 | 629 | A | C2-N3-C4 | 18.78 | 119.99 | 110.60 |
| 1 | 16S1 | 816 | A | N1-C6-N6 | -18.78 | 107.33 | 118.60 |
| 1 | 16S1 | 681 | A | N1-C6-N6 | -18.78 | 107.33 | 118.60 |
| 22 | 23S1 | 118 | A | N1-C6-N6 | -18.78 | 107.33 | 118.60 |
| 22 | 23S1 | 1650 | A | C2-N3-C4 | 18.78 | 119.99 | 110.60 |
| 22 | 23S1 | 1672 | A | C2-N3-C4 | 18.78 | 119.99 | 110.60 |
| 1 | 16S1 | 441 | A | C2-N3-C4 | 18.78 | 119.99 | 110.60 |
| 22 | 23S1 | 1276 | A | N1-C2-N3 | -18.78 | 119.91 | 129.30 |
| 1 | 16S1 | 456 | A | N1-C6-N6 | -18.78 | 107.33 | 118.60 |
| 1 | 16S1 | 1254 | A | N1-C6-N6 | -18.78 | 107.33 | 118.60 |
| 22 | 23S1 | 2052 | A | N1-C6-N6 | -18.77 | 107.34 | 118.60 |
| 22 | 23S1 | 155 | A | N1-C2-N3 | -18.77 | 119.91 | 129.30 |
| 22 | 23S1 | 449 | A | N1-C2-N3 | -18.77 | 119.91 | 129.30 |
| 1 | 16S1 | 906 | A | C2-N3-C4 | 18.77 | 119.98 | 110.60 |
| 22 | 23S1 | 959 | A | N1-C6-N6 | -18.77 | 107.34 | 118.60 |
| 22 | 23S1 | 1571 | A | C2-N3-C4 | 18.77 | 119.98 | 110.60 |
| 22 | 23S1 | 2088 | A | C2-N3-C4 | 18.77 | 119.99 | 110.60 |
| 1 | 16S1 | 1 | A | N1-C2-N3 | -18.77 | 119.92 | 129.30 |
| 1 | 16S1 | 205 | A | N1-C2-N3 | -18.77 | 119.92 | 129.30 |
| 1 | 16S1 | 315 | A | N1-C2-N3 | -18.77 | 119.92 | 129.30 |
| 1 | 16S1 | 790 | A | C2-N3-C4 | 18.77 | 119.98 | 110.60 |
| 22 | 23S1 | 582 | A | N1-C6-N6 | -18.77 | 107.34 | 118.60 |
| 1 | 16S1 | 509 | A | N1-C2-N3 | -18.77 | 119.92 | 129.30 |
| 22 | 23S1 | 2126 | A | N1-C6-N6 | -18.77 | 107.34 | 118.60 |
| 22 | 23S1 | 2670 | A | N1-C6-N6 | -18.77 | 107.34 | 118.60 |
| 1 | 16S1 | 363 | A | N1-C6-N6 | -18.77 | 107.34 | 118.60 |
| 1 | 16S1 | 579 | A | N1-C6-N6 | -18.77 | 107.34 | 118.60 |
| 1 | 16S1 | 729 | A | N1-C2-N3 | -18.77 | 119.92 | 129.30 |
| 22 | 23S1 | 453 | A | N1-C2-N3 | -18.77 | 119.92 | 129.30 |
| 23 | 05S1 | 119 | A | N1-C6-N6 | -18.77 | 107.34 | 118.60 |
| 1 | 16S1 | 236 | A | N1-C6-N6 | -18.76 | 107.34 | 118.60 |
| 22 | 23S1 | 299 | A | N1-C6-N6 | -18.76 | 107.34 | 118.60 |
| 22 | 23S1 | 637 | A | C2-N3-C4 | 18.76 | 119.98 | 110.60 |
| 22 | 23S1 | 896 | A | N1-C6-N6 | -18.76 | 107.34 | 118.60 |
| 1 | 16S1 | 1493 | A | C2-N3-C4 | 18.76 | 119.98 | 110.60 |
| 1 | 16S1 | 1375 | A | C2-N3-C4 | 18.76 | 119.98 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1469 | A | N1-C2-N3 | -18.76 | 119.92 | 129.30 |
| 22 | 23S1 | 2600 | A | N1-C6-N6 | -18.76 | 107.34 | 118.60 |
| 1 | 16S1 | 459 | A | C2-N3-C4 | 18.76 | 119.98 | 110.60 |
| 1 | 16S1 | 845 | A | C2-N3-C4 | 18.76 | 119.98 | 110.60 |
| 22 | 23S1 | 1783 | A | N1-C6-N6 | -18.76 | 107.35 | 118.60 |
| 1 | 16S1 | 120 | A | C2-N3-C4 | 18.75 | 119.98 | 110.60 |
| 22 | 23S1 | 582 | A | N1-C2-N3 | -18.75 | 119.92 | 129.30 |
| 22 | 23S1 | 1477 | A | C2-N3-C4 | 18.75 | 119.98 | 110.60 |
| 22 | 23S1 | 1549 | A | N1-C6-N6 | -18.75 | 107.35 | 118.60 |
| 22 | 23S1 | 1977 | A | C2-N3-C4 | 18.75 | 119.98 | 110.60 |
| 1 | 16S1 | 642 | A | C2-N3-C4 | 18.75 | 119.98 | 110.60 |
| 1 | 16S1 | 780 | A | N1-C2-N3 | -18.75 | 119.92 | 129.30 |
| 22 | 23S1 | 1532 | A | C2-N3-C4 | 18.75 | 119.97 | 110.60 |
| 1 | 16S1 | 282 | A | N1-C2-N3 | -18.75 | 119.92 | 129.30 |
| 1 | 16S1 | 609 | A | N1-C2-N3 | -18.75 | 119.92 | 129.30 |
| 1 | 16S1 | 1430 | A | C2-N3-C4 | 18.75 | 119.97 | 110.60 |
| 22 | 23S1 | 191 | A | C2-N3-C4 | 18.75 | 119.97 | 110.60 |
| 22 | 23S1 | 231 | A | C2-N3-C4 | 18.75 | 119.97 | 110.60 |
| 22 | 23S1 | 1151 | A | N1-C2-N3 | -18.75 | 119.93 | 129.30 |
| 22 | 23S1 | 38 | A | N1-C2-N3 | -18.75 | 119.93 | 129.30 |
| 22 | 23S1 | 497 | A | C2-N3-C4 | 18.75 | 119.97 | 110.60 |
| 1 | 16S1 | 596 | A | N1-C2-N3 | -18.75 | 119.93 | 129.30 |
| 22 | 23S1 | 282 | A | C2-N3-C4 | 18.75 | 119.97 | 110.60 |
| 22 | 23S1 | 344 | A | N1-C2-N3 | -18.75 | 119.93 | 129.30 |
| 1 | 16S1 | 573 | A | N1-C6-N6 | -18.74 | 107.36 | 118.60 |
| 1 | 16S1 | 1257 | A | C2-N3-C4 | 18.74 | 119.97 | 110.60 |
| 22 | 23S1 | 1359 | A | C2-N3-C4 | 18.74 | 119.97 | 110.60 |
| 55 | PTR1 | 42 | A | N1-C6-N6 | -18.74 | 107.35 | 118.60 |
| 1 | 16S1 | 8 | A | N1-C6-N6 | -18.74 | 107.36 | 118.60 |
| 1 | 16S1 | 535 | A | N1-C6-N6 | -18.74 | 107.36 | 118.60 |
| 22 | 23S1 | 2126 | A | C2-N3-C4 | 18.74 | 119.97 | 110.60 |
| 22 | 23S1 | 2736 | A | C2-N3-C4 | 18.74 | 119.97 | 110.60 |
| 22 | 23S1 | 63 | A | N1-C2-N3 | -18.74 | 119.93 | 129.30 |
| 22 | 23S1 | 1900 | A | C2-N3-C4 | 18.74 | 119.97 | 110.60 |
| 1 | 16S1 | 1111 | A | C2-N3-C4 | 18.73 | 119.97 | 110.60 |
| 22 | 23S1 | 2459 | A | N1-C2-N3 | -18.73 | 119.93 | 129.30 |
| 1 | 16S1 | 71 | A | C2-N3-C4 | 18.73 | 119.97 | 110.60 |
| 1 | 16S1 | 1288 | A | C2-N3-C4 | 18.73 | 119.97 | 110.60 |
| 1 | 16S1 | 1507 | A | N1-C2-N3 | -18.73 | 119.93 | 129.30 |
| 22 | 23S1 | 213 | A | N1-C2-N3 | -18.73 | 119.93 | 129.30 |
| 1 | 16S1 | 1236 | A | N1-C2-N3 | -18.73 | 119.93 | 129.30 |
| 22 | 23S1 | 1652 | A | C2-N3-C4 | 18.73 | 119.97 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1571 | A | N1-C2-N3 | -18.73 | 119.94 | 129.30 |
| 22 | 23S1 | 1953 | A | N1-C2-N3 | -18.73 | 119.94 | 129.30 |
| 22 | 23S1 | 1773 | A | N1-C2-N3 | -18.73 | 119.94 | 129.30 |
| 22 | 23S1 | 2711 | A | N1-C6-N6 | -18.73 | 107.36 | 118.60 |
| 22 | 23S1 | 2705 | A | N1-C6-N6 | -18.73 | 107.36 | 118.60 |
| 1 | 16S1 | 1447 | A | C2-N3-C4 | 18.72 | 119.96 | 110.60 |
| 22 | 23S1 | 751 | A | C2-N3-C4 | 18.72 | 119.96 | 110.60 |
| 1 | 16S1 | 1105 | A | N1-C6-N6 | -18.72 | 107.37 | 118.60 |
| 1 | 16S1 | 1456 | A | N1-C2-N3 | -18.72 | 119.94 | 129.30 |
| 22 | 23S1 | 1073 | A | N1-C2-N3 | -18.72 | 119.94 | 129.30 |
| 22 | 23S1 | 1505 | A | C2-N3-C4 | 18.72 | 119.96 | 110.60 |
| 22 | 23S1 | 2879 | A | N1-C2-N3 | -18.72 | 119.94 | 129.30 |
| 22 | 23S1 | 1111 | A | C2-N3-C4 | 18.72 | 119.96 | 110.60 |
| 1 | 16S1 | 908 | A | N1-C2-N3 | -18.71 | 119.94 | 129.30 |
| 22 | 23S1 | 1127 | A | C2-N3-C4 | 18.71 | 119.96 | 110.60 |
| 22 | 23S1 | 1495 | A | N1-C2-N3 | -18.71 | 119.94 | 129.30 |
| 22 | 23S1 | 1676 | A | C2-N3-C4 | 18.71 | 119.96 | 110.60 |
| 22 | 23S1 | 56 | A | C2-N3-C4 | 18.71 | 119.96 | 110.60 |
| 22 | 23S1 | 866 | A | C2-N3-C4 | 18.71 | 119.96 | 110.60 |
| 22 | 23S1 | 165 | A | N1-C2-N3 | -18.71 | 119.94 | 129.30 |
| 22 | 23S1 | 1787 | A | N1-C6-N6 | -18.71 | 107.37 | 118.60 |
| 22 | 23S1 | 152 | A | N1-C2-N3 | -18.71 | 119.95 | 129.30 |
| 22 | 23S1 | 1616 | A | N1-C6-N6 | -18.71 | 107.38 | 118.60 |
| 22 | 23S1 | 1876 | A | N1-C2-N3 | -18.71 | 119.94 | 129.30 |
| 22 | 23S1 | 1913 | A | N1-C2-N3 | -18.71 | 119.95 | 129.30 |
| 1 | 16S1 | 649 | A | N1-C2-N3 | -18.71 | 119.95 | 129.30 |
| 1 | 16S1 | 1152 | A | C2-N3-C4 | 18.71 | 119.95 | 110.60 |
| 22 | 23S1 | 833 | A | N1-C6-N6 | -18.71 | 107.38 | 118.60 |
| 22 | 23S1 | 2247 | A | N1-C2-N3 | -18.71 | 119.95 | 129.30 |
| 1 | 16S1 | 263 | A | N1-C2-N3 | -18.71 | 119.95 | 129.30 |
| 1 | 16S1 | 78 | A | C2-N3-C4 | 18.70 | 119.95 | 110.60 |
| 1 | 16S1 | 139 | A | C2-N3-C4 | 18.70 | 119.95 | 110.60 |
| 1 | 16S1 | 243 | A | N1-C6-N6 | -18.70 | 107.38 | 118.60 |
| 1 | 16S1 | 878 | A | C2-N3-C4 | 18.70 | 119.95 | 110.60 |
| 1 | 16S1 | 1377 | A | N1-C2-N3 | -18.70 | 119.95 | 129.30 |
| 22 | 23S1 | 609 | A | N1-C6-N6 | -18.70 | 107.38 | 118.60 |
| 22 | 23S1 | 2019 | A | N1-C2-N3 | -18.70 | 119.95 | 129.30 |
| 22 | 23S1 | 2358 | A | C2-N3-C4 | 18.70 | 119.95 | 110.60 |
| 22 | 23S1 | 2873 | A | N1-C6-N6 | -18.70 | 107.38 | 118.60 |
| 22 | 23S1 | 1307 | A | N1-C2-N3 | -18.70 | 119.95 | 129.30 |
| 22 | 23S1 | 1494 | A | C2-N3-C4 | 18.70 | 119.95 | 110.60 |
| 1 | 16S1 | 695 | A | N1-C2-N3 | -18.70 | 119.95 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1302 | A | C2-N3-C4 | 18.70 | 119.95 | 110.60 |
| 1 | 16S1 | 10 | A | N1-C6-N6 | -18.70 | 107.38 | 118.60 |
| 22 | 23S1 | 279 | A | C2-N3-C4 | 18.70 | 119.95 | 110.60 |
| 22 | 23S1 | 515 | A | C2-N3-C4 | 18.70 | 119.95 | 110.60 |
| 1 | 16S1 | 1092 | A | N1-C2-N3 | -18.70 | 119.95 | 129.30 |
| 22 | 23S1 | 2377 | A | C2-N3-C4 | 18.70 | 119.95 | 110.60 |
| 22 | 23S1 | 2792 | A | C2-N3-C4 | 18.70 | 119.95 | 110.60 |
| 1 | 16S1 | 1188 | A | N1-C6-N6 | -18.70 | 107.38 | 118.60 |
| 22 | 23S1 | 1953 | A | N1-C6-N6 | -18.70 | 107.38 | 118.60 |
| 22 | 23S1 | 218 | A | C2-N3-C4 | 18.70 | 119.95 | 110.60 |
| 1 | 16S1 | 1340 | A | C2-N3-C4 | 18.69 | 119.95 | 110.60 |
| 1 | 16S1 | 1513 | A | N1-C2-N3 | -18.69 | 119.95 | 129.30 |
| 22 | 23S1 | 401 | A | N1-C2-N3 | -18.69 | 119.95 | 129.30 |
| 22 | 23S1 | 471 | A | C2-N3-C4 | 18.69 | 119.95 | 110.60 |
| 22 | 23S1 | 1413 | A | N1-C6-N6 | -18.69 | 107.38 | 118.60 |
| 22 | 23S1 | 1169 | A | C2-N3-C4 | 18.69 | 119.95 | 110.60 |
| 1 | 16S1 | 1019 | A | C2-N3-C4 | 18.69 | 119.95 | 110.60 |
| 22 | 23S1 | 1269 | A | C2-N3-C4 | 18.69 | 119.94 | 110.60 |
| 22 | 23S1 | 2333 | A | N1-C6-N6 | -18.69 | 107.39 | 118.60 |
| 22 | 23S1 | 2542 | A | N1-C2-N3 | -18.69 | 119.95 | 129.30 |
| 23 | 05S1 | 104 | A | N1-C2-N3 | -18.69 | 119.95 | 129.30 |
| 1 | 16S1 | 238 | A | C2-N3-C4 | 18.69 | 119.94 | 110.60 |
| 22 | 23S1 | 689 | A | N1-C6-N6 | -18.69 | 107.39 | 118.60 |
| 1 | 16S1 | 349 | A | C2-N3-C4 | 18.69 | 119.94 | 110.60 |
| 1 | 16S1 | 1437 | A | N1-C6-N6 | -18.68 | 107.39 | 118.60 |
| 22 | 23S1 | 1284 | A | N1-C6-N6 | -18.68 | 107.39 | 118.60 |
| 22 | 23S1 | 2657 | A | N1-C6-N6 | -18.68 | 107.39 | 118.60 |
| 1 | 16S1 | 747 | A | N1-C6-N6 | -18.68 | 107.39 | 118.60 |
| 22 | 23S1 | 705 | A | C2-N3-C4 | 18.68 | 119.94 | 110.60 |
| 22 | 23S1 | 1365 | A | N1-C2-N3 | -18.68 | 119.96 | 129.30 |
| 1 | 16S1 | 1503 | A | C2-N3-C4 | 18.68 | 119.94 | 110.60 |
| 22 | 23S1 | 984 | A | N1-C2-N3 | -18.68 | 119.96 | 129.30 |
| 22 | 23S1 | 2482 | A | C2-N3-C4 | 18.68 | 119.94 | 110.60 |
| 22 | 23S1 | 348 | A | C2-N3-C4 | 18.68 | 119.94 | 110.60 |
| 23 | 05S1 | 109 | A | C2-N3-C4 | 18.68 | 119.94 | 110.60 |
| 1 | 16S1 | 499 | A | C2-N3-C4 | 18.68 | 119.94 | 110.60 |
| 1 | 16S1 | 1014 | A | C2-N3-C4 | 18.68 | 119.94 | 110.60 |
| 22 | 23S1 | 324 | A | N1-C2-N3 | -18.68 | 119.96 | 129.30 |
| 22 | 23S1 | 2534 | A | C2-N3-C4 | 18.68 | 119.94 | 110.60 |
| 22 | 23S1 | 911 | A | C2-N3-C4 | 18.68 | 119.94 | 110.60 |
| 1 | 16S1 | 1332 | A | C2-N3-C4 | 18.68 | 119.94 | 110.60 |
| 22 | 23S1 | 2706 | A | N1-C2-N3 | -18.68 | 119.96 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 2753 | A | N1-C2-N3 | -18.68 | 119.96 | 129.30 |
| 55 | PTR1 | 23 | A | N1-C2-N3 | -18.68 | 119.96 | 129.30 |
| 22 | 23S1 | 753 | A | N1-C6-N6 | -18.67 | 107.40 | 118.60 |
| 22 | 23S1 | 1549 | A | C2-N3-C4 | 18.67 | 119.94 | 110.60 |
| 22 | 23S1 | 928 | A | N1-C2-N3 | -18.67 | 119.96 | 129.30 |
| 22 | 23S1 | 1308 | A | N1-C2-N3 | -18.67 | 119.97 | 129.30 |
| 22 | 23S1 | 1614 | A | N1-C2-N3 | -18.67 | 119.96 | 129.30 |
| 22 | 23S1 | 2134 | A | C2-N3-C4 | 18.67 | 119.94 | 110.60 |
| 1 | 16S1 | 487 | A | N1-C6-N6 | -18.67 | 107.40 | 118.60 |
| 22 | 23S1 | 2882 | A | N1-C6-N6 | -18.67 | 107.40 | 118.60 |
| 22 | 23S1 | 1385 | A | C2-N3-C4 | 18.67 | 119.93 | 110.60 |
| 22 | 23S1 | 1637 | A | N1-C2-N3 | -18.67 | 119.97 | 129.30 |
| 22 | 23S1 | 1803 | A | N1-C2-N3 | -18.67 | 119.97 | 129.30 |
| 22 | 23S1 | 2058 | A | N1-C2-N3 | -18.67 | 119.97 | 129.30 |
| 1 | 16S1 | 787 | A | N1-C6-N6 | -18.67 | 107.40 | 118.60 |
| 22 | 23S1 | 28 | A | N1-C6-N6 | -18.67 | 107.40 | 118.60 |
| 1 | 16S1 | 864 | A | C2-N3-C4 | 18.66 | 119.93 | 110.60 |
| 22 | 23S1 | 1274 | A | N1-C2-N3 | -18.66 | 119.97 | 129.30 |
| 22 | 23S1 | 2736 | A | N1-C2-N3 | -18.66 | 119.97 | 129.30 |
| 1 | 16S1 | 238 | A | N1-C2-N3 | -18.66 | 119.97 | 129.30 |
| 1 | 16S1 | 554 | A | N1-C2-N3 | -18.66 | 119.97 | 129.30 |
| 22 | 23S1 | 632 | A | C2-N3-C4 | 18.66 | 119.93 | 110.60 |
| 22 | 23S1 | 2439 | A | N1-C2-N3 | -18.66 | 119.97 | 129.30 |
| 23 | 05S1 | 46 | A | N1-C2-N3 | -18.66 | 119.97 | 129.30 |
| 1 | 16S1 | 1196 | A | N1-C6-N6 | -18.66 | 107.41 | 118.60 |
| 22 | 23S1 | 2287 | A | N1-C6-N6 | -18.66 | 107.41 | 118.60 |
| 22 | 23S1 | 2654 | A | N1-C2-N3 | -18.66 | 119.97 | 129.30 |
| 22 | 23S1 | 750 | A | N1-C6-N6 | -18.65 | 107.41 | 118.60 |
| 22 | 23S1 | 1495 | A | C2-N3-C4 | 18.65 | 119.93 | 110.60 |
| 22 | 23S1 | 1815 | A | C2-N3-C4 | 18.65 | 119.93 | 110.60 |
| 1 | 16S1 | 309 | A | C2-N3-C4 | 18.65 | 119.93 | 110.60 |
| 22 | 23S1 | 2267 | A | N1-C2-N3 | -18.65 | 119.97 | 129.30 |
| 22 | 23S1 | 794 | A | N1-C2-N3 | -18.65 | 119.97 | 129.30 |
| 1 | 16S1 | 19 | A | N1-C6-N6 | -18.65 | 107.41 | 118.60 |
| 22 | 23S1 | 633 | A | N1-C2-N3 | -18.65 | 119.98 | 129.30 |
| 1 | 16S1 | 935 | A | C2-N3-C4 | 18.65 | 119.92 | 110.60 |
| 22 | 23S1 | 94 | A | C2-N3-C4 | 18.65 | 119.92 | 110.60 |
| 1 | 16S1 | 983 | A | N1-C6-N6 | -18.65 | 107.41 | 118.60 |
| 22 | 23S1 | 1096 | A | C2-N3-C4 | 18.65 | 119.92 | 110.60 |
| 22 | 23S1 | 2778 | A | N1-C6-N6 | -18.65 | 107.41 | 118.60 |
| 1 | 16S1 | 554 | A | C2-N3-C4 | 18.64 | 119.92 | 110.60 |
| 22 | 23S1 | 347 | A | N1-C6-N6 | -18.64 | 107.41 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 1155 | A | N1-C2-N3 | -18.64 | 119.98 | 129.30 |
| 22 | 23S1 | 167 | A | N1-C6-N6 | -18.64 | 107.41 | 118.60 |
| 22 | 23S1 | 278 | A | N1-C2-N3 | -18.64 | 119.98 | 129.30 |
| 22 | 23S1 | 2577 | A | C2-N3-C4 | 18.64 | 119.92 | 110.60 |
| 55 | PTR1 | 69 | A | C2-N3-C4 | 18.64 | 119.92 | 110.60 |
| 1 | 16S1 | 1480 | A | C2-N3-C4 | 18.64 | 119.92 | 110.60 |
| 22 | 23S1 | 49 | A | N1-C2-N3 | -18.64 | 119.98 | 129.30 |
| 22 | 23S1 | 917 | A | N1-C6-N6 | -18.64 | 107.42 | 118.60 |
| 22 | 23S1 | 1084 | A | C2-N3-C4 | 18.64 | 119.92 | 110.60 |
| 22 | 23S1 | 2589 | A | N1-C6-N6 | -18.64 | 107.42 | 118.60 |
| 22 | 23S1 | 95 | A | N1-C2-N3 | -18.64 | 119.98 | 129.30 |
| 22 | 23S1 | 900 | A | C2-N3-C4 | 18.64 | 119.92 | 110.60 |
| 22 | 23S1 | 2757 | A | N1-C6-N6 | -18.64 | 107.42 | 118.60 |
| 22 | 23S1 | 1509 | A | N1-C2-N3 | -18.64 | 119.98 | 129.30 |
| 22 | 23S1 | 2108 | A | C2-N3-C4 | 18.64 | 119.92 | 110.60 |
| 22 | 23S1 | 2435 | A | C2-N3-C4 | 18.64 | 119.92 | 110.60 |
| 22 | 23S1 | 756 | A | N1-C6-N6 | -18.64 | 107.42 | 118.60 |
| 1 | 16S1 | 1042 | A | N1-C2-N3 | -18.64 | 119.98 | 129.30 |
| 22 | 23S1 | 262 | A | N1-C2-N3 | -18.64 | 119.98 | 129.30 |
| 22 | 23S1 | 2600 | A | N1-C2-N3 | -18.64 | 119.98 | 129.30 |
| 22 | 23S1 | 2711 | A | C2-N3-C4 | 18.64 | 119.92 | 110.60 |
| 22 | 23S1 | 2886 | A | C2-N3-C4 | 18.64 | 119.92 | 110.60 |
| 22 | 23S1 | 661 | A | N1-C6-N6 | -18.63 | 107.42 | 118.60 |
| 1 | 16S1 | 195 | A | N1-C6-N6 | -18.63 | 107.42 | 118.60 |
| 1 | 16S1 | 938 | A | N1-C2-N3 | -18.63 | 119.98 | 129.30 |
| 1 | 16S1 | 1363 | A | N1-C2-N3 | -18.63 | 119.98 | 129.30 |
| 22 | 23S1 | 1819 | A | N1-C6-N6 | -18.63 | 107.42 | 118.60 |
| 1 | 16S1 | 792 | A | N1-C6-N6 | -18.63 | 107.42 | 118.60 |
| 22 | 23S1 | 1717 | A | C2-N3-C4 | 18.63 | 119.91 | 110.60 |
| 1 | 16S1 | 50 | A | C2-N3-C4 | 18.62 | 119.91 | 110.60 |
| 1 | 16S1 | 1179 | A | N1-C2-N3 | -18.62 | 119.99 | 129.30 |
| 22 | 23S1 | 528 | A | N1-C6-N6 | -18.62 | 107.42 | 118.60 |
| 22 | 23S1 | 1103 | A | C2-N3-C4 | 18.62 | 119.91 | 110.60 |
| 22 | 23S1 | 1960 | A | N1-C2-N3 | -18.62 | 119.99 | 129.30 |
| 22 | 23S1 | 2119 | A | C2-N3-C4 | 18.62 | 119.91 | 110.60 |
| 1 | 16S1 | 908 | A | C2-N3-C4 | 18.62 | 119.91 | 110.60 |
| 22 | 23S1 | 472 | A | N1-C2-N3 | -18.62 | 119.99 | 129.30 |
| 22 | 23S1 | 1048 | A | N1-C6-N6 | -18.62 | 107.43 | 118.60 |
| 22 | 23S1 | 2682 | A | N1-C6-N6 | -18.62 | 107.42 | 118.60 |
| 22 | 23S1 | 2741 | A | N1-C6-N6 | -18.62 | 107.43 | 118.60 |
| 22 | 23S1 | 2893 | A | C2-N3-C4 | 18.62 | 119.91 | 110.60 |
| 1 | 16S1 | 371 | A | N1-C2-N3 | -18.62 | 119.99 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 435 | A | N1-C2-N3 | -18.62 | 119.99 | 129.30 |
| 22 | 23S1 | 1095 | A | C2-N3-C4 | 18.62 | 119.91 | 110.60 |
| 22 | 23S1 | 2406 | A | N1-C6-N6 | -18.62 | 107.43 | 118.60 |
| 1 | 16S1 | 250 | A | N1-C2-N3 | -18.62 | 119.99 | 129.30 |
| 23 | 05S1 | 53 | A | C2-N3-C4 | 18.62 | 119.91 | 110.60 |
| 22 | 23S1 | 391 | A | N1-C6-N6 | -18.61 | 107.43 | 118.60 |
| 22 | 23S1 | 1505 | A | N1-C6-N6 | -18.61 | 107.43 | 118.60 |
| 22 | 23S1 | 2135 | A | C2-N3-C4 | 18.61 | 119.91 | 110.60 |
| 22 | 23S1 | 2077 | A | C2-N3-C4 | 18.61 | 119.91 | 110.60 |
| 22 | 23S1 | 2358 | A | N1-C2-N3 | -18.61 | 120.00 | 129.30 |
| 22 | 23S1 | 2727 | A | N1-C6-N6 | -18.61 | 107.43 | 118.60 |
| 22 | 23S1 | 2810 | A | N1-C6-N6 | -18.61 | 107.43 | 118.60 |
| 1 | 16S1 | 66 | A | N1-C2-N3 | -18.61 | 120.00 | 129.30 |
| 22 | 23S1 | 423 | A | N1-C2-N3 | -18.61 | 120.00 | 129.30 |
| 1 | 16S1 | 782 | A | C2-N3-C4 | 18.61 | 119.90 | 110.60 |
| 1 | 16S1 | 918 | A | N1-C2-N3 | -18.61 | 120.00 | 129.30 |
| 1 | 16S1 | 1248 | A | N1-C6-N6 | -18.61 | 107.44 | 118.60 |
| 1 | 16S1 | 1274 | A | N1-C2-N3 | -18.61 | 120.00 | 129.30 |
| 22 | 23S1 | 1700 | A | N1-C2-N3 | -18.61 | 120.00 | 129.30 |
| 22 | 23S1 | 2284 | A | N1-C6-N6 | -18.61 | 107.44 | 118.60 |
| 22 | 23S1 | 1096 | A | N1-C2-N3 | -18.60 | 120.00 | 129.30 |
| 22 | 23S1 | 1111 | A | N1-C2-N3 | -18.60 | 120.00 | 129.30 |
| 22 | 23S1 | 2377 | A | N1-C6-N6 | -18.60 | 107.44 | 118.60 |
| 22 | 23S1 | 428 | A | N1-C2-N3 | -18.60 | 120.00 | 129.30 |
| 22 | 23S1 | 1912 | A | N1-C6-N6 | -18.60 | 107.44 | 118.60 |
| 22 | 23S1 | 2378 | A | N1-C2-N3 | -18.60 | 120.00 | 129.30 |
| 1 | 16S1 | 139 | A | N1-C2-N3 | -18.60 | 120.00 | 129.30 |
| 22 | 23S1 | 2101 | A | N1-C2-N3 | -18.60 | 120.00 | 129.30 |
| 22 | 23S1 | 2721 | A | N1-C2-N3 | -18.60 | 120.00 | 129.30 |
| 1 | 16S1 | 907 | A | N1-C2-N3 | -18.60 | 120.00 | 129.30 |
| 1 | 16S1 | 1016 | A | N1-C6-N6 | -18.60 | 107.44 | 118.60 |
| 22 | 23S1 | 1014 | A | N1-C6-N6 | -18.60 | 107.44 | 118.60 |
| 22 | 23S1 | 1342 | A | C2-N3-C4 | 18.60 | 119.90 | 110.60 |
| 22 | 23S1 | 1545 | A | C2-N3-C4 | 18.60 | 119.90 | 110.60 |
| 22 | 23S1 | 819 | A | N1-C2-N3 | -18.60 | 120.00 | 129.30 |
| 22 | 23S1 | 2740 | A | N1-C6-N6 | -18.60 | 107.44 | 118.60 |
| 1 | 16S1 | 16 | A | C2-N3-C4 | 18.59 | 119.90 | 110.60 |
| 22 | 23S1 | 572 | A | N1-C6-N6 | -18.59 | 107.44 | 118.60 |
| 22 | 23S1 | 2748 | A | N1-C2-N3 | -18.59 | 120.00 | 129.30 |
| 23 | 05S1 | 78 | A | C2-N3-C4 | 18.59 | 119.90 | 110.60 |
| 22 | 23S1 | 735 | A | N1-C6-N6 | -18.59 | 107.44 | 118.60 |
| 1 | 16S1 | 1507 | A | C2-N3-C4 | 18.59 | 119.90 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 91 | A | N1-C6-N6 | -18.59 | 107.44 | 118.60 |
| 22 | 23S1 | 279 | A | N1-C2-N3 | -18.59 | 120.00 | 129.30 |
| 22 | 23S1 | 626 | A | C2-N3-C4 | 18.59 | 119.90 | 110.60 |
| 22 | 23S1 | 1096 | A | N1-C6-N6 | -18.59 | 107.44 | 118.60 |
| 1 | 16S1 | 298 | A | N1-C6-N6 | -18.59 | 107.45 | 118.60 |
| 22 | 23S1 | 1598 | A | N1-C2-N3 | -18.59 | 120.01 | 129.30 |
| 22 | 23S1 | 2733 | A | C2-N3-C4 | 18.59 | 119.89 | 110.60 |
| 22 | 23S1 | 1147 | A | N1-C2-N3 | -18.59 | 120.01 | 129.30 |
| 22 | 23S1 | 1821 | A | N1-C6-N6 | -18.59 | 107.45 | 118.60 |
| 1 | 16S1 | 807 | A | N1-C6-N6 | -18.58 | 107.45 | 118.60 |
| 22 | 23S1 | 311 | A | N1-C6-N6 | -18.58 | 107.45 | 118.60 |
| 1 | 16S1 | 1151 | A | N1-C6-N6 | -18.58 | 107.45 | 118.60 |
| 1 | 16S1 | 1236 | A | N1-C6-N6 | -18.58 | 107.45 | 118.60 |
| 22 | 23S1 | 2392 | A | C2-N3-C4 | 18.58 | 119.89 | 110.60 |
| 22 | 23S1 | 1156 | A | C2-N3-C4 | 18.58 | 119.89 | 110.60 |
| 22 | 23S1 | 2071 | A | C2-N3-C4 | 18.58 | 119.89 | 110.60 |
| 1 | 16S1 | 715 | A | C2-N3-C4 | 18.58 | 119.89 | 110.60 |
| 22 | 23S1 | 730 | A | N1-C2-N3 | -18.58 | 120.01 | 129.30 |
| 22 | 23S1 | 933 | A | N1-C6-N6 | -18.58 | 107.45 | 118.60 |
| 22 | 23S1 | 2733 | A | N1-C2-N3 | -18.58 | 120.01 | 129.30 |
| 22 | 23S1 | 2809 | A | N1-C6-N6 | -18.58 | 107.45 | 118.60 |
| 1 | 16S1 | 608 | A | N1-C2-N3 | -18.58 | 120.01 | 129.30 |
| 22 | 23S1 | 322 | A | C2-N3-C4 | 18.58 | 119.89 | 110.60 |
| 22 | 23S1 | 718 | A | C2-N3-C4 | 18.58 | 119.89 | 110.60 |
| 22 | 23S1 | 1597 | A | N1-C2-N3 | -18.58 | 120.01 | 129.30 |
| 1 | 16S1 | 1375 | A | N1-C2-N3 | -18.58 | 120.01 | 129.30 |
| 1 | 16S1 | 1188 | A | C2-N3-C4 | 18.57 | 119.89 | 110.60 |
| 22 | 23S1 | 1819 | A | N1-C2-N3 | -18.57 | 120.01 | 129.30 |
| 22 | 23S1 | 1899 | A | N1-C6-N6 | -18.57 | 107.45 | 118.60 |
| 1 | 16S1 | 753 | A | N1-C2-N3 | -18.57 | 120.01 | 129.30 |
| 1 | 16S1 | 1534 | A | C2-N3-C4 | 18.57 | 119.89 | 110.60 |
| 22 | 23S1 | 2748 | A | C2-N3-C4 | 18.57 | 119.89 | 110.60 |
| 23 | 05S1 | 73 | A | N1-C6-N6 | -18.57 | 107.46 | 118.60 |
| 22 | 23S1 | 95 | A | C2-N3-C4 | 18.57 | 119.89 | 110.60 |
| 22 | 23S1 | 863 | A | N1-C2-N3 | -18.57 | 120.02 | 129.30 |
| 22 | 23S1 | 1698 | A | N1-C2-N3 | -18.57 | 120.02 | 129.30 |
| 22 | 23S1 | 1877 | A | N1-C6-N6 | -18.57 | 107.46 | 118.60 |
| 22 | 23S1 | 344 | A | C2-N3-C4 | 18.57 | 119.88 | 110.60 |
| 22 | 23S1 | 705 | A | N1-C2-N3 | -18.57 | 120.02 | 129.30 |
| 22 | 23S1 | 1169 | A | N1-C2-N3 | -18.57 | 120.02 | 129.30 |
| 22 | 23S1 | 300 | A | N1-C6-N6 | -18.57 | 107.46 | 118.60 |
| 22 | 23S1 | 2317 | A | C2-N3-C4 | 18.57 | 119.88 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 2602 | A | C2-N3-C4 | 18.57 | 119.88 | 110.60 |
| 22 | 23S1 | 990 | A | N1-C6-N6 | -18.56 | 107.46 | 118.60 |
| 23 | 05S1 | 94 | A | N1-C2-N3 | -18.56 | 120.02 | 129.30 |
| 1 | 16S1 | 262 | A | N1-C6-N6 | -18.56 | 107.46 | 118.60 |
| 1 | 16S1 | 1252 | A | N1-C2-N3 | -18.56 | 120.02 | 129.30 |
| 22 | 23S1 | 1596 | A | C2-N3-C4 | 18.56 | 119.88 | 110.60 |
| 22 | 23S1 | 1088 | A | N1-C2-N3 | -18.56 | 120.02 | 129.30 |
| 22 | 23S1 | 1616 | A | C2-N3-C4 | 18.56 | 119.88 | 110.60 |
| 22 | 23S1 | 2434 | A | N1-C2-N3 | -18.56 | 120.02 | 129.30 |
| 1 | 16S1 | 1349 | A | N1-C6-N6 | -18.56 | 107.47 | 118.60 |
| 22 | 23S1 | 430 | A | N1-C2-N3 | -18.56 | 120.02 | 129.30 |
| 22 | 23S1 | 721 | A | C2-N3-C4 | 18.56 | 119.88 | 110.60 |
| 22 | 23S1 | 1008 | A | N1-C6-N6 | -18.56 | 107.47 | 118.60 |
| 22 | 23S1 | 2850 | A | N1-C6-N6 | -18.56 | 107.47 | 118.60 |
| 1 | 16S1 | 28 | A | N1-C2-N3 | -18.56 | 120.02 | 129.30 |
| 22 | 23S1 | 1641 | A | N1-C6-N6 | -18.56 | 107.47 | 118.60 |
| 1 | 16S1 | 382 | A | N1-C2-N3 | -18.55 | 120.02 | 129.30 |
| 1 | 16S1 | 374 | A | C2-N3-C4 | 18.55 | 119.88 | 110.60 |
| 1 | 16S1 | 482 | A | N1-C6-N6 | -18.55 | 107.47 | 118.60 |
| 1 | 16S1 | 609 | A | C2-N3-C4 | 18.55 | 119.88 | 110.60 |
| 22 | 23S1 | 990 | A | C2-N3-C4 | 18.55 | 119.88 | 110.60 |
| 1 | 16S1 | 182 | A | C2-N3-C4 | 18.55 | 119.88 | 110.60 |
| 1 | 16S1 | 831 | A | N1-C2-N3 | -18.55 | 120.02 | 129.30 |
| 1 | 16S1 | 1311 | A | N1-C2-N3 | -18.55 | 120.02 | 129.30 |
| 22 | 23S1 | 1677 | A | N1-C6-N6 | -18.55 | 107.47 | 118.60 |
| 22 | 23S1 | 2560 | A | N1-C6-N6 | -18.55 | 107.47 | 118.60 |
| 22 | 23S1 | 2435 | A | N1-C2-N3 | -18.55 | 120.03 | 129.30 |
| 22 | 23S1 | 483 | A | C2-N3-C4 | 18.55 | 119.87 | 110.60 |
| 22 | 23S1 | 1966 | A | N1-C6-N6 | -18.55 | 107.47 | 118.60 |
| 1 | 16S1 | 320 | A | N1-C2-N3 | -18.54 | 120.03 | 129.30 |
| 22 | 23S1 | 83 | A | N1-C2-N3 | -18.54 | 120.03 | 129.30 |
| 22 | 23S1 | 1689 | A | C2-N3-C4 | 18.54 | 119.87 | 110.60 |
| 1 | 16S1 | 860 | A | C2-N3-C4 | 18.54 | 119.87 | 110.60 |
| 22 | 23S1 | 1690 | A | N1-C6-N6 | -18.54 | 107.47 | 118.60 |
| 1 | 16S1 | 223 | A | N1-C2-N3 | -18.54 | 120.03 | 129.30 |
| 22 | 23S1 | 1070 | A | N1-C2-N3 | -18.54 | 120.03 | 129.30 |
| 22 | 23S1 | 95 | A | N1-C6-N6 | -18.54 | 107.48 | 118.60 |
| 22 | 23S1 | 1580 | A | C2-N3-C4 | 18.54 | 119.87 | 110.60 |
| 22 | 23S1 | 2810 | A | N1-C2-N3 | -18.54 | 120.03 | 129.30 |
| 1 | 16S1 | 356 | A | N1-C2-N3 | -18.53 | 120.03 | 129.30 |
| 1 | 16S1 | 1092 | A | C2-N3-C4 | 18.53 | 119.87 | 110.60 |
| 1 | 16S1 | 452 | A | N1-C2-N3 | -18.53 | 120.03 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 274 | A | N1-C6-N6 | -18.53 | 107.48 | 118.60 |
| 22 | 23S1 | 83 | A | N1-C6-N6 | -18.53 | 107.48 | 118.60 |
| 22 | 23S1 | 575 | A | C2-N3-C4 | 18.53 | 119.86 | 110.60 |
| 22 | 23S1 | 1260 | A | N1-C2-N3 | -18.53 | 120.03 | 129.30 |
| 22 | 23S1 | 1393 | A | N1-C6-N6 | -18.53 | 107.48 | 118.60 |
| 22 | 23S1 | 1509 | A | C2-N3-C4 | 18.53 | 119.86 | 110.60 |
| 1 | 16S1 | 160 | A | C2-N3-C4 | 18.53 | 119.86 | 110.60 |
| 1 | 16S1 | 431 | A | C2-N3-C4 | 18.53 | 119.86 | 110.60 |
| 22 | 23S1 | 391 | A | N1-C2-N3 | -18.53 | 120.04 | 129.30 |
| 22 | 23S1 | 1854 | A | C2-N3-C4 | 18.53 | 119.86 | 110.60 |
| 22 | 23S1 | 1877 | A | N1-C2-N3 | -18.53 | 120.04 | 129.30 |
| 1 | 16S1 | 1468 | A | N1-C2-N3 | -18.52 | 120.04 | 129.30 |
| 22 | 23S1 | 2814 | A | N1-C2-N3 | -18.52 | 120.04 | 129.30 |
| 22 | 23S1 | 2051 | A | N1-C6-N6 | -18.52 | 107.49 | 118.60 |
| 1 | 16S1 | 338 | A | C2-N3-C4 | 18.52 | 119.86 | 110.60 |
| 1 | 16S1 | 1021 | A | N1-C6-N6 | -18.52 | 107.49 | 118.60 |
| 22 | 23S1 | 182 | A | C2-N3-C4 | 18.52 | 119.86 | 110.60 |
| 22 | 23S1 | 789 | A | N1-C6-N6 | -18.52 | 107.49 | 118.60 |
| 1 | 16S1 | 199 | A | N1-C6-N6 | -18.52 | 107.49 | 118.60 |
| 22 | 23S1 | 655 | A | N1-C6-N6 | -18.52 | 107.49 | 118.60 |
| 1 | 16S1 | 1216 | A | N1-C6-N6 | -18.52 | 107.49 | 118.60 |
| 22 | 23S1 | 218 | A | N1-C2-N3 | -18.52 | 120.04 | 129.30 |
| 22 | 23S1 | 1322 | A | C2-N3-C4 | 18.52 | 119.86 | 110.60 |
| 22 | 23S1 | 2268 | A | C2-N3-C4 | 18.52 | 119.86 | 110.60 |
| 22 | 23S1 | 2679 | A | N1-C2-N3 | -18.52 | 120.04 | 129.30 |
| 22 | 23S1 | 2899 | A | C2-N3-C4 | 18.52 | 119.86 | 110.60 |
| 1 | 16S1 | 1431 | A | N1-C6-N6 | -18.52 | 107.49 | 118.60 |
| 22 | 23S1 | 1572 | A | N1-C2-N3 | -18.51 | 120.04 | 129.30 |
| 1 | 16S1 | 996 | A | N1-C6-N6 | -18.51 | 107.49 | 118.60 |
| 22 | 23S1 | 1194 | A | N1-C2-N3 | -18.51 | 120.05 | 129.30 |
| 22 | 23S1 | 2547 | A | N1-C2-N3 | -18.51 | 120.05 | 129.30 |
| 1 | 16S1 | 1483 | A | C2-N3-C4 | 18.51 | 119.85 | 110.60 |
| 22 | 23S1 | 368 | A | C2-N3-C4 | 18.51 | 119.85 | 110.60 |
| 22 | 23S1 | 633 | A | C2-N3-C4 | 18.51 | 119.85 | 110.60 |
| 22 | 23S1 | 2799 | A | C2-N3-C4 | 18.51 | 119.85 | 110.60 |
| 1 | 16S1 | 1261 | A | C2-N3-C4 | 18.51 | 119.85 | 110.60 |
| 22 | 23S1 | 756 | A | N1-C2-N3 | -18.50 | 120.05 | 129.30 |
| 22 | 23S1 | 1610 | A | N1-C6-N6 | -18.50 | 107.50 | 118.60 |
| 22 | 23S1 | 1028 | A | N1-C6-N6 | -18.50 | 107.50 | 118.60 |
| 22 | 23S1 | 2856 | A | N1-C2-N3 | -18.50 | 120.05 | 129.30 |
| 22 | 23S1 | 668 | A | C2-N3-C4 | 18.50 | 119.85 | 110.60 |
| 22 | 23S1 | 1608 | A | N1-C6-N6 | -18.50 | 107.50 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 1204 | A | C2-N3-C4 | 18.50 | 119.85 | 110.60 |
| 22 | 23S1 | 1086 | A | N1-C6-N6 | -18.50 | 107.50 | 118.60 |
| 1 | 16S1 | 325 | A | N1-C6-N6 | -18.50 | 107.50 | 118.60 |
| 1 | 16S1 | 1289 | A | C2-N3-C4 | 18.50 | 119.85 | 110.60 |
| 22 | 23S1 | 1134 | A | C2-N3-C4 | 18.50 | 119.85 | 110.60 |
| 22 | 23S1 | 1586 | A | N1-C2-N3 | -18.50 | 120.05 | 129.30 |
| 22 | 23S1 | 2856 | A | C2-N3-C4 | 18.50 | 119.85 | 110.60 |
| 1 | 16S1 | 66 | A | C2-N3-C4 | 18.49 | 119.85 | 110.60 |
| 1 | 16S1 | 1170 | A | C2-N3-C4 | 18.49 | 119.85 | 110.60 |
| 1 | 16S1 | 1394 | A | C2-N3-C4 | 18.49 | 119.85 | 110.60 |
| 22 | 23S1 | 735 | A | C2-N3-C4 | 18.49 | 119.84 | 110.60 |
| 22 | 23S1 | 1274 | A | C2-N3-C4 | 18.49 | 119.84 | 110.60 |
| 1 | 16S1 | 366 | A | C2-N3-C4 | 18.49 | 119.84 | 110.60 |
| 1 | 16S1 | 495 | A | N1-C6-N6 | -18.49 | 107.51 | 118.60 |
| 1 | 16S1 | 595 | A | N1-C6-N6 | -18.49 | 107.51 | 118.60 |
| 22 | 23S1 | 1383 | A | N1-C6-N6 | -18.49 | 107.51 | 118.60 |
| 22 | 23S1 | 1669 | A | N1-C2-N3 | -18.49 | 120.06 | 129.30 |
| 1 | 16S1 | 155 | A | N1-C2-N3 | -18.49 | 120.06 | 129.30 |
| 22 | 23S1 | 2565 | A | N1-C6-N6 | -18.49 | 107.51 | 118.60 |
| 1 | 16S1 | 600 | A | N1-C2-N3 | -18.49 | 120.06 | 129.30 |
| 1 | 16S1 | 878 | A | N1-C2-N3 | -18.49 | 120.06 | 129.30 |
| 1 | 16S1 | 878 | A | N1-C6-N6 | -18.49 | 107.51 | 118.60 |
| 22 | 23S1 | 2530 | A | C2-N3-C4 | 18.49 | 119.84 | 110.60 |
| 22 | 23S1 | 2135 | A | N1-C2-N3 | -18.48 | 120.06 | 129.30 |
| 22 | 23S1 | 2439 | A | N1-C6-N6 | -18.48 | 107.51 | 118.60 |
| 22 | 23S1 | 1010 | A | N1-C6-N6 | -18.48 | 107.51 | 118.60 |
| 22 | 23S1 | 1641 | A | N1-C2-N3 | -18.48 | 120.06 | 129.30 |
| 22 | 23S1 | 1664 | A | C2-N3-C4 | 18.48 | 119.84 | 110.60 |
| 1 | 16S1 | 873 | A | C2-N3-C4 | 18.48 | 119.84 | 110.60 |
| 1 | 16S1 | 1256 | A | N1-C2-N3 | -18.48 | 120.06 | 129.30 |
| 22 | 23S1 | 979 | A | C2-N3-C4 | 18.48 | 119.84 | 110.60 |
| 22 | 23S1 | 1054 | A | N1-C2-N3 | -18.48 | 120.06 | 129.30 |
| 1 | 16S1 | 1508 | A | N1-C6-N6 | -18.48 | 107.51 | 118.60 |
| 1 | 16S1 | 98 | A | N1-C6-N6 | -18.48 | 107.51 | 118.60 |
| 1 | 16S1 | 572 | A | C2-N3-C4 | 18.48 | 119.84 | 110.60 |
| 1 | 16S1 | 1430 | A | N1-C2-N3 | -18.48 | 120.06 | 129.30 |
| 22 | 23S1 | 920 | A | C2-N3-C4 | 18.48 | 119.84 | 110.60 |
| 1 | 16S1 | 1434 | A | N1-C6-N6 | -18.48 | 107.51 | 118.60 |
| 22 | 23S1 | 84 | A | C2-N3-C4 | 18.48 | 119.84 | 110.60 |
| 22 | 23S1 | 415 | A | N1-C2-N3 | -18.48 | 120.06 | 129.30 |
| 22 | 23S1 | 1580 | A | N1-C2-N3 | -18.48 | 120.06 | 129.30 |
| 22 | 23S1 | 2198 | A | N1-C6-N6 | -18.48 | 107.52 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1854 | A | N1-C2-N3 | -18.47 | 120.06 | 129.30 |
| 22 | 23S1 | 2058 | A | C2-N3-C4 | 18.47 | 119.84 | 110.60 |
| 1 | 16S1 | 1456 | A | C2-N3-C4 | 18.47 | 119.83 | 110.60 |
| 22 | 23S1 | 609 | A | N1-C2-N3 | -18.47 | 120.06 | 129.30 |
| 22 | 23S1 | 1504 | A | C2-N3-C4 | 18.47 | 119.83 | 110.60 |
| 22 | 23S1 | 1889 | A | N1-C6-N6 | -18.47 | 107.52 | 118.60 |
| 22 | 23S1 | 2273 | A | N1-C6-N6 | -18.47 | 107.52 | 118.60 |
| 22 | 23S1 | 2433 | A | N1-C2-N3 | -18.47 | 120.06 | 129.30 |
| 22 | 23S1 | 2887 | A | C2-N3-C4 | 18.47 | 119.83 | 110.60 |
| 1 | 16S1 | 968 | A | C2-N3-C4 | 18.47 | 119.83 | 110.60 |
| 22 | 23S1 | 439 | A | N1-C2-N3 | -18.47 | 120.07 | 129.30 |
| 22 | 23S1 | 2003 | A | N1-C2-N3 | -18.47 | 120.07 | 129.30 |
| 22 | 23S1 | 2336 | A | N1-C6-N6 | -18.47 | 107.52 | 118.60 |
| 22 | 23S1 | 2366 | A | N1-C2-N3 | -18.47 | 120.07 | 129.30 |
| 1 | 16S1 | 33 | A | N1-C2-N3 | -18.46 | 120.07 | 129.30 |
| 1 | 16S1 | 196 | A | N1-C2-N3 | -18.46 | 120.07 | 129.30 |
| 22 | 23S1 | 83 | A | C2-N3-C4 | 18.46 | 119.83 | 110.60 |
| 22 | 23S1 | 244 | A | N1-C6-N6 | -18.46 | 107.52 | 118.60 |
| 22 | 23S1 | 699 | A | N1-C6-N6 | -18.46 | 107.52 | 118.60 |
| 22 | 23S1 | 2241 | A | N1-C6-N6 | -18.46 | 107.52 | 118.60 |
| 22 | 23S1 | 721 | A | N1-C2-N3 | -18.46 | 120.07 | 129.30 |
| 1 | 16S1 | 205 | A | N1-C6-N6 | -18.46 | 107.52 | 118.60 |
| 1 | 16S1 | 430 | A | N1-C2-N3 | -18.46 | 120.07 | 129.30 |
| 22 | 23S1 | 492 | A | N1-C2-N3 | -18.46 | 120.07 | 129.30 |
| 22 | 23S1 | 1787 | A | N1-C2-N3 | -18.46 | 120.07 | 129.30 |
| 1 | 16S1 | 959 | A | C2-N3-C4 | 18.46 | 119.83 | 110.60 |
| 22 | 23S1 | 332 | A | C2-N3-C4 | 18.46 | 119.83 | 110.60 |
| 22 | 23S1 | 1596 | A | N1-C2-N3 | -18.46 | 120.07 | 129.30 |
| 22 | 23S1 | 2336 | A | C2-N3-C4 | 18.46 | 119.83 | 110.60 |
| 1 | 16S1 | 629 | A | N1-C2-N3 | -18.45 | 120.07 | 129.30 |
| 22 | 23S1 | 2170 | A | C2-N3-C4 | 18.45 | 119.83 | 110.60 |
| 22 | 23S1 | 1275 | A | C2-N3-C4 | 18.45 | 119.83 | 110.60 |
| 1 | 16S1 | 1219 | A | N1-C2-N3 | -18.45 | 120.07 | 129.30 |
| 22 | 23S1 | 2850 | A | C2-N3-C4 | 18.45 | 119.83 | 110.60 |
| 22 | 23S1 | 64 | A | N1-C2-N3 | -18.45 | 120.08 | 129.30 |
| 1 | 16S1 | 60 | A | C2-N3-C4 | 18.45 | 119.82 | 110.60 |
| 1 | 16S1 | 535 | A | C2-N3-C4 | 18.45 | 119.82 | 110.60 |
| 1 | 16S1 | 26 | A | N1-C6-N6 | -18.45 | 107.53 | 118.60 |
| 1 | 16S1 | 1179 | A | C2-N3-C4 | 18.45 | 119.82 | 110.60 |
| 22 | 23S1 | 1328 | A | N1-C2-N3 | -18.45 | 120.08 | 129.30 |
| 22 | 23S1 | 2451 | A | N1-C2-N3 | -18.45 | 120.08 | 129.30 |
| 1 | 16S1 | 78 | A | N1-C2-N3 | -18.44 | 120.08 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 479 | A | N1-C6-N6 | -18.44 | 107.53 | 118.60 |
| 1 | 16S1 | 366 | A | N1-C2-N3 | -18.44 | 120.08 | 129.30 |
| 22 | 23S1 | 1635 | A | N1-C6-N6 | -18.44 | 107.53 | 118.60 |
| 1 | 16S1 | 1257 | A | N1-C6-N6 | -18.44 | 107.54 | 118.60 |
| 1 | 16S1 | 181 | A | N1-C2-N3 | -18.44 | 120.08 | 129.30 |
| 1 | 16S1 | 696 | A | C2-N3-C4 | 18.44 | 119.82 | 110.60 |
| 1 | 16S1 | 766 | A | C2-N3-C4 | 18.44 | 119.82 | 110.60 |
| 1 | 16S1 | 1465 | A | N1-C2-N3 | -18.44 | 120.08 | 129.30 |
| 22 | 23S1 | 1505 | A | N1-C2-N3 | -18.44 | 120.08 | 129.30 |
| 22 | 23S1 | 1598 | A | N1-C6-N6 | -18.44 | 107.54 | 118.60 |
| 22 | 23S1 | 2657 | A | C2-N3-C4 | 18.43 | 119.82 | 110.60 |
| 1 | 16S1 | 253 | A | C2-N3-C4 | 18.43 | 119.82 | 110.60 |
| 22 | 23S1 | 2469 | A | C2-N3-C4 | 18.43 | 119.82 | 110.60 |
| 22 | 23S1 | 428 | A | N1-C6-N6 | -18.43 | 107.54 | 118.60 |
| 1 | 16S1 | 1349 | A | N1-C2-N3 | -18.43 | 120.09 | 129.30 |
| 1 | 16S1 | 1117 | A | N1-C6-N6 | -18.43 | 107.54 | 118.60 |
| 22 | 23S1 | 1698 | A | C2-N3-C4 | 18.43 | 119.81 | 110.60 |
| 22 | 23S1 | 1918 | A | N1-C2-N3 | -18.43 | 120.09 | 129.30 |
| 55 | PTR1 | 21 | A | N1-C6-N6 | -18.43 | 107.54 | 118.60 |
| 1 | 16S1 | 523 | A | N1-C2-N3 | -18.43 | 120.09 | 129.30 |
| 22 | 23S1 | 1029 | A | C2-N3-C4 | 18.43 | 119.81 | 110.60 |
| 55 | PTR1 | 69 | A | N1-C2-N3 | -18.43 | 120.09 | 129.30 |
| 22 | 23S1 | 422 | A | N1-C2-N3 | -18.42 | 120.09 | 129.30 |
| 22 | 23S1 | 2309 | A | N1-C6-N6 | -18.42 | 107.55 | 118.60 |
| 1 | 16S1 | 1036 | A | C2-N3-C4 | 18.42 | 119.81 | 110.60 |
| 1 | 16S1 | 487 | A | N1-C2-N3 | -18.42 | 120.09 | 129.30 |
| 22 | 23S1 | 2873 | A | N1-C2-N3 | -18.42 | 120.09 | 129.30 |
| 22 | 23S1 | 2900 | A | C2-N3-C4 | 18.42 | 119.81 | 110.60 |
| 1 | 16S1 | 914 | A | N1-C6-N6 | -18.42 | 107.55 | 118.60 |
| 1 | 16S1 | 949 | A | N1-C6-N6 | -18.41 | 107.55 | 118.60 |
| 1 | 16S1 | 743 | A | N1-C2-N3 | -18.41 | 120.09 | 129.30 |
| 22 | 23S1 | 2741 | A | C2-N3-C4 | 18.41 | 119.81 | 110.60 |
| 1 | 16S1 | 329 | A | N1-C2-N3 | -18.41 | 120.09 | 129.30 |
| 23 | 05S1 | 50 | A | N1-C6-N6 | -18.41 | 107.56 | 118.60 |
| 1 | 16S1 | 1285 | A | C2-N3-C4 | 18.41 | 119.80 | 110.60 |
| 22 | 23S1 | 213 | A | C2-N3-C4 | 18.41 | 119.80 | 110.60 |
| 22 | 23S1 | 1508 | A | C2-N3-C4 | 18.41 | 119.80 | 110.60 |
| 22 | 23S1 | 2070 | A | N1-C2-N3 | -18.41 | 120.10 | 129.30 |
| 22 | 23S1 | 988 | A | N1-C6-N6 | -18.40 | 107.56 | 118.60 |
| 1 | 16S1 | 7 | A | C2-N3-C4 | 18.40 | 119.80 | 110.60 |
| 22 | 23S1 | 1027 | A | N1-C2-N3 | -18.40 | 120.10 | 129.30 |
| 22 | 23S1 | 2868 | A | N1-C2-N3 | -18.40 | 120.10 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 1016 | A | C2-N3-C4 | 18.40 | 119.80 | 110.60 |
| 22 | 23S1 | 896 | A | C2-N3-C4 | 18.40 | 119.80 | 110.60 |
| 22 | 23S1 | 2660 | A | N1-C6-N6 | -18.40 | 107.56 | 118.60 |
| 22 | 23S1 | 1593 | A | N1-C6-N6 | -18.40 | 107.56 | 118.60 |
| 1 | 16S1 | 974 | A | C2-N3-C4 | 18.39 | 119.80 | 110.60 |
| 1 | 16S1 | 1410 | A | N1-C2-N3 | -18.39 | 120.10 | 129.30 |
| 1 | 16S1 | 1531 | A | N1-C2-N3 | -18.39 | 120.10 | 129.30 |
| 22 | 23S1 | 718 | A | N1-C6-N6 | -18.39 | 107.56 | 118.60 |
| 22 | 23S1 | 1665 | A | N1-C2-N3 | -18.39 | 120.10 | 129.30 |
| 22 | 23S1 | 1802 | A | N1-C2-N3 | -18.39 | 120.10 | 129.30 |
| 22 | 23S1 | 1285 | A | N1-C2-N3 | -18.39 | 120.10 | 129.30 |
| 22 | 23S1 | 2037 | A | N1-C6-N6 | -18.39 | 107.56 | 118.60 |
| 22 | 23S1 | 2753 | A | C2-N3-C4 | 18.39 | 119.80 | 110.60 |
| 1 | 16S1 | 1102 | A | N1-C2-N3 | -18.39 | 120.10 | 129.30 |
| 1 | 16S1 | 1254 | A | N1-C2-N3 | -18.39 | 120.11 | 129.30 |
| 22 | 23S1 | 574 | A | C2-N3-C4 | 18.39 | 119.79 | 110.60 |
| 22 | 23S1 | 1678 | A | C2-N3-C4 | 18.39 | 119.80 | 110.60 |
| 22 | 23S1 | 2059 | A | C2-N3-C4 | 18.39 | 119.80 | 110.60 |
| 22 | 23S1 | 2821 | A | N1-C6-N6 | -18.39 | 107.57 | 118.60 |
| 1 | 16S1 | 648 | A | N1-C2-N3 | -18.39 | 120.11 | 129.30 |
| 22 | 23S1 | 1393 | A | C2-N3-C4 | 18.39 | 119.79 | 110.60 |
| 22 | 23S1 | 2411 | A | N1-C2-N3 | -18.39 | 120.11 | 129.30 |
| 22 | 23S1 | 2534 | A | N1-C2-N3 | -18.39 | 120.11 | 129.30 |
| 22 | 23S1 | 1978 | A | N1-C6-N6 | -18.38 | 107.57 | 118.60 |
| 23 | 05S1 | 119 | A | N1-C2-N3 | -18.38 | 120.11 | 129.30 |
| 1 | 16S1 | 174 | A | N1-C2-N3 | -18.38 | 120.11 | 129.30 |
| 1 | 16S1 | 1274 | A | C2-N3-C4 | 18.38 | 119.79 | 110.60 |
| 1 | 16S1 | 974 | A | N1-C6-N6 | -18.38 | 107.57 | 118.60 |
| 22 | 23S1 | 1690 | A | C2-N3-C4 | 18.38 | 119.79 | 110.60 |
| 22 | 23S1 | 1803 | A | N1-C6-N6 | -18.38 | 107.57 | 118.60 |
| 1 | 16S1 | 160 | A | N1-C6-N6 | -18.38 | 107.57 | 118.60 |
| 1 | 16S1 | 1534 | A | N1-C2-N3 | -18.38 | 120.11 | 129.30 |
| 1 | 16S1 | 1180 | A | N1-C2-N3 | -18.38 | 120.11 | 129.30 |
| 22 | 23S1 | 1284 | A | C2-N3-C4 | 18.38 | 119.79 | 110.60 |
| 22 | 23S1 | 2590 | A | C2-N3-C4 | 18.38 | 119.79 | 110.60 |
| 1 | 16S1 | 1246 | A | N1-C6-N6 | -18.37 | 107.58 | 118.60 |
| 22 | 23S1 | 788 | A | C2-N3-C4 | 18.37 | 119.79 | 110.60 |
| 1 | 16S1 | 1492 | A | N1-C6-N6 | -18.37 | 107.58 | 118.60 |
| 1 | 16S1 | 630 | A | N1-C6-N6 | -18.37 | 107.58 | 118.60 |
| 1 | 16S1 | 782 | A | N1-C2-N3 | -18.37 | 120.11 | 129.30 |
| 22 | 23S1 | 1366 | A | N1-C6-N6 | -18.37 | 107.58 | 118.60 |
| 22 | 23S1 | 1987 | A | N1-C6-N6 | -18.37 | 107.58 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 256 | A | C2-N3-C4 | 18.37 | 119.78 | 110.60 |
| 1 | 16S1 | 74 | A | N1-C2-N3 | -18.37 | 120.12 | 129.30 |
| 22 | 23S1 | 670 | A | N1-C6-N6 | -18.37 | 107.58 | 118.60 |
| 22 | 23S1 | 715 | A | N1-C2-N3 | -18.37 | 120.12 | 129.30 |
| 1 | 16S1 | 996 | A | N1-C2-N3 | -18.36 | 120.12 | 129.30 |
| 22 | 23S1 | 2346 | A | C2-N3-C4 | 18.36 | 119.78 | 110.60 |
| 22 | 23S1 | 1272 | A | N1-C6-N6 | -18.36 | 107.58 | 118.60 |
| 22 | 23S1 | 2346 | A | N1-C2-N3 | -18.36 | 120.12 | 129.30 |
| 1 | 16S1 | 1044 | A | N1-C2-N3 | -18.36 | 120.12 | 129.30 |
| 22 | 23S1 | 255 | A | N1-C2-N3 | -18.36 | 120.12 | 129.30 |
| 22 | 23S1 | 782 | A | N1-C2-N3 | -18.36 | 120.12 | 129.30 |
| 1 | 16S1 | 139 | A | N1-C6-N6 | -18.36 | 107.58 | 118.60 |
| 22 | 23S1 | 44 | A | C2-N3-C4 | 18.36 | 119.78 | 110.60 |
| 22 | 23S1 | 368 | A | N1-C6-N6 | -18.36 | 107.58 | 118.60 |
| 22 | 23S1 | 1866 | A | C2-N3-C4 | 18.36 | 119.78 | 110.60 |
| 1 | 16S1 | 344 | A | C2-N3-C4 | 18.36 | 119.78 | 110.60 |
| 22 | 23S1 | 1070 | A | N1-C6-N6 | -18.36 | 107.59 | 118.60 |
| 22 | 23S1 | 1175 | A | N1-C6-N6 | -18.36 | 107.59 | 118.60 |
| 22 | 23S1 | 1970 | A | C2-N3-C4 | 18.36 | 119.78 | 110.60 |
| 1 | 16S1 | 547 | A | C2-N3-C4 | 18.35 | 119.78 | 110.60 |
| 22 | 23S1 | 146 | A | N1-C6-N6 | -18.35 | 107.59 | 118.60 |
| 22 | 23S1 | 2322 | A | C2-N3-C4 | 18.35 | 119.78 | 110.60 |
| 22 | 23S1 | 1677 | A | C2-N3-C4 | 18.35 | 119.78 | 110.60 |
| 22 | 23S1 | 2169 | A | N1-C6-N6 | -18.35 | 107.59 | 118.60 |
| 1 | 16S1 | 253 | A | N1-C2-N3 | -18.35 | 120.12 | 129.30 |
| 1 | 16S1 | 223 | A | N1-C6-N6 | -18.35 | 107.59 | 118.60 |
| 1 | 16S1 | 1117 | A | C2-N3-C4 | 18.35 | 119.77 | 110.60 |
| 22 | 23S1 | 2531 | A | C2-N3-C4 | 18.35 | 119.77 | 110.60 |
| 23 | 05S1 | 39 | A | N1-C6-N6 | -18.35 | 107.59 | 118.60 |
| 1 | 16S1 | 321 | A | C2-N3-C4 | 18.34 | 119.77 | 110.60 |
| 1 | 16S1 | 1428 | A | N1-C2-N3 | -18.34 | 120.13 | 129.30 |
| 22 | 23S1 | 1285 | A | C2-N3-C4 | 18.34 | 119.77 | 110.60 |
| 55 | PTR1 | 51 | A | N1-C2-N3 | -18.34 | 120.13 | 129.30 |
| 1 | 16S1 | 432 | A | N1-C2-N3 | -18.34 | 120.13 | 129.30 |
| 22 | 23S1 | 752 | A | N1-C2-N3 | -18.34 | 120.13 | 129.30 |
| 22 | 23S1 | 362 | A | C2-N3-C4 | 18.33 | 119.77 | 110.60 |
| 1 | 16S1 | 1157 | A | N1-C6-N6 | -18.33 | 107.60 | 118.60 |
| 22 | 23S1 | 71 | A | N1-C6-N6 | -18.33 | 107.60 | 118.60 |
| 1 | 16S1 | 579 | A | N1-C2-N3 | -18.33 | 120.14 | 129.30 |
| 22 | 23S1 | 342 | A | N1-C2-N3 | -18.33 | 120.14 | 129.30 |
| 22 | 23S1 | 654 | A | N1-C6-N6 | -18.33 | 107.60 | 118.60 |
| 22 | 23S1 | 310 | A | C2-N3-C4 | 18.33 | 119.76 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1913 | A | C2-N3-C4 | 18.33 | 119.76 | 110.60 |
| 22 | 23S1 | 1085 | A | N1-C2-N3 | -18.33 | 120.14 | 129.30 |
| 22 | 23S1 | 2750 | A | C2-N3-C4 | 18.33 | 119.76 | 110.60 |
| 23 | 05S1 | 29 | A | N1-C2-N3 | -18.33 | 120.14 | 129.30 |
| 22 | 23S1 | 877 | A | N1-C2-N3 | -18.32 | 120.14 | 129.30 |
| 22 | 23S1 | 1040 | A | N1-C6-N6 | -18.32 | 107.61 | 118.60 |
| 1 | 16S1 | 1197 | A | N1-C6-N6 | -18.32 | 107.61 | 118.60 |
| 55 | PTR1 | 21 | A | C2-N3-C4 | 18.32 | 119.76 | 110.60 |
| 1 | 16S1 | 1081 | A | C2-N3-C4 | 18.32 | 119.76 | 110.60 |
| 1 | 16S1 | 975 | A | N1-C6-N6 | -18.32 | 107.61 | 118.60 |
| 1 | 16S1 | 1093 | A | N1-C2-N3 | -18.32 | 120.14 | 129.30 |
| 22 | 23S1 | 753 | A | N1-C2-N3 | -18.32 | 120.14 | 129.30 |
| 22 | 23S1 | 1133 | A | C2-N3-C4 | 18.32 | 119.76 | 110.60 |
| 22 | 23S1 | 1321 | A | N1-C6-N6 | -18.32 | 107.61 | 118.60 |
| 22 | 23S1 | 1672 | A | N1-C6-N6 | -18.32 | 107.61 | 118.60 |
| 22 | 23S1 | 2654 | A | C2-N3-C4 | 18.32 | 119.76 | 110.60 |
| 22 | 23S1 | 101 | A | N1-C2-N3 | -18.31 | 120.14 | 129.30 |
| 22 | 23S1 | 900 | A | N1-C2-N3 | -18.31 | 120.14 | 129.30 |
| 23 | 05S1 | 57 | A | N1-C6-N6 | -18.31 | 107.61 | 118.60 |
| 1 | 16S1 | 72 | A | N1-C6-N6 | -18.31 | 107.61 | 118.60 |
| 22 | 23S1 | 1803 | A | C2-N3-C4 | 18.31 | 119.76 | 110.60 |
| 1 | 16S1 | 996 | A | C2-N3-C4 | 18.31 | 119.75 | 110.60 |
| 22 | 23S1 | 2369 | A | N1-C2-N3 | -18.31 | 120.14 | 129.30 |
| 22 | 23S1 | 127 | A | N1-C6-N6 | -18.31 | 107.61 | 118.60 |
| 22 | 23S1 | 507 | A | C2-N3-C4 | 18.31 | 119.75 | 110.60 |
| 22 | 23S1 | 2450 | A | C2-N3-C4 | 18.31 | 119.75 | 110.60 |
| 23 | 05S1 | 108 | A | N1-C6-N6 | -18.31 | 107.61 | 118.60 |
| 1 | 16S1 | 1513 | A | C2-N3-C4 | 18.31 | 119.75 | 110.60 |
| 1 | 16S1 | 1080 | A | C2-N3-C4 | 18.31 | 119.75 | 110.60 |
| 1 | 16S1 | 1480 | A | N1-C2-N3 | -18.31 | 120.15 | 129.30 |
| 22 | 23S1 | 2205 | A | N1-C2-N3 | -18.31 | 120.15 | 129.30 |
| 22 | 23S1 | 2297 | A | N1-C2-N3 | -18.31 | 120.15 | 129.30 |
| 22 | 23S1 | 829 | A | C2-N3-C4 | 18.30 | 119.75 | 110.60 |
| 1 | 16S1 | 397 | A | N1-C2-N3 | -18.30 | 120.15 | 129.30 |
| 22 | 23S1 | 401 | A | C2-N3-C4 | 18.30 | 119.75 | 110.60 |
| 22 | 23S1 | 666 | A | N1-C6-N6 | -18.30 | 107.62 | 118.60 |
| 1 | 16S1 | 77 | A | C2-N3-C4 | 18.30 | 119.75 | 110.60 |
| 1 | 16S1 | 523 | A | C2-N3-C4 | 18.30 | 119.75 | 110.60 |
| 22 | 23S1 | 256 | A | N1-C2-N3 | -18.29 | 120.15 | 129.30 |
| 22 | 23S1 | 2278 | A | N1-C6-N6 | -18.29 | 107.62 | 118.60 |
| 22 | 23S1 | 2560 | A | N1-C2-N3 | -18.29 | 120.15 | 129.30 |
| 22 | 23S1 | 2542 | A | C2-N3-C4 | 18.29 | 119.75 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 165 | A | C2-N3-C4 | 18.29 | 119.75 | 110.60 |
| 22 | 23S1 | 1711 | A | N1-C2-N3 | -18.29 | 120.16 | 129.30 |
| 22 | 23S1 | 2670 | A | N1-C2-N3 | -18.29 | 120.16 | 129.30 |
| 1 | 16S1 | 1014 | A | N1-C2-N3 | -18.29 | 120.16 | 129.30 |
| 1 | 16S1 | 1163 | A | N1-C2-N3 | -18.29 | 120.16 | 129.30 |
| 22 | 23S1 | 936 | A | N1-C6-N6 | -18.29 | 107.63 | 118.60 |
| 22 | 23S1 | 1151 | A | N1-C6-N6 | -18.29 | 107.63 | 118.60 |
| 22 | 23S1 | 1080 | A | N1-C2-N3 | -18.29 | 120.16 | 129.30 |
| 22 | 23S1 | 2386 | A | N1-C6-N6 | -18.29 | 107.63 | 118.60 |
| 1 | 16S1 | 715 | A | N1-C6-N6 | -18.28 | 107.63 | 118.60 |
| 22 | 23S1 | 2433 | A | C2-N3-C4 | 18.28 | 119.74 | 110.60 |
| 22 | 23S1 | 64 | A | N1-C6-N6 | -18.28 | 107.63 | 118.60 |
| 22 | 23S1 | 1928 | A | N1-C2-N3 | -18.28 | 120.16 | 129.30 |
| 22 | 23S1 | 2020 | A | C2-N3-C4 | 18.28 | 119.74 | 110.60 |
| 1 | 16S1 | 161 | A | C2-N3-C4 | 18.28 | 119.74 | 110.60 |
| 22 | 23S1 | 207 | A | N1-C6-N6 | -18.28 | 107.63 | 118.60 |
| 22 | 23S1 | 2198 | A | C2-N3-C4 | 18.28 | 119.74 | 110.60 |
| 22 | 23S1 | 2453 | A | N1-C2-N3 | -18.28 | 120.16 | 129.30 |
| 22 | 23S1 | 2482 | A | N1-C2-N3 | -18.28 | 120.16 | 129.30 |
| 23 | 05S1 | 115 | A | N1-C6-N6 | -18.28 | 107.63 | 118.60 |
| 1 | 16S1 | 1248 | A | C2-N3-C4 | 18.28 | 119.74 | 110.60 |
| 1 | 16S1 | 532 | A | C2-N3-C4 | 18.27 | 119.74 | 110.60 |
| 22 | 23S1 | 1050 | A | N1-C2-N3 | -18.27 | 120.16 | 129.30 |
| 22 | 23S1 | 2054 | A | N1-C6-N6 | -18.27 | 107.64 | 118.60 |
| 22 | 23S1 | 2346 | A | N1-C6-N6 | -18.27 | 107.64 | 118.60 |
| 1 | 16S1 | 155 | A | N1-C6-N6 | -18.27 | 107.64 | 118.60 |
| 1 | 16S1 | 978 | A | C2-N3-C4 | 18.27 | 119.73 | 110.60 |
| 22 | 23S1 | 1367 | A | C2-N3-C4 | 18.27 | 119.73 | 110.60 |
| 22 | 23S1 | 401 | A | N1-C6-N6 | -18.27 | 107.64 | 118.60 |
| 22 | 23S1 | 644 | A | N1-C6-N6 | -18.27 | 107.64 | 118.60 |
| 22 | 23S1 | 1773 | A | N1-C6-N6 | -18.27 | 107.64 | 118.60 |
| 22 | 23S1 | 2309 | A | C2-N3-C4 | 18.27 | 119.73 | 110.60 |
| 22 | 23S1 | 347 | A | N1-C2-N3 | -18.27 | 120.17 | 129.30 |
| 22 | 23S1 | 1502 | A | N1-C2-N3 | -18.27 | 120.17 | 129.30 |
| 22 | 23S1 | 190 | A | N1-C6-N6 | -18.27 | 107.64 | 118.60 |
| 22 | 23S1 | 1981 | A | N1-C2-N3 | -18.27 | 120.17 | 129.30 |
| 1 | 16S1 | 197 | A | C2-N3-C4 | 18.26 | 119.73 | 110.60 |
| 22 | 23S1 | 217 | A | N1-C6-N6 | -18.26 | 107.64 | 118.60 |
| 22 | 23S1 | 996 | A | N1-C2-N3 | -18.26 | 120.17 | 129.30 |
| 22 | 23S1 | 2406 | A | C2-N3-C4 | 18.26 | 119.73 | 110.60 |
| 22 | 23S1 | 505 | A | N1-C2-N3 | -18.26 | 120.17 | 129.30 |
| 22 | 23S1 | 131 | A | N1-C2-N3 | -18.25 | 120.17 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 749 | A | N1-C6-N6 | -18.25 | 107.65 | 118.60 |
| 22 | 23S1 | 2322 | A | N1-C2-N3 | -18.25 | 120.17 | 129.30 |
| 1 | 16S1 | 655 | A | N1-C6-N6 | -18.25 | 107.65 | 118.60 |
| 22 | 23S1 | 222 | A | N1-C6-N6 | -18.25 | 107.65 | 118.60 |
| 22 | 23S1 | 988 | A | N1-C2-N3 | -18.25 | 120.18 | 129.30 |
| 1 | 16S1 | 130 | A | N1-C6-N6 | -18.25 | 107.65 | 118.60 |
| 22 | 23S1 | 743 | A | N1-C6-N6 | -18.25 | 107.65 | 118.60 |
| 22 | 23S1 | 1610 | A | C2-N3-C4 | 18.25 | 119.72 | 110.60 |
| 22 | 23S1 | 2856 | A | N1-C6-N6 | -18.25 | 107.65 | 118.60 |
| 1 | 16S1 | 465 | A | N1-C6-N6 | -18.24 | 107.65 | 118.60 |
| 22 | 23S1 | 2211 | A | C2-N3-C4 | 18.24 | 119.72 | 110.60 |
| 22 | 23S1 | 2665 | A | N1-C6-N6 | -18.24 | 107.66 | 118.60 |
| 22 | 23S1 | 161 | A | N1-C2-N3 | -18.24 | 120.18 | 129.30 |
| 1 | 16S1 | 336 | A | C2-N3-C4 | 18.24 | 119.72 | 110.60 |
| 22 | 23S1 | 63 | A | C2-N3-C4 | 18.24 | 119.72 | 110.60 |
| 22 | 23S1 | 125 | A | N1-C6-N6 | -18.24 | 107.66 | 118.60 |
| 22 | 23S1 | 1367 | A | N1-C6-N6 | -18.24 | 107.66 | 118.60 |
| 1 | 16S1 | 366 | A | N1-C6-N6 | -18.24 | 107.66 | 118.60 |
| 1 | 16S1 | 408 | A | N1-C2-N3 | -18.24 | 120.18 | 129.30 |
| 22 | 23S1 | 172 | A | N1-C6-N6 | -18.24 | 107.66 | 118.60 |
| 22 | 23S1 | 272 | A | C2-N3-C4 | 18.24 | 119.72 | 110.60 |
| 55 | PTR1 | 51 | A | C2-N3-C4 | 18.24 | 119.72 | 110.60 |
| 1 | 16S1 | 807 | A | N1-C2-N3 | -18.23 | 120.18 | 129.30 |
| 1 | 16S1 | 1055 | A | C2-N3-C4 | 18.23 | 119.72 | 110.60 |
| 22 | 23S1 | 191 | A | N1-C2-N3 | -18.23 | 120.18 | 129.30 |
| 22 | 23S1 | 734 | A | C2-N3-C4 | 18.23 | 119.72 | 110.60 |
| 1 | 16S1 | 1476 | A | N1-C2-N3 | -18.23 | 120.18 | 129.30 |
| 22 | 23S1 | 49 | A | N1-C6-N6 | -18.23 | 107.66 | 118.60 |
| 1 | 16S1 | 1130 | A | N1-C2-N3 | -18.23 | 120.19 | 129.30 |
| 22 | 23S1 | 920 | A | N1-C6-N6 | -18.23 | 107.66 | 118.60 |
| 22 | 23S1 | 1246 | A | N1-C2-N3 | -18.23 | 120.19 | 129.30 |
| 1 | 16S1 | 1044 | A | N1-C6-N6 | -18.23 | 107.67 | 118.60 |
| 22 | 23S1 | 231 | A | N1-C6-N6 | -18.22 | 107.67 | 118.60 |
| 22 | 23S1 | 727 | A | C2-N3-C4 | 18.22 | 119.71 | 110.60 |
| 1 | 16S1 | 1176 | A | N1-C2-N3 | -18.22 | 120.19 | 129.30 |
| 22 | 23S1 | 1048 | A | C2-N3-C4 | 18.22 | 119.71 | 110.60 |
| 22 | 23S1 | 1572 | A | C2-N3-C4 | 18.22 | 119.71 | 110.60 |
| 23 | 05S1 | 104 | A | N1-C6-N6 | -18.22 | 107.67 | 118.60 |
| 1 | 16S1 | 1246 | A | N1-C2-N3 | -18.21 | 120.19 | 129.30 |
| 22 | 23S1 | 231 | A | N1-C2-N3 | -18.21 | 120.19 | 129.30 |
| 22 | 23S1 | 2082 | A | C2-N3-C4 | 18.21 | 119.71 | 110.60 |
| 1 | 16S1 | 1492 | A | N1-C2-N3 | -18.21 | 120.19 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 979 | A | N1-C6-N6 | -18.21 | 107.67 | 118.60 |
| 22 | 23S1 | 2278 | A | C2-N3-C4 | 18.21 | 119.71 | 110.60 |
| 22 | 23S1 | 2820 | A | C2-N3-C4 | 18.21 | 119.71 | 110.60 |
| 22 | 23S1 | 2721 | A | C2-N3-C4 | 18.21 | 119.71 | 110.60 |
| 1 | 16S1 | 329 | A | C2-N3-C4 | 18.21 | 119.70 | 110.60 |
| 1 | 16S1 | 1280 | A | C2-N3-C4 | 18.21 | 119.70 | 110.60 |
| 22 | 23S1 | 197 | A | N1-C2-N3 | -18.21 | 120.20 | 129.30 |
| 22 | 23S1 | 2366 | A | N1-C6-N6 | -18.21 | 107.68 | 118.60 |
| 22 | 23S1 | 1876 | A | N1-C6-N6 | -18.21 | 107.68 | 118.60 |
| 1 | 16S1 | 546 | A | N1-C6-N6 | -18.20 | 107.68 | 118.60 |
| 1 | 16S1 | 1319 | A | N1-C6-N6 | -18.20 | 107.68 | 118.60 |
| 1 | 16S1 | 172 | A | C2-N3-C4 | 18.20 | 119.70 | 110.60 |
| 1 | 16S1 | 466 | A | C2-N3-C4 | 18.20 | 119.70 | 110.60 |
| 22 | 23S1 | 2727 | A | N1-C2-N3 | -18.20 | 120.20 | 129.30 |
| 1 | 16S1 | 923 | A | N1-C2-N3 | -18.20 | 120.20 | 129.30 |
| 22 | 23S1 | 2887 | A | N1-C6-N6 | -18.20 | 107.68 | 118.60 |
| 23 | 05S1 | 15 | A | N1-C6-N6 | -18.20 | 107.68 | 118.60 |
| 1 | 16S1 | 1446 | A | N1-C6-N6 | -18.20 | 107.68 | 118.60 |
| 22 | 23S1 | 1548 | A | N1-C2-N3 | -18.20 | 120.20 | 129.30 |
| 22 | 23S1 | 2425 | A | N1-C6-N6 | -18.20 | 107.68 | 118.60 |
| 22 | 23S1 | 447 | A | C2-N3-C4 | 18.20 | 119.70 | 110.60 |
| 22 | 23S1 | 794 | A | N1-C6-N6 | -18.20 | 107.68 | 118.60 |
| 22 | 23S1 | 2199 | A | N1-C6-N6 | -18.19 | 107.68 | 118.60 |
| 22 | 23S1 | 2468 | A | N1-C6-N6 | -18.19 | 107.68 | 118.60 |
| 1 | 16S1 | 1169 | A | C2-N3-C4 | 18.19 | 119.70 | 110.60 |
| 22 | 23S1 | 1885 | A | N1-C6-N6 | -18.19 | 107.69 | 118.60 |
| 1 | 16S1 | 1362 | A | N1-C6-N6 | -18.19 | 107.69 | 118.60 |
| 1 | 16S1 | 80 | A | N1-C2-N3 | -18.19 | 120.21 | 129.30 |
| 1 | 16S1 | 430 | A | C2-N3-C4 | 18.19 | 119.69 | 110.60 |
| 22 | 23S1 | 2097 | A | N1-C6-N6 | -18.19 | 107.69 | 118.60 |
| 22 | 23S1 | 2761 | A | N1-C2-N3 | -18.19 | 120.20 | 129.30 |
| 55 | PTR1 | 14 | A | C2-N3-C4 | 18.19 | 119.69 | 110.60 |
| 1 | 16S1 | 74 | A | N1-C6-N6 | -18.19 | 107.69 | 118.60 |
| 22 | 23S1 | 1847 | A | N1-C2-N3 | -18.19 | 120.21 | 129.30 |
| 22 | 23S1 | 1735 | A | C2-N3-C4 | 18.18 | 119.69 | 110.60 |
| 22 | 23S1 | 1237 | A | C2-N3-C4 | 18.18 | 119.69 | 110.60 |
| 22 | 23S1 | 1938 | A | C2-N3-C4 | 18.18 | 119.69 | 110.60 |
| 1 | 16S1 | 432 | A | N1-C6-N6 | -18.18 | 107.69 | 118.60 |
| 23 | 05S1 | 34 | A | N1-C2-N3 | -18.18 | 120.21 | 129.30 |
| 22 | 23S1 | 718 | A | N1-C2-N3 | -18.18 | 120.21 | 129.30 |
| 22 | 23S1 | 1067 | A | N1-C6-N6 | -18.18 | 107.69 | 118.60 |
| 23 | 05S1 | 46 | A | C2-N3-C4 | 18.18 | 119.69 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 374 | A | N1-C6-N6 | -18.17 | 107.69 | 118.60 |
| 22 | 23S1 | 1237 | A | N1-C6-N6 | -18.17 | 107.70 | 118.60 |
| 22 | 23S1 | 2734 | A | N1-C6-N6 | -18.17 | 107.69 | 118.60 |
| 1 | 16S1 | 1418 | A | N1-C2-N3 | -18.17 | 120.21 | 129.30 |
| 22 | 23S1 | 945 | A | C2-N3-C4 | 18.17 | 119.69 | 110.60 |
| 1 | 16S1 | 1251 | A | N1-C6-N6 | -18.17 | 107.70 | 118.60 |
| 1 | 16S1 | 1357 | A | N1-C6-N6 | -18.17 | 107.70 | 118.60 |
| 22 | 23S1 | 538 | A | C2-N3-C4 | 18.17 | 119.69 | 110.60 |
| 22 | 23S1 | 547 | A | C2-N3-C4 | 18.17 | 119.69 | 110.60 |
| 22 | 23S1 | 2094 | A | N1-C2-N3 | -18.17 | 120.22 | 129.30 |
| 1 | 16S1 | 496 | A | N1-C6-N6 | -18.17 | 107.70 | 118.60 |
| 1 | 16S1 | 673 | A | N1-C6-N6 | -18.17 | 107.70 | 118.60 |
| 22 | 23S1 | 472 | A | C2-N3-C4 | 18.17 | 119.68 | 110.60 |
| 22 | 23S1 | 6 | A | N1-C6-N6 | -18.17 | 107.70 | 118.60 |
| 1 | 16S1 | 199 | A | N1-C2-N3 | -18.16 | 120.22 | 129.30 |
| 1 | 16S1 | 642 | A | N1-C2-N3 | -18.16 | 120.22 | 129.30 |
| 1 | 16S1 | 1157 | A | N1-C2-N3 | -18.16 | 120.22 | 129.30 |
| 22 | 23S1 | 2432 | A | N1-C6-N6 | -18.16 | 107.70 | 118.60 |
| 22 | 23S1 | 1134 | A | N1-C2-N3 | -18.16 | 120.22 | 129.30 |
| 22 | 23S1 | 1739 | A | N1-C2-N3 | -18.16 | 120.22 | 129.30 |
| 22 | 23S1 | 2317 | A | N1-C6-N6 | -18.16 | 107.71 | 118.60 |
| 22 | 23S1 | 2635 | A | N1-C2-N3 | -18.16 | 120.22 | 129.30 |
| 1 | 16S1 | 279 | A | N1-C2-N3 | -18.16 | 120.22 | 129.30 |
| 22 | 23S1 | 1783 | A | C2-N3-C4 | 18.16 | 119.68 | 110.60 |
| 22 | 23S1 | 2191 | A | N1-C6-N6 | -18.16 | 107.71 | 118.60 |
| 1 | 16S1 | 451 | A | C2-N3-C4 | 18.15 | 119.68 | 110.60 |
| 22 | 23S1 | 2088 | A | N1-C2-N3 | -18.15 | 120.22 | 129.30 |
| 22 | 23S1 | 2705 | A | N1-C2-N3 | -18.15 | 120.22 | 129.30 |
| 1 | 16S1 | 1441 | A | N1-C6-N6 | -18.15 | 107.71 | 118.60 |
| 22 | 23S1 | 1156 | A | N1-C6-N6 | -18.15 | 107.71 | 118.60 |
| 22 | 23S1 | 2860 | A | N1-C6-N6 | -18.15 | 107.71 | 118.60 |
| 22 | 23S1 | 716 | A | N1-C2-N3 | -18.15 | 120.22 | 129.30 |
| 22 | 23S1 | 156 | A | N1-C2-N3 | -18.15 | 120.23 | 129.30 |
| 22 | 23S1 | 2776 | A | C2-N3-C4 | 18.15 | 119.67 | 110.60 |
| 22 | 23S1 | 2412 | A | N1-C2-N3 | -18.14 | 120.23 | 129.30 |
| 1 | 16S1 | 143 | A | N1-C6-N6 | -18.14 | 107.71 | 118.60 |
| 1 | 16S1 | 353 | A | C2-N3-C4 | 18.14 | 119.67 | 110.60 |
| 1 | 16S1 | 189 | A | C2-N3-C4 | 18.14 | 119.67 | 110.60 |
| 1 | 16S1 | 1350 | A | N1-C2-N3 | -18.14 | 120.23 | 129.30 |
| 55 | PTR1 | 73 | A | C2-N3-C4 | 18.14 | 119.67 | 110.60 |
| 55 | PTR1 | 9 | A | N1-C2-N3 | -18.14 | 120.23 | 129.30 |
| 1 | 16S1 | 161 | A | N1-C2-N3 | -18.14 | 120.23 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 321 | A | N1-C2-N3 | -18.14 | 120.23 | 129.30 |
| 22 | 23S1 | 981 | A | C2-N3-C4 | 18.14 | 119.67 | 110.60 |
| 22 | 23S1 | 2378 | A | C2-N3-C4 | 18.14 | 119.67 | 110.60 |
| 22 | 23S1 | 734 | A | N1-C2-N3 | -18.13 | 120.23 | 129.30 |
| 22 | 23S1 | 2765 | A | N1-C6-N6 | -18.13 | 107.72 | 118.60 |
| 1 | 16S1 | 59 | A | N1-C6-N6 | -18.13 | 107.72 | 118.60 |
| 1 | 16S1 | 532 | A | N1-C2-N3 | -18.13 | 120.23 | 129.30 |
| 1 | 16S1 | 1418 | A | C2-N3-C4 | 18.13 | 119.67 | 110.60 |
| 22 | 23S1 | 1900 | A | N1-C6-N6 | -18.13 | 107.72 | 118.60 |
| 1 | 16S1 | 50 | A | N1-C6-N6 | -18.13 | 107.72 | 118.60 |
| 1 | 16S1 | 635 | A | C2-N3-C4 | 18.13 | 119.67 | 110.60 |
| 22 | 23S1 | 1801 | A | N1-C2-N3 | -18.13 | 120.23 | 129.30 |
| 22 | 23S1 | 2705 | A | C2-N3-C4 | 18.13 | 119.66 | 110.60 |
| 1 | 16S1 | 1229 | A | N1-C2-N3 | -18.13 | 120.24 | 129.30 |
| 1 | 16S1 | 642 | A | N1-C6-N6 | -18.12 | 107.72 | 118.60 |
| 1 | 16S1 | 236 | A | N1-C2-N3 | -18.12 | 120.24 | 129.30 |
| 1 | 16S1 | 1269 | A | N1-C6-N6 | -18.12 | 107.73 | 118.60 |
| 22 | 23S1 | 52 | A | N1-C2-N3 | -18.12 | 120.24 | 129.30 |
| 22 | 23S1 | 348 | A | N1-C6-N6 | -18.12 | 107.73 | 118.60 |
| 22 | 23S1 | 1899 | A | C2-N3-C4 | 18.12 | 119.66 | 110.60 |
| 22 | 23S1 | 1098 | A | N1-C2-N3 | -18.12 | 120.24 | 129.30 |
| 22 | 23S1 | 2042 | A | N1-C6-N6 | -18.12 | 107.73 | 118.60 |
| 22 | 23S1 | 146 | A | N1-C2-N3 | -18.12 | 120.24 | 129.30 |
| 22 | 23S1 | 866 | A | N1-C6-N6 | -18.12 | 107.73 | 118.60 |
| 1 | 16S1 | 1227 | A | N1-C2-N3 | -18.11 | 120.24 | 129.30 |
| 22 | 23S1 | 182 | A | N1-C2-N3 | -18.11 | 120.24 | 129.30 |
| 23 | 05S1 | 58 | A | N1-C6-N6 | -18.11 | 107.73 | 118.60 |
| 22 | 23S1 | 104 | A | N1-C6-N6 | -18.11 | 107.73 | 118.60 |
| 22 | 23S1 | 1745 | A | N1-C2-N3 | -18.11 | 120.25 | 129.30 |
| 22 | 23S1 | 2602 | A | N1-C2-N3 | -18.11 | 120.25 | 129.30 |
| 1 | 16S1 | 1042 | A | N1-C6-N6 | -18.11 | 107.74 | 118.60 |
| 22 | 23S1 | 2090 | A | N1-C6-N6 | -18.10 | 107.74 | 118.60 |
| 1 | 16S1 | 974 | A | N1-C2-N3 | -18.10 | 120.25 | 129.30 |
| 1 | 16S1 | 1105 | A | N1-C2-N3 | -18.10 | 120.25 | 129.30 |
| 22 | 23S1 | 223 | A | C2-N3-C4 | 18.10 | 119.65 | 110.60 |
| 22 | 23S1 | 1783 | A | N1-C2-N3 | -18.09 | 120.25 | 129.30 |
| 22 | 23S1 | 13 | A | N1-C2-N3 | -18.09 | 120.25 | 129.30 |
| 22 | 23S1 | 73 | A | C2-N3-C4 | 18.09 | 119.65 | 110.60 |
| 22 | 23S1 | 590 | A | N1-C2-N3 | -18.09 | 120.25 | 129.30 |
| 22 | 23S1 | 1801 | A | C2-N3-C4 | 18.09 | 119.65 | 110.60 |
| 22 | 23S1 | 2792 | A | N1-C2-N3 | -18.09 | 120.25 | 129.30 |
| 22 | 23S1 | 1626 | A | C2-N3-C4 | 18.09 | 119.64 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 716 | A | N1-C6-N6 | -18.09 | 107.75 | 118.60 |
| 22 | 23S1 | 1142 | A | N1-C2-N3 | -18.09 | 120.26 | 129.30 |
| 1 | 16S1 | 1019 | A | N1-C6-N6 | -18.08 | 107.75 | 118.60 |
| 22 | 23S1 | 127 | A | C2-N3-C4 | 18.08 | 119.64 | 110.60 |
| 1 | 16S1 | 1256 | A | C2-N3-C4 | 18.08 | 119.64 | 110.60 |
| 22 | 23S1 | 1495 | A | N1-C6-N6 | -18.08 | 107.75 | 118.60 |
| 22 | 23S1 | 1784 | A | N1-C6-N6 | -18.08 | 107.75 | 118.60 |
| 22 | 23S1 | 2352 | A | N1-C2-N3 | -18.08 | 120.26 | 129.30 |
| 55 | PTR1 | 76 | A | C2-N3-C4 | 18.08 | 119.64 | 110.60 |
| 1 | 16S1 | 1012 | A | N1-C6-N6 | -18.08 | 107.75 | 118.60 |
| 1 | 16S1 | 1502 | A | C2-N3-C4 | 18.08 | 119.64 | 110.60 |
| 1 | 16S1 | 303 | A | N1-C6-N6 | -18.07 | 107.75 | 118.60 |
| 22 | 23S1 | 505 | A | C2-N3-C4 | 18.07 | 119.64 | 110.60 |
| 22 | 23S1 | 1535 | A | N1-C2-N3 | -18.07 | 120.26 | 129.30 |
| 22 | 23S1 | 52 | A | C2-N3-C4 | 18.07 | 119.64 | 110.60 |
| 22 | 23S1 | 251 | A | C2-N3-C4 | 18.07 | 119.64 | 110.60 |
| 22 | 23S1 | 423 | A | C2-N3-C4 | 18.07 | 119.64 | 110.60 |
| 1 | 16S1 | 676 | A | N1-C2-N3 | -18.07 | 120.27 | 129.30 |
| 22 | 23S1 | 574 | A | N1-C6-N6 | -18.07 | 107.76 | 118.60 |
| 1 | 16S1 | 228 | A | N1-C6-N6 | -18.07 | 107.76 | 118.60 |
| 22 | 23S1 | 2738 | A | N1-C6-N6 | -18.07 | 107.76 | 118.60 |
| 1 | 16S1 | 949 | A | N1-C2-N3 | -18.06 | 120.27 | 129.30 |
| 22 | 23S1 | 947 | A | N1-C6-N6 | -18.06 | 107.77 | 118.60 |
| 22 | 23S1 | 2288 | A | N1-C6-N6 | -18.06 | 107.77 | 118.60 |
| 1 | 16S1 | 1155 | A | N1-C6-N6 | -18.06 | 107.77 | 118.60 |
| 1 | 16S1 | 1429 | A | N1-C2-N3 | -18.06 | 120.27 | 129.30 |
| 1 | 16S1 | 246 | A | C2-N3-C4 | 18.06 | 119.63 | 110.60 |
| 1 | 16S1 | 448 | A | N1-C6-N6 | -18.06 | 107.77 | 118.60 |
| 22 | 23S1 | 1549 | A | N1-C2-N3 | -18.05 | 120.27 | 129.30 |
| 1 | 16S1 | 1346 | A | C2-N3-C4 | 18.05 | 119.63 | 110.60 |
| 1 | 16S1 | 901 | A | C2-N3-C4 | 18.05 | 119.62 | 110.60 |
| 1 | 16S1 | 1167 | A | C2-N3-C4 | 18.05 | 119.62 | 110.60 |
| 1 | 16S1 | 1 | A | C2-N3-C4 | 18.05 | 119.62 | 110.60 |
| 1 | 16S1 | 865 | A | N1-C6-N6 | -18.04 | 107.77 | 118.60 |
| 22 | 23S1 | 1077 | A | N1-C6-N6 | -18.04 | 107.77 | 118.60 |
| 1 | 16S1 | 143 | A | C2-N3-C4 | 18.04 | 119.62 | 110.60 |
| 22 | 23S1 | 2314 | A | N1-C6-N6 | -18.04 | 107.78 | 118.60 |
| 1 | 16S1 | 845 | A | N1-C2-N3 | -18.04 | 120.28 | 129.30 |
| 1 | 16S1 | 1531 | A | C2-N3-C4 | 18.04 | 119.62 | 110.60 |
| 22 | 23S1 | 2298 | A | N1-C6-N6 | -18.04 | 107.78 | 118.60 |
| 22 | 23S1 | 156 | A | N1-C6-N6 | -18.04 | 107.78 | 118.60 |
| 22 | 23S1 | 2679 | A | N1-C6-N6 | -18.04 | 107.78 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 502 | A | N1-C2-N3 | -18.04 | 120.28 | 129.30 |
| 22 | 23S1 | 538 | A | N1-C6-N6 | -18.04 | 107.78 | 118.60 |
| 22 | 23S1 | 1144 | A | N1-C6-N6 | -18.04 | 107.78 | 118.60 |
| 22 | 23S1 | 2748 | A | N1-C6-N6 | -18.04 | 107.78 | 118.60 |
| 22 | 23S1 | 1373 | A | N1-C2-N3 | -18.03 | 120.28 | 129.30 |
| 22 | 23S1 | 457 | A | C2-N3-C4 | 18.03 | 119.61 | 110.60 |
| 22 | 23S1 | 1008 | A | C2-N3-C4 | 18.03 | 119.61 | 110.60 |
| 22 | 23S1 | 73 | A | N1-C6-N6 | -18.03 | 107.78 | 118.60 |
| 22 | 23S1 | 689 | A | N1-C2-N3 | -18.03 | 120.29 | 129.30 |
| 22 | 23S1 | 829 | A | N1-C6-N6 | -18.03 | 107.78 | 118.60 |
| 1 | 16S1 | 51 | A | N1-C2-N3 | -18.02 | 120.29 | 129.30 |
| 1 | 16S1 | 695 | A | N1-C6-N6 | -18.02 | 107.79 | 118.60 |
| 22 | 23S1 | 1244 | A | N1-C6-N6 | -18.02 | 107.78 | 118.60 |
| 1 | 16S1 | 192 | A | N1-C2-N3 | -18.02 | 120.29 | 129.30 |
| 22 | 23S1 | 251 | A | N1-C2-N3 | -18.02 | 120.29 | 129.30 |
| 22 | 23S1 | 1713 | A | C2-N3-C4 | 18.02 | 119.61 | 110.60 |
| 22 | 23S1 | 2482 | A | N1-C6-N6 | -18.02 | 107.79 | 118.60 |
| 1 | 16S1 | 510 | A | C2-N3-C4 | 18.02 | 119.61 | 110.60 |
| 1 | 16S1 | 602 | A | N1-C2-N3 | -18.02 | 120.29 | 129.30 |
| 23 | 05S1 | 109 | A | N1-C6-N6 | -18.02 | 107.79 | 118.60 |
| 22 | 23S1 | 1700 | A | C2-N3-C4 | 18.02 | 119.61 | 110.60 |
| 22 | 23S1 | 1916 | A | N1-C2-N3 | -18.02 | 120.29 | 129.30 |
| 22 | 23S1 | 2392 | A | N1-C2-N3 | -18.02 | 120.29 | 129.30 |
| 1 | 16S1 | 1000 | A | N1-C2-N3 | -18.01 | 120.29 | 129.30 |
| 1 | 16S1 | 303 | A | C2-N3-C4 | 18.01 | 119.61 | 110.60 |
| 22 | 23S1 | 2883 | A | C2-N3-C4 | 18.01 | 119.61 | 110.60 |
| 1 | 16S1 | 1398 | A | C2-N3-C4 | 18.01 | 119.60 | 110.60 |
| 22 | 23S1 | 131 | A | N1-C6-N6 | -18.01 | 107.80 | 118.60 |
| 23 | 05S1 | 52 | A | C2-N3-C4 | 18.01 | 119.60 | 110.60 |
| 22 | 23S1 | 1552 | A | N1-C6-N6 | -18.01 | 107.80 | 118.60 |
| 22 | 23S1 | 1953 | A | C2-N3-C4 | 18.01 | 119.60 | 110.60 |
| 1 | 16S1 | 1299 | A | N1-C2-N3 | -18.00 | 120.30 | 129.30 |
| 22 | 23S1 | 2700 | A | N1-C6-N6 | -18.00 | 107.80 | 118.60 |
| 22 | 23S1 | 603 | A | C2-N3-C4 | 18.00 | 119.60 | 110.60 |
| 22 | 23S1 | 616 | A | N1-C6-N6 | -18.00 | 107.80 | 118.60 |
| 22 | 23S1 | 1754 | A | C2-N3-C4 | 18.00 | 119.60 | 110.60 |
| 22 | 23S1 | 2448 | A | N1-C2-N3 | -18.00 | 120.30 | 129.30 |
| 1 | 16S1 | 901 | A | N1-C2-N3 | -18.00 | 120.30 | 129.30 |
| 1 | 16S1 | 1152 | A | N1-C2-N3 | -18.00 | 120.30 | 129.30 |
| 22 | 23S1 | 6 | A | N1-C2-N3 | -18.00 | 120.30 | 129.30 |
| 22 | 23S1 | 320 | A | N1-C6-N6 | -18.00 | 107.80 | 118.60 |
| 22 | 23S1 | 2412 | A | C2-N3-C4 | 18.00 | 119.60 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 913 | A | C2-N3-C4 | 18.00 | 119.60 | 110.60 |
| 22 | 23S1 | 2060 | A | C2-N3-C4 | 18.00 | 119.60 | 110.60 |
| 1 | 16S1 | 675 | A | C2-N3-C4 | 17.99 | 119.60 | 110.60 |
| 55 | PTR1 | 26 | A | N1-C6-N6 | -17.99 | 107.80 | 118.60 |
| 22 | 23S1 | 2317 | A | N1-C2-N3 | -17.99 | 120.31 | 129.30 |
| 1 | 16S1 | 243 | A | C2-N3-C4 | 17.99 | 119.59 | 110.60 |
| 22 | 23S1 | 2654 | A | N1-C6-N6 | -17.99 | 107.81 | 118.60 |
| 1 | 16S1 | 702 | A | C2-N3-C4 | 17.99 | 119.59 | 110.60 |
| 1 | 16S1 | 131 | A | C2-N3-C4 | 17.98 | 119.59 | 110.60 |
| 1 | 16S1 | 451 | A | N1-C2-N3 | -17.98 | 120.31 | 129.30 |
| 22 | 23S1 | 2738 | A | C2-N3-C4 | 17.98 | 119.59 | 110.60 |
| 22 | 23S1 | 1829 | A | N1-C2-N3 | -17.98 | 120.31 | 129.30 |
| 22 | 23S1 | 2328 | A | N1-C6-N6 | -17.98 | 107.81 | 118.60 |
| 22 | 23S1 | 2126 | A | N1-C2-N3 | -17.98 | 120.31 | 129.30 |
| 1 | 16S1 | 1130 | A | C2-N3-C4 | 17.98 | 119.59 | 110.60 |
| 22 | 23S1 | 2799 | A | N1-C2-N3 | -17.97 | 120.31 | 129.30 |
| 22 | 23S1 | 181 | A | N1-C6-N6 | -17.97 | 107.82 | 118.60 |
| 22 | 23S1 | 354 | A | C2-N3-C4 | 17.97 | 119.59 | 110.60 |
| 22 | 23S1 | 2425 | A | C2-N3-C4 | 17.97 | 119.59 | 110.60 |
| 22 | 23S1 | 2170 | A | N1-C2-N3 | -17.97 | 120.31 | 129.30 |
| 1 | 16S1 | 687 | A | C2-N3-C4 | 17.97 | 119.58 | 110.60 |
| 22 | 23S1 | 1532 | A | N1-C6-N6 | -17.96 | 107.82 | 118.60 |
| 22 | 23S1 | 2015 | A | N1-C6-N6 | -17.96 | 107.82 | 118.60 |
| 22 | 23S1 | 2411 | A | C2-N3-C4 | 17.96 | 119.58 | 110.60 |
| 1 | 16S1 | 303 | A | N1-C2-N3 | -17.96 | 120.32 | 129.30 |
| 22 | 23S1 | 2335 | A | N1-C6-N6 | -17.96 | 107.83 | 118.60 |
| 22 | 23S1 | 2662 | A | C2-N3-C4 | 17.96 | 119.58 | 110.60 |
| 1 | 16S1 | 1332 | A | N1-C2-N3 | -17.95 | 120.32 | 129.30 |
| 22 | 23S1 | 1084 | A | N1-C2-N3 | -17.95 | 120.32 | 129.30 |
| 22 | 23S1 | 1866 | A | N1-C2-N3 | -17.95 | 120.32 | 129.30 |
| 22 | 23S1 | 149 | A | N1-C6-N6 | -17.95 | 107.83 | 118.60 |
| 22 | 23S1 | 608 | A | N1-C6-N6 | -17.95 | 107.83 | 118.60 |
| 55 | PTR1 | 26 | A | C2-N3-C4 | 17.95 | 119.58 | 110.60 |
| 22 | 23S1 | 1095 | A | N1-C2-N3 | -17.95 | 120.33 | 129.30 |
| 1 | 16S1 | 101 | A | N1-C2-N3 | -17.95 | 120.33 | 129.30 |
| 1 | 16S1 | 382 | A | N1-C6-N6 | -17.95 | 107.83 | 118.60 |
| 22 | 23S1 | 541 | A | N1-C2-N3 | -17.94 | 120.33 | 129.30 |
| 22 | 23S1 | 227 | A | C2-N3-C4 | 17.94 | 119.57 | 110.60 |
| 22 | 23S1 | 2340 | A | N1-C2-N3 | -17.94 | 120.33 | 129.30 |
| 22 | 23S1 | 2814 | A | C2-N3-C4 | 17.94 | 119.57 | 110.60 |
| 1 | 16S1 | 600 | A | N1-C6-N6 | -17.94 | 107.84 | 118.60 |
| 22 | 23S1 | 480 | A | N1-C2-N3 | -17.94 | 120.33 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1739 | A | C2-N3-C4 | 17.93 | 119.57 | 110.60 |
| 22 | 23S1 | 2284 | A | N1-C2-N3 | -17.93 | 120.33 | 129.30 |
| 22 | 23S1 | 42 | A | N1-C6-N6 | -17.93 | 107.84 | 118.60 |
| 22 | 23S1 | 2577 | A | N1-C2-N3 | -17.93 | 120.34 | 129.30 |
| 1 | 16S1 | 250 | A | C2-N3-C4 | 17.92 | 119.56 | 110.60 |
| 22 | 23S1 | 2461 | A | N1-C2-N3 | -17.92 | 120.34 | 129.30 |
| 22 | 23S1 | 2471 | A | N1-C2-N3 | -17.92 | 120.34 | 129.30 |
| 22 | 23S1 | 2886 | A | N1-C6-N6 | -17.92 | 107.85 | 118.60 |
| 1 | 16S1 | 1 | A | N1-C6-N6 | -17.92 | 107.85 | 118.60 |
| 1 | 16S1 | 192 | A | N1-C6-N6 | -17.92 | 107.85 | 118.60 |
| 1 | 16S1 | 663 | A | N1-C2-N3 | -17.92 | 120.34 | 129.30 |
| 22 | 23S1 | 2154 | A | N1-C2-N3 | -17.92 | 120.34 | 129.30 |
| 1 | 16S1 | 655 | A | N1-C2-N3 | -17.92 | 120.34 | 129.30 |
| 22 | 23S1 | 203 | A | N1-C6-N6 | -17.92 | 107.85 | 118.60 |
| 22 | 23S1 | 1496 | A | N1-C6-N6 | -17.92 | 107.85 | 118.60 |
| 22 | 23S1 | 2328 | A | N1-C2-N3 | -17.91 | 120.34 | 129.30 |
| 22 | 23S1 | 1336 | A | N1-C2-N3 | -17.91 | 120.35 | 129.30 |
| 22 | 23S1 | 1077 | A | C2-N3-C4 | 17.91 | 119.55 | 110.60 |
| 22 | 23S1 | 2095 | A | N1-C2-N3 | -17.91 | 120.35 | 129.30 |
| 22 | 23S1 | 2225 | A | N1-C6-N6 | -17.91 | 107.86 | 118.60 |
| 1 | 16S1 | 3 | A | C2-N3-C4 | 17.90 | 119.55 | 110.60 |
| 22 | 23S1 | 2900 | A | N1-C2-N3 | -17.90 | 120.35 | 129.30 |
| 1 | 16S1 | 1374 | A | N1-C6-N6 | -17.90 | 107.86 | 118.60 |
| 22 | 23S1 | 482 | A | C2-N3-C4 | 17.90 | 119.55 | 110.60 |
| 1 | 16S1 | 860 | A | N1-C2-N3 | -17.90 | 120.35 | 129.30 |
| 22 | 23S1 | 63 | A | N1-C6-N6 | -17.89 | 107.86 | 118.60 |
| 22 | 23S1 | 480 | A | N1-C6-N6 | -17.89 | 107.86 | 118.60 |
| 22 | 23S1 | 2171 | A | C2-N3-C4 | 17.89 | 119.55 | 110.60 |
| 22 | 23S1 | 2412 | A | N1-C6-N6 | -17.89 | 107.87 | 118.60 |
| 22 | 23S1 | 1848 | A | N1-C2-N3 | -17.89 | 120.36 | 129.30 |
| 22 | 23S1 | 2169 | A | N1-C2-N3 | -17.89 | 120.36 | 129.30 |
| 1 | 16S1 | 1005 | A | N1-C6-N6 | -17.88 | 107.87 | 118.60 |
| 22 | 23S1 | 2814 | A | N1-C6-N6 | -17.88 | 107.87 | 118.60 |
| 1 | 16S1 | 1256 | A | N1-C6-N6 | -17.88 | 107.87 | 118.60 |
| 1 | 16S1 | 914 | A | C2-N3-C4 | 17.88 | 119.54 | 110.60 |
| 22 | 23S1 | 2800 | A | C2-N3-C4 | 17.88 | 119.54 | 110.60 |
| 22 | 23S1 | 1871 | A | N1-C2-N3 | -17.87 | 120.36 | 129.30 |
| 1 | 16S1 | 349 | A | N1-C6-N6 | -17.87 | 107.88 | 118.60 |
| 22 | 23S1 | 2082 | A | N1-C2-N3 | -17.87 | 120.36 | 129.30 |
| 22 | 23S1 | 751 | A | N1-C6-N6 | -17.87 | 107.88 | 118.60 |
| 1 | 16S1 | 1111 | A | N1-C6-N6 | -17.87 | 107.88 | 118.60 |
| 1 | 16S1 | 1261 | A | N1-C6-N6 | -17.87 | 107.88 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 352 | A | C2-N3-C4 | 17.87 | 119.53 | 110.60 |
| 22 | 23S1 | 1134 | A | N1-C6-N6 | -17.87 | 107.88 | 118.60 |
| 1 | 16S1 | 629 | A | N1-C6-N6 | -17.86 | 107.88 | 118.60 |
| 22 | 23S1 | 2059 | A | N1-C2-N3 | -17.86 | 120.37 | 129.30 |
| 22 | 23S1 | 2080 | A | N1-C6-N6 | -17.86 | 107.89 | 118.60 |
| 22 | 23S1 | 743 | A | N1-C2-N3 | -17.86 | 120.37 | 129.30 |
| 23 | 05S1 | 78 | A | N1-C6-N6 | -17.86 | 107.89 | 118.60 |
| 1 | 16S1 | 780 | A | N1-C6-N6 | -17.85 | 107.89 | 118.60 |
| 22 | 23S1 | 1126 | A | N1-C2-N3 | -17.85 | 120.38 | 129.30 |
| 22 | 23S1 | 2281 | A | N1-C2-N3 | -17.85 | 120.38 | 129.30 |
| 1 | 16S1 | 98 | A | N1-C2-N3 | -17.84 | 120.38 | 129.30 |
| 1 | 16S1 | 622 | A | C2-N3-C4 | 17.84 | 119.52 | 110.60 |
| 1 | 16S1 | 864 | A | N1-C2-N3 | -17.84 | 120.38 | 129.30 |
| 1 | 16S1 | 1339 | A | N1-C2-N3 | -17.84 | 120.38 | 129.30 |
| 22 | 23S1 | 2750 | A | N1-C2-N3 | -17.84 | 120.38 | 129.30 |
| 22 | 23S1 | 2883 | A | N1-C6-N6 | -17.84 | 107.89 | 118.60 |
| 1 | 16S1 | 675 | A | N1-C6-N6 | -17.84 | 107.89 | 118.60 |
| 1 | 16S1 | 55 | A | N1-C2-N3 | -17.84 | 120.38 | 129.30 |
| 1 | 16S1 | 1483 | A | N1-C2-N3 | -17.84 | 120.38 | 129.30 |
| 22 | 23S1 | 272 | A | N1-C2-N3 | -17.84 | 120.38 | 129.30 |
| 22 | 23S1 | 1241 | A | N1-C2-N3 | -17.84 | 120.38 | 129.30 |
| 22 | 23S1 | 1307 | A | N1-C6-N6 | -17.84 | 107.90 | 118.60 |
| 1 | 16S1 | 466 | A | N1-C2-N3 | -17.83 | 120.38 | 129.30 |
| 22 | 23S1 | 466 | A | C2-N3-C4 | 17.83 | 119.52 | 110.60 |
| 22 | 23S1 | 1679 | A | C2-N3-C4 | 17.83 | 119.52 | 110.60 |
| 22 | 23S1 | 2147 | A | N1-C6-N6 | -17.83 | 107.90 | 118.60 |
| 22 | 23S1 | 1808 | A | C2-N3-C4 | 17.83 | 119.51 | 110.60 |
| 22 | 23S1 | 362 | A | N1-C2-N3 | -17.82 | 120.39 | 129.30 |
| 22 | 23S1 | 1609 | A | N1-C6-N6 | -17.82 | 107.91 | 118.60 |
| 1 | 16S1 | 1216 | A | N1-C2-N3 | -17.82 | 120.39 | 129.30 |
| 22 | 23S1 | 1608 | A | N1-C2-N3 | -17.82 | 120.39 | 129.30 |
| 22 | 23S1 | 56 | A | N1-C2-N3 | -17.82 | 120.39 | 129.30 |
| 22 | 23S1 | 2176 | A | C2-N3-C4 | 17.82 | 119.51 | 110.60 |
| 23 | 05S1 | 34 | A | N1-C6-N6 | -17.82 | 107.91 | 118.60 |
| 1 | 16S1 | 959 | A | N1-C2-N3 | -17.81 | 120.39 | 129.30 |
| 1 | 16S1 | 1204 | A | N1-C2-N3 | -17.81 | 120.39 | 129.30 |
| 22 | 23S1 | 2352 | A | N1-C6-N6 | -17.80 | 107.92 | 118.60 |
| 1 | 16S1 | 1339 | A | C2-N3-C4 | 17.80 | 119.50 | 110.60 |
| 1 | 16S1 | 608 | A | N1-C6-N6 | -17.80 | 107.92 | 118.60 |
| 22 | 23S1 | 402 | A | C2-N3-C4 | 17.80 | 119.50 | 110.60 |
| 1 | 16S1 | 694 | A | N1-C6-N6 | -17.80 | 107.92 | 118.60 |
| 1 | 16S1 | 55 | A | N1-C6-N6 | -17.80 | 107.92 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 56 | A | N1-C6-N6 | -17.80 | 107.92 | 118.60 |
| 55 | PTR1 | 3 | A | N1-C6-N6 | -17.80 | 107.92 | 118.60 |
| 1 | 16S1 | 681 | A | N1-C2-N3 | -17.79 | 120.40 | 129.30 |
| 22 | 23S1 | 1969 | A | C2-N3-C4 | 17.79 | 119.50 | 110.60 |
| 1 | 16S1 | 279 | A | N1-C6-N6 | -17.79 | 107.92 | 118.60 |
| 1 | 16S1 | 743 | A | N1-C6-N6 | -17.79 | 107.92 | 118.60 |
| 22 | 23S1 | 19 | A | N1-C6-N6 | -17.79 | 107.92 | 118.60 |
| 22 | 23S1 | 382 | A | N1-C2-N3 | -17.79 | 120.40 | 129.30 |
| 22 | 23S1 | 2059 | A | N1-C6-N6 | -17.79 | 107.92 | 118.60 |
| 22 | 23S1 | 2634 | A | N1-C2-N3 | -17.79 | 120.40 | 129.30 |
| 22 | 23S1 | 1230 | A | N1-C2-N3 | -17.79 | 120.41 | 129.30 |
| 1 | 16S1 | 131 | A | N1-C2-N3 | -17.79 | 120.41 | 129.30 |
| 22 | 23S1 | 404 | A | N1-C6-N6 | -17.79 | 107.93 | 118.60 |
| 22 | 23S1 | 144 | A | N1-C6-N6 | -17.79 | 107.93 | 118.60 |
| 22 | 23S1 | 547 | A | N1-C6-N6 | -17.79 | 107.93 | 118.60 |
| 22 | 23S1 | 2433 | A | N1-C6-N6 | -17.78 | 107.93 | 118.60 |
| 22 | 23S1 | 439 | A | N1-C6-N6 | -17.78 | 107.93 | 118.60 |
| 22 | 23S1 | 716 | A | C2-N3-C4 | 17.78 | 119.49 | 110.60 |
| 22 | 23S1 | 2095 | A | C2-N3-C4 | 17.78 | 119.49 | 110.60 |
| 1 | 16S1 | 80 | A | N1-C6-N6 | -17.78 | 107.93 | 118.60 |
| 1 | 16S1 | 946 | A | N1-C2-N3 | -17.77 | 120.41 | 129.30 |
| 22 | 23S1 | 1226 | A | C2-N3-C4 | 17.77 | 119.49 | 110.60 |
| 22 | 23S1 | 1387 | A | N1-C2-N3 | -17.77 | 120.41 | 129.30 |
| 22 | 23S1 | 1913 | A | N1-C6-N6 | -17.77 | 107.94 | 118.60 |
| 1 | 16S1 | 1081 | A | N1-C6-N6 | -17.77 | 107.94 | 118.60 |
| 1 | 16S1 | 338 | A | N1-C6-N6 | -17.77 | 107.94 | 118.60 |
| 1 | 16S1 | 1534 | A | N1-C6-N6 | -17.77 | 107.94 | 118.60 |
| 1 | 16S1 | 174 | A | N1-C6-N6 | -17.77 | 107.94 | 118.60 |
| 1 | 16S1 | 182 | A | N1-C6-N6 | -17.77 | 107.94 | 118.60 |
| 22 | 23S1 | 2274 | A | C2-N3-C4 | 17.77 | 119.48 | 110.60 |
| 22 | 23S1 | 1027 | A | C2-N3-C4 | 17.77 | 119.48 | 110.60 |
| 1 | 16S1 | 189 | A | N1-C2-N3 | -17.77 | 120.42 | 129.30 |
| 22 | 23S1 | 2176 | A | N1-C2-N3 | -17.77 | 120.42 | 129.30 |
| 1 | 16S1 | 607 | A | C2-N3-C4 | 17.76 | 119.48 | 110.60 |
| 22 | 23S1 | 348 | A | N1-C2-N3 | -17.76 | 120.42 | 129.30 |
| 22 | 23S1 | 2340 | A | C2-N3-C4 | 17.76 | 119.48 | 110.60 |
| 1 | 16S1 | 1531 | A | N1-C6-N6 | -17.76 | 107.95 | 118.60 |
| 22 | 23S1 | 1689 | A | N1-C2-N3 | -17.76 | 120.42 | 129.30 |
| 23 | 05S1 | 52 | A | N1-C6-N6 | -17.76 | 107.95 | 118.60 |
| 1 | 16S1 | 1171 | A | N1-C2-N3 | -17.75 | 120.42 | 129.30 |
| 22 | 23S1 | 1268 | A | N1-C6-N6 | -17.75 | 107.95 | 118.60 |
| 22 | 23S1 | 1373 | A | N1-C6-N6 | -17.75 | 107.95 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 729 | A | N1-C6-N6 | -17.75 | 107.95 | 118.60 |
| 1 | 16S1 | 344 | A | N1-C6-N6 | -17.75 | 107.95 | 118.60 |
| 22 | 23S1 | 2425 | A | N1-C2-N3 | -17.75 | 120.43 | 129.30 |
| 1 | 16S1 | 196 | A | C2-N3-C4 | 17.74 | 119.47 | 110.60 |
| 22 | 23S1 | 471 | A | N1-C6-N6 | -17.74 | 107.95 | 118.60 |
| 22 | 23S1 | 1810 | A | C2-N3-C4 | 17.74 | 119.47 | 110.60 |
| 1 | 16S1 | 1360 | A | N1-C2-N3 | -17.74 | 120.43 | 129.30 |
| 1 | 16S1 | 864 | A | N1-C6-N6 | -17.74 | 107.96 | 118.60 |
| 22 | 23S1 | 602 | A | N1-C6-N6 | -17.74 | 107.96 | 118.60 |
| 22 | 23S1 | 1287 | A | N1-C6-N6 | -17.73 | 107.96 | 118.60 |
| 1 | 16S1 | 65 | A | N1-C6-N6 | -17.73 | 107.96 | 118.60 |
| 1 | 16S1 | 1171 | A | N1-C6-N6 | -17.73 | 107.96 | 118.60 |
| 22 | 23S1 | 1057 | A | N1-C6-N6 | -17.73 | 107.96 | 118.60 |
| 22 | 23S1 | 2134 | A | N1-C2-N3 | -17.73 | 120.44 | 129.30 |
| 22 | 23S1 | 91 | A | C2-N3-C4 | 17.72 | 119.46 | 110.60 |
| 1 | 16S1 | 640 | A | N1-C2-N3 | -17.72 | 120.44 | 129.30 |
| 22 | 23S1 | 1302 | A | N1-C6-N6 | -17.72 | 107.97 | 118.60 |
| 1 | 16S1 | 663 | A | N1-C6-N6 | -17.72 | 107.97 | 118.60 |
| 1 | 16S1 | 635 | A | N1-C2-N3 | -17.72 | 120.44 | 129.30 |
| 22 | 23S1 | 1433 | A | N1-C2-N3 | -17.72 | 120.44 | 129.30 |
| 22 | 23S1 | 2634 | A | N1-C6-N6 | -17.72 | 107.97 | 118.60 |
| 55 | PTR1 | 9 | A | C2-N3-C4 | 17.72 | 119.46 | 110.60 |
| 1 | 16S1 | 65 | A | C2-N3-C4 | 17.71 | 119.46 | 110.60 |
| 22 | 23S1 | 182 | A | N1-C6-N6 | -17.71 | 107.97 | 118.60 |
| 22 | 23S1 | 2154 | A | N1-C6-N6 | -17.71 | 107.97 | 118.60 |
| 22 | 23S1 | 2860 | A | C2-N3-C4 | 17.71 | 119.45 | 110.60 |
| 1 | 16S1 | 383 | A | C2-N3-C4 | 17.71 | 119.45 | 110.60 |
| 22 | 23S1 | 2893 | A | N1-C6-N6 | -17.71 | 107.97 | 118.60 |
| 22 | 23S1 | 572 | A | N1-C2-N3 | -17.71 | 120.45 | 129.30 |
| 22 | 23S1 | 1327 | A | N1-C6-N6 | -17.71 | 107.98 | 118.60 |
| 22 | 23S1 | 255 | A | N1-C6-N6 | -17.70 | 107.98 | 118.60 |
| 22 | 23S1 | 2071 | A | N1-C2-N3 | -17.70 | 120.45 | 129.30 |
| 1 | 16S1 | 415 | A | N1-C2-N3 | -17.70 | 120.45 | 129.30 |
| 1 | 16S1 | 968 | A | N1-C6-N6 | -17.70 | 107.98 | 118.60 |
| 22 | 23S1 | 960 | A | C2-N3-C4 | 17.70 | 119.45 | 110.60 |
| 1 | 16S1 | 1102 | A | N1-C6-N6 | -17.70 | 107.98 | 118.60 |
| 22 | 23S1 | 2430 | A | N1-C6-N6 | -17.69 | 107.98 | 118.60 |
| 23 | 05S1 | 66 | A | N1-C2-N3 | -17.69 | 120.45 | 129.30 |
| 1 | 16S1 | 1513 | A | N1-C6-N6 | -17.69 | 107.98 | 118.60 |
| 22 | 23S1 | 1938 | A | N1-C6-N6 | -17.69 | 107.99 | 118.60 |
| 1 | 16S1 | 1306 | A | N1-C6-N6 | -17.69 | 107.99 | 118.60 |
| 22 | 23S1 | 1046 | A | N1-C6-N6 | -17.69 | 107.99 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1127 | A | N1-C6-N6 | -17.69 | 107.99 | 118.60 |
| 22 | 23S1 | 2411 | A | N1-C6-N6 | -17.69 | 107.99 | 118.60 |
| 1 | 16S1 | 1324 | A | N1-C2-N3 | -17.68 | 120.46 | 129.30 |
| 22 | 23S1 | 928 | A | N1-C6-N6 | -17.68 | 107.99 | 118.60 |
| 22 | 23S1 | 1508 | A | N1-C6-N6 | -17.68 | 107.99 | 118.60 |
| 1 | 16S1 | 493 | A | C2-N3-C4 | 17.68 | 119.44 | 110.60 |
| 1 | 16S1 | 120 | A | N1-C6-N6 | -17.68 | 107.99 | 118.60 |
| 1 | 16S1 | 1167 | A | N1-C6-N6 | -17.67 | 108.00 | 118.60 |
| 22 | 23S1 | 1566 | A | N1-C6-N6 | -17.67 | 108.00 | 118.60 |
| 22 | 23S1 | 1745 | A | C2-N3-C4 | 17.67 | 119.43 | 110.60 |
| 22 | 23S1 | 1899 | A | N1-C2-N3 | -17.67 | 120.47 | 129.30 |
| 22 | 23S1 | 1470 | A | N1-C6-N6 | -17.66 | 108.00 | 118.60 |
| 22 | 23S1 | 2531 | A | N1-C2-N3 | -17.66 | 120.47 | 129.30 |
| 22 | 23S1 | 1169 | A | N1-C6-N6 | -17.66 | 108.00 | 118.60 |
| 22 | 23S1 | 1387 | A | N1-C6-N6 | -17.66 | 108.00 | 118.60 |
| 22 | 23S1 | 899 | A | N1-C2-N3 | -17.66 | 120.47 | 129.30 |
| 22 | 23S1 | 1039 | A | N1-C6-N6 | -17.66 | 108.00 | 118.60 |
| 1 | 16S1 | 935 | A | N1-C2-N3 | -17.66 | 120.47 | 129.30 |
| 1 | 16S1 | 919 | A | N1-C6-N6 | -17.66 | 108.01 | 118.60 |
| 22 | 23S1 | 2278 | A | N1-C2-N3 | -17.65 | 120.47 | 129.30 |
| 22 | 23S1 | 1848 | A | C2-N3-C4 | 17.65 | 119.42 | 110.60 |
| 23 | 05S1 | 45 | A | N1-C6-N6 | -17.64 | 108.02 | 118.60 |
| 1 | 16S1 | 1508 | A | N1-C2-N3 | -17.64 | 120.48 | 129.30 |
| 22 | 23S1 | 155 | A | N1-C6-N6 | -17.64 | 108.02 | 118.60 |
| 22 | 23S1 | 2439 | A | C2-N3-C4 | 17.63 | 119.41 | 110.60 |
| 22 | 23S1 | 2114 | A | N1-C2-N3 | -17.63 | 120.49 | 129.30 |
| 1 | 16S1 | 706 | A | N1-C6-N6 | -17.63 | 108.02 | 118.60 |
| 1 | 16S1 | 790 | A | N1-C6-N6 | -17.63 | 108.02 | 118.60 |
| 22 | 23S1 | 44 | A | N1-C6-N6 | -17.63 | 108.02 | 118.60 |
| 1 | 16S1 | 77 | A | N1-C6-N6 | -17.62 | 108.03 | 118.60 |
| 22 | 23S1 | 943 | A | N1-C6-N6 | -17.62 | 108.03 | 118.60 |
| 22 | 23S1 | 1403 | A | N1-C6-N6 | -17.62 | 108.03 | 118.60 |
| 22 | 23S1 | 2407 | A | N1-C6-N6 | -17.62 | 108.03 | 118.60 |
| 22 | 23S1 | 1354 | A | N1-C6-N6 | -17.62 | 108.03 | 118.60 |
| 22 | 23S1 | 742 | A | N1-C6-N6 | -17.62 | 108.03 | 118.60 |
| 22 | 23S1 | 152 | A | N1-C6-N6 | -17.62 | 108.03 | 118.60 |
| 22 | 23S1 | 1073 | A | N1-C6-N6 | -17.62 | 108.03 | 118.60 |
| 22 | 23S1 | 586 | A | C2-N3-C4 | 17.61 | 119.41 | 110.60 |
| 1 | 16S1 | 190 | A | C2-N3-C4 | 17.61 | 119.41 | 110.60 |
| 1 | 16S1 | 1022 | A | N1-C6-N6 | -17.61 | 108.03 | 118.60 |
| 22 | 23S1 | 2407 | A | N1-C2-N3 | -17.61 | 120.50 | 129.30 |
| 1 | 16S1 | 327 | A | N1-C6-N6 | -17.61 | 108.04 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 1191 | A | N1-C6-N6 | -17.61 | 108.04 | 118.60 |
| 22 | 23S1 | 2077 | A | N1-C2-N3 | -17.61 | 120.50 | 129.30 |
| 22 | 23S1 | 1088 | A | N1-C6-N6 | -17.60 | 108.04 | 118.60 |
| 22 | 23S1 | 1705 | A | N1-C6-N6 | -17.60 | 108.04 | 118.60 |
| 1 | 16S1 | 101 | A | N1-C6-N6 | -17.60 | 108.04 | 118.60 |
| 22 | 23S1 | 2534 | A | N1-C6-N6 | -17.60 | 108.04 | 118.60 |
| 1 | 16S1 | 53 | A | N1-C6-N6 | -17.59 | 108.04 | 118.60 |
| 22 | 23S1 | 2378 | A | N1-C6-N6 | -17.59 | 108.04 | 118.60 |
| 1 | 16S1 | 1012 | A | C2-N3-C4 | 17.59 | 119.40 | 110.60 |
| 22 | 23S1 | 1579 | A | N1-C6-N6 | -17.59 | 108.05 | 118.60 |
| 22 | 23S1 | 2448 | A | C2-N3-C4 | 17.59 | 119.39 | 110.60 |
| 22 | 23S1 | 1431 | A | N1-C6-N6 | -17.59 | 108.05 | 118.60 |
| 22 | 23S1 | 1810 | A | N1-C2-N3 | -17.59 | 120.51 | 129.30 |
| 22 | 23S1 | 1504 | A | N1-C6-N6 | -17.58 | 108.05 | 118.60 |
| 22 | 23S1 | 2516 | A | N1-C6-N6 | -17.57 | 108.06 | 118.60 |
| 22 | 23S1 | 1548 | A | N1-C6-N6 | -17.57 | 108.06 | 118.60 |
| 22 | 23S1 | 1477 | A | N1-C6-N6 | -17.57 | 108.06 | 118.60 |
| 22 | 23S1 | 2071 | A | N1-C6-N6 | -17.57 | 108.06 | 118.60 |
| 22 | 23S1 | 477 | A | C2-N3-C4 | 17.56 | 119.38 | 110.60 |
| 22 | 23S1 | 482 | A | N1-C2-N3 | -17.56 | 120.52 | 129.30 |
| 22 | 23S1 | 218 | A | N1-C6-N6 | -17.56 | 108.06 | 118.60 |
| 22 | 23S1 | 1336 | A | N1-C6-N6 | -17.56 | 108.06 | 118.60 |
| 22 | 23S1 | 1711 | A | N1-C6-N6 | -17.56 | 108.06 | 118.60 |
| 22 | 23S1 | 1735 | A | N1-C2-N3 | -17.56 | 120.52 | 129.30 |
| 22 | 23S1 | 142 | A | C2-N3-C4 | 17.55 | 119.38 | 110.60 |
| 22 | 23S1 | 233 | A | N1-C6-N6 | -17.54 | 108.07 | 118.60 |
| 22 | 23S1 | 1998 | A | N1-C2-N3 | -17.54 | 120.53 | 129.30 |
| 22 | 23S1 | 900 | A | N1-C6-N6 | -17.54 | 108.08 | 118.60 |
| 22 | 23S1 | 1614 | A | C2-N3-C4 | 17.54 | 119.37 | 110.60 |
| 22 | 23S1 | 1713 | A | N1-C6-N6 | -17.54 | 108.08 | 118.60 |
| 22 | 23S1 | 2469 | A | N1-C6-N6 | -17.53 | 108.08 | 118.60 |
| 1 | 16S1 | 532 | A | N1-C6-N6 | -17.53 | 108.08 | 118.60 |
| 22 | 23S1 | 1626 | A | N1-C6-N6 | -17.53 | 108.08 | 118.60 |
| 1 | 16S1 | 109 | A | N1-C6-N6 | -17.53 | 108.08 | 118.60 |
| 22 | 23S1 | 1679 | A | N1-C2-N3 | -17.53 | 120.54 | 129.30 |
| 1 | 16S1 | 81 | A | C2-N3-C4 | 17.52 | 119.36 | 110.60 |
| 1 | 16S1 | 353 | A | N1-C6-N6 | -17.51 | 108.10 | 118.60 |
| 1 | 16S1 | 673 | A | N1-C2-N3 | -17.50 | 120.55 | 129.30 |
| 22 | 23S1 | 2598 | A | N1-C6-N6 | -17.50 | 108.10 | 118.60 |
| 1 | 16S1 | 336 | A | N1-C6-N6 | -17.50 | 108.10 | 118.60 |
| 1 | 16S1 | 466 | A | N1-C6-N6 | -17.50 | 108.10 | 118.60 |
| 22 | 23S1 | 2792 | A | N1-C6-N6 | -17.50 | 108.10 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 609 | A | N1-C6-N6 | -17.49 | 108.11 | 118.60 |
| 22 | 23S1 | 586 | A | N1-C6-N6 | -17.49 | 108.11 | 118.60 |
| 1 | 16S1 | 1318 | A | N1-C6-N6 | -17.48 | 108.11 | 118.60 |
| 1 | 16S1 | 687 | A | N1-C6-N6 | -17.48 | 108.11 | 118.60 |
| 1 | 16S1 | 1081 | A | N1-C2-N3 | -17.48 | 120.56 | 129.30 |
| 22 | 23S1 | 613 | A | N1-C6-N6 | -17.48 | 108.11 | 118.60 |
| 22 | 23S1 | 2281 | A | N1-C6-N6 | -17.48 | 108.11 | 118.60 |
| 22 | 23S1 | 522 | A | N1-C2-N3 | -17.47 | 120.57 | 129.30 |
| 22 | 23S1 | 1269 | A | N1-C2-N3 | -17.46 | 120.57 | 129.30 |
| 1 | 16S1 | 1022 | A | N1-C2-N3 | -17.46 | 120.57 | 129.30 |
| 22 | 23S1 | 404 | A | C2-N3-C4 | 17.46 | 119.33 | 110.60 |
| 22 | 23S1 | 1590 | A | N1-C6-N6 | -17.46 | 108.12 | 118.60 |
| 22 | 23S1 | 142 | A | N1-C2-N3 | -17.45 | 120.57 | 129.30 |
| 22 | 23S1 | 2142 | A | N1-C2-N3 | -17.45 | 120.57 | 129.30 |
| 1 | 16S1 | 539 | A | N1-C6-N6 | -17.45 | 108.13 | 118.60 |
| 22 | 23S1 | 53 | A | N1-C6-N6 | -17.45 | 108.13 | 118.60 |
| 22 | 23S1 | 221 | A | C2-N3-C4 | 17.45 | 119.33 | 110.60 |
| 1 | 16S1 | 1324 | A | N1-C6-N6 | -17.45 | 108.13 | 118.60 |
| 22 | 23S1 | 161 | A | C2-N3-C4 | 17.45 | 119.32 | 110.60 |
| 1 | 16S1 | 270 | A | N1-C6-N6 | -17.44 | 108.14 | 118.60 |
| 22 | 23S1 | 781 | A | N1-C2-N3 | -17.44 | 120.58 | 129.30 |
| 22 | 23S1 | 282 | A | N1-C6-N6 | -17.44 | 108.14 | 118.60 |
| 1 | 16S1 | 935 | A | N1-C6-N6 | -17.44 | 108.14 | 118.60 |
| 22 | 23S1 | 1143 | A | C2-N3-C4 | 17.43 | 119.32 | 110.60 |
| 1 | 16S1 | 373 | A | N1-C6-N6 | -17.43 | 108.14 | 118.60 |
| 22 | 23S1 | 721 | A | N1-C6-N6 | -17.43 | 108.14 | 118.60 |
| 22 | 23S1 | 227 | A | N1-C6-N6 | -17.41 | 108.15 | 118.60 |
| 22 | 23S1 | 2565 | A | C2-N3-C4 | 17.41 | 119.30 | 110.60 |
| 22 | 23S1 | 975 | A | N1-C6-N6 | -17.41 | 108.16 | 118.60 |
| 1 | 16S1 | 635 | A | N1-C6-N6 | -17.40 | 108.16 | 118.60 |
| 1 | 16S1 | 1169 | A | N1-C6-N6 | -17.40 | 108.16 | 118.60 |
| 1 | 16S1 | 116 | A | N1-C6-N6 | -17.39 | 108.16 | 118.60 |
| 22 | 23S1 | 1603 | A | N1-C6-N6 | -17.39 | 108.17 | 118.60 |
| 55 | PTR1 | 76 | A | N1-C6-N6 | -17.39 | 108.17 | 118.60 |
| 1 | 16S1 | 908 | A | N1-C6-N6 | -17.39 | 108.17 | 118.60 |
| 1 | 16S1 | 74 | A | C2-N3-C4 | 17.38 | 119.29 | 110.60 |
| 55 | PTR1 | 73 | A | N1-C6-N6 | -17.38 | 108.17 | 118.60 |
| 22 | 23S1 | 503 | A | N1-C6-N6 | -17.37 | 108.18 | 118.60 |
| 22 | 23S1 | 1420 | A | N1-C6-N6 | -17.37 | 108.18 | 118.60 |
| 1 | 16S1 | 1271 | A | N1-C6-N6 | -17.37 | 108.18 | 118.60 |
| 1 | 16S1 | 1275 | A | N1-C6-N6 | -17.37 | 108.18 | 118.60 |
| 22 | 23S1 | 2117 | A | C2-N3-C4 | 17.37 | 119.28 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 66 | A | N1-C6-N6 | -17.36 | 108.18 | 118.60 |
| 22 | 23S1 | 644 | A | N1-C2-N3 | -17.36 | 120.62 | 129.30 |
| 1 | 16S1 | 263 | A | N1-C6-N6 | -17.36 | 108.18 | 118.60 |
| 22 | 23S1 | 1403 | A | N1-C2-N3 | -17.36 | 120.62 | 129.30 |
| 22 | 23S1 | 2820 | A | N1-C6-N6 | -17.36 | 108.18 | 118.60 |
| 22 | 23S1 | 342 | A | N1-C6-N6 | -17.36 | 108.19 | 118.60 |
| 22 | 23S1 | 1735 | A | N1-C6-N6 | -17.36 | 108.19 | 118.60 |
| 22 | 23S1 | 503 | A | N1-C2-N3 | -17.35 | 120.62 | 129.30 |
| 22 | 23S1 | 627 | A | N1-C6-N6 | -17.35 | 108.19 | 118.60 |
| 22 | 23S1 | 173 | A | N1-C6-N6 | -17.35 | 108.19 | 118.60 |
| 22 | 23S1 | 2900 | A | N1-C6-N6 | -17.35 | 108.19 | 118.60 |
| 1 | 16S1 | 32 | A | N1-C2-N3 | -17.34 | 120.63 | 129.30 |
| 1 | 16S1 | 300 | A | C2-N3-C4 | 17.34 | 119.27 | 110.60 |
| 22 | 23S1 | 863 | A | N1-C6-N6 | -17.34 | 108.20 | 118.60 |
| 22 | 23S1 | 599 | A | N1-C6-N6 | -17.33 | 108.20 | 118.60 |
| 22 | 23S1 | 2530 | A | N1-C6-N6 | -17.32 | 108.20 | 118.60 |
| 1 | 16S1 | 78 | A | N1-C6-N6 | -17.32 | 108.21 | 118.60 |
| 22 | 23S1 | 632 | A | N1-C6-N6 | -17.32 | 108.21 | 118.60 |
| 22 | 23S1 | 272 | A | N1-C6-N6 | -17.32 | 108.21 | 118.60 |
| 1 | 16S1 | 1219 | A | N1-C6-N6 | -17.32 | 108.21 | 118.60 |
| 1 | 16S1 | 510 | A | N1-C6-N6 | -17.31 | 108.21 | 118.60 |
| 22 | 23S1 | 1528 | A | C2-N3-C4 | 17.31 | 119.26 | 110.60 |
| 22 | 23S1 | 101 | A | N1-C6-N6 | -17.31 | 108.22 | 118.60 |
| 22 | 23S1 | 256 | A | N1-C6-N6 | -17.31 | 108.22 | 118.60 |
| 22 | 23S1 | 477 | A | N1-C2-N3 | -17.31 | 120.65 | 129.30 |
| 22 | 23S1 | 1847 | A | N1-C6-N6 | -17.30 | 108.22 | 118.60 |
| 1 | 16S1 | 1319 | A | C2-N3-C4 | 17.30 | 119.25 | 110.60 |
| 22 | 23S1 | 677 | A | N1-C6-N6 | -17.29 | 108.22 | 118.60 |
| 1 | 16S1 | 374 | A | N1-C6-N6 | -17.29 | 108.23 | 118.60 |
| 1 | 16S1 | 1080 | A | N1-C6-N6 | -17.29 | 108.23 | 118.60 |
| 1 | 16S1 | 71 | A | N1-C6-N6 | -17.28 | 108.23 | 118.60 |
| 22 | 23S1 | 861 | A | N1-C6-N6 | -17.28 | 108.23 | 118.60 |
| 22 | 23S1 | 94 | A | N1-C6-N6 | -17.28 | 108.23 | 118.60 |
| 22 | 23S1 | 344 | A | N1-C6-N6 | -17.28 | 108.23 | 118.60 |
| 22 | 23S1 | 677 | A | N1-C2-N3 | -17.28 | 120.66 | 129.30 |
| 1 | 16S1 | 1012 | A | N1-C2-N3 | -17.27 | 120.66 | 129.30 |
| 22 | 23S1 | 1717 | A | N1-C6-N6 | -17.27 | 108.24 | 118.60 |
| 22 | 23S1 | 191 | A | N1-C6-N6 | -17.26 | 108.24 | 118.60 |
| 22 | 23S1 | 1614 | A | N1-C6-N6 | -17.26 | 108.24 | 118.60 |
| 1 | 16S1 | 356 | A | N1-C6-N6 | -17.26 | 108.24 | 118.60 |
| 1 | 16S1 | 975 | A | C2-N3-C4 | 17.26 | 119.23 | 110.60 |
| 22 | 23S1 | 447 | A | N1-C6-N6 | -17.26 | 108.25 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1650 | A | N1-C6-N6 | -17.26 | 108.25 | 118.60 |
| 1 | 16S1 | 250 | A | N1-C6-N6 | -17.25 | 108.25 | 118.60 |
| 1 | 16S1 | 1274 | A | N1-C6-N6 | -17.25 | 108.25 | 118.60 |
| 22 | 23S1 | 1808 | A | N1-C6-N6 | -17.25 | 108.25 | 118.60 |
| 1 | 16S1 | 919 | A | N1-C2-N3 | -17.25 | 120.68 | 129.30 |
| 22 | 23S1 | 575 | A | N1-C6-N6 | -17.24 | 108.25 | 118.60 |
| 1 | 16S1 | 1036 | A | N1-C2-N3 | -17.24 | 120.68 | 129.30 |
| 22 | 23S1 | 2108 | A | N1-C2-N3 | -17.24 | 120.68 | 129.30 |
| 1 | 16S1 | 162 | A | N1-C2-N3 | -17.23 | 120.68 | 129.30 |
| 1 | 16S1 | 279 | A | C2-N3-C4 | 17.23 | 119.22 | 110.60 |
| 1 | 16S1 | 767 | A | N1-C6-N6 | -17.23 | 108.26 | 118.60 |
| 1 | 16S1 | 1000 | A | N1-C6-N6 | -17.23 | 108.26 | 118.60 |
| 22 | 23S1 | 1553 | A | N1-C6-N6 | -17.22 | 108.27 | 118.60 |
| 22 | 23S1 | 2721 | A | N1-C6-N6 | -17.22 | 108.27 | 118.60 |
| 1 | 16S1 | 435 | A | N1-C6-N6 | -17.21 | 108.27 | 118.60 |
| 22 | 23S1 | 2094 | A | N1-C6-N6 | -17.21 | 108.27 | 118.60 |
| 22 | 23S1 | 972 | A | N1-C6-N6 | -17.21 | 108.27 | 118.60 |
| 22 | 23S1 | 1189 | A | N1-C6-N6 | -17.21 | 108.27 | 118.60 |
| 1 | 16S1 | 460 | A | N1-C6-N6 | -17.20 | 108.28 | 118.60 |
| 1 | 16S1 | 1014 | A | N1-C6-N6 | -17.20 | 108.28 | 118.60 |
| 22 | 23S1 | 2088 | A | N1-C6-N6 | -17.20 | 108.28 | 118.60 |
| 1 | 16S1 | 959 | A | N1-C6-N6 | -17.20 | 108.28 | 118.60 |
| 22 | 23S1 | 1020 | A | C2-N3-C4 | 17.20 | 119.20 | 110.60 |
| 1 | 16S1 | 189 | A | N1-C6-N6 | -17.20 | 108.28 | 118.60 |
| 22 | 23S1 | 1001 | A | C2-N3-C4 | 17.20 | 119.20 | 110.60 |
| 1 | 16S1 | 246 | A | N1-C6-N6 | -17.19 | 108.28 | 118.60 |
| 22 | 23S1 | 960 | A | N1-C2-N3 | -17.19 | 120.71 | 129.30 |
| 22 | 23S1 | 1080 | A | N1-C6-N6 | -17.18 | 108.29 | 118.60 |
| 22 | 23S1 | 1722 | A | C2-N3-C4 | 17.18 | 119.19 | 110.60 |
| 22 | 23S1 | 1205 | A | C2-N3-C4 | 17.18 | 119.19 | 110.60 |
| 1 | 16S1 | 1503 | A | N1-C6-N6 | -17.18 | 108.30 | 118.60 |
| 1 | 16S1 | 461 | A | N1-C6-N6 | -17.17 | 108.30 | 118.60 |
| 1 | 16S1 | 33 | A | N1-C6-N6 | -17.17 | 108.30 | 118.60 |
| 23 | 05S1 | 66 | A | N1-C6-N6 | -17.17 | 108.30 | 118.60 |
| 22 | 23S1 | 2675 | A | N1-C6-N6 | -17.16 | 108.30 | 118.60 |
| 1 | 16S1 | 1093 | A | N1-C6-N6 | -17.15 | 108.31 | 118.60 |
| 22 | 23S1 | 2725 | A | N1-C6-N6 | -17.15 | 108.31 | 118.60 |
| 22 | 23S1 | 415 | A | N1-C6-N6 | -17.15 | 108.31 | 118.60 |
| 22 | 23S1 | 945 | A | N1-C2-N3 | -17.15 | 120.72 | 129.30 |
| 1 | 16S1 | 493 | A | N1-C6-N6 | -17.15 | 108.31 | 118.60 |
| 22 | 23S1 | 2662 | A | N1-C2-N3 | -17.15 | 120.73 | 129.30 |
| 1 | 16S1 | 523 | A | N1-C6-N6 | -17.15 | 108.31 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 2117 | A | N1-C6-N6 | -17.15 | 108.31 | 118.60 |
| 22 | 23S1 | 1722 | A | N1-C2-N3 | -17.13 | 120.73 | 129.30 |
| 22 | 23S1 | 472 | A | N1-C6-N6 | -17.13 | 108.32 | 118.60 |
| 22 | 23S1 | 89 | A | N1-C6-N6 | -17.12 | 108.33 | 118.60 |
| 22 | 23S1 | 1746 | A | N1-C2-N3 | -17.12 | 120.74 | 129.30 |
| 22 | 23S1 | 1103 | A | N1-C6-N6 | -17.12 | 108.33 | 118.60 |
| 1 | 16S1 | 1170 | A | N1-C2-N3 | -17.11 | 120.75 | 129.30 |
| 1 | 16S1 | 431 | A | C5-C6-N6 | 17.11 | 137.39 | 123.70 |
| 22 | 23S1 | 1745 | A | N1-C6-N6 | -17.10 | 108.34 | 118.60 |
| 22 | 23S1 | 788 | A | N1-C6-N6 | -17.10 | 108.34 | 118.60 |
| 22 | 23S1 | 1272 | A | C2-N3-C4 | 17.10 | 119.15 | 110.60 |
| 55 | PTR1 | 14 | A | N1-C2-N3 | -17.10 | 120.75 | 129.30 |
| 22 | 23S1 | 2014 | A | N1-C6-N6 | -17.09 | 108.34 | 118.60 |
| 22 | 23S1 | 1928 | A | C2-N3-C4 | 17.09 | 119.15 | 110.60 |
| 23 | 05S1 | 66 | A | C2-N3-C4 | 17.09 | 119.14 | 110.60 |
| 22 | 23S1 | 1586 | A | N1-C6-N6 | -17.08 | 108.35 | 118.60 |
| 22 | 23S1 | 2781 | A | N1-C6-N6 | -17.07 | 108.36 | 118.60 |
| 22 | 23S1 | 2837 | A | N1-C6-N6 | -17.06 | 108.36 | 118.60 |
| 1 | 16S1 | 907 | A | N1-C6-N6 | -17.06 | 108.36 | 118.60 |
| 22 | 23S1 | 2268 | A | N1-C6-N6 | -17.05 | 108.37 | 118.60 |
| 55 | PTR1 | 9 | A | N1-C6-N6 | -17.05 | 108.37 | 118.60 |
| 22 | 23S1 | 693 | A | N1-C6-N6 | -17.03 | 108.38 | 118.60 |
| 22 | 23S1 | 1936 | A | N1-C6-N6 | -17.03 | 108.38 | 118.60 |
| 22 | 23S1 | 2158 | A | N1-C6-N6 | -17.03 | 108.39 | 118.60 |
| 22 | 23S1 | 2781 | A | C2-N3-C4 | 17.02 | 119.11 | 110.60 |
| 22 | 23S1 | 1866 | A | N1-C6-N6 | -17.02 | 108.39 | 118.60 |
| 1 | 16S1 | 1483 | A | N1-C6-N6 | -17.02 | 108.39 | 118.60 |
| 22 | 23S1 | 1054 | A | N1-C6-N6 | -17.02 | 108.39 | 118.60 |
| 22 | 23S1 | 1111 | A | N1-C6-N6 | -17.01 | 108.39 | 118.60 |
| 23 | 05S1 | 94 | A | N1-C6-N6 | -17.00 | 108.40 | 118.60 |
| 22 | 23S1 | 1226 | A | N1-C6-N6 | -17.00 | 108.40 | 118.60 |
| 22 | 23S1 | 460 | A | N1-C6-N6 | -17.00 | 108.40 | 118.60 |
| 22 | 23S1 | 2476 | A | N1-C6-N6 | -16.99 | 108.41 | 118.60 |
| 22 | 23S1 | 1276 | A | N1-C6-N6 | -16.98 | 108.41 | 118.60 |
| 1 | 16S1 | 865 | A | N1-C2-N3 | -16.98 | 120.81 | 129.30 |
| 22 | 23S1 | 324 | A | N1-C6-N6 | -16.98 | 108.41 | 118.60 |
| 22 | 23S1 | 2706 | A | N1-C6-N6 | -16.97 | 108.42 | 118.60 |
| 22 | 23S1 | 626 | A | N1-C6-N6 | -16.97 | 108.42 | 118.60 |
| 22 | 23S1 | 2135 | A | N1-C6-N6 | -16.96 | 108.42 | 118.60 |
| 1 | 16S1 | 712 | A | N1-C2-N3 | -16.96 | 120.82 | 129.30 |
| 1 | 16S1 | 452 | A | N1-C6-N6 | -16.96 | 108.42 | 118.60 |
| 22 | 23S1 | 1689 | A | N1-C6-N6 | -16.95 | 108.43 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 451 | A | N1-C6-N6 | -16.94 | 108.43 | 118.60 |
| 22 | 23S1 | 1981 | A | C2-N3-C4 | 16.94 | 119.07 | 110.60 |
| 22 | 23S1 | 1027 | A | N1-C6-N6 | -16.94 | 108.44 | 118.60 |
| 1 | 16S1 | 1288 | A | N1-C6-N6 | -16.94 | 108.44 | 118.60 |
| 1 | 16S1 | 1201 | A | N1-C6-N6 | -16.93 | 108.44 | 118.60 |
| 1 | 16S1 | 1227 | A | C2-N3-C4 | 16.93 | 119.06 | 110.60 |
| 22 | 23S1 | 2598 | A | C2-N3-C4 | 16.93 | 119.06 | 110.60 |
| 1 | 16S1 | 161 | A | N1-C6-N6 | -16.93 | 108.44 | 118.60 |
| 1 | 16S1 | 51 | A | C2-N3-C4 | 16.91 | 119.05 | 110.60 |
| 22 | 23S1 | 727 | A | N1-C6-N6 | -16.90 | 108.46 | 118.60 |
| 1 | 16S1 | 1216 | A | C2-N3-C4 | 16.90 | 119.05 | 110.60 |
| 1 | 16S1 | 964 | A | N1-C6-N6 | -16.89 | 108.46 | 118.60 |
| 22 | 23S1 | 1801 | A | N1-C6-N6 | -16.89 | 108.47 | 118.60 |
| 1 | 16S1 | 994 | A | N1-C6-N6 | -16.88 | 108.47 | 118.60 |
| 22 | 23S1 | 1969 | A | N1-C6-N6 | -16.88 | 108.47 | 118.60 |
| 22 | 23S1 | 633 | A | N1-C6-N6 | -16.87 | 108.48 | 118.60 |
| 22 | 23S1 | 1528 | A | N1-C2-N3 | -16.86 | 120.87 | 129.30 |
| 22 | 23S1 | 2392 | A | N1-C6-N6 | -16.84 | 108.50 | 118.60 |
| 22 | 23S1 | 470 | A | N1-C6-N6 | -16.83 | 108.50 | 118.60 |
| 22 | 23S1 | 2176 | A | N1-C6-N6 | -16.83 | 108.50 | 118.60 |
| 1 | 16S1 | 706 | A | N1-C2-N3 | -16.82 | 120.89 | 129.30 |
| 1 | 16S1 | 411 | A | N1-C6-N6 | -16.82 | 108.51 | 118.60 |
| 22 | 23S1 | 1821 | A | C2-N3-C4 | 16.82 | 119.01 | 110.60 |
| 22 | 23S1 | 1848 | A | N1-C6-N6 | -16.82 | 108.51 | 118.60 |
| 1 | 16S1 | 746 | A | N1-C2-N3 | -16.82 | 120.89 | 129.30 |
| 22 | 23S1 | 2082 | A | N1-C6-N6 | -16.81 | 108.51 | 118.60 |
| 1 | 16S1 | 300 | A | N1-C2-N3 | -16.80 | 120.90 | 129.30 |
| 22 | 23S1 | 522 | A | N1-C6-N6 | -16.80 | 108.52 | 118.60 |
| 22 | 23S1 | 52 | A | N1-C6-N6 | -16.80 | 108.52 | 118.60 |
| 22 | 23S1 | 221 | A | N1-C6-N6 | -16.80 | 108.52 | 118.60 |
| 1 | 16S1 | 563 | A | N1-C6-N6 | -16.79 | 108.53 | 118.60 |
| 1 | 16S1 | 383 | A | N1-C2-N3 | -16.79 | 120.91 | 129.30 |
| 1 | 16S1 | 1394 | A | N1-C6-N6 | -16.78 | 108.53 | 118.60 |
| 22 | 23S1 | 2766 | A | N1-C6-N6 | -16.76 | 108.54 | 118.60 |
| 22 | 23S1 | 213 | A | N1-C6-N6 | -16.75 | 108.55 | 118.60 |
| 22 | 23S1 | 1791 | A | N1-C6-N6 | -16.74 | 108.56 | 118.60 |
| 22 | 23S1 | 504 | A | C2-N3-C4 | 16.73 | 118.96 | 110.60 |
| 22 | 23S1 | 1821 | A | N1-C2-N3 | -16.70 | 120.95 | 129.30 |
| 1 | 16S1 | 51 | A | N1-C6-N6 | -16.70 | 108.58 | 118.60 |
| 22 | 23S1 | 1676 | A | N1-C6-N6 | -16.69 | 108.59 | 118.60 |
| 22 | 23S1 | 1098 | A | N1-C6-N6 | -16.66 | 108.61 | 118.60 |
| 1 | 16S1 | 919 | A | C2-N3-C4 | 16.66 | 118.93 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 1163 | A | N1-C6-N6 | -16.64 | 108.61 | 118.60 |
| 22 | 23S1 | 2879 | A | N1-C6-N6 | -16.63 | 108.62 | 118.60 |
| 22 | 23S1 | 466 | A | N1-C6-N6 | -16.62 | 108.62 | 118.60 |
| 22 | 23S1 | 1872 | A | N1-C2-N3 | -16.62 | 120.99 | 129.30 |
| 55 | PTR1 | 14 | A | N1-C6-N6 | -16.61 | 108.63 | 118.60 |
| 1 | 16S1 | 502 | A | N1-C6-N6 | -16.59 | 108.65 | 118.60 |
| 55 | PTR1 | 69 | A | N1-C6-N6 | -16.59 | 108.65 | 118.60 |
| 22 | 23S1 | 1977 | A | N1-C6-N6 | -16.57 | 108.66 | 118.60 |
| 1 | 16S1 | 77 | A | N1-C2-N3 | -16.56 | 121.02 | 129.30 |
| 1 | 16S1 | 329 | A | N1-C6-N6 | -16.56 | 108.66 | 118.60 |
| 22 | 23S1 | 730 | A | N1-C6-N6 | -16.55 | 108.67 | 118.60 |
| 1 | 16S1 | 430 | A | N1-C6-N6 | -16.55 | 108.67 | 118.60 |
| 1 | 16S1 | 1375 | A | N1-C6-N6 | -16.54 | 108.67 | 118.60 |
| 22 | 23S1 | 2800 | A | N1-C6-N6 | -16.54 | 108.68 | 118.60 |
| 22 | 23S1 | 2899 | A | N1-C6-N6 | -16.50 | 108.70 | 118.60 |
| 1 | 16S1 | 1152 | A | N1-C6-N6 | -16.44 | 108.74 | 118.60 |
| 1 | 16S1 | 1055 | A | N1-C6-N6 | -16.41 | 108.75 | 118.60 |
| 22 | 23S1 | 1802 | A | N1-C6-N6 | -16.38 | 108.77 | 118.60 |
| 1 | 16S1 | 1201 | A | N1-C2-N3 | -16.36 | 121.12 | 129.30 |
| 22 | 23S1 | 505 | A | N1-C6-N6 | -16.34 | 108.80 | 118.60 |
| 22 | 23S1 | 1580 | A | N1-C6-N6 | -16.34 | 108.80 | 118.60 |
| 22 | 23S1 | 477 | A | N1-C6-N6 | -16.32 | 108.81 | 118.60 |
| 22 | 23S1 | 844 | A | N1-C6-N6 | -16.32 | 108.81 | 118.60 |
| 22 | 23S1 | 422 | A | N1-C6-N6 | -16.31 | 108.81 | 118.60 |
| 22 | 23S1 | 1469 | A | N1-C6-N6 | -16.28 | 108.83 | 118.60 |
| 22 | 23S1 | 1572 | A | N1-C6-N6 | -16.26 | 108.84 | 118.60 |
| 1 | 16S1 | 32 | A | N1-C6-N6 | -16.24 | 108.86 | 118.60 |
| 22 | 23S1 | 1241 | A | N1-C6-N6 | -16.24 | 108.86 | 118.60 |
| 1 | 16S1 | 923 | A | N1-C6-N6 | -16.23 | 108.86 | 118.60 |
| 22 | 23S1 | 1664 | A | N1-C2-N3 | -16.23 | 121.19 | 129.30 |
| 1 | 16S1 | 190 | A | N1-C2-N3 | -16.21 | 121.19 | 129.30 |
| 22 | 23S1 | 2369 | A | N1-C6-N6 | -16.21 | 108.88 | 118.60 |
| 22 | 23S1 | 2459 | A | N1-C6-N6 | -16.19 | 108.89 | 118.60 |
| 1 | 16S1 | 1507 | A | N1-C6-N6 | -16.18 | 108.89 | 118.60 |
| 22 | 23S1 | 2340 | A | N1-C6-N6 | -16.17 | 108.90 | 118.60 |
| 22 | 23S1 | 1434 | A | C5-C6-N6 | 16.16 | 136.63 | 123.70 |
| 1 | 16S1 | 1396 | A | N1-C6-N6 | -16.15 | 108.91 | 118.60 |
| 22 | 23S1 | 722 | A | N1-C6-N6 | -16.14 | 108.91 | 118.60 |
| 1 | 16S1 | 441 | A | N1-C6-N6 | -16.14 | 108.92 | 118.60 |
| 1 | 16S1 | 1252 | A | N1-C6-N6 | -16.10 | 108.94 | 118.60 |
| 22 | 23S1 | 911 | A | N1-C6-N6 | -16.09 | 108.95 | 118.60 |
| 55 | PTR1 | 38 | A | N1-C6-N6 | -16.06 | 108.96 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 925 | A | N1-C6-N6 | -16.06 | 108.97 | 118.60 |
| 22 | 23S1 | 1020 | A | N1-C6-N6 | -16.05 | 108.97 | 118.60 |
| 1 | 16S1 | 397 | A | N1-C6-N6 | -16.03 | 108.98 | 118.60 |
| 22 | 23S1 | 492 | A | N1-C6-N6 | -15.95 | 109.03 | 118.60 |
| 22 | 23S1 | 2426 | A | N1-C6-N6 | -15.94 | 109.03 | 118.60 |
| 1 | 16S1 | 459 | A | N1-C6-N6 | -15.93 | 109.04 | 118.60 |
| 22 | 23S1 | 1970 | A | N1-C6-N6 | -15.91 | 109.05 | 118.60 |
| 22 | 23S1 | 1213 | A | N1-C6-N6 | -15.90 | 109.06 | 118.60 |
| 22 | 23S1 | 1591 | A | N1-C6-N6 | -15.90 | 109.06 | 118.60 |
| 22 | 23S1 | 1029 | A | N1-C6-N6 | -15.86 | 109.08 | 118.60 |
| 1 | 16S1 | 533 | A | N1-C2-N3 | -15.86 | 121.37 | 129.30 |
| 1 | 16S1 | 873 | A | N1-C6-N6 | -15.76 | 109.14 | 118.60 |
| 1 | 16S1 | 181 | A | N1-C6-N6 | -15.76 | 109.14 | 118.60 |
| 1 | 16S1 | 1339 | A | N1-C6-N6 | -15.73 | 109.16 | 118.60 |
| 1 | 16S1 | 1418 | A | N1-C6-N6 | -15.69 | 109.19 | 118.60 |
| 22 | 23S1 | 2077 | A | N1-C6-N6 | -15.65 | 109.21 | 118.60 |
| 22 | 23S1 | 1143 | A | N1-C6-N6 | -15.62 | 109.23 | 118.60 |
| 1 | 16S1 | 520 | A | C5-C6-N6 | 15.46 | 136.07 | 123.70 |
| 1 | 16S1 | 1468 | A | N1-C6-N6 | -15.42 | 109.35 | 118.60 |
| 22 | 23S1 | 819 | A | N1-C6-N6 | -15.39 | 109.37 | 118.60 |
| 22 | 23S1 | 1937 | A | C5-C6-N6 | 15.37 | 135.99 | 123.70 |
| 22 | 23S1 | 2799 | A | N1-C6-N6 | -15.37 | 109.38 | 118.60 |
| 22 | 23S1 | 2614 | A | N1-C2-N3 | -15.36 | 121.62 | 129.30 |
| 22 | 23S1 | 1739 | A | N1-C6-N6 | -15.35 | 109.39 | 118.60 |
| 22 | 23S1 | 504 | A | N1-C6-N6 | -15.32 | 109.41 | 118.60 |
| 1 | 16S1 | 81 | A | N1-C2-N3 | -15.29 | 121.66 | 129.30 |
| 22 | 23S1 | 2142 | A | N1-C6-N6 | -15.25 | 109.45 | 118.60 |
| 22 | 23S1 | 820 | A | N1-C6-N6 | -15.14 | 109.52 | 118.60 |
| 1 | 16S1 | 1046 | A | N1-C2-N3 | -15.14 | 121.73 | 129.30 |
| 22 | 23S1 | 705 | A | N1-C6-N6 | -15.03 | 109.58 | 118.60 |
| 22 | 23S1 | 504 | A | N7-C8-N9 | -14.98 | 106.31 | 113.80 |
| 1 | 16S1 | 498 | A | N1-C2-N3 | -14.92 | 121.84 | 129.30 |
| 1 | 16S1 | 499 | A | N1-C6-N6 | -14.74 | 109.76 | 118.60 |
| 1 | 16S1 | 554 | A | C5-C6-N6 | 14.60 | 135.38 | 123.70 |
| 22 | 23S1 | 1872 | A | N1-C6-N6 | -14.59 | 109.85 | 118.60 |
| 1 | 16S1 | 1213 | A | C5-C6-N6 | 14.56 | 135.35 | 123.70 |
| 22 | 23S1 | 1571 | A | N1-C6-N6 | -14.41 | 109.95 | 118.60 |
| 22 | 23S1 | 2119 | A | N7-C8-N9 | -14.40 | 106.60 | 113.80 |
| 23 | 05S1 | 59 | A | N3-C4-C5 | -14.36 | 116.75 | 126.80 |
| 22 | 23S1 | 1854 | A | N1-C6-N6 | -14.36 | 109.99 | 118.60 |
| 22 | 23S1 | 513 | A | N1-C6-N6 | -14.32 | 110.01 | 118.60 |
| 1 | 16S1 | 696 | A | N1-C6-N6 | -14.29 | 110.02 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 23 | 05S1 | 101 | A | N3-C4-C5 | -14.16 | 116.89 | 126.80 |
| 22 | 23S1 | 2566 | A | N7-C8-N9 | -14.12 | 106.74 | 113.80 |
| 1 | 16S1 | 498 | A | N3-C4-C5 | -13.96 | 117.03 | 126.80 |
| 22 | 23S1 | 960 | A | N1-C6-N6 | -13.89 | 110.27 | 118.60 |
| 1 | 16S1 | 1004 | A | N7-C8-N9 | -13.81 | 106.89 | 113.80 |
| 1 | 16S1 | 1227 | A | N1-C6-N6 | -13.74 | 110.36 | 118.60 |
| 22 | 23S1 | 2662 | A | N1-C6-N6 | -13.59 | 110.44 | 118.60 |
| 22 | 23S1 | 1722 | A | N1-C6-N6 | -13.59 | 110.44 | 118.60 |
| 1 | 16S1 | 704 | A | C5-C6-N6 | 13.56 | 134.55 | 123.70 |
| 23 | 05S1 | 59 | A | N1-C2-N3 | -13.51 | 122.54 | 129.30 |
| 1 | 16S1 | 978 | A | C5-C6-N6 | 13.49 | 134.49 | 123.70 |
| 22 | 23S1 | 783 | A | N3-C4-C5 | -13.42 | 117.41 | 126.80 |
| 22 | 23S1 | 1528 | A | N1-C6-N6 | -13.41 | 110.55 | 118.60 |
| 22 | 23S1 | 2171 | A | N1-C6-N6 | -13.38 | 110.57 | 118.60 |
| 1 | 16S1 | 815 | A | N7-C8-N9 | -13.31 | 107.14 | 113.80 |
| 22 | 23S1 | 2101 | A | C5-C6-N6 | 13.31 | 134.35 | 123.70 |
| 22 | 23S1 | 2572 | A | N7-C8-N9 | -13.26 | 107.17 | 113.80 |
| 22 | 23S1 | 981 | A | C5-C6-N6 | 13.18 | 134.24 | 123.70 |
| 22 | 23S1 | 845 | A | N3-C4-C5 | -13.17 | 117.58 | 126.80 |
| 1 | 16S1 | 860 | A | C5-C6-N6 | 13.17 | 134.23 | 123.70 |
| 1 | 16S1 | 19 | A | N7-C8-N9 | -13.16 | 107.22 | 113.80 |
| 22 | 23S1 | 142 | A | N1-C6-N6 | -13.15 | 110.71 | 118.60 |
| 1 | 16S1 | 694 | A | N7-C8-N9 | -13.11 | 107.24 | 113.80 |
| 22 | 23S1 | 1630 | A | N7-C8-N9 | -13.10 | 107.25 | 113.80 |
| 1 | 16S1 | 1170 | A | N1-C6-N6 | -13.10 | 110.74 | 118.60 |
| 22 | 23S1 | 752 | A | C5-C6-N6 | 13.10 | 134.18 | 123.70 |
| 22 | 23S1 | 2469 | A | N7-C8-N9 | -13.08 | 107.26 | 113.80 |
| 1 | 16S1 | 81 | A | C5-C6-N6 | 13.08 | 134.16 | 123.70 |
| 1 | 16S1 | 533 | A | N3-C4-C5 | -13.08 | 117.64 | 126.80 |
| 1 | 16S1 | 411 | A | N7-C8-N9 | -13.07 | 107.26 | 113.80 |
| 1 | 16S1 | 622 | A | C5-C6-N6 | 13.07 | 134.16 | 123.70 |
| 22 | 23S1 | 1755 | A | C5-C6-N6 | 13.06 | 134.15 | 123.70 |
| 22 | 23S1 | 1021 | A | N3-C4-C5 | -13.06 | 117.66 | 126.80 |
| 22 | 23S1 | 1872 | A | N3-C4-C5 | -13.06 | 117.66 | 126.80 |
| 22 | 23S1 | 2590 | A | N7-C8-N9 | -13.06 | 107.27 | 113.80 |
| 22 | 23S1 | 2632 | A | N7-C8-N9 | -13.04 | 107.28 | 113.80 |
| 22 | 23S1 | 167 | A | N7-C8-N9 | -13.03 | 107.29 | 113.80 |
| 1 | 16S1 | 572 | A | N7-C8-N9 | -13.01 | 107.29 | 113.80 |
| 1 | 16S1 | 1441 | A | N7-C8-N9 | -13.01 | 107.30 | 113.80 |
| 22 | 23S1 | 1515 | A | C5-C6-N6 | 12.99 | 134.09 | 123.70 |
| 1 | 16S1 | 397 | A | N3-C4-C5 | -12.97 | 117.72 | 126.80 |
| 1 | 16S1 | 572 | A | C5-C6-N6 | 12.95 | 134.06 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 16 | A | C5-C6-N6 | 12.95 | 134.06 | 123.70 |
| 22 | 23S1 | 362 | A | N1-C6-N6 | -12.94 | 110.83 | 118.60 |
| 1 | 16S1 | 607 | A | C5-C6-N6 | 12.94 | 134.05 | 123.70 |
| 1 | 16S1 | 179 | A | C5-C6-N6 | 12.92 | 134.04 | 123.70 |
| 22 | 23S1 | 2449 | U | C5-C6-N1 | -12.91 | 116.25 | 122.70 |
| 1 | 16S1 | 8 | A | N7-C8-N9 | -12.89 | 107.35 | 113.80 |
| 1 | 16S1 | 1503 | A | N7-C8-N9 | -12.89 | 107.35 | 113.80 |
| 1 | 16S1 | 913 | A | C5-C6-N6 | 12.89 | 134.01 | 123.70 |
| 1 | 16S1 | 794 | A | N7-C8-N9 | -12.89 | 107.36 | 113.80 |
| 22 | 23S1 | 457 | A | N7-C8-N9 | -12.87 | 107.36 | 113.80 |
| 1 | 16S1 | 16 | A | N7-C8-N9 | -12.87 | 107.37 | 113.80 |
| 22 | 23S1 | 1754 | A | C5-C6-N6 | 12.87 | 134.00 | 123.70 |
| 22 | 23S1 | 800 | A | C5-C6-N6 | 12.86 | 133.99 | 123.70 |
| 22 | 23S1 | 2031 | A | N7-C8-N9 | -12.84 | 107.38 | 113.80 |
| 1 | 16S1 | 162 | A | N3-C4-C5 | -12.82 | 117.82 | 126.80 |
| 1 | 16S1 | 499 | A | N7-C8-N9 | -12.81 | 107.40 | 113.80 |
| 1 | 16S1 | 151 | A | C5-C6-N6 | 12.80 | 133.94 | 123.70 |
| 22 | 23S1 | 195 | A | C5-C6-N6 | 12.80 | 133.94 | 123.70 |
| 22 | 23S1 | 1597 | A | C5-C6-N6 | 12.79 | 133.93 | 123.70 |
| 22 | 23S1 | 278 | A | N3-C4-C5 | -12.79 | 117.85 | 126.80 |
| 1 | 16S1 | 1398 | A | C5-C6-N6 | 12.78 | 133.93 | 123.70 |
| 22 | 23S1 | 2117 | A | N7-C8-N9 | -12.78 | 107.41 | 113.80 |
| 22 | 23S1 | 2837 | A | N7-C8-N9 | -12.77 | 107.41 | 113.80 |
| 22 | 23S1 | 910 | A | C5-C6-N6 | 12.77 | 133.92 | 123.70 |
| 22 | 23S1 | 2114 | A | N3-C4-C5 | -12.77 | 117.86 | 126.80 |
| 1 | 16S1 | 996 | A | N7-C8-N9 | -12.76 | 107.42 | 113.80 |
| 22 | 23S1 | 2388 | A | C5-C6-N6 | 12.76 | 133.91 | 123.70 |
| 1 | 16S1 | 274 | A | N7-C8-N9 | -12.75 | 107.42 | 113.80 |
| 22 | 23S1 | 1050 | A | N7-C8-N9 | -12.75 | 107.42 | 113.80 |
| 22 | 23S1 | 1912 | A | N7-C8-N9 | -12.73 | 107.44 | 113.80 |
| 22 | 23S1 | 270 | A | N7-C8-N9 | -12.72 | 107.44 | 113.80 |
| 1 | 16S1 | 55 | A | N7-C8-N9 | -12.72 | 107.44 | 113.80 |
| 22 | 23S1 | 84 | A | C5-C6-N6 | 12.69 | 133.85 | 123.70 |
| 22 | 23S1 | 821 | A | C5-C6-N6 | 12.69 | 133.85 | 123.70 |
| 22 | 23S1 | 1504 | A | N7-C8-N9 | -12.67 | 107.47 | 113.80 |
| 22 | 23S1 | 1669 | A | N3-C4-C5 | -12.67 | 117.93 | 126.80 |
| 22 | 23S1 | 251 | A | N1-C6-N6 | -12.65 | 111.01 | 118.60 |
| 1 | 16S1 | 1280 | A | N7-C8-N9 | -12.65 | 107.47 | 113.80 |
| 22 | 23S1 | 1328 | A | C5-C6-N6 | 12.65 | 133.82 | 123.70 |
| 1 | 16S1 | 1201 | A | N3-C4-C5 | -12.64 | 117.95 | 126.80 |
| 22 | 23S1 | 1420 | A | N7-C8-N9 | -12.64 | 107.48 | 113.80 |
| 23 | 05S1 | 101 | A | N1-C2-N3 | -12.64 | 122.98 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 55 | PTR1 | 14 | A | N7-C8-N9 | -12.62 | 107.49 | 113.80 |
| 22 | 23S1 | 2060 | A | N7-C8-N9 | -12.61 | 107.49 | 113.80 |
| 22 | 23S1 | 2572 | A | C5-C6-N6 | 12.61 | 133.79 | 123.70 |
| 22 | 23S1 | 1308 | A | C5-C6-N6 | 12.60 | 133.78 | 123.70 |
| 1 | 16S1 | 1257 | A | N7-C8-N9 | -12.59 | 107.50 | 113.80 |
| 22 | 23S1 | 454 | A | C5-C6-N6 | 12.58 | 133.77 | 123.70 |
| 1 | 16S1 | 246 | A | N7-C8-N9 | -12.58 | 107.51 | 113.80 |
| 22 | 23S1 | 1668 | A | C5-C6-N6 | 12.57 | 133.76 | 123.70 |
| 22 | 23S1 | 213 | A | N7-C8-N9 | -12.56 | 107.52 | 113.80 |
| 22 | 23S1 | 1069 | A | N7-C8-N9 | -12.56 | 107.52 | 113.80 |
| 22 | 23S1 | 2682 | A | N7-C8-N9 | -12.56 | 107.52 | 113.80 |
| 23 | 05S1 | 109 | A | N7-C8-N9 | -12.53 | 107.53 | 113.80 |
| 1 | 16S1 | 143 | A | N7-C8-N9 | -12.53 | 107.53 | 113.80 |
| 22 | 23S1 | 1395 | A | C5-C6-N6 | 12.53 | 133.72 | 123.70 |
| 22 | 23S1 | 1597 | A | N7-C8-N9 | -12.53 | 107.54 | 113.80 |
| 22 | 23S1 | 1020 | A | N7-C8-N9 | -12.53 | 107.54 | 113.80 |
| 22 | 23S1 | 2602 | A | N7-C8-N9 | -12.52 | 107.54 | 113.80 |
| 22 | 23S1 | 1583 | A | N7-C8-N9 | -12.51 | 107.54 | 113.80 |
| 55 | PTR1 | 76 | A | N7-C8-N9 | -12.51 | 107.55 | 113.80 |
| 1 | 16S1 | 596 | A | N7-C8-N9 | -12.51 | 107.55 | 113.80 |
| 1 | 16S1 | 309 | A | N7-C8-N9 | -12.50 | 107.55 | 113.80 |
| 22 | 23S1 | 983 | A | C5-C6-N6 | 12.50 | 133.70 | 123.70 |
| 22 | 23S1 | 1655 | A | N7-C8-N9 | -12.50 | 107.55 | 113.80 |
| 22 | 23S1 | 2800 | A | N7-C8-N9 | -12.48 | 107.56 | 113.80 |
| 1 | 16S1 | 1145 | A | N7-C8-N9 | -12.48 | 107.56 | 113.80 |
| 22 | 23S1 | 10 | A | C5-C6-N6 | 12.48 | 133.68 | 123.70 |
| 22 | 23S1 | 2298 | A | N7-C8-N9 | -12.48 | 107.56 | 113.80 |
| 22 | 23S1 | 1919 | A | C5-C6-N6 | 12.48 | 133.68 | 123.70 |
| 29 | L091 | 68 | ARG | NE-CZ-NH2 | -12.48 | 114.06 | 120.30 |
| 23 | 05S1 | 108 | A | N7-C8-N9 | -12.47 | 107.57 | 113.80 |
| 1 | 16S1 | 389 | A | N3-C4-C5 | -12.47 | 118.07 | 126.80 |
| 22 | 23S1 | 749 | A | C5-C6-N6 | 12.46 | 133.67 | 123.70 |
| 22 | 23S1 | 1700 | A | N7-C8-N9 | -12.47 | 107.57 | 113.80 |
| 1 | 16S1 | 1004 | A | C5-N7-C8 | 12.46 | 110.13 | 103.90 |
| 22 | 23S1 | 1652 | A | C5-C6-N6 | 12.46 | 133.67 | 123.70 |
| 22 | 23S1 | 2823 | A | C5-C6-N6 | 12.46 | 133.67 | 123.70 |
| 22 | 23S1 | 196 | A | C5-C6-N6 | 12.45 | 133.66 | 123.70 |
| 1 | 16S1 | 1346 | A | C5-C6-N6 | 12.45 | 133.66 | 123.70 |
| 22 | 23S1 | 2542 | A | C5-C6-N6 | 12.44 | 133.65 | 123.70 |
| 1 | 16S1 | 915 | A | N7-C8-N9 | -12.44 | 107.58 | 113.80 |
| 22 | 23S1 | 2660 | A | N7-C8-N9 | -12.43 | 107.58 | 113.80 |
| 1 | 16S1 | 1340 | A | N7-C8-N9 | -12.43 | 107.58 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 574 | A | C5-C6-N6 | 12.43 | 133.64 | 123.70 |
| 22 | 23S1 | 1570 | A | C5-C6-N6 | 12.43 | 133.64 | 123.70 |
| 22 | 23S1 | 101 | A | N3-C4-C5 | -12.42 | 118.10 | 126.80 |
| 22 | 23S1 | 482 | A | N1-C6-N6 | -12.42 | 111.14 | 118.60 |
| 22 | 23S1 | 2726 | A | C5-C6-N6 | 12.42 | 133.63 | 123.70 |
| 22 | 23S1 | 160 | A | C5-C6-N6 | 12.41 | 133.63 | 123.70 |
| 22 | 23S1 | 1237 | A | N7-C8-N9 | -12.40 | 107.60 | 113.80 |
| 22 | 23S1 | 1580 | A | N7-C8-N9 | -12.40 | 107.60 | 113.80 |
| 22 | 23S1 | 2614 | A | N3-C4-C5 | -12.40 | 118.12 | 126.80 |
| 22 | 23S1 | 2406 | A | N7-C8-N9 | -12.39 | 107.60 | 113.80 |
| 22 | 23S1 | 1359 | A | C5-C6-N6 | 12.39 | 133.61 | 123.70 |
| 1 | 16S1 | 1004 | A | N3-C4-C5 | -12.38 | 118.13 | 126.80 |
| 22 | 23S1 | 2274 | A | C5-C6-N6 | 12.38 | 133.60 | 123.70 |
| 22 | 23S1 | 655 | A | N7-C8-N9 | -12.37 | 107.61 | 113.80 |
| 1 | 16S1 | 1101 | A | N7-C8-N9 | -12.37 | 107.62 | 113.80 |
| 22 | 23S1 | 227 | A | N7-C8-N9 | -12.36 | 107.62 | 113.80 |
| 55 | PTR1 | 51 | A | N7-C8-N9 | -12.36 | 107.62 | 113.80 |
| 22 | 23S1 | 2776 | A | N7-C8-N9 | -12.36 | 107.62 | 113.80 |
| 22 | 23S1 | 371 | A | N7-C8-N9 | -12.36 | 107.62 | 113.80 |
| 22 | 23S1 | 804 | A | C5-C6-N6 | 12.35 | 133.58 | 123.70 |
| 22 | 23S1 | 2882 | A | N7-C8-N9 | -12.35 | 107.63 | 113.80 |
| 55 | PTR1 | 59 | A | N7-C8-N9 | -12.34 | 107.63 | 113.80 |
| 1 | 16S1 | 1299 | A | N3-C4-C5 | -12.34 | 118.17 | 126.80 |
| 22 | 23S1 | 497 | A | C5-C6-N6 | 12.34 | 133.57 | 123.70 |
| 22 | 23S1 | 2883 | A | N7-C8-N9 | -12.34 | 107.63 | 113.80 |
| 22 | 23S1 | 1652 | A | N7-C8-N9 | -12.33 | 107.63 | 113.80 |
| 22 | 23S1 | 161 | A | C5-C6-N6 | 12.33 | 133.56 | 123.70 |
| 22 | 23S1 | 1001 | A | C5-C6-N6 | 12.33 | 133.56 | 123.70 |
| 22 | 23S1 | 1342 | A | N7-C8-N9 | -12.33 | 107.64 | 113.80 |
| 1 | 16S1 | 901 | A | N1-C6-N6 | -12.32 | 111.21 | 118.60 |
| 22 | 23S1 | 344 | A | N7-C8-N9 | -12.32 | 107.64 | 113.80 |
| 1 | 16S1 | 831 | A | N7-C8-N9 | -12.32 | 107.64 | 113.80 |
| 22 | 23S1 | 1014 | A | N7-C8-N9 | -12.32 | 107.64 | 113.80 |
| 22 | 23S1 | 1439 | A | N7-C8-N9 | -12.32 | 107.64 | 113.80 |
| 1 | 16S1 | 554 | A | N7-C8-N9 | -12.31 | 107.64 | 113.80 |
| 1 | 16S1 | 1346 | A | N7-C8-N9 | -12.31 | 107.64 | 113.80 |
| 22 | 23S1 | 821 | A | N7-C8-N9 | -12.31 | 107.64 | 113.80 |
| 22 | 23S1 | 1274 | A | C5-C6-N6 | 12.31 | 133.55 | 123.70 |
| 1 | 16S1 | 60 | A | C5-C6-N6 | 12.31 | 133.55 | 123.70 |
| 22 | 23S1 | 1040 | A | N7-C8-N9 | -12.30 | 107.65 | 113.80 |
| 22 | 23S1 | 10 | A | N7-C8-N9 | -12.30 | 107.65 | 113.80 |
| 22 | 23S1 | 878 | A | N7-C8-N9 | -12.30 | 107.65 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 547 | A | N7-C8-N9 | -12.30 | 107.65 | 113.80 |
| 23 | 05S1 | 34 | A | N7-C8-N9 | -12.30 | 107.65 | 113.80 |
| 1 | 16S1 | 1101 | A | C5-C6-N6 | 12.29 | 133.53 | 123.70 |
| 22 | 23S1 | 2711 | A | N7-C8-N9 | -12.29 | 107.65 | 113.80 |
| 1 | 16S1 | 74 | A | N7-C8-N9 | -12.29 | 107.66 | 113.80 |
| 22 | 23S1 | 165 | A | C5-C6-N6 | 12.29 | 133.53 | 123.70 |
| 22 | 23S1 | 322 | A | N7-C8-N9 | -12.29 | 107.66 | 113.80 |
| 22 | 23S1 | 2726 | A | N7-C8-N9 | -12.29 | 107.66 | 113.80 |
| 22 | 23S1 | 2765 | A | N3-C4-C5 | -12.28 | 118.20 | 126.80 |
| 22 | 23S1 | 1304 | A | N7-C8-N9 | -12.28 | 107.66 | 113.80 |
| 22 | 23S1 | 2736 | A | N7-C8-N9 | -12.28 | 107.66 | 113.80 |
| 1 | 16S1 | 383 | A | C4-C5-C6 | 12.28 | 123.14 | 117.00 |
| 55 | PTR1 | 58 | A | N7-C8-N9 | -12.28 | 107.66 | 113.80 |
| 22 | 23S1 | 2566 | A | C5-C6-N6 | 12.27 | 133.52 | 123.70 |
| 22 | 23S1 | 204 | A | N7-C8-N9 | -12.27 | 107.67 | 113.80 |
| 22 | 23S1 | 1304 | A | C5-C6-N6 | 12.27 | 133.52 | 123.70 |
| 1 | 16S1 | 44 | A | C5-C6-N6 | 12.26 | 133.51 | 123.70 |
| 1 | 16S1 | 1005 | A | N7-C8-N9 | -12.26 | 107.67 | 113.80 |
| 1 | 16S1 | 1105 | A | N7-C8-N9 | -12.26 | 107.67 | 113.80 |
| 1 | 16S1 | 1117 | A | N7-C8-N9 | -12.26 | 107.67 | 113.80 |
| 22 | 23S1 | 752 | A | N7-C8-N9 | -12.26 | 107.67 | 113.80 |
| 1 | 16S1 | 182 | A | N7-C8-N9 | -12.26 | 107.67 | 113.80 |
| 1 | 16S1 | 197 | A | C5-C6-N6 | 12.26 | 133.50 | 123.70 |
| 1 | 16S1 | 1225 | A | N3-C4-C5 | -12.26 | 118.22 | 126.80 |
| 22 | 23S1 | 1272 | A | N7-C8-N9 | -12.24 | 107.68 | 113.80 |
| 22 | 23S1 | 2311 | A | N7-C8-N9 | -12.24 | 107.68 | 113.80 |
| 22 | 23S1 | 783 | A | C5-C6-N6 | 12.24 | 133.49 | 123.70 |
| 22 | 23S1 | 2142 | A | N7-C8-N9 | -12.24 | 107.68 | 113.80 |
| 23 | 05S1 | 119 | A | N7-C8-N9 | -12.24 | 107.68 | 113.80 |
| 1 | 16S1 | 782 | A | N7-C8-N9 | -12.23 | 107.68 | 113.80 |
| 22 | 23S1 | 196 | A | N3-C4-C5 | -12.23 | 118.24 | 126.80 |
| 22 | 23S1 | 529 | A | C5-C6-N6 | 12.23 | 133.48 | 123.70 |
| 1 | 16S1 | 3 | A | C5-C6-N6 | 12.23 | 133.48 | 123.70 |
| 22 | 23S1 | 1090 | A | N7-C8-N9 | -12.22 | 107.69 | 113.80 |
| 1 | 16S1 | 383 | A | N3-C4-C5 | -12.22 | 118.25 | 126.80 |
| 1 | 16S1 | 1179 | A | C5-C6-N6 | 12.22 | 133.48 | 123.70 |
| 22 | 23S1 | 111 | A | N7-C8-N9 | -12.22 | 107.69 | 113.80 |
| 1 | 16S1 | 435 | A | N7-C8-N9 | -12.22 | 107.69 | 113.80 |
| 55 | PTR1 | 38 | A | N7-C8-N9 | -12.22 | 107.69 | 113.80 |
| 22 | 23S1 | 221 | A | N7-C8-N9 | -12.21 | 107.69 | 113.80 |
| 22 | 23S1 | 354 | A | N7-C8-N9 | -12.21 | 107.69 | 113.80 |
| 1 | 16S1 | 321 | A | N7-C8-N9 | -12.21 | 107.70 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 661 | A | N7-C8-N9 | -12.21 | 107.70 | 113.80 |
| 22 | 23S1 | 2297 | A | C5-C6-N6 | 12.21 | 133.46 | 123.70 |
| 22 | 23S1 | 352 | A | N7-C8-N9 | -12.20 | 107.70 | 113.80 |
| 22 | 23S1 | 1134 | A | N7-C8-N9 | -12.20 | 107.70 | 113.80 |
| 22 | 23S1 | 2516 | A | N7-C8-N9 | -12.20 | 107.70 | 113.80 |
| 22 | 23S1 | 2450 | A | C5-C6-N6 | 12.20 | 133.46 | 123.70 |
| 22 | 23S1 | 84 | A | N7-C8-N9 | -12.19 | 107.70 | 113.80 |
| 22 | 23S1 | 125 | A | N7-C8-N9 | -12.19 | 107.70 | 113.80 |
| 22 | 23S1 | 2577 | A | N7-C8-N9 | -12.19 | 107.70 | 113.80 |
| 1 | 16S1 | 1004 | A | C5-C6-N6 | 12.19 | 133.45 | 123.70 |
| 22 | 23S1 | 402 | A | C5-C6-N6 | 12.18 | 133.44 | 123.70 |
| 1 | 16S1 | 149 | A | C5-C6-N6 | 12.18 | 133.44 | 123.70 |
| 1 | 16S1 | 349 | A | N7-C8-N9 | -12.18 | 107.71 | 113.80 |
| 22 | 23S1 | 2311 | A | C5-C6-N6 | 12.18 | 133.44 | 123.70 |
| 1 | 16S1 | 1042 | A | N7-C8-N9 | -12.17 | 107.71 | 113.80 |
| 1 | 16S1 | 130 | A | N7-C8-N9 | -12.17 | 107.72 | 113.80 |
| 22 | 23S1 | 1469 | A | N7-C8-N9 | -12.16 | 107.72 | 113.80 |
| 22 | 23S1 | 1785 | A | C5-C6-N6 | 12.16 | 133.43 | 123.70 |
| 22 | 23S1 | 1532 | A | N7-C8-N9 | -12.16 | 107.72 | 113.80 |
| 22 | 23S1 | 1966 | A | N7-C8-N9 | -12.16 | 107.72 | 113.80 |
| 1 | 16S1 | 553 | A | N7-C8-N9 | -12.16 | 107.72 | 113.80 |
| 22 | 23S1 | 2753 | A | C5-C6-N6 | 12.16 | 133.43 | 123.70 |
| 1 | 16S1 | 535 | A | N7-C8-N9 | -12.15 | 107.72 | 113.80 |
| 22 | 23S1 | 1244 | A | N7-C8-N9 | -12.15 | 107.73 | 113.80 |
| 22 | 23S1 | 2388 | A | N7-C8-N9 | -12.15 | 107.73 | 113.80 |
| 1 | 16S1 | 1408 | A | N7-C8-N9 | -12.14 | 107.73 | 113.80 |
| 22 | 23S1 | 1591 | A | N7-C8-N9 | -12.14 | 107.73 | 113.80 |
| 22 | 23S1 | 2060 | A | C5-C6-N6 | 12.14 | 133.41 | 123.70 |
| 23 | 05S1 | 52 | A | N7-C8-N9 | -12.14 | 107.73 | 113.80 |
| 1 | 16S1 | 983 | A | N3-C4-C5 | -12.13 | 118.31 | 126.80 |
| 1 | 16S1 | 1188 | A | N7-C8-N9 | -12.13 | 107.73 | 113.80 |
| 1 | 16S1 | 1306 | A | N7-C8-N9 | -12.13 | 107.73 | 113.80 |
| 22 | 23S1 | 1057 | A | N7-C8-N9 | -12.14 | 107.73 | 113.80 |
| 22 | 23S1 | 2094 | A | N7-C8-N9 | -12.13 | 107.73 | 113.80 |
| 22 | 23S1 | 644 | A | N3-C4-C5 | -12.13 | 118.31 | 126.80 |
| 22 | 23S1 | 1535 | A | C5-C6-N6 | 12.13 | 133.40 | 123.70 |
| 1 | 16S1 | 547 | A | C5-C6-N6 | 12.13 | 133.40 | 123.70 |
| 22 | 23S1 | 706 | A | N7-C8-N9 | -12.13 | 107.74 | 113.80 |
| 22 | 23S1 | 119 | A | C5-C6-N6 | 12.12 | 133.40 | 123.70 |
| 22 | 23S1 | 2887 | A | N7-C8-N9 | -12.12 | 107.74 | 113.80 |
| 22 | 23S1 | 1205 | A | N7-C8-N9 | -12.12 | 107.74 | 113.80 |
| 22 | 23S1 | 1970 | A | N7-C8-N9 | -12.12 | 107.74 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 2095 | A | N7-C8-N9 | -12.12 | 107.74 | 113.80 |
| 22 | 23S1 | 1204 | A | C5-C6-N6 | 12.11 | 133.39 | 123.70 |
| 22 | 23S1 | 233 | A | N7-C8-N9 | -12.11 | 107.75 | 113.80 |
| 22 | 23S1 | 1713 | A | N7-C8-N9 | -12.10 | 107.75 | 113.80 |
| 1 | 16S1 | 1447 | A | C5-C6-N6 | 12.10 | 133.38 | 123.70 |
| 22 | 23S1 | 155 | A | N7-C8-N9 | -12.10 | 107.75 | 113.80 |
| 1 | 16S1 | 1239 | A | N7-C8-N9 | -12.10 | 107.75 | 113.80 |
| 22 | 23S1 | 340 | A | N7-C8-N9 | -12.10 | 107.75 | 113.80 |
| 22 | 23S1 | 2564 | A | C5-C6-N6 | 12.09 | 133.38 | 123.70 |
| 1 | 16S1 | 977 | A | N3-C4-C5 | -12.09 | 118.34 | 126.80 |
| 22 | 23S1 | 614 | A | N7-C8-N9 | -12.09 | 107.75 | 113.80 |
| 1 | 16S1 | 1250 | A | N7-C8-N9 | -12.09 | 107.76 | 113.80 |
| 22 | 23S1 | 2247 | A | N7-C8-N9 | -12.09 | 107.76 | 113.80 |
| 22 | 23S1 | 2333 | A | N7-C8-N9 | -12.08 | 107.76 | 113.80 |
| 22 | 23S1 | 2013 | A | N7-C8-N9 | -12.08 | 107.76 | 113.80 |
| 22 | 23S1 | 1378 | A | C5-C6-N6 | 12.08 | 133.36 | 123.70 |
| 1 | 16S1 | 787 | A | N7-C8-N9 | -12.07 | 107.76 | 113.80 |
| 22 | 23S1 | 574 | A | N7-C8-N9 | -12.07 | 107.76 | 113.80 |
| 22 | 23S1 | 2513 | A | C5-C6-N6 | 12.07 | 133.36 | 123.70 |
| 22 | 23S1 | 627 | A | N7-C8-N9 | -12.07 | 107.76 | 113.80 |
| 1 | 16S1 | 300 | A | C4-C5-C6 | 12.07 | 123.03 | 117.00 |
| 1 | 16S1 | 702 | A | C5-C6-N6 | 12.07 | 133.35 | 123.70 |
| 22 | 23S1 | 925 | A | N7-C8-N9 | -12.07 | 107.77 | 113.80 |
| 22 | 23S1 | 1302 | A | N7-C8-N9 | -12.07 | 107.77 | 113.80 |
| 1 | 16S1 | 1145 | A | C5-C6-N6 | 12.07 | 133.35 | 123.70 |
| 22 | 23S1 | 1427 | A | C5-C6-N6 | 12.06 | 133.35 | 123.70 |
| 1 | 16S1 | 1225 | A | C5-C6-N6 | 12.05 | 133.34 | 123.70 |
| 22 | 23S1 | 1205 | A | C5-C6-N6 | 12.05 | 133.34 | 123.70 |
| 22 | 23S1 | 1928 | A | C5-C6-N6 | 12.06 | 133.34 | 123.70 |
| 22 | 23S1 | 1913 | A | N7-C8-N9 | -12.05 | 107.77 | 113.80 |
| 1 | 16S1 | 448 | A | N7-C8-N9 | -12.05 | 107.77 | 113.80 |
| 1 | 16S1 | 889 | A | C5-C6-N6 | 12.05 | 133.34 | 123.70 |
| 1 | 16S1 | 1067 | A | C5-C6-N6 | 12.05 | 133.34 | 123.70 |
| 22 | 23S1 | 866 | A | N7-C8-N9 | -12.05 | 107.78 | 113.80 |
| 22 | 23S1 | 2227 | A | C5-C6-N6 | 12.05 | 133.34 | 123.70 |
| 22 | 23S1 | 14 | A | C5-C6-N6 | 12.04 | 133.34 | 123.70 |
| 1 | 16S1 | 353 | A | N7-C8-N9 | -12.04 | 107.78 | 113.80 |
| 22 | 23S1 | 693 | A | N7-C8-N9 | -12.04 | 107.78 | 113.80 |
| 1 | 16S1 | 1333 | A | C5-C6-N6 | 12.04 | 133.33 | 123.70 |
| 22 | 23S1 | 2432 | A | N7-C8-N9 | -12.04 | 107.78 | 113.80 |
| 1 | 16S1 | 1413 | A | N7-C8-N9 | -12.04 | 107.78 | 113.80 |
| 1 | 16S1 | 356 | A | N7-C8-N9 | -12.03 | 107.78 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 465 | A | N3-C4-C5 | -12.03 | 118.38 | 126.80 |
| 1 | 16S1 | 1360 | A | C5-C6-N6 | 12.03 | 133.32 | 123.70 |
| 22 | 23S1 | 789 | A | N7-C8-N9 | -12.03 | 107.78 | 113.80 |
| 1 | 16S1 | 1196 | A | N7-C8-N9 | -12.03 | 107.79 | 113.80 |
| 22 | 23S1 | 1353 | A | C5-C6-N6 | 12.03 | 133.32 | 123.70 |
| 22 | 23S1 | 2750 | A | N7-C8-N9 | -12.03 | 107.79 | 113.80 |
| 1 | 16S1 | 190 | A | N3-C4-C5 | -12.03 | 118.38 | 126.80 |
| 1 | 16S1 | 1329 | A | N7-C8-N9 | -12.03 | 107.79 | 113.80 |
| 22 | 23S1 | 127 | A | C5-C6-N6 | 12.03 | 133.32 | 123.70 |
| 22 | 23S1 | 2309 | A | N7-C8-N9 | -12.03 | 107.79 | 113.80 |
| 23 | 05S1 | 46 | A | C5-C6-N6 | 12.03 | 133.32 | 123.70 |
| 1 | 16S1 | 602 | A | N7-C8-N9 | -12.02 | 107.79 | 113.80 |
| 22 | 23S1 | 412 | A | N7-C8-N9 | -12.02 | 107.79 | 113.80 |
| 1 | 16S1 | 197 | A | N7-C8-N9 | -12.02 | 107.79 | 113.80 |
| 22 | 23S1 | 936 | A | N7-C8-N9 | -12.02 | 107.79 | 113.80 |
| 22 | 23S1 | 2565 | A | C5-C6-N6 | 12.02 | 133.31 | 123.70 |
| 1 | 16S1 | 44 | A | N7-C8-N9 | -12.02 | 107.79 | 113.80 |
| 22 | 23S1 | 2014 | A | N7-C8-N9 | -12.01 | 107.79 | 113.80 |
| 22 | 23S1 | 2590 | A | C5-C6-N6 | 12.01 | 133.31 | 123.70 |
| 1 | 16S1 | 946 | A | N7-C8-N9 | -12.01 | 107.80 | 113.80 |
| 22 | 23S1 | 979 | A | N7-C8-N9 | -12.00 | 107.80 | 113.80 |
| 1 | 16S1 | 432 | A | N7-C8-N9 | -12.00 | 107.80 | 113.80 |
| 22 | 23S1 | 1596 | A | N7-C8-N9 | -11.99 | 107.80 | 113.80 |
| 1 | 16S1 | 65 | A | N7-C8-N9 | -11.99 | 107.80 | 113.80 |
| 1 | 16S1 | 1275 | A | N7-C8-N9 | -11.99 | 107.81 | 113.80 |
| 22 | 23S1 | 1028 | A | N7-C8-N9 | -11.99 | 107.81 | 113.80 |
| 22 | 23S1 | 1650 | A | N7-C8-N9 | -11.99 | 107.81 | 113.80 |
| 1 | 16S1 | 1447 | A | N7-C8-N9 | -11.98 | 107.81 | 113.80 |
| 1 | 16S1 | 1499 | A | N7-C8-N9 | -11.98 | 107.81 | 113.80 |
| 22 | 23S1 | 616 | A | N7-C8-N9 | -11.98 | 107.81 | 113.80 |
| 22 | 23S1 | 644 | A | N7-C8-N9 | -11.98 | 107.81 | 113.80 |
| 22 | 23S1 | 2434 | A | C5-C6-N6 | 11.98 | 133.28 | 123.70 |
| 1 | 16S1 | 1500 | A | C5-C6-N6 | 11.98 | 133.28 | 123.70 |
| 1 | 16S1 | 461 | A | N7-C8-N9 | -11.98 | 107.81 | 113.80 |
| 22 | 23S1 | 1129 | A | C5-C6-N6 | 11.98 | 133.28 | 123.70 |
| 22 | 23S1 | 637 | A | C5-C6-N6 | 11.97 | 133.28 | 123.70 |
| 22 | 23S1 | 1634 | A | C5-C6-N6 | 11.97 | 133.28 | 123.70 |
| 23 | 05S1 | 53 | A | N7-C8-N9 | -11.97 | 107.81 | 113.80 |
| 1 | 16S1 | 914 | A | C5-C6-N6 | 11.97 | 133.27 | 123.70 |
| 1 | 16S1 | 914 | A | N7-C8-N9 | -11.96 | 107.82 | 113.80 |
| 1 | 16S1 | 1311 | A | N7-C8-N9 | -11.96 | 107.82 | 113.80 |
| 22 | 23S1 | 1630 | A | C5-C6-N6 | 11.96 | 133.27 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 364 | A | N7-C8-N9 | -11.95 | 107.82 | 113.80 |
| 22 | 23S1 | 1808 | A | N7-C8-N9 | -11.95 | 107.83 | 113.80 |
| 22 | 23S1 | 2095 | A | C5-C6-N6 | 11.95 | 133.26 | 123.70 |
| 22 | 23S1 | 176 | A | N7-C8-N9 | -11.95 | 107.83 | 113.80 |
| 1 | 16S1 | 1204 | A | C5-C6-N6 | 11.95 | 133.26 | 123.70 |
| 1 | 16S1 | 675 | A | N7-C8-N9 | -11.95 | 107.83 | 113.80 |
| 1 | 16S1 | 768 | A | C5-C6-N6 | 11.95 | 133.26 | 123.70 |
| 22 | 23S1 | 792 | A | N7-C8-N9 | -11.95 | 107.83 | 113.80 |
| 22 | 23S1 | 1927 | A | C5-C6-N6 | 11.94 | 133.25 | 123.70 |
| 1 | 16S1 | 468 | A | N7-C8-N9 | -11.94 | 107.83 | 113.80 |
| 22 | 23S1 | 38 | A | C5-C6-N6 | 11.94 | 133.25 | 123.70 |
| 22 | 23S1 | 1635 | A | N7-C8-N9 | -11.94 | 107.83 | 113.80 |
| 22 | 23S1 | 2577 | A | C5-C6-N6 | 11.94 | 133.25 | 123.70 |
| 22 | 23S1 | 443 | A | C5-C6-N6 | 11.93 | 133.25 | 123.70 |
| 22 | 23S1 | 1640 | A | C5-C6-N6 | 11.93 | 133.25 | 123.70 |
| 22 | 23S1 | 2171 | A | N7-C8-N9 | -11.93 | 107.84 | 113.80 |
| 22 | 23S1 | 1490 | A | N3-C4-C5 | -11.92 | 118.45 | 126.80 |
| 22 | 23S1 | 2183 | A | C5-C6-N6 | 11.92 | 133.24 | 123.70 |
| 22 | 23S1 | 2297 | A | N7-C8-N9 | -11.92 | 107.84 | 113.80 |
| 22 | 23S1 | 2003 | A | N7-C8-N9 | -11.92 | 107.84 | 113.80 |
| 1 | 16S1 | 1256 | A | N7-C8-N9 | -11.92 | 107.84 | 113.80 |
| 22 | 23S1 | 1494 | A | C5-C6-N6 | 11.92 | 133.23 | 123.70 |
| 22 | 23S1 | 1285 | A | C5-C6-N6 | 11.91 | 133.23 | 123.70 |
| 22 | 23S1 | 2740 | A | N7-C8-N9 | -11.91 | 107.84 | 113.80 |
| 22 | 23S1 | 2033 | A | C5-C6-N6 | 11.91 | 133.23 | 123.70 |
| 1 | 16S1 | 1480 | A | C5-C6-N6 | 11.90 | 133.22 | 123.70 |
| 22 | 23S1 | 332 | A | N7-C8-N9 | -11.90 | 107.85 | 113.80 |
| 22 | 23S1 | 2850 | A | N7-C8-N9 | -11.90 | 107.85 | 113.80 |
| 22 | 23S1 | 2734 | A | N7-C8-N9 | -11.90 | 107.85 | 113.80 |
| 1 | 16S1 | 728 | A | C5-C6-N6 | 11.90 | 133.22 | 123.70 |
| 22 | 23S1 | 2657 | A | N7-C8-N9 | -11.90 | 107.85 | 113.80 |
| 23 | 05S1 | 39 | A | N7-C8-N9 | -11.90 | 107.85 | 113.80 |
| 1 | 16S1 | 152 | A | C5-C6-N6 | 11.90 | 133.22 | 123.70 |
| 22 | 23S1 | 354 | A | C5-C6-N6 | 11.89 | 133.22 | 123.70 |
| 1 | 16S1 | 300 | A | N3-C4-C5 | -11.89 | 118.47 | 126.80 |
| 1 | 16S1 | 781 | A | N7-C8-N9 | -11.89 | 107.86 | 113.80 |
| 1 | 16S1 | 1016 | A | N7-C8-N9 | -11.89 | 107.85 | 113.80 |
| 23 | 05S1 | 29 | A | C5-C6-N6 | 11.89 | 133.21 | 123.70 |
| 22 | 23S1 | 829 | A | N7-C8-N9 | -11.89 | 107.86 | 113.80 |
| 22 | 23S1 | 1308 | A | N7-C8-N9 | -11.89 | 107.86 | 113.80 |
| 22 | 23S1 | 2005 | A | N7-C8-N9 | -11.89 | 107.86 | 113.80 |
| 22 | 23S1 | 2173 | A | N3-C4-C5 | -11.89 | 118.48 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 984 | A | N3-C4-C5 | -11.89 | 118.48 | 126.80 |
| 1 | 16S1 | 1332 | A | C5-C6-N6 | 11.88 | 133.20 | 123.70 |
| 1 | 16S1 | 2 | A | N3-C4-C5 | -11.88 | 118.48 | 126.80 |
| 1 | 16S1 | 1092 | A | C5-C6-N6 | 11.88 | 133.20 | 123.70 |
| 22 | 23S1 | 207 | A | N7-C8-N9 | -11.88 | 107.86 | 113.80 |
| 22 | 23S1 | 2826 | A | N7-C8-N9 | -11.88 | 107.86 | 113.80 |
| 22 | 23S1 | 1938 | A | N7-C8-N9 | -11.88 | 107.86 | 113.80 |
| 1 | 16S1 | 975 | A | C5-C6-N6 | 11.88 | 133.20 | 123.70 |
| 22 | 23S1 | 668 | A | N7-C8-N9 | -11.88 | 107.86 | 113.80 |
| 22 | 23S1 | 933 | A | N3-C4-C5 | -11.87 | 118.49 | 126.80 |
| 22 | 23S1 | 1322 | A | N7-C8-N9 | -11.87 | 107.86 | 113.80 |
| 1 | 16S1 | 563 | A | N3-C4-C5 | -11.87 | 118.49 | 126.80 |
| 22 | 23S1 | 2766 | A | N3-C4-C5 | -11.87 | 118.49 | 126.80 |
| 1 | 16S1 | 51 | A | N7-C8-N9 | -11.87 | 107.87 | 113.80 |
| 1 | 16S1 | 1239 | A | C5-C6-N6 | 11.87 | 133.19 | 123.70 |
| 1 | 16S1 | 298 | A | N7-C8-N9 | -11.86 | 107.87 | 113.80 |
| 22 | 23S1 | 63 | A | N7-C8-N9 | -11.86 | 107.87 | 113.80 |
| 1 | 16S1 | 665 | A | C5-C6-N6 | 11.86 | 133.19 | 123.70 |
| 22 | 23S1 | 1275 | A | N7-C8-N9 | -11.86 | 107.87 | 113.80 |
| 1 | 16S1 | 315 | A | N7-C8-N9 | -11.86 | 107.87 | 113.80 |
| 22 | 23S1 | 2632 | A | C5-C6-N6 | 11.86 | 133.19 | 123.70 |
| 1 | 16S1 | 1167 | A | N7-C8-N9 | -11.85 | 107.88 | 113.80 |
| 22 | 23S1 | 1175 | A | N3-C4-C5 | -11.85 | 118.51 | 126.80 |
| 22 | 23S1 | 2764 | A | N7-C8-N9 | -11.85 | 107.88 | 113.80 |
| 22 | 23S1 | 1165 | A | N7-C8-N9 | -11.84 | 107.88 | 113.80 |
| 1 | 16S1 | 1151 | A | N7-C8-N9 | -11.84 | 107.88 | 113.80 |
| 1 | 16S1 | 1236 | A | N7-C8-N9 | -11.84 | 107.88 | 113.80 |
| 22 | 23S1 | 1784 | A | N7-C8-N9 | -11.84 | 107.88 | 113.80 |
| 23 | 05S1 | 15 | A | N7-C8-N9 | -11.84 | 107.88 | 113.80 |
| 1 | 16S1 | 1280 | A | C5-C6-N6 | 11.83 | 133.16 | 123.70 |
| 22 | 23S1 | 2872 | A | N7-C8-N9 | -11.83 | 107.88 | 113.80 |
| 22 | 23S1 | 1544 | A | C5-C6-N6 | 11.83 | 133.16 | 123.70 |
| 1 | 16S1 | 1502 | A | C5-C6-N6 | 11.82 | 133.16 | 123.70 |
| 22 | 23S1 | 13 | A | C5-C6-N6 | 11.82 | 133.16 | 123.70 |
| 22 | 23S1 | 374 | A | N7-C8-N9 | -11.82 | 107.89 | 113.80 |
| 22 | 23S1 | 1392 | A | N3-C4-C5 | -11.82 | 118.52 | 126.80 |
| 22 | 23S1 | 1393 | A | C5-C6-N6 | 11.82 | 133.16 | 123.70 |
| 22 | 23S1 | 2042 | A | N7-C8-N9 | -11.82 | 107.89 | 113.80 |
| 22 | 23S1 | 515 | A | C5-C6-N6 | 11.82 | 133.16 | 123.70 |
| 22 | 23S1 | 1853 | A | N7-C8-N9 | -11.82 | 107.89 | 113.80 |
| 22 | 23S1 | 2565 | A | N7-C8-N9 | -11.82 | 107.89 | 113.80 |
| 22 | 23S1 | 2657 | A | C5-C6-N6 | 11.82 | 133.15 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 792 | A | N7-C8-N9 | -11.81 | 107.89 | 113.80 |
| 22 | 23S1 | 1419 | A | N7-C8-N9 | -11.81 | 107.89 | 113.80 |
| 1 | 16S1 | 1500 | A | N7-C8-N9 | -11.81 | 107.89 | 113.80 |
| 1 | 16S1 | 825 | A | N7-C8-N9 | -11.81 | 107.89 | 113.80 |
| 55 | PTR1 | 51 | A | C5-C6-N6 | 11.81 | 133.15 | 123.70 |
| 22 | 23S1 | 716 | A | N7-C8-N9 | -11.81 | 107.90 | 113.80 |
| 23 | 05S1 | 78 | A | N7-C8-N9 | -11.81 | 107.90 | 113.80 |
| 55 | PTR1 | 58 | A | C5-C6-N6 | 11.81 | 133.15 | 123.70 |
| 1 | 16S1 | 364 | A | C5-C6-N6 | 11.81 | 133.14 | 123.70 |
| 1 | 16S1 | 949 | A | N7-C8-N9 | -11.80 | 107.90 | 113.80 |
| 1 | 16S1 | 1170 | A | N3-C4-C5 | -11.81 | 118.54 | 126.80 |
| 1 | 16S1 | 715 | A | N7-C8-N9 | -11.80 | 107.90 | 113.80 |
| 23 | 05S1 | 115 | A | N7-C8-N9 | -11.80 | 107.90 | 113.80 |
| 55 | PTR1 | 20 | U | C5-C6-N1 | -11.80 | 116.80 | 122.70 |
| 1 | 16S1 | 327 | A | N7-C8-N9 | -11.80 | 107.90 | 113.80 |
| 1 | 16S1 | 243 | A | C5-C6-N6 | 11.80 | 133.14 | 123.70 |
| 22 | 23S1 | 262 | A | N7-C8-N9 | -11.80 | 107.90 | 113.80 |
| 1 | 16S1 | 1036 | A | C5-C6-N6 | 11.80 | 133.14 | 123.70 |
| 1 | 16S1 | 1157 | A | N7-C8-N9 | -11.80 | 107.90 | 113.80 |
| 22 | 23S1 | 278 | A | C5-C6-N6 | 11.79 | 133.13 | 123.70 |
| 22 | 23S1 | 2020 | A | N7-C8-N9 | -11.79 | 107.90 | 113.80 |
| 22 | 23S1 | 479 | A | N7-C8-N9 | -11.79 | 107.91 | 113.80 |
| 22 | 23S1 | 920 | A | N7-C8-N9 | -11.79 | 107.91 | 113.80 |
| 22 | 23S1 | 1080 | A | N7-C8-N9 | -11.78 | 107.91 | 113.80 |
| 22 | 23S1 | 1086 | A | N3-C4-C5 | -11.79 | 118.55 | 126.80 |
| 22 | 23S1 | 538 | A | N7-C8-N9 | -11.78 | 107.91 | 113.80 |
| 1 | 16S1 | 172 | A | C5-C6-N6 | 11.78 | 133.12 | 123.70 |
| 1 | 16S1 | 969 | A | C5-C6-N6 | 11.78 | 133.12 | 123.70 |
| 22 | 23S1 | 2453 | A | C5-C6-N6 | 11.78 | 133.12 | 123.70 |
| 1 | 16S1 | 969 | A | N7-C8-N9 | -11.78 | 107.91 | 113.80 |
| 22 | 23S1 | 905 | A | N7-C8-N9 | -11.77 | 107.91 | 113.80 |
| 22 | 23S1 | 1711 | A | N7-C8-N9 | -11.77 | 107.91 | 113.80 |
| 22 | 23S1 | 1579 | A | N7-C8-N9 | -11.77 | 107.91 | 113.80 |
| 22 | 23S1 | 352 | A | C5-C6-N6 | 11.77 | 133.12 | 123.70 |
| 22 | 23S1 | 794 | A | N3-C4-C5 | -11.77 | 118.56 | 126.80 |
| 22 | 23S1 | 532 | A | N3-C4-C5 | -11.77 | 118.56 | 126.80 |
| 1 | 16S1 | 1429 | A | N7-C8-N9 | -11.77 | 107.92 | 113.80 |
| 22 | 23S1 | 483 | A | N7-C8-N9 | -11.76 | 107.92 | 113.80 |
| 22 | 23S1 | 2119 | A | C5-C6-N6 | 11.76 | 133.11 | 123.70 |
| 1 | 16S1 | 498 | A | C5-C6-N1 | 11.76 | 123.58 | 117.70 |
| 22 | 23S1 | 505 | A | N7-C8-N9 | -11.76 | 107.92 | 113.80 |
| 1 | 16S1 | 1413 | A | C5-C6-N6 | 11.76 | 133.11 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 371 | A | C5-C6-N6 | 11.76 | 133.11 | 123.70 |
| 22 | 23S1 | 497 | A | N7-C8-N9 | -11.76 | 107.92 | 113.80 |
| 1 | 16S1 | 179 | A | N7-C8-N9 | -11.76 | 107.92 | 113.80 |
| 22 | 23S1 | 2212 | A | N7-C8-N9 | -11.75 | 107.92 | 113.80 |
| 22 | 23S1 | 1654 | A | C5-C6-N6 | 11.75 | 133.10 | 123.70 |
| 1 | 16S1 | 784 | A | N7-C8-N9 | -11.75 | 107.93 | 113.80 |
| 1 | 16S1 | 1363 | A | N3-C4-C5 | -11.74 | 118.58 | 126.80 |
| 1 | 16S1 | 915 | A | C5-C6-N6 | 11.74 | 133.09 | 123.70 |
| 22 | 23S1 | 103 | A | C5-C6-N6 | 11.74 | 133.09 | 123.70 |
| 22 | 23S1 | 1665 | A | N7-C8-N9 | -11.74 | 107.93 | 113.80 |
| 22 | 23S1 | 973 | A | C5-C6-N6 | 11.74 | 133.09 | 123.70 |
| 22 | 23S1 | 2381 | A | N7-C8-N9 | -11.74 | 107.93 | 113.80 |
| 22 | 23S1 | 2821 | A | N7-C8-N9 | -11.74 | 107.93 | 113.80 |
| 1 | 16S1 | 199 | A | N7-C8-N9 | -11.74 | 107.93 | 113.80 |
| 22 | 23S1 | 1566 | A | N7-C8-N9 | -11.74 | 107.93 | 113.80 |
| 22 | 23S1 | 727 | A | N7-C8-N9 | -11.73 | 107.94 | 113.80 |
| 1 | 16S1 | 250 | A | N7-C8-N9 | -11.73 | 107.94 | 113.80 |
| 1 | 16S1 | 313 | A | C5-C6-N6 | 11.72 | 133.08 | 123.70 |
| 1 | 16S1 | 1437 | A | N7-C8-N9 | -11.72 | 107.94 | 113.80 |
| 22 | 23S1 | 256 | A | N7-C8-N9 | -11.72 | 107.94 | 113.80 |
| 22 | 23S1 | 2435 | A | C5-C6-N6 | 11.72 | 133.08 | 123.70 |
| 22 | 23S1 | 2448 | A | C5-C6-N6 | 11.72 | 133.08 | 123.70 |
| 22 | 23S1 | 28 | A | N7-C8-N9 | -11.72 | 107.94 | 113.80 |
| 22 | 23S1 | 2753 | A | N7-C8-N9 | -11.72 | 107.94 | 113.80 |
| 22 | 23S1 | 1247 | A | N7-C8-N9 | -11.72 | 107.94 | 113.80 |
| 22 | 23S1 | 2288 | A | N7-C8-N9 | -11.72 | 107.94 | 113.80 |
| 22 | 23S1 | 91 | A | N7-C8-N9 | -11.72 | 107.94 | 113.80 |
| 1 | 16S1 | 681 | A | N7-C8-N9 | -11.71 | 107.94 | 113.80 |
| 22 | 23S1 | 1275 | A | C5-C6-N6 | 11.71 | 133.07 | 123.70 |
| 23 | 05S1 | 46 | A | N7-C8-N9 | -11.71 | 107.94 | 113.80 |
| 1 | 16S1 | 451 | A | N7-C8-N9 | -11.71 | 107.95 | 113.80 |
| 1 | 16S1 | 802 | A | C5-C6-N6 | 11.71 | 133.07 | 123.70 |
| 22 | 23S1 | 449 | A | N3-C4-C5 | -11.71 | 118.60 | 126.80 |
| 22 | 23S1 | 643 | A | C5-C6-N6 | 11.71 | 133.07 | 123.70 |
| 22 | 23S1 | 1129 | A | N7-C8-N9 | -11.71 | 107.94 | 113.80 |
| 22 | 23S1 | 2278 | A | N7-C8-N9 | -11.71 | 107.94 | 113.80 |
| 1 | 16S1 | 414 | A | C5-C6-N6 | 11.70 | 133.06 | 123.70 |
| 22 | 23S1 | 526 | A | C5-C6-N6 | 11.71 | 133.06 | 123.70 |
| 22 | 23S1 | 1383 | A | N7-C8-N9 | -11.71 | 107.95 | 113.80 |
| 22 | 23S1 | 1937 | A | N7-C8-N9 | -11.70 | 107.95 | 113.80 |
| 1 | 16S1 | 28 | A | N7-C8-N9 | -11.70 | 107.95 | 113.80 |
| 22 | 23S1 | 1570 | A | N7-C8-N9 | -11.70 | 107.95 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1230 | A | N7-C8-N9 | -11.70 | 107.95 | 113.80 |
| 1 | 16S1 | 171 | A | N7-C8-N9 | -11.70 | 107.95 | 113.80 |
| 22 | 23S1 | 637 | A | N7-C8-N9 | -11.70 | 107.95 | 113.80 |
| 22 | 23S1 | 677 | A | N3-C4-C5 | -11.70 | 118.61 | 126.80 |
| 1 | 16S1 | 559 | A | C5-C6-N6 | 11.70 | 133.06 | 123.70 |
| 22 | 23S1 | 900 | A | N7-C8-N9 | -11.70 | 107.95 | 113.80 |
| 22 | 23S1 | 1147 | A | N7-C8-N9 | -11.70 | 107.95 | 113.80 |
| 22 | 23S1 | 2426 | A | N7-C8-N9 | -11.70 | 107.95 | 113.80 |
| 22 | 23S1 | 172 | A | N7-C8-N9 | -11.69 | 107.95 | 113.80 |
| 1 | 16S1 | 749 | A | N7-C8-N9 | -11.69 | 107.95 | 113.80 |
| 55 | PTR1 | 73 | A | N7-C8-N9 | -11.69 | 107.95 | 113.80 |
| 22 | 23S1 | 428 | A | N7-C8-N9 | -11.69 | 107.96 | 113.80 |
| 22 | 23S1 | 1032 | A | N7-C8-N9 | -11.69 | 107.96 | 113.80 |
| 22 | 23S1 | 1276 | A | N7-C8-N9 | -11.69 | 107.96 | 113.80 |
| 22 | 23S1 | 1347 | A | N7-C8-N9 | -11.69 | 107.96 | 113.80 |
| 22 | 23S1 | 2471 | A | N7-C8-N9 | -11.69 | 107.96 | 113.80 |
| 22 | 23S1 | 223 | A | C5-C6-N6 | 11.68 | 133.05 | 123.70 |
| 22 | 23S1 | 1085 | A | C5-C6-N6 | 11.68 | 133.05 | 123.70 |
| 22 | 23S1 | 1347 | A | C5-C6-N6 | 11.68 | 133.05 | 123.70 |
| 22 | 23S1 | 734 | A | N7-C8-N9 | -11.68 | 107.96 | 113.80 |
| 22 | 23S1 | 761 | A | C5-C6-N6 | 11.68 | 133.04 | 123.70 |
| 22 | 23S1 | 1265 | A | C5-C6-N6 | 11.68 | 133.04 | 123.70 |
| 22 | 23S1 | 1981 | A | N7-C8-N9 | -11.68 | 107.96 | 113.80 |
| 22 | 23S1 | 2634 | A | N7-C8-N9 | -11.68 | 107.96 | 113.80 |
| 1 | 16S1 | 373 | A | N7-C8-N9 | -11.68 | 107.96 | 113.80 |
| 22 | 23S1 | 603 | A | C5-C6-N6 | 11.68 | 133.04 | 123.70 |
| 22 | 23S1 | 502 | A | C5-C6-N6 | 11.67 | 133.04 | 123.70 |
| 22 | 23S1 | 721 | A | N7-C8-N9 | -11.67 | 107.97 | 113.80 |
| 1 | 16S1 | 1046 | A | N3-C4-C5 | -11.67 | 118.63 | 126.80 |
| 22 | 23S1 | 1583 | A | C5-C6-N6 | 11.67 | 133.03 | 123.70 |
| 22 | 23S1 | 1780 | A | C5-C6-N6 | 11.66 | 133.03 | 123.70 |
| 23 | 05S1 | 104 | A | N7-C8-N9 | -11.66 | 107.97 | 113.80 |
| 1 | 16S1 | 243 | A | N7-C8-N9 | -11.66 | 107.97 | 113.80 |
| 1 | 16S1 | 1340 | A | C5-C6-N6 | 11.66 | 133.03 | 123.70 |
| 1 | 16S1 | 139 | A | N7-C8-N9 | -11.66 | 107.97 | 113.80 |
| 22 | 23S1 | 668 | A | C5-C6-N6 | 11.66 | 133.03 | 123.70 |
| 22 | 23S1 | 1871 | A | C5-C6-N6 | 11.66 | 133.03 | 123.70 |
| 1 | 16S1 | 815 | A | C5-C6-N6 | 11.65 | 133.02 | 123.70 |
| 1 | 16S1 | 1216 | A | C5-C6-N6 | 11.65 | 133.02 | 123.70 |
| 22 | 23S1 | 792 | A | C5-C6-N6 | 11.65 | 133.02 | 123.70 |
| 22 | 23S1 | 2183 | A | N7-C8-N9 | -11.65 | 107.97 | 113.80 |
| 22 | 23S1 | 2530 | A | N7-C8-N9 | -11.65 | 107.97 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1853 | A | C5-C6-N6 | 11.65 | 133.02 | 123.70 |
| 1 | 16S1 | 306 | A | N7-C8-N9 | -11.65 | 107.97 | 113.80 |
| 22 | 23S1 | 330 | A | C5-C6-N6 | 11.65 | 133.02 | 123.70 |
| 22 | 23S1 | 2173 | A | C5-C6-N6 | 11.65 | 133.02 | 123.70 |
| 22 | 23S1 | 984 | A | C5-C6-N6 | 11.65 | 133.02 | 123.70 |
| 1 | 16S1 | 1285 | A | N7-C8-N9 | -11.65 | 107.98 | 113.80 |
| 22 | 23S1 | 1046 | A | N7-C8-N9 | -11.65 | 107.98 | 113.80 |
| 1 | 16S1 | 913 | A | N7-C8-N9 | -11.64 | 107.98 | 113.80 |
| 1 | 16S1 | 935 | A | N7-C8-N9 | -11.64 | 107.98 | 113.80 |
| 22 | 23S1 | 1805 | A | N7-C8-N9 | -11.64 | 107.98 | 113.80 |
| 22 | 23S1 | 602 | A | N7-C8-N9 | -11.63 | 107.98 | 113.80 |
| 1 | 16S1 | 441 | A | N7-C8-N9 | -11.63 | 107.98 | 113.80 |
| 1 | 16S1 | 1408 | A | C5-C6-N6 | 11.63 | 133.01 | 123.70 |
| 22 | 23S1 | 152 | A | N7-C8-N9 | -11.63 | 107.98 | 113.80 |
| 22 | 23S1 | 2776 | A | C5-C6-N6 | 11.63 | 133.01 | 123.70 |
| 1 | 16S1 | 583 | A | C5-C6-N6 | 11.63 | 133.00 | 123.70 |
| 1 | 16S1 | 900 | A | C5-C6-N6 | 11.63 | 133.00 | 123.70 |
| 22 | 23S1 | 2435 | A | N7-C8-N9 | -11.63 | 107.98 | 113.80 |
| 22 | 23S1 | 800 | A | N7-C8-N9 | -11.63 | 107.99 | 113.80 |
| 22 | 23S1 | 2270 | A | N7-C8-N9 | -11.63 | 107.98 | 113.80 |
| 22 | 23S1 | 2468 | A | N7-C8-N9 | -11.63 | 107.99 | 113.80 |
| 55 | PTR1 | 26 | A | N7-C8-N9 | -11.63 | 107.99 | 113.80 |
| 1 | 16S1 | 167 | A | N7-C8-N9 | -11.62 | 107.99 | 113.80 |
| 22 | 23S1 | 735 | A | N7-C8-N9 | -11.62 | 107.99 | 113.80 |
| 22 | 23S1 | 1953 | A | C5-C6-N6 | 11.62 | 133.00 | 123.70 |
| 1 | 16S1 | 371 | A | N7-C8-N9 | -11.62 | 107.99 | 113.80 |
| 22 | 23S1 | 1077 | A | N7-C8-N9 | -11.62 | 107.99 | 113.80 |
| 1 | 16S1 | 1374 | A | N7-C8-N9 | -11.62 | 107.99 | 113.80 |
| 22 | 23S1 | 1088 | A | N3-C4-C5 | -11.62 | 118.67 | 126.80 |
| 22 | 23S1 | 507 | A | C5-C6-N6 | 11.62 | 132.99 | 123.70 |
| 1 | 16S1 | 1067 | A | N7-C8-N9 | -11.61 | 108.00 | 113.80 |
| 1 | 16S1 | 1493 | A | N7-C8-N9 | -11.61 | 108.00 | 113.80 |
| 22 | 23S1 | 322 | A | C5-C6-N6 | 11.61 | 132.99 | 123.70 |
| 22 | 23S1 | 346 | A | C5-C6-N6 | 11.61 | 132.98 | 123.70 |
| 22 | 23S1 | 429 | A | C5-C6-N6 | 11.60 | 132.98 | 123.70 |
| 22 | 23S1 | 2758 | A | C5-C6-N6 | 11.60 | 132.98 | 123.70 |
| 1 | 16S1 | 509 | A | N7-C8-N9 | -11.60 | 108.00 | 113.80 |
| 22 | 23S1 | 1786 | A | C5-C6-N6 | 11.60 | 132.98 | 123.70 |
| 22 | 23S1 | 878 | A | C5-C6-N6 | 11.60 | 132.98 | 123.70 |
| 1 | 16S1 | 98 | A | N3-C4-C5 | -11.60 | 118.68 | 126.80 |
| 22 | 23S1 | 892 | A | N3-C4-C5 | -11.60 | 118.68 | 126.80 |
| 1 | 16S1 | 1499 | A | C5-C6-N6 | 11.60 | 132.98 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1569 | A | C5-C6-N6 | 11.60 | 132.98 | 123.70 |
| 22 | 23S1 | 927 | A | C5-C6-N6 | 11.60 | 132.98 | 123.70 |
| 1 | 16S1 | 129 | A | N7-C8-N9 | -11.59 | 108.00 | 113.80 |
| 1 | 16S1 | 1271 | A | N7-C8-N9 | -11.59 | 108.00 | 113.80 |
| 22 | 23S1 | 614 | A | C5-C6-N6 | 11.59 | 132.97 | 123.70 |
| 22 | 23S1 | 1084 | A | C5-C6-N6 | 11.59 | 132.97 | 123.70 |
| 1 | 16S1 | 958 | A | N7-C8-N9 | -11.59 | 108.00 | 113.80 |
| 22 | 23S1 | 165 | A | N7-C8-N9 | -11.59 | 108.00 | 113.80 |
| 22 | 23S1 | 332 | A | C5-C6-N6 | 11.59 | 132.97 | 123.70 |
| 1 | 16S1 | 635 | A | N7-C8-N9 | -11.59 | 108.00 | 113.80 |
| 22 | 23S1 | 1262 | A | C5-C6-N6 | 11.59 | 132.97 | 123.70 |
| 1 | 16S1 | 33 | A | N7-C8-N9 | -11.59 | 108.01 | 113.80 |
| 1 | 16S1 | 923 | A | N3-C4-C5 | -11.59 | 118.69 | 126.80 |
| 22 | 23S1 | 348 | A | N7-C8-N9 | -11.58 | 108.01 | 113.80 |
| 22 | 23S1 | 226 | A | C5-C6-N6 | 11.58 | 132.97 | 123.70 |
| 22 | 23S1 | 1144 | A | N7-C8-N9 | -11.57 | 108.01 | 113.80 |
| 22 | 23S1 | 1829 | A | C5-C6-N6 | 11.57 | 132.96 | 123.70 |
| 1 | 16S1 | 253 | A | N7-C8-N9 | -11.57 | 108.01 | 113.80 |
| 1 | 16S1 | 766 | A | C5-C6-N6 | 11.57 | 132.96 | 123.70 |
| 22 | 23S1 | 2346 | A | N7-C8-N9 | -11.57 | 108.01 | 113.80 |
| 22 | 23S1 | 2542 | A | N7-C8-N9 | -11.57 | 108.01 | 113.80 |
| 1 | 16S1 | 1434 | A | N7-C8-N9 | -11.57 | 108.01 | 113.80 |
| 22 | 23S1 | 504 | A | C5-C6-N6 | 11.57 | 132.96 | 123.70 |
| 22 | 23S1 | 1155 | A | C5-C6-N6 | 11.57 | 132.96 | 123.70 |
| 22 | 23S1 | 1890 | A | N7-C8-N9 | -11.57 | 108.02 | 113.80 |
| 1 | 16S1 | 814 | A | N7-C8-N9 | -11.57 | 108.02 | 113.80 |
| 22 | 23S1 | 73 | A | C5-C6-N6 | 11.57 | 132.95 | 123.70 |
| 22 | 23S1 | 1439 | A | C5-C6-N6 | 11.57 | 132.96 | 123.70 |
| 22 | 23S1 | 1772 | A | N7-C8-N9 | -11.57 | 108.02 | 113.80 |
| 1 | 16S1 | 728 | A | N3-C4-C5 | -11.56 | 118.70 | 126.80 |
| 22 | 23S1 | 1287 | A | N7-C8-N9 | -11.56 | 108.02 | 113.80 |
| 22 | 23S1 | 279 | A | C5-C6-N6 | 11.56 | 132.95 | 123.70 |
| 22 | 23S1 | 1147 | A | C5-C6-N6 | 11.56 | 132.95 | 123.70 |
| 22 | 23S1 | 1700 | A | C5-C6-N6 | 11.56 | 132.95 | 123.70 |
| 22 | 23S1 | 1981 | A | C5-C6-N6 | 11.56 | 132.95 | 123.70 |
| 1 | 16S1 | 794 | A | C5-C6-N6 | 11.56 | 132.95 | 123.70 |
| 1 | 16S1 | 190 | A | C4-C5-C6 | 11.56 | 122.78 | 117.00 |
| 1 | 16S1 | 1456 | A | C5-C6-N6 | 11.56 | 132.95 | 123.70 |
| 22 | 23S1 | 1819 | A | N7-C8-N9 | -11.56 | 108.02 | 113.80 |
| 1 | 16S1 | 174 | A | N7-C8-N9 | -11.55 | 108.02 | 113.80 |
| 1 | 16S1 | 1035 | A | C5-C6-N6 | 11.55 | 132.94 | 123.70 |
| 22 | 23S1 | 1525 | A | N7-C8-N9 | -11.55 | 108.02 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 2009 | A | N7-C8-N9 | -11.55 | 108.02 | 113.80 |
| 22 | 23S1 | 631 | A | C5-C6-N6 | 11.55 | 132.94 | 123.70 |
| 22 | 23S1 | 718 | A | N7-C8-N9 | -11.55 | 108.02 | 113.80 |
| 22 | 23S1 | 2411 | A | N7-C8-N9 | -11.55 | 108.02 | 113.80 |
| 1 | 16S1 | 621 | A | N3-C4-C5 | -11.55 | 118.72 | 126.80 |
| 1 | 16S1 | 649 | A | N7-C8-N9 | -11.55 | 108.03 | 113.80 |
| 22 | 23S1 | 2019 | A | N7-C8-N9 | -11.55 | 108.03 | 113.80 |
| 22 | 23S1 | 2270 | A | C5-C6-N6 | 11.55 | 132.94 | 123.70 |
| 22 | 23S1 | 1169 | A | N7-C8-N9 | -11.54 | 108.03 | 113.80 |
| 22 | 23S1 | 1885 | A | N7-C8-N9 | -11.55 | 108.03 | 113.80 |
| 22 | 23S1 | 1889 | A | N7-C8-N9 | -11.54 | 108.03 | 113.80 |
| 22 | 23S1 | 1969 | A | N7-C8-N9 | -11.54 | 108.03 | 113.80 |
| 22 | 23S1 | 947 | A | N7-C8-N9 | -11.54 | 108.03 | 113.80 |
| 22 | 23S1 | 2227 | A | N7-C8-N9 | -11.54 | 108.03 | 113.80 |
| 22 | 23S1 | 1509 | A | N7-C8-N9 | -11.54 | 108.03 | 113.80 |
| 1 | 16S1 | 1394 | A | N7-C8-N9 | -11.54 | 108.03 | 113.80 |
| 22 | 23S1 | 56 | A | N7-C8-N9 | -11.54 | 108.03 | 113.80 |
| 22 | 23S1 | 2813 | A | C5-C6-N6 | 11.54 | 132.93 | 123.70 |
| 55 | PTR1 | 3 | A | N7-C8-N9 | -11.54 | 108.03 | 113.80 |
| 22 | 23S1 | 1502 | A | N7-C8-N9 | -11.54 | 108.03 | 113.80 |
| 22 | 23S1 | 1821 | A | C5-C6-N6 | 11.54 | 132.93 | 123.70 |
| 1 | 16S1 | 196 | A | C5-C6-N6 | 11.54 | 132.93 | 123.70 |
| 22 | 23S1 | 764 | A | C5-C6-N6 | 11.54 | 132.93 | 123.70 |
| 22 | 23S1 | 1253 | A | C5-C6-N6 | 11.54 | 132.93 | 123.70 |
| 22 | 23S1 | 2547 | A | C5-C6-N6 | 11.54 | 132.93 | 123.70 |
| 22 | 23S1 | 1189 | A | N7-C8-N9 | -11.53 | 108.03 | 113.80 |
| 22 | 23S1 | 1111 | A | N7-C8-N9 | -11.53 | 108.03 | 113.80 |
| 1 | 16S1 | 743 | A | N7-C8-N9 | -11.53 | 108.03 | 113.80 |
| 22 | 23S1 | 1998 | A | N3-C4-C5 | -11.53 | 118.73 | 126.80 |
| 1 | 16S1 | 1150 | A | N7-C8-N9 | -11.53 | 108.04 | 113.80 |
| 22 | 23S1 | 1254 | A | N7-C8-N9 | -11.53 | 108.04 | 113.80 |
| 22 | 23S1 | 1551 | A | N7-C8-N9 | -11.53 | 108.03 | 113.80 |
| 22 | 23S1 | 1858 | A | N7-C8-N9 | -11.53 | 108.03 | 113.80 |
| 1 | 16S1 | 1021 | A | N7-C8-N9 | -11.53 | 108.04 | 113.80 |
| 22 | 23S1 | 126 | A | C5-C6-N6 | 11.53 | 132.92 | 123.70 |
| 1 | 16S1 | 162 | A | N1-C6-N6 | -11.53 | 111.69 | 118.60 |
| 22 | 23S1 | 265 | A | N7-C8-N9 | -11.53 | 108.04 | 113.80 |
| 1 | 16S1 | 363 | A | N7-C8-N9 | -11.52 | 108.04 | 113.80 |
| 22 | 23S1 | 2088 | A | N7-C8-N9 | -11.52 | 108.04 | 113.80 |
| 1 | 16S1 | 282 | A | C5-C6-N6 | 11.52 | 132.92 | 123.70 |
| 1 | 16S1 | 1019 | A | N7-C8-N9 | -11.52 | 108.04 | 113.80 |
| 22 | 23S1 | 621 | A | C5-C6-N6 | 11.52 | 132.91 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 685 | A | N7-C8-N9 | -11.52 | 108.04 | 113.80 |
| 22 | 23S1 | 1809 | A | N3-C4-C5 | -11.52 | 118.74 | 126.80 |
| 22 | 23S1 | 1918 | A | C5-C6-N6 | 11.52 | 132.91 | 123.70 |
| 1 | 16S1 | 155 | A | N7-C8-N9 | -11.51 | 108.04 | 113.80 |
| 22 | 23S1 | 5 | A | N7-C8-N9 | -11.51 | 108.04 | 113.80 |
| 22 | 23S1 | 2851 | A | C5-C6-N6 | 11.51 | 132.91 | 123.70 |
| 23 | 05S1 | 45 | A | N7-C8-N9 | -11.51 | 108.05 | 113.80 |
| 1 | 16S1 | 116 | A | N7-C8-N9 | -11.51 | 108.05 | 113.80 |
| 1 | 16S1 | 478 | A | N3-C4-C5 | -11.51 | 118.74 | 126.80 |
| 22 | 23S1 | 432 | A | N7-C8-N9 | -11.51 | 108.05 | 113.80 |
| 22 | 23S1 | 1365 | A | C5-C6-N6 | 11.51 | 132.91 | 123.70 |
| 1 | 16S1 | 320 | A | N7-C8-N9 | -11.51 | 108.05 | 113.80 |
| 1 | 16S1 | 563 | A | N7-C8-N9 | -11.50 | 108.05 | 113.80 |
| 22 | 23S1 | 599 | A | N7-C8-N9 | -11.50 | 108.05 | 113.80 |
| 22 | 23S1 | 1032 | A | C5-C6-N6 | 11.50 | 132.90 | 123.70 |
| 1 | 16S1 | 1093 | A | N7-C8-N9 | -11.50 | 108.05 | 113.80 |
| 1 | 16S1 | 238 | A | N7-C8-N9 | -11.50 | 108.05 | 113.80 |
| 22 | 23S1 | 216 | A | C5-C6-N6 | 11.50 | 132.90 | 123.70 |
| 22 | 23S1 | 1272 | A | C5-C6-N6 | 11.50 | 132.90 | 123.70 |
| 22 | 23S1 | 2893 | A | N7-C8-N9 | -11.50 | 108.05 | 113.80 |
| 1 | 16S1 | 1410 | A | N7-C8-N9 | -11.49 | 108.05 | 113.80 |
| 22 | 23S1 | 563 | A | N7-C8-N9 | -11.49 | 108.05 | 113.80 |
| 22 | 23S1 | 1385 | A | C5-C6-N6 | 11.49 | 132.89 | 123.70 |
| 22 | 23S1 | 1569 | A | N7-C8-N9 | -11.49 | 108.05 | 113.80 |
| 22 | 23S1 | 825 | A | C5-C6-N6 | 11.49 | 132.89 | 123.70 |
| 22 | 23S1 | 118 | A | C5-C6-N6 | 11.49 | 132.89 | 123.70 |
| 22 | 23S1 | 423 | A | C5-C6-N6 | 11.48 | 132.89 | 123.70 |
| 22 | 23S1 | 1336 | A | N7-C8-N9 | -11.48 | 108.06 | 113.80 |
| 1 | 16S1 | 53 | A | N7-C8-N9 | -11.48 | 108.06 | 113.80 |
| 22 | 23S1 | 1876 | A | N7-C8-N9 | -11.48 | 108.06 | 113.80 |
| 22 | 23S1 | 2009 | A | C5-C6-N6 | 11.48 | 132.89 | 123.70 |
| 23 | 05S1 | 50 | A | N7-C8-N9 | -11.48 | 108.06 | 113.80 |
| 22 | 23S1 | 1757 | A | N7-C8-N9 | -11.48 | 108.06 | 113.80 |
| 22 | 23S1 | 1901 | A | C5-C6-N6 | 11.48 | 132.88 | 123.70 |
| 22 | 23S1 | 2051 | A | N3-C4-C5 | -11.48 | 118.76 | 126.80 |
| 22 | 23S1 | 2199 | A | N7-C8-N9 | -11.48 | 108.06 | 113.80 |
| 1 | 16S1 | 162 | A | C4-C5-C6 | 11.48 | 122.74 | 117.00 |
| 22 | 23S1 | 1616 | A | N7-C8-N9 | -11.48 | 108.06 | 113.80 |
| 22 | 23S1 | 1678 | A | C5-C6-N6 | 11.48 | 132.88 | 123.70 |
| 1 | 16S1 | 1465 | A | N7-C8-N9 | -11.47 | 108.06 | 113.80 |
| 22 | 23S1 | 324 | A | N7-C8-N9 | -11.47 | 108.06 | 113.80 |
| 22 | 23S1 | 1286 | A | N7-C8-N9 | -11.47 | 108.06 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 21 | A | N7-C8-N9 | -11.47 | 108.06 | 113.80 |
| 22 | 23S1 | 504 | A | C8-N9-C4 | 11.47 | 110.39 | 105.80 |
| 22 | 23S1 | 1783 | A | N7-C8-N9 | -11.47 | 108.06 | 113.80 |
| 22 | 23S1 | 2430 | A | C2-N3-C4 | 11.47 | 116.34 | 110.60 |
| 22 | 23S1 | 2635 | A | C5-C6-N6 | 11.47 | 132.88 | 123.70 |
| 22 | 23S1 | 1772 | A | C5-C6-N6 | 11.47 | 132.88 | 123.70 |
| 22 | 23S1 | 1328 | A | N7-C8-N9 | -11.47 | 108.07 | 113.80 |
| 22 | 23S1 | 2317 | A | N7-C8-N9 | -11.47 | 108.07 | 113.80 |
| 22 | 23S1 | 2497 | A | C5-C6-N6 | 11.47 | 132.88 | 123.70 |
| 22 | 23S1 | 294 | A | N7-C8-N9 | -11.46 | 108.07 | 113.80 |
| 22 | 23S1 | 1039 | A | N7-C8-N9 | -11.46 | 108.07 | 113.80 |
| 22 | 23S1 | 1453 | A | N7-C8-N9 | -11.46 | 108.07 | 113.80 |
| 22 | 23S1 | 2052 | A | N7-C8-N9 | -11.47 | 108.07 | 113.80 |
| 22 | 23S1 | 918 | A | C5-C6-N6 | 11.46 | 132.87 | 123.70 |
| 22 | 23S1 | 49 | A | N7-C8-N9 | -11.46 | 108.07 | 113.80 |
| 22 | 23S1 | 342 | A | N7-C8-N9 | -11.46 | 108.07 | 113.80 |
| 22 | 23S1 | 1780 | A | N7-C8-N9 | -11.46 | 108.07 | 113.80 |
| 22 | 23S1 | 1890 | A | C5-C6-N6 | 11.46 | 132.87 | 123.70 |
| 22 | 23S1 | 2134 | A | C5-C6-N6 | 11.46 | 132.87 | 123.70 |
| 1 | 16S1 | 1287 | A | N7-C8-N9 | -11.46 | 108.07 | 113.80 |
| 22 | 23S1 | 2418 | A | C5-C6-N6 | 11.46 | 132.87 | 123.70 |
| 22 | 23S1 | 2635 | A | N7-C8-N9 | -11.46 | 108.07 | 113.80 |
| 1 | 16S1 | 1274 | A | N7-C8-N9 | -11.46 | 108.07 | 113.80 |
| 22 | 23S1 | 391 | A | N7-C8-N9 | -11.46 | 108.07 | 113.80 |
| 22 | 23S1 | 2358 | A | C5-C6-N6 | 11.45 | 132.86 | 123.70 |
| 22 | 23S1 | 2872 | A | N9-C4-C5 | 11.45 | 110.38 | 105.80 |
| 1 | 16S1 | 1000 | A | N7-C8-N9 | -11.45 | 108.08 | 113.80 |
| 22 | 23S1 | 2322 | A | N7-C8-N9 | -11.45 | 108.08 | 113.80 |
| 22 | 23S1 | 2336 | A | C5-C6-N6 | 11.45 | 132.86 | 123.70 |
| 22 | 23S1 | 181 | A | N7-C8-N9 | -11.45 | 108.08 | 113.80 |
| 22 | 23S1 | 1525 | A | C5-C6-N6 | 11.45 | 132.86 | 123.70 |
| 22 | 23S1 | 1815 | A | C5-C6-N6 | 11.45 | 132.86 | 123.70 |
| 22 | 23S1 | 294 | A | C5-C6-N6 | 11.44 | 132.85 | 123.70 |
| 22 | 23S1 | 1095 | A | N7-C8-N9 | -11.44 | 108.08 | 113.80 |
| 22 | 23S1 | 231 | A | N7-C8-N9 | -11.44 | 108.08 | 113.80 |
| 22 | 23S1 | 804 | A | N7-C8-N9 | -11.44 | 108.08 | 113.80 |
| 22 | 23S1 | 1810 | A | N3-C4-C5 | -11.44 | 118.79 | 126.80 |
| 1 | 16S1 | 119 | A | C5-C6-N6 | 11.44 | 132.85 | 123.70 |
| 22 | 23S1 | 53 | A | N7-C8-N9 | -11.44 | 108.08 | 113.80 |
| 22 | 23S1 | 1090 | A | C5-C6-N6 | 11.44 | 132.85 | 123.70 |
| 22 | 23S1 | 1952 | A | C5-C6-N6 | 11.44 | 132.85 | 123.70 |
| 1 | 16S1 | 389 | A | C5-C6-N6 | 11.44 | 132.85 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 1250 | A | C5-C6-N6 | 11.44 | 132.85 | 123.70 |
| 22 | 23S1 | 382 | A | N7-C8-N9 | -11.44 | 108.08 | 113.80 |
| 22 | 23S1 | 2835 | A | C5-C6-N6 | 11.43 | 132.85 | 123.70 |
| 1 | 16S1 | 131 | A | N7-C8-N9 | -11.43 | 108.08 | 113.80 |
| 22 | 23S1 | 849 | A | C5-C6-N6 | 11.43 | 132.84 | 123.70 |
| 1 | 16S1 | 1238 | A | C5-C6-N6 | 11.43 | 132.84 | 123.70 |
| 22 | 23S1 | 896 | A | C5-C6-N6 | 11.43 | 132.84 | 123.70 |
| 22 | 23S1 | 1085 | A | N3-C4-C5 | -11.43 | 118.80 | 126.80 |
| 22 | 23S1 | 1783 | A | C5-C6-N6 | 11.43 | 132.84 | 123.70 |
| 22 | 23S1 | 1156 | A | N7-C8-N9 | -11.43 | 108.09 | 113.80 |
| 22 | 23S1 | 2665 | A | N7-C8-N9 | -11.43 | 108.09 | 113.80 |
| 22 | 23S1 | 788 | A | N7-C8-N9 | -11.43 | 108.09 | 113.80 |
| 1 | 16S1 | 687 | A | C5-C6-N6 | 11.42 | 132.84 | 123.70 |
| 1 | 16S1 | 889 | A | N7-C8-N9 | -11.42 | 108.09 | 113.80 |
| 22 | 23S1 | 1545 | A | C5-C6-N6 | 11.42 | 132.84 | 123.70 |
| 22 | 23S1 | 2856 | A | N7-C8-N9 | -11.42 | 108.09 | 113.80 |
| 22 | 23S1 | 42 | A | N7-C8-N9 | -11.42 | 108.09 | 113.80 |
| 22 | 23S1 | 1073 | A | N7-C8-N9 | -11.42 | 108.09 | 113.80 |
| 1 | 16S1 | 72 | A | N7-C8-N9 | -11.42 | 108.09 | 113.80 |
| 22 | 23S1 | 2733 | A | C5-C6-N6 | 11.42 | 132.83 | 123.70 |
| 1 | 16S1 | 321 | A | C5-C6-N6 | 11.41 | 132.83 | 123.70 |
| 1 | 16S1 | 1289 | A | C5-C6-N6 | 11.41 | 132.83 | 123.70 |
| 22 | 23S1 | 945 | A | C5-C6-N6 | 11.41 | 132.83 | 123.70 |
| 22 | 23S1 | 310 | A | C5-C6-N6 | 11.41 | 132.83 | 123.70 |
| 22 | 23S1 | 1637 | A | C5-C6-N6 | 11.41 | 132.83 | 123.70 |
| 22 | 23S1 | 608 | A | N7-C8-N9 | -11.41 | 108.10 | 113.80 |
| 22 | 23S1 | 675 | A | C5-C6-N6 | 11.41 | 132.83 | 123.70 |
| 22 | 23S1 | 2459 | A | N7-C8-N9 | -11.41 | 108.09 | 113.80 |
| 1 | 16S1 | 160 | A | N7-C8-N9 | -11.41 | 108.10 | 113.80 |
| 1 | 16S1 | 1055 | A | N7-C8-N9 | -11.41 | 108.10 | 113.80 |
| 22 | 23S1 | 756 | A | N7-C8-N9 | -11.41 | 108.10 | 113.80 |
| 22 | 23S1 | 1010 | A | C5-C6-N6 | 11.41 | 132.82 | 123.70 |
| 22 | 23S1 | 1367 | A | N7-C8-N9 | -11.41 | 108.10 | 113.80 |
| 1 | 16S1 | 487 | A | N7-C8-N9 | -11.40 | 108.10 | 113.80 |
| 1 | 16S1 | 640 | A | N7-C8-N9 | -11.40 | 108.10 | 113.80 |
| 22 | 23S1 | 1214 | A | C5-C6-N6 | 11.40 | 132.82 | 123.70 |
| 1 | 16S1 | 547 | A | N7-C8-N9 | -11.40 | 108.10 | 113.80 |
| 22 | 23S1 | 2587 | A | C5-C6-N6 | 11.40 | 132.82 | 123.70 |
| 22 | 23S1 | 2589 | A | N7-C8-N9 | -11.40 | 108.10 | 113.80 |
| 1 | 16S1 | 1349 | A | N7-C8-N9 | -11.40 | 108.10 | 113.80 |
| 22 | 23S1 | 1987 | A | N7-C8-N9 | -11.40 | 108.10 | 113.80 |
| 22 | 23S1 | 2267 | A | N3-C4-C5 | -11.40 | 118.82 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 1468 | A | N3-C4-C5 | -11.40 | 118.82 | 126.80 |
| 22 | 23S1 | 64 | A | N7-C8-N9 | -11.40 | 108.10 | 113.80 |
| 22 | 23S1 | 2198 | A | C5-C6-N6 | 11.40 | 132.82 | 123.70 |
| 23 | 05S1 | 53 | A | C5-C6-N6 | 11.40 | 132.82 | 123.70 |
| 1 | 16S1 | 120 | A | N7-C8-N9 | -11.39 | 108.10 | 113.80 |
| 22 | 23S1 | 2820 | A | N7-C8-N9 | -11.39 | 108.10 | 113.80 |
| 22 | 23S1 | 2899 | A | N7-C8-N9 | -11.39 | 108.10 | 113.80 |
| 1 | 16S1 | 502 | A | N3-C4-C5 | -11.39 | 118.83 | 126.80 |
| 22 | 23S1 | 83 | A | N7-C8-N9 | -11.39 | 108.11 | 113.80 |
| 22 | 23S1 | 1434 | A | N7-C8-N9 | -11.39 | 108.11 | 113.80 |
| 22 | 23S1 | 844 | A | N7-C8-N9 | -11.38 | 108.11 | 113.80 |
| 22 | 23S1 | 1133 | A | C5-C6-N6 | 11.39 | 132.81 | 123.70 |
| 22 | 23S1 | 2019 | A | C5-C6-N6 | 11.39 | 132.81 | 123.70 |
| 22 | 23S1 | 2327 | A | C5-C6-N6 | 11.39 | 132.81 | 123.70 |
| 22 | 23S1 | 927 | A | N7-C8-N9 | -11.38 | 108.11 | 113.80 |
| 22 | 23S1 | 1194 | A | C5-C6-N6 | 11.38 | 132.81 | 123.70 |
| 1 | 16S1 | 60 | A | N7-C8-N9 | -11.38 | 108.11 | 113.80 |
| 1 | 16S1 | 872 | A | C5-C6-N6 | 11.38 | 132.81 | 123.70 |
| 22 | 23S1 | 1522 | A | N7-C8-N9 | -11.38 | 108.11 | 113.80 |
| 22 | 23S1 | 2090 | A | N7-C8-N9 | -11.38 | 108.11 | 113.80 |
| 22 | 23S1 | 2284 | A | N7-C8-N9 | -11.38 | 108.11 | 113.80 |
| 22 | 23S1 | 89 | A | N7-C8-N9 | -11.38 | 108.11 | 113.80 |
| 22 | 23S1 | 2741 | A | N7-C8-N9 | -11.38 | 108.11 | 113.80 |
| 1 | 16S1 | 303 | A | N7-C8-N9 | -11.38 | 108.11 | 113.80 |
| 1 | 16S1 | 802 | A | N7-C8-N9 | -11.38 | 108.11 | 113.80 |
| 22 | 23S1 | 197 | A | N7-C8-N9 | -11.38 | 108.11 | 113.80 |
| 22 | 23S1 | 715 | A | N7-C8-N9 | -11.38 | 108.11 | 113.80 |
| 22 | 23S1 | 1503 | A | N7-C8-N9 | -11.38 | 108.11 | 113.80 |
| 22 | 23S1 | 1614 | A | N7-C8-N9 | -11.38 | 108.11 | 113.80 |
| 22 | 23S1 | 71 | A | N7-C8-N9 | -11.38 | 108.11 | 113.80 |
| 22 | 23S1 | 402 | A | N7-C8-N9 | -11.38 | 108.11 | 113.80 |
| 22 | 23S1 | 892 | A | C5-C6-N6 | 11.38 | 132.80 | 123.70 |
| 1 | 16S1 | 1261 | A | N7-C8-N9 | -11.37 | 108.11 | 113.80 |
| 22 | 23S1 | 453 | A | C5-C6-N6 | 11.37 | 132.80 | 123.70 |
| 22 | 23S1 | 1384 | A | C5-C6-N6 | 11.37 | 132.80 | 123.70 |
| 22 | 23S1 | 2158 | A | N7-C8-N9 | -11.37 | 108.11 | 113.80 |
| 22 | 23S1 | 241 | A | N7-C8-N9 | -11.37 | 108.11 | 113.80 |
| 22 | 23S1 | 345 | A | N7-C8-N9 | -11.37 | 108.12 | 113.80 |
| 23 | 05S1 | 99 | A | C5-C6-N6 | 11.37 | 132.79 | 123.70 |
| 1 | 16S1 | 509 | A | C5-C6-N6 | 11.36 | 132.79 | 123.70 |
| 22 | 23S1 | 819 | A | N3-C4-C5 | -11.36 | 118.85 | 126.80 |
| 22 | 23S1 | 1359 | A | N7-C8-N9 | -11.36 | 108.12 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 2184 | A | N7-C8-N9 | -11.36 | 108.12 | 113.80 |
| 22 | 23S1 | 103 | A | N7-C8-N9 | -11.36 | 108.12 | 113.80 |
| 22 | 23S1 | 265 | A | C5-C6-N6 | 11.36 | 132.79 | 123.70 |
| 22 | 23S1 | 2829 | A | N7-C8-N9 | -11.36 | 108.12 | 113.80 |
| 1 | 16S1 | 807 | A | N7-C8-N9 | -11.36 | 108.12 | 113.80 |
| 22 | 23S1 | 44 | A | N7-C8-N9 | -11.36 | 108.12 | 113.80 |
| 22 | 23S1 | 1126 | A | C5-C6-N6 | 11.36 | 132.78 | 123.70 |
| 22 | 23S1 | 1672 | A | N7-C8-N9 | -11.36 | 108.12 | 113.80 |
| 22 | 23S1 | 91 | A | C5-C6-N6 | 11.35 | 132.78 | 123.70 |
| 22 | 23S1 | 1048 | A | C5-C6-N6 | 11.35 | 132.78 | 123.70 |
| 22 | 23S1 | 1762 | A | C5-C6-N6 | 11.35 | 132.78 | 123.70 |
| 1 | 16S1 | 151 | A | N7-C8-N9 | -11.35 | 108.12 | 113.80 |
| 1 | 16S1 | 595 | A | N7-C8-N9 | -11.35 | 108.13 | 113.80 |
| 22 | 23S1 | 1048 | A | N7-C8-N9 | -11.35 | 108.12 | 113.80 |
| 22 | 23S1 | 1241 | A | N7-C8-N9 | -11.35 | 108.12 | 113.80 |
| 22 | 23S1 | 204 | A | C5-C6-N6 | 11.35 | 132.78 | 123.70 |
| 22 | 23S1 | 1155 | A | N7-C8-N9 | -11.35 | 108.13 | 113.80 |
| 22 | 23S1 | 279 | A | N7-C8-N9 | -11.35 | 108.13 | 113.80 |
| 22 | 23S1 | 2170 | A | C5-C6-N6 | 11.35 | 132.78 | 123.70 |
| 1 | 16S1 | 1213 | A | N7-C8-N9 | -11.34 | 108.13 | 113.80 |
| 1 | 16S1 | 533 | A | N7-C8-N9 | -11.34 | 108.13 | 113.80 |
| 1 | 16S1 | 560 | A | N7-C8-N9 | -11.34 | 108.13 | 113.80 |
| 22 | 23S1 | 1387 | A | N3-C4-C5 | -11.34 | 118.86 | 126.80 |
| 22 | 23S1 | 454 | A | N7-C8-N9 | -11.34 | 108.13 | 113.80 |
| 22 | 23S1 | 1677 | A | C5-C6-N6 | 11.34 | 132.77 | 123.70 |
| 22 | 23S1 | 1241 | A | N3-C4-C5 | -11.34 | 118.87 | 126.80 |
| 22 | 23S1 | 2031 | A | C5-C6-N6 | 11.34 | 132.77 | 123.70 |
| 22 | 23S1 | 1284 | A | N7-C8-N9 | -11.33 | 108.13 | 113.80 |
| 22 | 23S1 | 1717 | A | N7-C8-N9 | -11.33 | 108.13 | 113.80 |
| 22 | 23S1 | 2476 | A | N7-C8-N9 | -11.33 | 108.13 | 113.80 |
| 22 | 23S1 | 2757 | A | C5-C6-N6 | 11.33 | 132.77 | 123.70 |
| 22 | 23S1 | 2873 | A | C5-C6-N6 | 11.33 | 132.77 | 123.70 |
| 1 | 16S1 | 223 | A | N7-C8-N9 | -11.33 | 108.14 | 113.80 |
| 1 | 16S1 | 1428 | A | C5-C6-N6 | 11.33 | 132.76 | 123.70 |
| 22 | 23S1 | 2054 | A | N7-C8-N9 | -11.33 | 108.14 | 113.80 |
| 22 | 23S1 | 2679 | A | N7-C8-N9 | -11.33 | 108.14 | 113.80 |
| 22 | 23S1 | 272 | A | N7-C8-N9 | -11.33 | 108.14 | 113.80 |
| 22 | 23S1 | 666 | A | N7-C8-N9 | -11.33 | 108.14 | 113.80 |
| 22 | 23S1 | 1095 | A | C5-C6-N6 | 11.32 | 132.76 | 123.70 |
| 22 | 23S1 | 74 | A | C5-C6-N6 | 11.32 | 132.76 | 123.70 |
| 22 | 23S1 | 1757 | A | C5-C6-N6 | 11.32 | 132.76 | 123.70 |
| 22 | 23S1 | 2314 | A | N7-C8-N9 | -11.32 | 108.14 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 1163 | A | N7-C8-N9 | -11.32 | 108.14 | 113.80 |
| 1 | 16S1 | 1246 | A | N7-C8-N9 | -11.32 | 108.14 | 113.80 |
| 1 | 16S1 | 1176 | A | N7-C8-N9 | -11.32 | 108.14 | 113.80 |
| 1 | 16S1 | 80 | A | N3-C4-C5 | -11.32 | 118.88 | 126.80 |
| 1 | 16S1 | 1201 | A | N7-C8-N9 | -11.32 | 108.14 | 113.80 |
| 1 | 16S1 | 1363 | A | N7-C8-N9 | -11.32 | 108.14 | 113.80 |
| 22 | 23S1 | 310 | A | N7-C8-N9 | -11.32 | 108.14 | 113.80 |
| 1 | 16S1 | 523 | A | N7-C8-N9 | -11.31 | 108.14 | 113.80 |
| 22 | 23S1 | 1354 | A | N7-C8-N9 | -11.31 | 108.14 | 113.80 |
| 22 | 23S1 | 346 | A | N7-C8-N9 | -11.31 | 108.14 | 113.80 |
| 1 | 16S1 | 1180 | A | C5-C6-N6 | 11.31 | 132.75 | 123.70 |
| 1 | 16S1 | 1204 | A | N7-C8-N9 | -11.31 | 108.14 | 113.80 |
| 22 | 23S1 | 2386 | A | N7-C8-N9 | -11.31 | 108.14 | 113.80 |
| 1 | 16S1 | 1216 | A | N7-C8-N9 | -11.31 | 108.15 | 113.80 |
| 22 | 23S1 | 118 | A | N7-C8-N9 | -11.31 | 108.15 | 113.80 |
| 22 | 23S1 | 449 | A | N7-C8-N9 | -11.31 | 108.15 | 113.80 |
| 22 | 23S1 | 2378 | A | N7-C8-N9 | -11.31 | 108.15 | 113.80 |
| 22 | 23S1 | 2835 | A | N7-C8-N9 | -11.31 | 108.15 | 113.80 |
| 1 | 16S1 | 768 | A | N7-C8-N9 | -11.31 | 108.15 | 113.80 |
| 22 | 23S1 | 2005 | A | C5-C6-N6 | 11.31 | 132.75 | 123.70 |
| 1 | 16S1 | 676 | A | C5-C6-N6 | 11.30 | 132.74 | 123.70 |
| 22 | 23S1 | 751 | A | N7-C8-N9 | -11.30 | 108.15 | 113.80 |
| 22 | 23S1 | 1000 | A | C5-C6-N6 | 11.30 | 132.74 | 123.70 |
| 22 | 23S1 | 2602 | A | C5-C6-N6 | 11.30 | 132.74 | 123.70 |
| 22 | 23S1 | 1322 | A | C5-C6-N6 | 11.30 | 132.74 | 123.70 |
| 22 | 23S1 | 825 | A | N7-C8-N9 | -11.30 | 108.15 | 113.80 |
| 22 | 23S1 | 1544 | A | N3-C4-C5 | -11.30 | 118.89 | 126.80 |
| 22 | 23S1 | 1960 | A | N7-C8-N9 | -11.30 | 108.15 | 113.80 |
| 22 | 23S1 | 863 | A | N3-C4-C5 | -11.30 | 118.89 | 126.80 |
| 22 | 23S1 | 2598 | A | C5-C6-N6 | 11.30 | 132.74 | 123.70 |
| 1 | 16S1 | 1428 | A | N7-C8-N9 | -11.30 | 108.15 | 113.80 |
| 1 | 16S1 | 1431 | A | N7-C8-N9 | -11.30 | 108.15 | 113.80 |
| 22 | 23S1 | 2198 | A | N7-C8-N9 | -11.30 | 108.15 | 113.80 |
| 22 | 23S1 | 582 | A | N7-C8-N9 | -11.29 | 108.15 | 113.80 |
| 22 | 23S1 | 2340 | A | N7-C8-N9 | -11.29 | 108.15 | 113.80 |
| 22 | 23S1 | 2792 | A | N7-C8-N9 | -11.29 | 108.15 | 113.80 |
| 1 | 16S1 | 1493 | A | C5-C6-N6 | 11.29 | 132.73 | 123.70 |
| 22 | 23S1 | 501 | A | C5-C6-N6 | 11.29 | 132.73 | 123.70 |
| 1 | 16S1 | 1130 | A | C5-C6-N6 | 11.29 | 132.73 | 123.70 |
| 22 | 23S1 | 1679 | A | C5-C6-N6 | 11.29 | 132.73 | 123.70 |
| 23 | 05S1 | 73 | A | N3-C4-C5 | -11.29 | 118.90 | 126.80 |
| 1 | 16S1 | 767 | A | N7-C8-N9 | -11.29 | 108.16 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 384 | A | C5-C6-N6 | 11.29 | 132.73 | 123.70 |
| 22 | 23S1 | 513 | A | N3-C4-C5 | -11.29 | 118.90 | 126.80 |
| 22 | 23S1 | 94 | A | N7-C8-N9 | -11.29 | 108.16 | 113.80 |
| 22 | 23S1 | 504 | A | C6-N1-C2 | 11.29 | 125.37 | 118.60 |
| 1 | 16S1 | 1319 | A | C5-C6-N6 | 11.28 | 132.73 | 123.70 |
| 22 | 23S1 | 1086 | A | N7-C8-N9 | -11.28 | 108.16 | 113.80 |
| 1 | 16S1 | 415 | A | N7-C8-N9 | -11.28 | 108.16 | 113.80 |
| 22 | 23S1 | 19 | A | N7-C8-N9 | -11.28 | 108.16 | 113.80 |
| 22 | 23S1 | 119 | A | N7-C8-N9 | -11.28 | 108.16 | 113.80 |
| 22 | 23S1 | 2225 | A | N7-C8-N9 | -11.28 | 108.16 | 113.80 |
| 22 | 23S1 | 2736 | A | C5-C6-N6 | 11.28 | 132.72 | 123.70 |
| 22 | 23S1 | 161 | A | N7-C8-N9 | -11.28 | 108.16 | 113.80 |
| 22 | 23S1 | 590 | A | C5-C6-N6 | 11.28 | 132.72 | 123.70 |
| 22 | 23S1 | 1000 | A | N7-C8-N9 | -11.28 | 108.16 | 113.80 |
| 22 | 23S1 | 1698 | A | C5-C6-N6 | 11.28 | 132.72 | 123.70 |
| 22 | 23S1 | 793 | A | C5-C6-N6 | 11.28 | 132.72 | 123.70 |
| 22 | 23S1 | 1899 | A | C5-C6-N6 | 11.28 | 132.72 | 123.70 |
| 22 | 23S1 | 905 | A | C5-C6-N6 | 11.28 | 132.72 | 123.70 |
| 22 | 23S1 | 1730 | C | N1-C2-O2 | 11.28 | 125.67 | 118.90 |
| 22 | 23S1 | 1194 | A | N7-C8-N9 | -11.27 | 108.16 | 113.80 |
| 1 | 16S1 | 1082 | A | C5-C6-N6 | 11.27 | 132.72 | 123.70 |
| 22 | 23S1 | 241 | A | C5-C6-N6 | 11.27 | 132.72 | 123.70 |
| 22 | 23S1 | 311 | A | N7-C8-N9 | -11.27 | 108.16 | 113.80 |
| 22 | 23S1 | 471 | A | N7-C8-N9 | -11.27 | 108.16 | 113.80 |
| 22 | 23S1 | 706 | A | C5-C6-N6 | 11.27 | 132.72 | 123.70 |
| 22 | 23S1 | 1321 | A | N7-C8-N9 | -11.27 | 108.17 | 113.80 |
| 22 | 23S1 | 522 | A | N7-C8-N9 | -11.27 | 108.17 | 113.80 |
| 22 | 23S1 | 2639 | A | C5-C6-N6 | 11.27 | 132.72 | 123.70 |
| 22 | 23S1 | 2126 | A | C5-C6-N6 | 11.27 | 132.71 | 123.70 |
| 1 | 16S1 | 702 | A | N7-C8-N9 | -11.27 | 108.17 | 113.80 |
| 22 | 23S1 | 2430 | A | C5-C6-N6 | 11.27 | 132.71 | 123.70 |
| 22 | 23S1 | 1342 | A | C5-C6-N6 | 11.27 | 132.71 | 123.70 |
| 1 | 16S1 | 1285 | A | C5-C6-N6 | 11.26 | 132.71 | 123.70 |
| 22 | 23S1 | 382 | A | C5-C6-N6 | 11.26 | 132.71 | 123.70 |
| 22 | 23S1 | 1385 | A | N7-C8-N9 | -11.26 | 108.17 | 113.80 |
| 22 | 23S1 | 1632 | A | C5-C6-N6 | 11.26 | 132.71 | 123.70 |
| 22 | 23S1 | 1641 | A | C5-C6-N6 | 11.26 | 132.71 | 123.70 |
| 22 | 23S1 | 2721 | A | N7-C8-N9 | -11.26 | 108.17 | 113.80 |
| 22 | 23S1 | 1678 | A | N7-C8-N9 | -11.26 | 108.17 | 113.80 |
| 22 | 23S1 | 861 | A | N7-C8-N9 | -11.26 | 108.17 | 113.80 |
| 1 | 16S1 | 171 | A | C5-C6-N6 | 11.26 | 132.71 | 123.70 |
| 1 | 16S1 | 288 | A | C5-C6-N6 | 11.26 | 132.70 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 2518 | A | N3-C4-C5 | -11.26 | 118.92 | 126.80 |
| 1 | 16S1 | 706 | A | N3-C4-C5 | -11.25 | 118.92 | 126.80 |
| 22 | 23S1 | 1009 | A | C5-C6-N6 | 11.25 | 132.70 | 123.70 |
| 22 | 23S1 | 1690 | A | N7-C8-N9 | -11.25 | 108.17 | 113.80 |
| 22 | 23S1 | 2154 | A | N7-C8-N9 | -11.25 | 108.17 | 113.80 |
| 22 | 23S1 | 219 | A | N7-C8-N9 | -11.25 | 108.18 | 113.80 |
| 1 | 16S1 | 649 | A | C5-C6-N6 | 11.25 | 132.70 | 123.70 |
| 1 | 16S1 | 1495 | U | N1-C2-O2 | 11.25 | 130.67 | 122.80 |
| 22 | 23S1 | 401 | A | N7-C8-N9 | -11.25 | 108.18 | 113.80 |
| 22 | 23S1 | 1610 | A | C5-C6-N6 | 11.25 | 132.70 | 123.70 |
| 22 | 23S1 | 670 | A | N7-C8-N9 | -11.25 | 108.18 | 113.80 |
| 1 | 16S1 | 918 | A | C5-C6-N6 | 11.24 | 132.70 | 123.70 |
| 22 | 23S1 | 586 | A | C5-C6-N6 | 11.24 | 132.69 | 123.70 |
| 22 | 23S1 | 863 | A | N7-C8-N9 | -11.24 | 108.18 | 113.80 |
| 22 | 23S1 | 1008 | A | C5-C6-N6 | 11.24 | 132.70 | 123.70 |
| 1 | 16S1 | 816 | A | C5-C6-N6 | 11.24 | 132.69 | 123.70 |
| 1 | 16S1 | 1238 | A | N7-C8-N9 | -11.24 | 108.18 | 113.80 |
| 22 | 23S1 | 2711 | A | C5-C6-N6 | 11.24 | 132.69 | 123.70 |
| 22 | 23S1 | 2758 | A | N7-C8-N9 | -11.24 | 108.18 | 113.80 |
| 1 | 16S1 | 1150 | A | C5-C6-N6 | 11.24 | 132.69 | 123.70 |
| 22 | 23S1 | 2425 | A | N7-C8-N9 | -11.24 | 108.18 | 113.80 |
| 1 | 16S1 | 759 | A | C5-C6-N6 | 11.23 | 132.69 | 123.70 |
| 1 | 16S1 | 766 | A | N7-C8-N9 | -11.23 | 108.18 | 113.80 |
| 22 | 23S1 | 222 | A | N7-C8-N9 | -11.23 | 108.18 | 113.80 |
| 22 | 23S1 | 443 | A | N7-C8-N9 | -11.23 | 108.18 | 113.80 |
| 22 | 23S1 | 1626 | A | N7-C8-N9 | -11.23 | 108.18 | 113.80 |
| 22 | 23S1 | 457 | A | C5-C6-N6 | 11.23 | 132.68 | 123.70 |
| 1 | 16S1 | 10 | A | N7-C8-N9 | -11.23 | 108.19 | 113.80 |
| 1 | 16S1 | 50 | A | N7-C8-N9 | -11.23 | 108.19 | 113.80 |
| 22 | 23S1 | 739 | A | N3-C4-C5 | -11.23 | 118.94 | 126.80 |
| 22 | 23S1 | 1088 | A | N7-C8-N9 | -11.22 | 108.19 | 113.80 |
| 22 | 23S1 | 1384 | A | N7-C8-N9 | -11.22 | 108.19 | 113.80 |
| 22 | 23S1 | 1953 | A | N7-C8-N9 | -11.22 | 108.19 | 113.80 |
| 22 | 23S1 | 1246 | A | N7-C8-N9 | -11.22 | 108.19 | 113.80 |
| 1 | 16S1 | 131 | A | C5-C6-N6 | 11.22 | 132.67 | 123.70 |
| 22 | 23S1 | 262 | A | C5-C6-N6 | 11.22 | 132.68 | 123.70 |
| 22 | 23S1 | 802 | A | C5-C6-N6 | 11.22 | 132.67 | 123.70 |
| 22 | 23S1 | 1096 | A | C5-C6-N6 | 11.22 | 132.67 | 123.70 |
| 22 | 23S1 | 430 | A | C5-C6-N6 | 11.21 | 132.67 | 123.70 |
| 1 | 16S1 | 687 | A | N7-C8-N9 | -11.21 | 108.19 | 113.80 |
| 1 | 16S1 | 1197 | A | N7-C8-N9 | -11.21 | 108.19 | 113.80 |
| 22 | 23S1 | 270 | A | C5-C6-N6 | 11.21 | 132.67 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 522 | A | N3-C4-C5 | -11.21 | 118.95 | 126.80 |
| 1 | 16S1 | 363 | A | C5-C6-N6 | 11.21 | 132.67 | 123.70 |
| 1 | 16S1 | 648 | A | N7-C8-N9 | -11.21 | 108.20 | 113.80 |
| 1 | 16S1 | 1146 | A | C5-C6-N6 | 11.21 | 132.67 | 123.70 |
| 1 | 16S1 | 1169 | A | N7-C8-N9 | -11.21 | 108.20 | 113.80 |
| 1 | 16S1 | 1476 | A | N7-C8-N9 | -11.21 | 108.20 | 113.80 |
| 1 | 16S1 | 1430 | A | C5-C6-N6 | 11.21 | 132.66 | 123.70 |
| 22 | 23S1 | 251 | A | N3-C4-C5 | -11.21 | 118.96 | 126.80 |
| 22 | 23S1 | 1403 | A | N7-C8-N9 | -11.21 | 108.20 | 113.80 |
| 22 | 23S1 | 613 | A | N3-C4-C5 | -11.20 | 118.96 | 126.80 |
| 22 | 23S1 | 2860 | A | C5-C6-N6 | 11.21 | 132.66 | 123.70 |
| 55 | PTR1 | 17 | U | N3-C2-O2 | -11.21 | 114.36 | 122.20 |
| 22 | 23S1 | 2675 | A | N7-C8-N9 | -11.20 | 108.20 | 113.80 |
| 1 | 16S1 | 1287 | A | C5-C6-N6 | 11.20 | 132.66 | 123.70 |
| 22 | 23S1 | 676 | A | C5-C6-N6 | 11.20 | 132.66 | 123.70 |
| 22 | 23S1 | 910 | A | N7-C8-N9 | -11.20 | 108.20 | 113.80 |
| 22 | 23S1 | 1431 | A | N7-C8-N9 | -11.20 | 108.20 | 113.80 |
| 1 | 16S1 | 790 | A | N7-C8-N9 | -11.20 | 108.20 | 113.80 |
| 1 | 16S1 | 7 | A | C5-C6-N6 | 11.19 | 132.66 | 123.70 |
| 1 | 16S1 | 777 | A | N7-C8-N9 | -11.19 | 108.20 | 113.80 |
| 1 | 16S1 | 908 | A | N7-C8-N9 | -11.20 | 108.20 | 113.80 |
| 1 | 16S1 | 968 | A | N7-C8-N9 | -11.20 | 108.20 | 113.80 |
| 22 | 23S1 | 2376 | A | N7-C8-N9 | -11.19 | 108.20 | 113.80 |
| 22 | 23S1 | 2781 | A | C5-C6-N6 | 11.20 | 132.66 | 123.70 |
| 22 | 23S1 | 603 | A | N7-C8-N9 | -11.19 | 108.20 | 113.80 |
| 22 | 23S1 | 718 | A | C5-C6-N6 | 11.19 | 132.65 | 123.70 |
| 22 | 23S1 | 2829 | A | C5-C6-N6 | 11.19 | 132.65 | 123.70 |
| 1 | 16S1 | 579 | A | N7-C8-N9 | -11.19 | 108.21 | 113.80 |
| 22 | 23S1 | 749 | A | N7-C8-N9 | -11.19 | 108.20 | 113.80 |
| 22 | 23S1 | 1509 | A | C5-C6-N6 | 11.19 | 132.65 | 123.70 |
| 1 | 16S1 | 1110 | A | C5-C6-N6 | 11.19 | 132.65 | 123.70 |
| 22 | 23S1 | 541 | A | N7-C8-N9 | -11.19 | 108.21 | 113.80 |
| 22 | 23S1 | 2287 | A | C5-C6-N6 | 11.19 | 132.65 | 123.70 |
| 22 | 23S1 | 2406 | A | C5-C6-N6 | 11.19 | 132.65 | 123.70 |
| 1 | 16S1 | 74 | A | C5-C6-N6 | 11.18 | 132.65 | 123.70 |
| 22 | 23S1 | 330 | A | N3-C4-C5 | -11.18 | 118.97 | 126.80 |
| 22 | 23S1 | 1204 | A | N7-C8-N9 | -11.18 | 108.21 | 113.80 |
| 22 | 23S1 | 1545 | A | N7-C8-N9 | -11.18 | 108.21 | 113.80 |
| 1 | 16S1 | 777 | A | C5-C6-N6 | 11.18 | 132.65 | 123.70 |
| 1 | 16S1 | 718 | A | C5-C6-N6 | 11.18 | 132.64 | 123.70 |
| 1 | 16S1 | 1289 | A | N7-C8-N9 | -11.18 | 108.21 | 113.80 |
| 1 | 16S1 | 1429 | A | C5-C6-N6 | 11.18 | 132.64 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1378 | A | N7-C8-N9 | -11.18 | 108.21 | 113.80 |
| 22 | 23S1 | 1705 | A | N7-C8-N9 | -11.18 | 108.21 | 113.80 |
| 22 | 23S1 | 2037 | A | N7-C8-N9 | -11.18 | 108.21 | 113.80 |
| 1 | 16S1 | 1362 | A | N7-C8-N9 | -11.18 | 108.21 | 113.80 |
| 22 | 23S1 | 572 | A | N3-C4-C5 | -11.18 | 118.98 | 126.80 |
| 22 | 23S1 | 1085 | A | N7-C8-N9 | -11.18 | 108.21 | 113.80 |
| 22 | 23S1 | 2163 | A | C5-C6-N6 | 11.18 | 132.64 | 123.70 |
| 22 | 23S1 | 2322 | A | C5-C6-N6 | 11.18 | 132.64 | 123.70 |
| 22 | 23S1 | 320 | A | N7-C8-N9 | -11.17 | 108.21 | 113.80 |
| 22 | 23S1 | 2070 | A | N7-C8-N9 | -11.17 | 108.21 | 113.80 |
| 1 | 16S1 | 937 | A | N7-C8-N9 | -11.17 | 108.21 | 113.80 |
| 22 | 23S1 | 1269 | A | C5-C6-N6 | 11.17 | 132.64 | 123.70 |
| 22 | 23S1 | 2407 | A | N3-C4-C5 | -11.17 | 118.98 | 126.80 |
| 22 | 23S1 | 2564 | A | N7-C8-N9 | -11.17 | 108.21 | 113.80 |
| 1 | 16S1 | 1044 | A | N7-C8-N9 | -11.17 | 108.22 | 113.80 |
| 1 | 16S1 | 32 | A | N7-C8-N9 | -11.17 | 108.22 | 113.80 |
| 22 | 23S1 | 1366 | A | N7-C8-N9 | -11.17 | 108.22 | 113.80 |
| 22 | 23S1 | 1755 | A | N7-C8-N9 | -11.17 | 108.22 | 113.80 |
| 1 | 16S1 | 974 | A | N7-C8-N9 | -11.16 | 108.22 | 113.80 |
| 22 | 23S1 | 782 | A | N3-C4-C5 | -11.16 | 118.98 | 126.80 |
| 22 | 23S1 | 2705 | A | C5-C6-N6 | 11.16 | 132.63 | 123.70 |
| 22 | 23S1 | 1264 | A | C5-C6-N6 | 11.16 | 132.63 | 123.70 |
| 22 | 23S1 | 1655 | A | C5-C6-N6 | 11.16 | 132.63 | 123.70 |
| 22 | 23S1 | 515 | A | N7-C8-N9 | -11.16 | 108.22 | 113.80 |
| 1 | 16S1 | 478 | A | C5-C6-N6 | 11.16 | 132.63 | 123.70 |
| 22 | 23S1 | 219 | A | C5-C6-N6 | 11.16 | 132.62 | 123.70 |
| 22 | 23S1 | 592 | A | C5-C6-N6 | 11.16 | 132.63 | 123.70 |
| 22 | 23S1 | 781 | A | N7-C8-N9 | -11.16 | 108.22 | 113.80 |
| 22 | 23S1 | 1098 | A | N3-C4-C5 | -11.16 | 118.99 | 126.80 |
| 22 | 23S1 | 2211 | A | N7-C8-N9 | -11.16 | 108.22 | 113.80 |
| 22 | 23S1 | 960 | A | N3-C4-C5 | -11.15 | 118.99 | 126.80 |
| 22 | 23S1 | 1054 | A | N7-C8-N9 | -11.15 | 108.22 | 113.80 |
| 22 | 23S1 | 2205 | A | C5-C6-N6 | 11.15 | 132.62 | 123.70 |
| 22 | 23S1 | 2813 | A | N7-C8-N9 | -11.15 | 108.22 | 113.80 |
| 55 | PTR1 | 9 | A | N7-C8-N9 | -11.15 | 108.22 | 113.80 |
| 1 | 16S1 | 919 | A | C5-C6-N6 | 11.15 | 132.62 | 123.70 |
| 1 | 16S1 | 1319 | A | N7-C8-N9 | -11.15 | 108.22 | 113.80 |
| 22 | 23S1 | 49 | A | C5-C6-N6 | 11.15 | 132.62 | 123.70 |
| 1 | 16S1 | 414 | A | N7-C8-N9 | -11.15 | 108.22 | 113.80 |
| 1 | 16S1 | 909 | A | C5-C6-N6 | 11.15 | 132.62 | 123.70 |
| 22 | 23S1 | 753 | A | N7-C8-N9 | -11.15 | 108.23 | 113.80 |
| 22 | 23S1 | 2281 | A | N7-C8-N9 | -11.15 | 108.23 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 2439 | A | C5-C6-N6 | 11.15 | 132.62 | 123.70 |
| 22 | 23S1 | 1548 | A | N7-C8-N9 | -11.15 | 108.23 | 113.80 |
| 22 | 23S1 | 2412 | A | N7-C8-N9 | -11.15 | 108.23 | 113.80 |
| 22 | 23S1 | 2851 | A | N7-C8-N9 | -11.15 | 108.23 | 113.80 |
| 1 | 16S1 | 1146 | A | N7-C8-N9 | -11.14 | 108.23 | 113.80 |
| 22 | 23S1 | 1069 | A | C5-C6-N6 | 11.14 | 132.62 | 123.70 |
| 22 | 23S1 | 2433 | A | N7-C8-N9 | -11.14 | 108.23 | 113.80 |
| 22 | 23S1 | 1609 | A | N7-C8-N9 | -11.14 | 108.23 | 113.80 |
| 1 | 16S1 | 673 | A | N3-C4-C5 | -11.14 | 119.00 | 126.80 |
| 22 | 23S1 | 362 | A | N7-C8-N9 | -11.14 | 108.23 | 113.80 |
| 22 | 23S1 | 654 | A | N3-C4-C5 | -11.14 | 119.00 | 126.80 |
| 55 | PTR1 | 14 | A | N3-C4-C5 | -11.14 | 119.00 | 126.80 |
| 1 | 16S1 | 655 | A | N3-C4-C5 | -11.13 | 119.00 | 126.80 |
| 1 | 16S1 | 1368 | A | C5-C6-N6 | 11.14 | 132.61 | 123.70 |
| 1 | 16S1 | 865 | A | N3-C4-C5 | -11.13 | 119.01 | 126.80 |
| 22 | 23S1 | 2101 | A | N7-C8-N9 | -11.13 | 108.23 | 113.80 |
| 22 | 23S1 | 2377 | A | N7-C8-N9 | -11.14 | 108.23 | 113.80 |
| 22 | 23S1 | 2418 | A | N7-C8-N9 | -11.13 | 108.23 | 113.80 |
| 1 | 16S1 | 746 | A | N3-C4-C5 | -11.13 | 119.01 | 126.80 |
| 22 | 23S1 | 226 | A | N7-C8-N9 | -11.13 | 108.23 | 113.80 |
| 22 | 23S1 | 1735 | A | N7-C8-N9 | -11.13 | 108.23 | 113.80 |
| 1 | 16S1 | 1329 | A | C5-C6-N6 | 11.13 | 132.60 | 123.70 |
| 22 | 23S1 | 2439 | A | N7-C8-N9 | -11.13 | 108.23 | 113.80 |
| 1 | 16S1 | 782 | A | C5-C6-N6 | 11.13 | 132.60 | 123.70 |
| 22 | 23S1 | 144 | A | N7-C8-N9 | -11.13 | 108.23 | 113.80 |
| 22 | 23S1 | 156 | A | N7-C8-N9 | -11.13 | 108.24 | 113.80 |
| 22 | 23S1 | 676 | A | N7-C8-N9 | -11.13 | 108.24 | 113.80 |
| 22 | 23S1 | 705 | A | N7-C8-N9 | -11.13 | 108.24 | 113.80 |
| 22 | 23S1 | 996 | A | N7-C8-N9 | -11.13 | 108.23 | 113.80 |
| 22 | 23S1 | 1789 | A | C5-C6-N6 | 11.13 | 132.60 | 123.70 |
| 22 | 23S1 | 1872 | A | C4-C5-C6 | 11.13 | 122.56 | 117.00 |
| 22 | 23S1 | 2451 | A | C5-C6-N6 | 11.13 | 132.60 | 123.70 |
| 22 | 23S1 | 2461 | A | N7-C8-N9 | -11.13 | 108.24 | 113.80 |
| 1 | 16S1 | 1248 | A | N7-C8-N9 | -11.12 | 108.24 | 113.80 |
| 22 | 23S1 | 1086 | A | C5-C6-N6 | 11.12 | 132.60 | 123.70 |
| 22 | 23S1 | 2706 | A | N3-C4-C5 | -11.12 | 119.01 | 126.80 |
| 1 | 16S1 | 781 | A | C5-C6-N6 | 11.12 | 132.60 | 123.70 |
| 22 | 23S1 | 988 | A | N7-C8-N9 | -11.12 | 108.24 | 113.80 |
| 22 | 23S1 | 1254 | A | C5-C6-N6 | 11.12 | 132.60 | 123.70 |
| 22 | 23S1 | 1932 | A | N7-C8-N9 | -11.12 | 108.24 | 113.80 |
| 22 | 23S1 | 2126 | A | N7-C8-N9 | -11.12 | 108.24 | 113.80 |
| 22 | 23S1 | 528 | A | N7-C8-N9 | -11.12 | 108.24 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 2453 | A | N3-C4-C5 | -11.12 | 119.02 | 126.80 |
| 22 | 23S1 | 2058 | A | C5-C6-N6 | 11.12 | 132.59 | 123.70 |
| 1 | 16S1 | 535 | A | C5-C6-N6 | 11.11 | 132.59 | 123.70 |
| 22 | 23S1 | 1810 | A | C4-C5-C6 | 11.12 | 122.56 | 117.00 |
| 22 | 23S1 | 2062 | A | C5-C6-N6 | 11.12 | 132.59 | 123.70 |
| 22 | 23S1 | 503 | A | N3-C4-C5 | -11.11 | 119.02 | 126.80 |
| 1 | 16S1 | 845 | A | N7-C8-N9 | -11.11 | 108.25 | 113.80 |
| 1 | 16S1 | 906 | A | N7-C8-N9 | -11.11 | 108.25 | 113.80 |
| 22 | 23S1 | 2273 | A | N3-C4-C5 | -11.11 | 119.03 | 126.80 |
| 22 | 23S1 | 508 | A | C5-C6-N6 | 11.10 | 132.58 | 123.70 |
| 22 | 23S1 | 1744 | A | C5-C6-N6 | 11.10 | 132.58 | 123.70 |
| 22 | 23S1 | 2654 | A | N7-C8-N9 | -11.10 | 108.25 | 113.80 |
| 1 | 16S1 | 495 | A | N7-C8-N9 | -11.10 | 108.25 | 113.80 |
| 1 | 16S1 | 1035 | A | N7-C8-N9 | -11.10 | 108.25 | 113.80 |
| 1 | 16S1 | 1180 | A | N7-C8-N9 | -11.10 | 108.25 | 113.80 |
| 22 | 23S1 | 750 | A | N7-C8-N9 | -11.10 | 108.25 | 113.80 |
| 22 | 23S1 | 1494 | A | N7-C8-N9 | -11.10 | 108.25 | 113.80 |
| 1 | 16S1 | 309 | A | C5-C6-N6 | 11.09 | 132.57 | 123.70 |
| 22 | 23S1 | 432 | A | C5-C6-N6 | 11.09 | 132.57 | 123.70 |
| 22 | 23S1 | 216 | A | N7-C8-N9 | -11.09 | 108.25 | 113.80 |
| 1 | 16S1 | 129 | A | C5-C6-N6 | 11.09 | 132.57 | 123.70 |
| 1 | 16S1 | 270 | A | N7-C8-N9 | -11.09 | 108.25 | 113.80 |
| 22 | 23S1 | 14 | A | N7-C8-N9 | -11.09 | 108.25 | 113.80 |
| 22 | 23S1 | 223 | A | N7-C8-N9 | -11.09 | 108.25 | 113.80 |
| 22 | 23S1 | 675 | A | N7-C8-N9 | -11.09 | 108.25 | 113.80 |
| 22 | 23S1 | 1165 | A | C5-C6-N6 | 11.09 | 132.57 | 123.70 |
| 22 | 23S1 | 1503 | A | C5-C6-N6 | 11.09 | 132.57 | 123.70 |
| 22 | 23S1 | 1453 | A | C5-C6-N6 | 11.09 | 132.57 | 123.70 |
| 22 | 23S1 | 538 | A | C5-C6-N6 | 11.09 | 132.57 | 123.70 |
| 22 | 23S1 | 563 | A | C5-C6-N6 | 11.09 | 132.57 | 123.70 |
| 22 | 23S1 | 1787 | A | N3-C4-C5 | -11.09 | 119.04 | 126.80 |
| 22 | 23S1 | 2327 | A | N7-C8-N9 | -11.09 | 108.26 | 113.80 |
| 1 | 16S1 | 288 | A | N7-C8-N9 | -11.08 | 108.26 | 113.80 |
| 22 | 23S1 | 1502 | A | C5-C6-N6 | 11.08 | 132.57 | 123.70 |
| 55 | PTR1 | 23 | A | N7-C8-N9 | -11.08 | 108.26 | 113.80 |
| 1 | 16S1 | 694 | A | C5-C6-N6 | 11.08 | 132.56 | 123.70 |
| 22 | 23S1 | 340 | A | C5-C6-N6 | 11.08 | 132.57 | 123.70 |
| 22 | 23S1 | 2531 | A | C5-C6-N6 | 11.08 | 132.57 | 123.70 |
| 1 | 16S1 | 1456 | A | N7-C8-N9 | -11.08 | 108.26 | 113.80 |
| 22 | 23S1 | 941 | A | C5-C6-N6 | 11.08 | 132.56 | 123.70 |
| 22 | 23S1 | 1789 | A | N7-C8-N9 | -11.08 | 108.26 | 113.80 |
| 1 | 16S1 | 546 | A | N7-C8-N9 | -11.07 | 108.26 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 937 | A | C5-C6-N6 | 11.07 | 132.56 | 123.70 |
| 22 | 23S1 | 1786 | A | N7-C8-N9 | -11.07 | 108.26 | 113.80 |
| 22 | 23S1 | 2560 | A | N7-C8-N9 | -11.07 | 108.26 | 113.80 |
| 22 | 23S1 | 2886 | A | N7-C8-N9 | -11.07 | 108.26 | 113.80 |
| 1 | 16S1 | 59 | A | N7-C8-N9 | -11.07 | 108.27 | 113.80 |
| 22 | 23S1 | 38 | A | N7-C8-N9 | -11.07 | 108.27 | 113.80 |
| 23 | 05S1 | 29 | A | N7-C8-N9 | -11.07 | 108.27 | 113.80 |
| 22 | 23S1 | 146 | A | N3-C4-C5 | -11.07 | 119.05 | 126.80 |
| 22 | 23S1 | 782 | A | C5-C6-N6 | 11.07 | 132.56 | 123.70 |
| 22 | 23S1 | 1077 | A | C5-C6-N6 | 11.07 | 132.56 | 123.70 |
| 22 | 23S1 | 2700 | A | N7-C8-N9 | -11.07 | 108.27 | 113.80 |
| 22 | 23S1 | 1496 | A | N7-C8-N9 | -11.07 | 108.27 | 113.80 |
| 55 | PTR1 | 21 | A | C5-C6-N6 | 11.07 | 132.55 | 123.70 |
| 1 | 16S1 | 374 | A | N7-C8-N9 | -11.06 | 108.27 | 113.80 |
| 22 | 23S1 | 1535 | A | N7-C8-N9 | -11.06 | 108.27 | 113.80 |
| 22 | 23S1 | 1794 | A | N7-C8-N9 | -11.06 | 108.27 | 113.80 |
| 22 | 23S1 | 2273 | A | C5-C6-N6 | 11.06 | 132.55 | 123.70 |
| 1 | 16S1 | 1502 | A | N7-C8-N9 | -11.06 | 108.27 | 113.80 |
| 22 | 23S1 | 899 | A | C5-C6-N6 | 11.06 | 132.55 | 123.70 |
| 22 | 23S1 | 1899 | A | N3-C4-C5 | -11.06 | 119.06 | 126.80 |
| 1 | 16S1 | 1360 | A | N7-C8-N9 | -11.06 | 108.27 | 113.80 |
| 22 | 23S1 | 144 | A | N3-C4-C5 | -11.06 | 119.06 | 126.80 |
| 23 | 05S1 | 29 | A | N3-C4-C5 | -11.06 | 119.06 | 126.80 |
| 1 | 16S1 | 7 | A | N7-C8-N9 | -11.06 | 108.27 | 113.80 |
| 1 | 16S1 | 1377 | A | N7-C8-N9 | -11.06 | 108.27 | 113.80 |
| 22 | 23S1 | 975 | A | N7-C8-N9 | -11.06 | 108.27 | 113.80 |
| 22 | 23S1 | 1640 | A | N7-C8-N9 | -11.06 | 108.27 | 113.80 |
| 22 | 23S1 | 1552 | A | N7-C8-N9 | -11.06 | 108.27 | 113.80 |
| 1 | 16S1 | 977 | A | C5-C6-N6 | 11.05 | 132.54 | 123.70 |
| 22 | 23S1 | 2587 | A | N7-C8-N9 | -11.05 | 108.27 | 113.80 |
| 1 | 16S1 | 408 | A | C5-C6-N6 | 11.05 | 132.54 | 123.70 |
| 22 | 23S1 | 715 | A | C5-C6-N6 | 11.05 | 132.54 | 123.70 |
| 22 | 23S1 | 2108 | A | C5-C6-N6 | 11.05 | 132.54 | 123.70 |
| 22 | 23S1 | 449 | A | C5-C6-N6 | 11.05 | 132.54 | 123.70 |
| 22 | 23S1 | 2170 | A | N7-C8-N9 | -11.05 | 108.28 | 113.80 |
| 22 | 23S1 | 556 | A | C5-C6-N6 | 11.05 | 132.54 | 123.70 |
| 22 | 23S1 | 2191 | A | C5-C6-N6 | 11.05 | 132.54 | 123.70 |
| 22 | 23S1 | 2247 | A | C5-C6-N6 | 11.05 | 132.54 | 123.70 |
| 22 | 23S1 | 2328 | A | N3-C4-C5 | -11.05 | 119.07 | 126.80 |
| 22 | 23S1 | 959 | A | C5-C6-N6 | 11.04 | 132.53 | 123.70 |
| 22 | 23S1 | 2748 | A | N7-C8-N9 | -11.04 | 108.28 | 113.80 |
| 22 | 23S1 | 1805 | A | C5-C6-N6 | 11.04 | 132.53 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1 | 16S1 | 901 | A | N3-C4-C5 | -11.04 | 119.07 | 126.80 |
| 1 | 16S1 | 1476 | A | C5-C6-N6 | 11.04 | 132.53 | 123.70 |
| 22 | 23S1 | 2682 | A | C5-C6-N6 | 11.04 | 132.53 | 123.70 |
| 22 | 23S1 | 735 | A | C5-C6-N6 | 11.04 | 132.53 | 123.70 |
| 22 | 23S1 | 1701 | A | N7-C8-N9 | -11.04 | 108.28 | 113.80 |
| 22 | 23S1 | 2033 | A | N7-C8-N9 | -11.04 | 108.28 | 113.80 |
| 22 | 23S1 | 2778 | A | C5-C6-N6 | 11.04 | 132.53 | 123.70 |
| 22 | 23S1 | 1829 | A | N7-C8-N9 | -11.03 | 108.28 | 113.80 |
| 1 | 16S1 | 1 | A | N7-C8-N9 | -11.03 | 108.28 | 113.80 |
| 22 | 23S1 | 131 | A | N3-C4-C5 | -11.03 | 119.08 | 126.80 |
| 22 | 23S1 | 2662 | A | N3-C4-C5 | -11.03 | 119.08 | 126.80 |
| 22 | 23S1 | 2284 | A | N3-C4-C5 | -11.03 | 119.08 | 126.80 |
| 22 | 23S1 | 877 | A | C5-C6-N6 | 11.03 | 132.52 | 123.70 |
| 22 | 23S1 | 1970 | A | O5'-P-OP1 | -11.03 | 95.77 | 105.70 |
| 22 | 23S1 | 1433 | A | C5-C6-N6 | 11.03 | 132.52 | 123.70 |
| 22 | 23S1 | 2335 | A | N7-C8-N9 | -11.03 | 108.29 | 113.80 |
| 22 | 23S1 | 347 | A | N7-C8-N9 | -11.02 | 108.29 | 113.80 |
| 1 | 16S1 | 3 | A | N7-C8-N9 | -11.02 | 108.29 | 113.80 |
| 1 | 16S1 | 1508 | A | N3-C4-C5 | -11.02 | 119.09 | 126.80 |
| 22 | 23S1 | 1336 | A | N3-C4-C5 | -11.02 | 119.09 | 126.80 |
| 22 | 23S1 | 1871 | A | N3-C4-C5 | -11.02 | 119.09 | 126.80 |
| 22 | 23S1 | 2212 | A | C5-C6-N6 | 11.02 | 132.51 | 123.70 |
| 22 | 23S1 | 2733 | A | N7-C8-N9 | -11.02 | 108.29 | 113.80 |
| 1 | 16S1 | 320 | A | C5-C6-N6 | 11.02 | 132.51 | 123.70 |
| 1 | 16S1 | 1022 | A | N3-C4-C5 | -11.02 | 119.09 | 126.80 |
| 22 | 23S1 | 492 | A | N3-C4-C5 | -11.02 | 119.09 | 126.80 |
| 22 | 23S1 | 221 | A | C5-C6-N6 | 11.02 | 132.51 | 123.70 |
| 1 | 16S1 | 452 | A | N7-C8-N9 | -11.01 | 108.29 | 113.80 |
| 1 | 16S1 | 482 | A | N7-C8-N9 | -11.01 | 108.29 | 113.80 |
| 22 | 23S1 | 104 | A | N7-C8-N9 | -11.01 | 108.29 | 113.80 |
| 22 | 23S1 | 1977 | A | N7-C8-N9 | -11.01 | 108.29 | 113.80 |
| 22 | 23S1 | 734 | A | C5-C6-N6 | 11.01 | 132.51 | 123.70 |
| 22 | 23S1 | 2205 | A | N7-C8-N9 | -11.01 | 108.30 | 113.80 |
| 22 | 23S1 | 655 | A | C5-C6-N6 | 11.01 | 132.51 | 123.70 |
| 22 | 23S1 | 1070 | A | N7-C8-N9 | -11.01 | 108.30 | 113.80 |
| 22 | 23S1 | 1327 | A | N7-C8-N9 | -11.01 | 108.30 | 113.80 |
| 22 | 23S1 | 2433 | A | C5-C6-N6 | 11.01 | 132.51 | 123.70 |
| 22 | 23S1 | 1998 | A | N7-C8-N9 | -11.01 | 108.30 | 113.80 |
| 1 | 16S1 | 892 | A | C5-C6-N6 | 11.00 | 132.50 | 123.70 |
| 22 | 23S1 | 592 | A | N7-C8-N9 | -11.00 | 108.30 | 113.80 |
| 22 | 23S1 | 1419 | A | C5-C6-N6 | 11.00 | 132.50 | 123.70 |
| 22 | 23S1 | 460 | A | N7-C8-N9 | -11.00 | 108.30 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 2287 | A | N7-C8-N9 | -11.00 | 108.30 | 113.80 |
| 1 | 16S1 | 468 | A | C5-C6-N6 | 11.00 | 132.50 | 123.70 |
| 1 | 16S1 | 1229 | A | N7-C8-N9 | -11.00 | 108.30 | 113.80 |
| 1 | 16S1 | 1433 | A | C5-C6-N6 | 11.00 | 132.50 | 123.70 |
| 22 | 23S1 | 941 | A | N7-C8-N9 | -11.00 | 108.30 | 113.80 |
| 1 | 16S1 | 819 | A | C5-C6-N6 | 11.00 | 132.50 | 123.70 |
| 1 | 16S1 | 1021 | A | C5-C6-N6 | 11.00 | 132.50 | 123.70 |
| 22 | 23S1 | 1505 | A | N7-C8-N9 | -11.00 | 108.30 | 113.80 |
| 22 | 23S1 | 689 | A | N3-C4-C5 | -11.00 | 119.10 | 126.80 |
| 1 | 16S1 | 596 | A | C5-C6-N6 | 10.99 | 132.50 | 123.70 |
| 1 | 16S1 | 892 | A | N7-C8-N9 | -10.99 | 108.30 | 113.80 |
| 1 | 16S1 | 907 | A | N7-C8-N9 | -10.99 | 108.30 | 113.80 |
| 22 | 23S1 | 412 | A | C5-C6-N6 | 10.99 | 132.50 | 123.70 |
| 1 | 16S1 | 873 | A | N7-C8-N9 | -10.99 | 108.31 | 113.80 |
| 1 | 16S1 | 560 | A | C5-C6-N6 | 10.99 | 132.49 | 123.70 |
| 22 | 23S1 | 528 | A | C5-C6-N6 | 10.99 | 132.49 | 123.70 |
| 1 | 16S1 | 900 | A | N7-C8-N9 | -10.99 | 108.31 | 113.80 |
| 1 | 16S1 | 906 | A | C5-C6-N6 | 10.99 | 132.49 | 123.70 |
| 22 | 23S1 | 5 | A | N3-C4-C5 | -10.99 | 119.11 | 126.80 |
| 22 | 23S1 | 439 | A | N7-C8-N9 | -10.99 | 108.31 | 113.80 |
| 22 | 23S1 | 2810 | A | C5-C6-N6 | 10.99 | 132.49 | 123.70 |
| 22 | 23S1 | 2531 | A | N7-C8-N9 | -10.99 | 108.31 | 113.80 |
| 22 | 23S1 | 2589 | A | C5-C6-N6 | 10.99 | 132.49 | 123.70 |
| 22 | 23S1 | 2727 | A | N7-C8-N9 | -10.99 | 108.31 | 113.80 |
| 1 | 16S1 | 510 | A | N7-C8-N9 | -10.98 | 108.31 | 113.80 |
| 1 | 16S1 | 1248 | A | C5-C6-N6 | 10.98 | 132.49 | 123.70 |
| 22 | 23S1 | 422 | A | N3-C4-C5 | -10.98 | 119.11 | 126.80 |
| 1 | 16S1 | 415 | A | C5-C6-N6 | 10.98 | 132.49 | 123.70 |
| 22 | 23S1 | 470 | A | N3-C4-C5 | -10.98 | 119.11 | 126.80 |
| 22 | 23S1 | 925 | A | N3-C4-C5 | -10.98 | 119.11 | 126.80 |
| 22 | 23S1 | 2366 | A | N7-C8-N9 | -10.98 | 108.31 | 113.80 |
| 23 | 05S1 | 57 | A | N7-C8-N9 | -10.98 | 108.31 | 113.80 |
| 22 | 23S1 | 1084 | A | N7-C8-N9 | -10.98 | 108.31 | 113.80 |
| 22 | 23S1 | 2541 | A | C5-C6-N6 | 10.98 | 132.48 | 123.70 |
| 1 | 16S1 | 495 | A | C5-C6-N6 | 10.98 | 132.48 | 123.70 |
| 1 | 16S1 | 600 | A | N7-C8-N9 | -10.98 | 108.31 | 113.80 |
| 1 | 16S1 | 729 | A | N7-C8-N9 | -10.98 | 108.31 | 113.80 |
| 22 | 23S1 | 532 | A | C5-C6-N6 | 10.98 | 132.48 | 123.70 |
| 1 | 16S1 | 1480 | A | N7-C8-N9 | -10.98 | 108.31 | 113.80 |
| 22 | 23S1 | 996 | A | C5-C6-N6 | 10.97 | 132.48 | 123.70 |
| 22 | 23S1 | 1477 | A | N7-C8-N9 | -10.97 | 108.31 | 113.80 |
| 22 | 23S1 | 2117 | A | C5-C6-N6 | 10.97 | 132.48 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 1170 | A | N7-C8-N9 | -10.97 | 108.31 | 113.80 |
| 22 | 23S1 | 1001 | A | N7-C8-N9 | -10.97 | 108.31 | 113.80 |
| 22 | 23S1 | 2169 | A | N7-C8-N9 | -10.97 | 108.31 | 113.80 |
| 22 | 23S1 | 1952 | A | N7-C8-N9 | -10.97 | 108.32 | 113.80 |
| 1 | 16S1 | 181 | A | N7-C8-N9 | -10.97 | 108.32 | 113.80 |
| 1 | 16S1 | 460 | A | N7-C8-N9 | -10.97 | 108.32 | 113.80 |
| 22 | 23S1 | 483 | A | C5-C6-N6 | 10.97 | 132.47 | 123.70 |
| 1 | 16S1 | 2 | A | C5-C6-N6 | 10.96 | 132.47 | 123.70 |
| 22 | 23S1 | 1916 | A | C5-C6-N6 | 10.96 | 132.47 | 123.70 |
| 22 | 23S1 | 190 | A | C5-C6-N6 | 10.96 | 132.47 | 123.70 |
| 22 | 23S1 | 345 | A | C5-C6-N6 | 10.96 | 132.47 | 123.70 |
| 22 | 23S1 | 716 | A | C5-C6-N6 | 10.96 | 132.47 | 123.70 |
| 1 | 16S1 | 199 | A | N3-C4-C5 | -10.96 | 119.13 | 126.80 |
| 1 | 16S1 | 994 | A | N7-C8-N9 | -10.96 | 108.32 | 113.80 |
| 22 | 23S1 | 52 | A | N7-C8-N9 | -10.96 | 108.32 | 113.80 |
| 1 | 16S1 | 71 | A | N7-C8-N9 | -10.96 | 108.32 | 113.80 |
| 22 | 23S1 | 1021 | A | C5-C6-N6 | 10.96 | 132.47 | 123.70 |
| 22 | 23S1 | 1847 | A | N3-C4-C5 | -10.96 | 119.13 | 126.80 |
| 22 | 23S1 | 2900 | A | N7-C8-N9 | -10.96 | 108.32 | 113.80 |
| 22 | 23S1 | 2868 | A | C5-C6-N6 | 10.96 | 132.47 | 123.70 |
| 22 | 23S1 | 199 | A | C5-C6-N6 | 10.95 | 132.46 | 123.70 |
| 22 | 23S1 | 1746 | A | C5-C6-N6 | 10.96 | 132.46 | 123.70 |
| 1 | 16S1 | 32 | A | N3-C4-C5 | -10.95 | 119.13 | 126.80 |
| 22 | 23S1 | 802 | A | N7-C8-N9 | -10.95 | 108.32 | 113.80 |
| 22 | 23S1 | 1246 | A | N3-C4-C5 | -10.95 | 119.13 | 126.80 |
| 22 | 23S1 | 2809 | A | N3-C4-C5 | -10.95 | 119.13 | 126.80 |
| 22 | 23S1 | 2823 | A | N7-C8-N9 | -10.95 | 108.32 | 113.80 |
| 1 | 16S1 | 160 | A | C5-C6-N6 | 10.95 | 132.46 | 123.70 |
| 1 | 16S1 | 238 | A | C5-C6-N6 | 10.94 | 132.45 | 123.70 |
| 1 | 16S1 | 1333 | A | N7-C8-N9 | -10.94 | 108.33 | 113.80 |
| 22 | 23S1 | 384 | A | N7-C8-N9 | -10.94 | 108.33 | 113.80 |
| 22 | 23S1 | 1978 | A | C5-C6-N6 | 10.94 | 132.45 | 123.70 |
| 22 | 23S1 | 2670 | A | N7-C8-N9 | -10.94 | 108.33 | 113.80 |
| 22 | 23S1 | 2826 | A | C5-C6-N6 | 10.94 | 132.45 | 123.70 |
| 1 | 16S1 | 716 | A | N3-C4-C5 | -10.94 | 119.14 | 126.80 |
| 1 | 16S1 | 845 | A | C5-C6-N6 | 10.94 | 132.45 | 123.70 |
| 22 | 23S1 | 1495 | A | N7-C8-N9 | -10.94 | 108.33 | 113.80 |
| 22 | 23S1 | 2211 | A | C5-C6-N6 | 10.94 | 132.45 | 123.70 |
| 22 | 23S1 | 2749 | A | C5-C6-N6 | 10.94 | 132.45 | 123.70 |
| 1 | 16S1 | 1430 | A | N7-C8-N9 | -10.94 | 108.33 | 113.80 |
| 22 | 23S1 | 1285 | A | N7-C8-N9 | -10.94 | 108.33 | 113.80 |
| 22 | 23S1 | 2741 | A | C5-C6-N6 | 10.94 | 132.45 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 2850 | A | C5-C6-N6 | 10.94 | 132.45 | 123.70 |
| 22 | 23S1 | 1156 | A | C5-C6-N6 | 10.93 | 132.45 | 123.70 |
| 1 | 16S1 | 344 | A | N7-C8-N9 | -10.93 | 108.33 | 113.80 |
| 1 | 16S1 | 393 | A | N7-C8-N9 | -10.93 | 108.33 | 113.80 |
| 22 | 23S1 | 2518 | A | N7-C8-N9 | -10.93 | 108.33 | 113.80 |
| 1 | 16S1 | 553 | A | C5-C6-N6 | 10.93 | 132.44 | 123.70 |
| 1 | 16S1 | 1396 | A | N7-C8-N9 | -10.93 | 108.33 | 113.80 |
| 1 | 16S1 | 949 | A | N3-C4-C5 | -10.93 | 119.15 | 126.80 |
| 1 | 16S1 | 1446 | A | N3-C4-C5 | -10.93 | 119.15 | 126.80 |
| 22 | 23S1 | 1586 | A | N3-C4-C5 | -10.93 | 119.15 | 126.80 |
| 22 | 23S1 | 362 | A | N3-C4-C5 | -10.93 | 119.15 | 126.80 |
| 22 | 23S1 | 1669 | A | C5-C6-N6 | 10.93 | 132.44 | 123.70 |
| 22 | 23S1 | 1701 | A | C5-C6-N6 | 10.93 | 132.44 | 123.70 |
| 22 | 23S1 | 2560 | A | N3-C4-C5 | -10.92 | 119.15 | 126.80 |
| 1 | 16S1 | 1082 | A | N7-C8-N9 | -10.92 | 108.34 | 113.80 |
| 22 | 23S1 | 347 | A | C5-C6-N6 | 10.92 | 132.44 | 123.70 |
| 22 | 23S1 | 2241 | A | N3-C4-C5 | -10.92 | 119.16 | 126.80 |
| 22 | 23S1 | 2453 | A | N7-C8-N9 | -10.92 | 108.34 | 113.80 |
| 22 | 23S1 | 2764 | A | C5-C6-N6 | 10.92 | 132.44 | 123.70 |
| 1 | 16S1 | 279 | A | C5-C6-N6 | 10.92 | 132.43 | 123.70 |
| 1 | 16S1 | 456 | A | C5-C6-N6 | 10.92 | 132.43 | 123.70 |
| 55 | PTR1 | 69 | A | N7-C8-N9 | -10.92 | 108.34 | 113.80 |
| 22 | 23S1 | 38 | A | N3-C4-C5 | -10.92 | 119.16 | 126.80 |
| 22 | 23S1 | 146 | A | N7-C8-N9 | -10.92 | 108.34 | 113.80 |
| 22 | 23S1 | 541 | A | C5-C6-N6 | 10.92 | 132.43 | 123.70 |
| 22 | 23S1 | 917 | A | C5-C6-N6 | 10.92 | 132.43 | 123.70 |
| 22 | 23S1 | 1307 | A | N7-C8-N9 | -10.92 | 108.34 | 113.80 |
| 22 | 23S1 | 1749 | A | N7-C8-N9 | -10.92 | 108.34 | 113.80 |
| 22 | 23S1 | 1508 | A | N7-C8-N9 | -10.91 | 108.34 | 113.80 |
| 55 | PTR1 | 42 | A | N7-C8-N9 | -10.91 | 108.34 | 113.80 |
| 22 | 23S1 | 1932 | A | C5-C6-N6 | 10.91 | 132.43 | 123.70 |
| 1 | 16S1 | 814 | A | C5-C6-N6 | 10.91 | 132.43 | 123.70 |
| 22 | 23S1 | 917 | A | N7-C8-N9 | -10.91 | 108.34 | 113.80 |
| 22 | 23S1 | 2478 | A | N7-C8-N9 | -10.91 | 108.34 | 113.80 |
| 1 | 16S1 | 262 | A | C5-C6-N6 | 10.91 | 132.43 | 123.70 |
| 22 | 23S1 | 1668 | A | N7-C8-N9 | -10.91 | 108.35 | 113.80 |
| 1 | 16S1 | 825 | A | C5-C6-N6 | 10.91 | 132.43 | 123.70 |
| 22 | 23S1 | 480 | A | N3-C4-C5 | -10.91 | 119.17 | 126.80 |
| 1 | 16S1 | 1375 | A | N7-C8-N9 | -10.90 | 108.35 | 113.80 |
| 22 | 23S1 | 1127 | A | N7-C8-N9 | -10.90 | 108.35 | 113.80 |
| 22 | 23S1 | 1353 | A | N3-C4-C5 | -10.90 | 119.17 | 126.80 |
| 1 | 16S1 | 712 | A | N3-C4-C5 | -10.90 | 119.17 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 716 | A | C5-C6-N6 | 10.90 | 132.42 | 123.70 |
| 1 | 16S1 | 994 | A | N3-C4-C5 | -10.90 | 119.17 | 126.80 |
| 22 | 23S1 | 781 | A | C5-C6-N6 | 10.90 | 132.42 | 123.70 |
| 22 | 23S1 | 1260 | A | C5-C6-N6 | 10.90 | 132.42 | 123.70 |
| 1 | 16S1 | 532 | A | N7-C8-N9 | -10.90 | 108.35 | 113.80 |
| 1 | 16S1 | 663 | A | N3-C4-C5 | -10.90 | 119.17 | 126.80 |
| 1 | 16S1 | 759 | A | N7-C8-N9 | -10.90 | 108.35 | 113.80 |
| 22 | 23S1 | 1103 | A | N7-C8-N9 | -10.90 | 108.35 | 113.80 |
| 22 | 23S1 | 2070 | A | C5-C6-N6 | 10.90 | 132.42 | 123.70 |
| 22 | 23S1 | 2184 | A | C5-C6-N6 | 10.90 | 132.42 | 123.70 |
| 22 | 23S1 | 2461 | A | N3-C4-C5 | -10.90 | 119.17 | 126.80 |
| 22 | 23S1 | 404 | A | C5-C6-N6 | 10.89 | 132.42 | 123.70 |
| 22 | 23S1 | 1664 | A | N3-C4-C5 | -10.89 | 119.17 | 126.80 |
| 22 | 23S1 | 2097 | A | N7-C8-N9 | -10.89 | 108.35 | 113.80 |
| 22 | 23S1 | 742 | A | N7-C8-N9 | -10.89 | 108.36 | 113.80 |
| 22 | 23S1 | 643 | A | N7-C8-N9 | -10.89 | 108.36 | 113.80 |
| 1 | 16S1 | 807 | A | N3-C4-C5 | -10.88 | 119.18 | 126.80 |
| 22 | 23S1 | 556 | A | N7-C8-N9 | -10.88 | 108.36 | 113.80 |
| 22 | 23S1 | 917 | A | N3-C4-C5 | -10.88 | 119.18 | 126.80 |
| 1 | 16S1 | 236 | A | C5-C6-N6 | 10.88 | 132.41 | 123.70 |
| 1 | 16S1 | 520 | A | N7-C8-N9 | -10.88 | 108.36 | 113.80 |
| 22 | 23S1 | 2750 | A | C5-C6-N6 | 10.88 | 132.41 | 123.70 |
| 22 | 23S1 | 1858 | A | C5-C6-N6 | 10.88 | 132.40 | 123.70 |
| 22 | 23S1 | 1096 | A | N7-C8-N9 | -10.88 | 108.36 | 113.80 |
| 22 | 23S1 | 2062 | A | N3-C4-C5 | -10.88 | 119.19 | 126.80 |
| 22 | 23S1 | 2169 | A | N3-C4-C5 | -10.88 | 119.18 | 126.80 |
| 23 | 05S1 | 59 | A | N7-C8-N9 | -10.88 | 108.36 | 113.80 |
| 1 | 16S1 | 1299 | A | C5-C6-N6 | 10.88 | 132.40 | 123.70 |
| 22 | 23S1 | 1383 | A | C5-C6-N6 | 10.88 | 132.40 | 123.70 |
| 22 | 23S1 | 1803 | A | C5-C6-N6 | 10.88 | 132.40 | 123.70 |
| 1 | 16S1 | 1171 | A | N3-C4-C5 | -10.87 | 119.19 | 126.80 |
| 1 | 16S1 | 746 | A | N7-C8-N9 | -10.87 | 108.36 | 113.80 |
| 22 | 23S1 | 1010 | A | N7-C8-N9 | -10.87 | 108.36 | 113.80 |
| 1 | 16S1 | 263 | A | N3-C4-C5 | -10.87 | 119.19 | 126.80 |
| 22 | 23S1 | 575 | A | N7-C8-N9 | -10.87 | 108.36 | 113.80 |
| 22 | 23S1 | 1900 | A | N7-C8-N9 | -10.87 | 108.36 | 113.80 |
| 22 | 23S1 | 959 | A | N7-C8-N9 | -10.87 | 108.36 | 113.80 |
| 22 | 23S1 | 892 | A | N7-C8-N9 | -10.87 | 108.37 | 113.80 |
| 22 | 23S1 | 1214 | A | N7-C8-N9 | -10.87 | 108.36 | 113.80 |
| 22 | 23S1 | 1936 | A | N3-C4-C5 | -10.87 | 119.19 | 126.80 |
| 22 | 23S1 | 2471 | A | C5-C6-N6 | 10.87 | 132.39 | 123.70 |
| 1 | 16S1 | 1229 | A | N3-C4-C5 | -10.87 | 119.19 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 255 | A | N3-C4-C5 | -10.86 | 119.19 | 126.80 |
| 22 | 23S1 | 1151 | A | N7-C8-N9 | -10.86 | 108.37 | 113.80 |
| 22 | 23S1 | 1284 | A | C5-C6-N6 | 10.86 | 132.39 | 123.70 |
| 22 | 23S1 | 1413 | A | C5-C6-N6 | 10.86 | 132.39 | 123.70 |
| 22 | 23S1 | 1522 | A | C5-C6-N6 | 10.87 | 132.39 | 123.70 |
| 1 | 16S1 | 393 | A | N3-C4-C5 | -10.86 | 119.20 | 126.80 |
| 1 | 16S1 | 1111 | A | N7-C8-N9 | -10.86 | 108.37 | 113.80 |
| 1 | 16S1 | 1251 | A | N7-C8-N9 | -10.86 | 108.37 | 113.80 |
| 1 | 16S1 | 1377 | A | C5-C6-N6 | 10.86 | 132.39 | 123.70 |
| 22 | 23S1 | 2135 | A | N7-C8-N9 | -10.86 | 108.37 | 113.80 |
| 22 | 23S1 | 2266 | A | C5-C6-N6 | 10.86 | 132.39 | 123.70 |
| 23 | 05S1 | 66 | A | N7-C8-N9 | -10.86 | 108.37 | 113.80 |
| 1 | 16S1 | 706 | A | N7-C8-N9 | -10.86 | 108.37 | 113.80 |
| 1 | 16S1 | 938 | A | N7-C8-N9 | -10.86 | 108.37 | 113.80 |
| 1 | 16S1 | 1492 | A | N7-C8-N9 | -10.86 | 108.37 | 113.80 |
| 22 | 23S1 | 2534 | A | N7-C8-N9 | -10.86 | 108.37 | 113.80 |
| 22 | 23S1 | 217 | A | N7-C8-N9 | -10.86 | 108.37 | 113.80 |
| 22 | 23S1 | 2883 | A | C5-C6-N6 | 10.86 | 132.38 | 123.70 |
| 1 | 16S1 | 415 | A | N3-C4-C5 | -10.86 | 119.20 | 126.80 |
| 22 | 23S1 | 1089 | A | C5-C6-N6 | 10.85 | 132.38 | 123.70 |
| 22 | 23S1 | 1505 | A | C5-C6-N6 | 10.85 | 132.38 | 123.70 |
| 1 | 16S1 | 143 | A | C5-C6-N6 | 10.85 | 132.38 | 123.70 |
| 1 | 16S1 | 579 | A | C5-C6-N6 | 10.85 | 132.38 | 123.70 |
| 22 | 23S1 | 2358 | A | N7-C8-N9 | -10.85 | 108.37 | 113.80 |
| 1 | 16S1 | 329 | A | N7-C8-N9 | -10.85 | 108.38 | 113.80 |
| 22 | 23S1 | 197 | A | C5-C6-N6 | 10.85 | 132.38 | 123.70 |
| 22 | 23S1 | 299 | A | N3-C4-C5 | -10.85 | 119.20 | 126.80 |
| 22 | 23S1 | 478 | A | C5-C6-N6 | 10.85 | 132.38 | 123.70 |
| 1 | 16S1 | 408 | A | N3-C4-C5 | -10.85 | 119.21 | 126.80 |
| 1 | 16S1 | 432 | A | C5-C6-N6 | 10.85 | 132.38 | 123.70 |
| 1 | 16S1 | 964 | A | N3-C4-C5 | -10.85 | 119.21 | 126.80 |
| 22 | 23S1 | 1098 | A | N7-C8-N9 | -10.85 | 108.38 | 113.80 |
| 22 | 23S1 | 2119 | A | C5-N7-C8 | 10.85 | 109.32 | 103.90 |
| 1 | 16S1 | 630 | A | C5-C6-N6 | 10.84 | 132.37 | 123.70 |
| 22 | 23S1 | 2749 | A | N7-C8-N9 | -10.84 | 108.38 | 113.80 |
| 22 | 23S1 | 2761 | A | C5-C6-N6 | 10.84 | 132.37 | 123.70 |
| 1 | 16S1 | 51 | A | C5-C6-N6 | 10.84 | 132.37 | 123.70 |
| 22 | 23S1 | 6 | A | N3-C4-C5 | -10.84 | 119.22 | 126.80 |
| 22 | 23S1 | 1759 | A | N7-C8-N9 | -10.84 | 108.38 | 113.80 |
| 22 | 23S1 | 190 | A | N3-C4-C5 | -10.84 | 119.22 | 126.80 |
| 1 | 16S1 | 695 | A | N3-C4-C5 | -10.83 | 119.22 | 126.80 |
| 1 | 16S1 | 1176 | A | C5-C6-N6 | 10.83 | 132.37 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 872 | A | N3-C4-C5 | -10.83 | 119.22 | 126.80 |
| 22 | 23S1 | 1787 | A | C5-C6-N6 | 10.83 | 132.37 | 123.70 |
| 1 | 16S1 | 55 | A | N3-C4-C5 | -10.83 | 119.22 | 126.80 |
| 1 | 16S1 | 621 | A | C5-C6-N6 | 10.83 | 132.36 | 123.70 |
| 22 | 23S1 | 1142 | A | N3-C4-C5 | -10.83 | 119.22 | 126.80 |
| 22 | 23S1 | 1802 | A | N7-C8-N9 | -10.83 | 108.39 | 113.80 |
| 22 | 23S1 | 2287 | A | N3-C4-C5 | -10.83 | 119.22 | 126.80 |
| 22 | 23S1 | 2369 | A | N3-C4-C5 | -10.83 | 119.22 | 126.80 |
| 22 | 23S1 | 825 | A | N3-C4-C5 | -10.83 | 119.22 | 126.80 |
| 1 | 16S1 | 270 | A | N3-C4-C5 | -10.83 | 119.22 | 126.80 |
| 22 | 23S1 | 1794 | A | C5-C6-N6 | 10.83 | 132.36 | 123.70 |
| 23 | 05S1 | 15 | A | C5-C6-N6 | 10.83 | 132.36 | 123.70 |
| 22 | 23S1 | 689 | A | N7-C8-N9 | -10.82 | 108.39 | 113.80 |
| 22 | 23S1 | 1759 | A | C5-C6-N6 | 10.82 | 132.36 | 123.70 |
| 22 | 23S1 | 1794 | A | N3-C4-C5 | -10.82 | 119.22 | 126.80 |
| 22 | 23S1 | 1998 | A | C5-C6-N6 | 10.82 | 132.36 | 123.70 |
| 1 | 16S1 | 1179 | A | N7-C8-N9 | -10.82 | 108.39 | 113.80 |
| 22 | 23S1 | 311 | A | C5-C6-N6 | 10.82 | 132.35 | 123.70 |
| 22 | 23S1 | 1593 | A | N7-C8-N9 | -10.82 | 108.39 | 113.80 |
| 22 | 23S1 | 1027 | A | N7-C8-N9 | -10.82 | 108.39 | 113.80 |
| 22 | 23S1 | 1262 | A | N7-C8-N9 | -10.82 | 108.39 | 113.80 |
| 22 | 23S1 | 2335 | A | C5-C6-N6 | 10.82 | 132.35 | 123.70 |
| 22 | 23S1 | 609 | A | C5-C6-N6 | 10.81 | 132.35 | 123.70 |
| 22 | 23S1 | 866 | A | C5-C6-N6 | 10.81 | 132.35 | 123.70 |
| 22 | 23S1 | 1301 | A | N3-C4-C5 | -10.81 | 119.23 | 126.80 |
| 22 | 23S1 | 1367 | A | C5-C6-N6 | 10.81 | 132.35 | 123.70 |
| 22 | 23S1 | 1477 | A | C5-C6-N6 | 10.81 | 132.35 | 123.70 |
| 22 | 23S1 | 1912 | A | C5-C6-N6 | 10.81 | 132.35 | 123.70 |
| 22 | 23S1 | 572 | A | C5-C6-N6 | 10.81 | 132.35 | 123.70 |
| 22 | 23S1 | 1773 | A | C5-C6-N6 | 10.81 | 132.35 | 123.70 |
| 55 | PTR1 | 59 | A | C5-C6-N6 | 10.81 | 132.35 | 123.70 |
| 1 | 16S1 | 607 | A | N7-C8-N9 | -10.80 | 108.40 | 113.80 |
| 1 | 16S1 | 878 | A | C5-C6-N6 | 10.80 | 132.34 | 123.70 |
| 22 | 23S1 | 244 | A | N7-C8-N9 | -10.80 | 108.40 | 113.80 |
| 22 | 23S1 | 849 | A | N3-C4-C5 | -10.80 | 119.24 | 126.80 |
| 22 | 23S1 | 1598 | A | C5-C6-N6 | 10.80 | 132.34 | 123.70 |
| 22 | 23S1 | 502 | A | N7-C8-N9 | -10.80 | 108.40 | 113.80 |
| 22 | 23S1 | 1246 | A | C5-C6-N6 | 10.80 | 132.34 | 123.70 |
| 1 | 16S1 | 246 | A | C5-C6-N6 | 10.80 | 132.34 | 123.70 |
| 22 | 23S1 | 309 | A | N7-C8-N9 | -10.80 | 108.40 | 113.80 |
| 22 | 23S1 | 1528 | A | N3-C4-C5 | -10.80 | 119.24 | 126.80 |
| 22 | 23S1 | 1553 | A | N7-C8-N9 | -10.80 | 108.40 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1230 | A | C5-C6-N6 | 10.80 | 132.34 | 123.70 |
| 1 | 16S1 | 595 | A | C5-C6-N6 | 10.79 | 132.34 | 123.70 |
| 1 | 16S1 | 573 | A | N3-C4-C5 | -10.79 | 119.25 | 126.80 |
| 22 | 23S1 | 447 | A | N7-C8-N9 | -10.79 | 108.40 | 113.80 |
| 22 | 23S1 | 988 | A | C5-C6-N6 | 10.79 | 132.33 | 123.70 |
| 22 | 23S1 | 1762 | A | N3-C4-C5 | -10.79 | 119.25 | 126.80 |
| 22 | 23S1 | 439 | A | N3-C4-C5 | -10.79 | 119.25 | 126.80 |
| 22 | 23S1 | 1960 | A | C5-C6-N6 | 10.79 | 132.33 | 123.70 |
| 1 | 16S1 | 630 | A | N7-C8-N9 | -10.79 | 108.41 | 113.80 |
| 22 | 23S1 | 972 | A | N3-C4-C5 | -10.79 | 119.25 | 126.80 |
| 22 | 23S1 | 1802 | A | N3-C4-C5 | -10.79 | 119.25 | 126.80 |
| 22 | 23S1 | 2547 | A | N7-C8-N9 | -10.79 | 108.41 | 113.80 |
| 1 | 16S1 | 1311 | A | C5-C6-N6 | 10.78 | 132.33 | 123.70 |
| 22 | 23S1 | 632 | A | N7-C8-N9 | -10.78 | 108.41 | 113.80 |
| 22 | 23S1 | 1142 | A | N7-C8-N9 | -10.78 | 108.41 | 113.80 |
| 22 | 23S1 | 2425 | A | C5-C6-N6 | 10.78 | 132.32 | 123.70 |
| 1 | 16S1 | 1363 | A | C5-C6-N6 | 10.78 | 132.32 | 123.70 |
| 22 | 23S1 | 1495 | A | C5-C6-N6 | 10.78 | 132.32 | 123.70 |
| 1 | 16S1 | 831 | A | C5-C6-N6 | 10.78 | 132.32 | 123.70 |
| 22 | 23S1 | 677 | A | N7-C8-N9 | -10.78 | 108.41 | 113.80 |
| 22 | 23S1 | 631 | A | N7-C8-N9 | -10.78 | 108.41 | 113.80 |
| 22 | 23S1 | 1353 | A | N7-C8-N9 | -10.78 | 108.41 | 113.80 |
| 22 | 23S1 | 1392 | A | C5-C6-N6 | 10.78 | 132.32 | 123.70 |
| 1 | 16S1 | 704 | A | N7-C8-N9 | -10.77 | 108.41 | 113.80 |
| 1 | 16S1 | 1513 | A | N7-C8-N9 | -10.77 | 108.41 | 113.80 |
| 22 | 23S1 | 28 | A | C5-C6-N6 | 10.77 | 132.31 | 123.70 |
| 1 | 16S1 | 8 | A | C5-C6-N6 | 10.77 | 132.31 | 123.70 |
| 1 | 16S1 | 1155 | A | N7-C8-N9 | -10.77 | 108.42 | 113.80 |
| 22 | 23S1 | 391 | A | C5-C6-N6 | 10.77 | 132.31 | 123.70 |
| 22 | 23S1 | 781 | A | N3-C4-C5 | -10.77 | 119.27 | 126.80 |
| 22 | 23S1 | 1672 | A | C5-C6-N6 | 10.77 | 132.31 | 123.70 |
| 22 | 23S1 | 2761 | A | N7-C8-N9 | -10.77 | 108.42 | 113.80 |
| 1 | 16S1 | 493 | A | C5-C6-N6 | 10.76 | 132.31 | 123.70 |
| 1 | 16S1 | 1254 | A | C5-C6-N6 | 10.76 | 132.31 | 123.70 |
| 22 | 23S1 | 609 | A | N7-C8-N9 | -10.76 | 108.42 | 113.80 |
| 1 | 16S1 | 77 | A | N3-C4-C5 | -10.76 | 119.27 | 126.80 |
| 22 | 23S1 | 2173 | A | N7-C8-N9 | -10.76 | 108.42 | 113.80 |
| 1 | 16S1 | 189 | A | N7-C8-N9 | -10.76 | 108.42 | 113.80 |
| 22 | 23S1 | 111 | A | C5-C6-N6 | 10.76 | 132.31 | 123.70 |
| 22 | 23S1 | 160 | A | N7-C8-N9 | -10.76 | 108.42 | 113.80 |
| 22 | 23S1 | 368 | A | N7-C8-N9 | -10.76 | 108.42 | 113.80 |
| 22 | 23S1 | 1635 | A | C5-C6-N6 | 10.76 | 132.31 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 2352 | A | C5-C6-N6 | 10.76 | 132.31 | 123.70 |
| 22 | 23S1 | 1070 | A | C5-C6-N6 | 10.76 | 132.31 | 123.70 |
| 1 | 16S1 | 673 | A | N7-C8-N9 | -10.76 | 108.42 | 113.80 |
| 1 | 16S1 | 1105 | A | C5-C6-N6 | 10.76 | 132.31 | 123.70 |
| 1 | 16S1 | 1269 | A | C5-C6-N6 | 10.76 | 132.31 | 123.70 |
| 1 | 16S1 | 1433 | A | N7-C8-N9 | -10.76 | 108.42 | 113.80 |
| 1 | 16S1 | 262 | A | N7-C8-N9 | -10.75 | 108.42 | 113.80 |
| 1 | 16S1 | 393 | A | C5-C6-N6 | 10.75 | 132.30 | 123.70 |
| 1 | 16S1 | 1350 | A | N3-C4-C5 | -10.75 | 119.27 | 126.80 |
| 22 | 23S1 | 1690 | A | C5-C6-N6 | 10.75 | 132.30 | 123.70 |
| 22 | 23S1 | 2778 | A | N7-C8-N9 | -10.75 | 108.42 | 113.80 |
| 1 | 16S1 | 313 | A | N7-C8-N9 | -10.75 | 108.42 | 113.80 |
| 1 | 16S1 | 325 | A | N7-C8-N9 | -10.75 | 108.42 | 113.80 |
| 22 | 23S1 | 478 | A | N3-C4-C5 | -10.75 | 119.28 | 126.80 |
| 22 | 23S1 | 2346 | A | C5-C6-N6 | 10.75 | 132.30 | 123.70 |
| 1 | 16S1 | 205 | A | C5-C6-N6 | 10.75 | 132.30 | 123.70 |
| 22 | 23S1 | 1677 | A | N7-C8-N9 | -10.75 | 108.43 | 113.80 |
| 1 | 16S1 | 487 | A | C5-C6-N6 | 10.75 | 132.30 | 123.70 |
| 22 | 23S1 | 928 | A | N3-C4-C5 | -10.75 | 119.28 | 126.80 |
| 22 | 23S1 | 1548 | A | N3-C4-C5 | -10.75 | 119.28 | 126.80 |
| 22 | 23S1 | 1746 | A | N3-C4-C5 | -10.75 | 119.28 | 126.80 |
| 1 | 16S1 | 676 | A | N7-C8-N9 | -10.74 | 108.43 | 113.80 |
| 22 | 23S1 | 282 | A | N7-C8-N9 | -10.74 | 108.43 | 113.80 |
| 22 | 23S1 | 751 | A | C5-C6-N6 | 10.74 | 132.29 | 123.70 |
| 22 | 23S1 | 1637 | A | N7-C8-N9 | -10.74 | 108.43 | 113.80 |
| 1 | 16S1 | 1016 | A | C5-C6-N6 | 10.74 | 132.29 | 123.70 |
| 23 | 05S1 | 101 | A | C5-C6-N1 | 10.74 | 123.07 | 117.70 |
| 1 | 16S1 | 456 | A | N7-C8-N9 | -10.74 | 108.43 | 113.80 |
| 1 | 16S1 | 59 | A | N3-C4-C5 | -10.74 | 119.28 | 126.80 |
| 22 | 23S1 | 1829 | A | N3-C4-C5 | -10.74 | 119.28 | 126.80 |
| 22 | 23S1 | 2288 | A | C5-C6-N6 | 10.74 | 132.29 | 123.70 |
| 1 | 16S1 | 19 | A | C5-C6-N6 | 10.73 | 132.29 | 123.70 |
| 22 | 23S1 | 391 | A | N3-C4-C5 | -10.73 | 119.29 | 126.80 |
| 22 | 23S1 | 980 | A | C5-C6-N6 | 10.73 | 132.29 | 123.70 |
| 22 | 23S1 | 1759 | A | N3-C4-C5 | -10.73 | 119.29 | 126.80 |
| 1 | 16S1 | 101 | A | N3-C4-C5 | -10.73 | 119.29 | 126.80 |
| 1 | 16S1 | 718 | A | N3-C4-C5 | -10.73 | 119.29 | 126.80 |
| 22 | 23S1 | 699 | A | C5-C6-N6 | 10.73 | 132.29 | 123.70 |
| 22 | 23S1 | 2377 | A | C5-C6-N6 | 10.73 | 132.28 | 123.70 |
| 1 | 16S1 | 629 | A | C5-C6-N6 | 10.73 | 132.28 | 123.70 |
| 22 | 23S1 | 981 | A | N7-C8-N9 | -10.73 | 108.44 | 113.80 |
| 22 | 23S1 | 2518 | A | C5-C6-N6 | 10.73 | 132.28 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 753 | A | C5-C6-N6 | 10.73 | 132.28 | 123.70 |
| 22 | 23S1 | 896 | A | N7-C8-N9 | -10.73 | 108.44 | 113.80 |
| 1 | 16S1 | 1507 | A | N7-C8-N9 | -10.72 | 108.44 | 113.80 |
| 1 | 16S1 | 1130 | A | N7-C8-N9 | -10.72 | 108.44 | 113.80 |
| 22 | 23S1 | 685 | A | C5-C6-N6 | 10.72 | 132.28 | 123.70 |
| 22 | 23S1 | 1722 | A | N7-C8-N9 | -10.72 | 108.44 | 113.80 |
| 22 | 23S1 | 2336 | A | N7-C8-N9 | -10.72 | 108.44 | 113.80 |
| 1 | 16S1 | 1117 | A | C5-C6-N6 | 10.72 | 132.28 | 123.70 |
| 22 | 23S1 | 368 | A | C5-C6-N6 | 10.72 | 132.28 | 123.70 |
| 22 | 23S1 | 670 | A | C5-C6-N6 | 10.72 | 132.28 | 123.70 |
| 1 | 16S1 | 1152 | A | N3-C4-C5 | -10.72 | 119.30 | 126.80 |
| 22 | 23S1 | 299 | A | C5-C6-N6 | 10.72 | 132.28 | 123.70 |
| 22 | 23S1 | 1274 | A | N7-C8-N9 | -10.72 | 108.44 | 113.80 |
| 22 | 23S1 | 1821 | A | N7-C8-N9 | -10.72 | 108.44 | 113.80 |
| 22 | 23S1 | 1858 | A | N3-C4-C5 | -10.72 | 119.30 | 126.80 |
| 1 | 16S1 | 1368 | A | N7-C8-N9 | -10.72 | 108.44 | 113.80 |
| 22 | 23S1 | 909 | A | C5-C6-N6 | 10.72 | 132.28 | 123.70 |
| 22 | 23S1 | 1515 | A | N7-C8-N9 | -10.72 | 108.44 | 113.80 |
| 22 | 23S1 | 2191 | A | N3-C4-C5 | -10.72 | 119.30 | 126.80 |
| 22 | 23S1 | 2600 | A | C5-C6-N6 | 10.72 | 132.28 | 123.70 |
| 22 | 23S1 | 2020 | A | C5-C6-N6 | 10.71 | 132.27 | 123.70 |
| 22 | 23S1 | 2513 | A | N3-C4-C5 | -10.71 | 119.30 | 126.80 |
| 1 | 16S1 | 482 | A | C5-C6-N6 | 10.71 | 132.27 | 123.70 |
| 1 | 16S1 | 1188 | A | C5-C6-N6 | 10.71 | 132.27 | 123.70 |
| 22 | 23S1 | 126 | A | N7-C8-N9 | -10.71 | 108.44 | 113.80 |
| 22 | 23S1 | 1809 | A | C5-C6-N6 | 10.71 | 132.27 | 123.70 |
| 1 | 16S1 | 356 | A | N3-C4-C5 | -10.71 | 119.30 | 126.80 |
| 22 | 23S1 | 526 | A | N7-C8-N9 | -10.71 | 108.44 | 113.80 |
| 22 | 23S1 | 2013 | A | C5-C6-N6 | 10.71 | 132.27 | 123.70 |
| 22 | 23S1 | 2412 | A | C5-C6-N6 | 10.71 | 132.27 | 123.70 |
| 1 | 16S1 | 371 | A | C5-C6-N6 | 10.71 | 132.27 | 123.70 |
| 1 | 16S1 | 119 | A | N7-C8-N9 | -10.71 | 108.45 | 113.80 |
| 1 | 16S1 | 780 | A | C5-C6-N6 | 10.71 | 132.27 | 123.70 |
| 1 | 16S1 | 1046 | A | N7-C8-N9 | -10.71 | 108.45 | 113.80 |
| 22 | 23S1 | 1286 | A | C5-C6-N6 | 10.71 | 132.26 | 123.70 |
| 1 | 16S1 | 109 | A | N7-C8-N9 | -10.71 | 108.45 | 113.80 |
| 1 | 16S1 | 1251 | A | C5-C6-N6 | 10.71 | 132.26 | 123.70 |
| 22 | 23S1 | 990 | A | C5-C6-N6 | 10.71 | 132.26 | 123.70 |
| 22 | 23S1 | 743 | A | N3-C4-C5 | -10.70 | 119.31 | 126.80 |
| 22 | 23S1 | 1009 | A | N3-C4-C5 | -10.70 | 119.31 | 126.80 |
| 22 | 23S1 | 2541 | A | N7-C8-N9 | -10.70 | 108.45 | 113.80 |
| 1 | 16S1 | 573 | A | N7-C8-N9 | -10.70 | 108.45 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 695 | A | C5-C6-N6 | 10.70 | 132.26 | 123.70 |
| 1 | 16S1 | 1171 | A | N7-C8-N9 | -10.70 | 108.45 | 113.80 |
| 22 | 23S1 | 309 | A | C5-C6-N6 | 10.70 | 132.26 | 123.70 |
| 22 | 23S1 | 2163 | A | N7-C8-N9 | -10.70 | 108.45 | 113.80 |
| 22 | 23S1 | 2352 | A | N3-C4-C5 | -10.70 | 119.31 | 126.80 |
| 23 | 05S1 | 57 | A | C5-C6-N6 | 10.70 | 132.26 | 123.70 |
| 22 | 23S1 | 730 | A | N3-C4-C5 | -10.70 | 119.31 | 126.80 |
| 22 | 23S1 | 1144 | A | N3-C4-C5 | -10.70 | 119.31 | 126.80 |
| 22 | 23S1 | 1698 | A | N7-C8-N9 | -10.70 | 108.45 | 113.80 |
| 1 | 16S1 | 223 | A | N3-C4-C5 | -10.70 | 119.31 | 126.80 |
| 22 | 23S1 | 1809 | A | N7-C8-N9 | -10.70 | 108.45 | 113.80 |
| 22 | 23S1 | 693 | A | N3-C4-C5 | -10.69 | 119.31 | 126.80 |
| 22 | 23S1 | 2309 | A | C5-C6-N6 | 10.69 | 132.25 | 123.70 |
| 1 | 16S1 | 1219 | A | N3-C4-C5 | -10.69 | 119.32 | 126.80 |
| 22 | 23S1 | 1610 | A | N7-C8-N9 | -10.69 | 108.45 | 113.80 |
| 22 | 23S1 | 1634 | A | N7-C8-N9 | -10.69 | 108.45 | 113.80 |
| 22 | 23S1 | 1746 | A | N7-C8-N9 | -10.69 | 108.45 | 113.80 |
| 22 | 23S1 | 1366 | A | C5-C6-N6 | 10.69 | 132.25 | 123.70 |
| 22 | 23S1 | 2882 | A | C5-C6-N6 | 10.69 | 132.25 | 123.70 |
| 1 | 16S1 | 753 | A | N7-C8-N9 | -10.69 | 108.46 | 113.80 |
| 22 | 23S1 | 2738 | A | C5-C6-N6 | 10.69 | 132.25 | 123.70 |
| 1 | 16S1 | 747 | A | C5-C6-N6 | 10.68 | 132.25 | 123.70 |
| 22 | 23S1 | 793 | A | N7-C8-N9 | -10.68 | 108.46 | 113.80 |
| 1 | 16S1 | 583 | A | N7-C8-N9 | -10.68 | 108.46 | 113.80 |
| 1 | 16S1 | 1157 | A | N3-C4-C5 | -10.68 | 119.32 | 126.80 |
| 1 | 16S1 | 172 | A | N7-C8-N9 | -10.68 | 108.46 | 113.80 |
| 22 | 23S1 | 910 | A | N3-C4-C5 | -10.68 | 119.33 | 126.80 |
| 1 | 16S1 | 366 | A | C5-C6-N6 | 10.68 | 132.24 | 123.70 |
| 22 | 23S1 | 1608 | A | C5-C6-N6 | 10.68 | 132.24 | 123.70 |
| 1 | 16S1 | 573 | A | C5-C6-N6 | 10.68 | 132.24 | 123.70 |
| 22 | 23S1 | 71 | A | C5-C6-N6 | 10.68 | 132.24 | 123.70 |
| 22 | 23S1 | 722 | A | N7-C8-N9 | -10.68 | 108.46 | 113.80 |
| 1 | 16S1 | 1196 | A | C5-C6-N6 | 10.67 | 132.24 | 123.70 |
| 23 | 05S1 | 58 | A | N3-C4-C5 | -10.67 | 119.33 | 126.80 |
| 22 | 23S1 | 1632 | A | N7-C8-N9 | -10.67 | 108.47 | 113.80 |
| 22 | 23S1 | 2199 | A | N3-C4-C5 | -10.67 | 119.33 | 126.80 |
| 22 | 23S1 | 2814 | A | N7-C8-N9 | -10.67 | 108.47 | 113.80 |
| 1 | 16S1 | 353 | A | C5-C6-N6 | 10.67 | 132.23 | 123.70 |
| 1 | 16S1 | 1012 | A | N7-C8-N9 | -10.67 | 108.47 | 113.80 |
| 1 | 16S1 | 1350 | A | C5-C6-N6 | 10.67 | 132.23 | 123.70 |
| 1 | 16S1 | 1360 | A | N3-C4-C5 | -10.67 | 119.33 | 126.80 |
| 22 | 23S1 | 13 | A | N3-C4-C5 | -10.67 | 119.33 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1287 | A | C5-C6-N6 | 10.67 | 132.23 | 123.70 |
| 22 | 23S1 | 1469 | A | N3-C4-C5 | -10.67 | 119.33 | 126.80 |
| 1 | 16S1 | 66 | A | C5-C6-N6 | 10.66 | 132.23 | 123.70 |
| 1 | 16S1 | 306 | A | C5-C6-N6 | 10.66 | 132.23 | 123.70 |
| 1 | 16S1 | 716 | A | N7-C8-N9 | -10.66 | 108.47 | 113.80 |
| 1 | 16S1 | 816 | A | N7-C8-N9 | -10.66 | 108.47 | 113.80 |
| 22 | 23S1 | 1302 | A | C5-C6-N6 | 10.66 | 132.23 | 123.70 |
| 22 | 23S1 | 1395 | A | N7-C8-N9 | -10.66 | 108.47 | 113.80 |
| 22 | 23S1 | 1632 | A | N3-C4-C5 | -10.66 | 119.33 | 126.80 |
| 1 | 16S1 | 325 | A | C5-C6-N6 | 10.66 | 132.23 | 123.70 |
| 1 | 16S1 | 1146 | A | N3-C4-C5 | -10.66 | 119.34 | 126.80 |
| 22 | 23S1 | 125 | A | C5-C6-N6 | 10.66 | 132.23 | 123.70 |
| 1 | 16S1 | 366 | A | N7-C8-N9 | -10.66 | 108.47 | 113.80 |
| 1 | 16S1 | 712 | A | N7-C8-N9 | -10.66 | 108.47 | 113.80 |
| 22 | 23S1 | 95 | A | N7-C8-N9 | -10.66 | 108.47 | 113.80 |
| 22 | 23S1 | 613 | A | N7-C8-N9 | -10.66 | 108.47 | 113.80 |
| 22 | 23S1 | 943 | A | N7-C8-N9 | -10.66 | 108.47 | 113.80 |
| 1 | 16S1 | 155 | A | N3-C4-C5 | -10.65 | 119.34 | 126.80 |
| 22 | 23S1 | 2665 | A | C5-C6-N6 | 10.65 | 132.22 | 123.70 |
| 1 | 16S1 | 192 | A | N7-C8-N9 | -10.65 | 108.47 | 113.80 |
| 1 | 16S1 | 978 | A | N7-C8-N9 | -10.65 | 108.47 | 113.80 |
| 1 | 16S1 | 1167 | A | C5-C6-N6 | 10.65 | 132.22 | 123.70 |
| 22 | 23S1 | 508 | A | N7-C8-N9 | -10.65 | 108.47 | 113.80 |
| 22 | 23S1 | 1900 | A | C5-C6-N6 | 10.65 | 132.22 | 123.70 |
| 1 | 16S1 | 253 | A | C5-C6-N6 | 10.65 | 132.22 | 123.70 |
| 1 | 16S1 | 382 | A | N3-C4-C5 | -10.65 | 119.35 | 126.80 |
| 1 | 16S1 | 648 | A | C5-C6-N6 | 10.65 | 132.22 | 123.70 |
| 22 | 23S1 | 300 | A | C5-C6-N6 | 10.65 | 132.22 | 123.70 |
| 1 | 16S1 | 787 | A | C5-C6-N6 | 10.64 | 132.21 | 123.70 |
| 22 | 23S1 | 1008 | A | N7-C8-N9 | -10.64 | 108.48 | 113.80 |
| 22 | 23S1 | 1403 | A | N3-C4-C5 | -10.64 | 119.35 | 126.80 |
| 1 | 16S1 | 465 | A | N7-C8-N9 | -10.64 | 108.48 | 113.80 |
| 22 | 23S1 | 1470 | A | N7-C8-N9 | -10.64 | 108.48 | 113.80 |
| 1 | 16S1 | 814 | A | N3-C4-C5 | -10.64 | 119.35 | 126.80 |
| 22 | 23S1 | 49 | A | N3-C4-C5 | -10.64 | 119.35 | 126.80 |
| 22 | 23S1 | 575 | A | C5-C6-N6 | 10.64 | 132.21 | 123.70 |
| 22 | 23S1 | 608 | A | N3-C4-C5 | -10.64 | 119.35 | 126.80 |
| 22 | 23S1 | 1089 | A | N7-C8-N9 | -10.64 | 108.48 | 113.80 |
| 22 | 23S1 | 1230 | A | N3-C4-C5 | -10.64 | 119.35 | 126.80 |
| 23 | 05S1 | 73 | A | C5-C6-N6 | 10.64 | 132.21 | 123.70 |
| 22 | 23S1 | 2169 | A | C5-C6-N6 | 10.63 | 132.21 | 123.70 |
| 22 | 23S1 | 2814 | A | C5-C6-N6 | 10.63 | 132.21 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 878 | A | N7-C8-N9 | -10.63 | 108.48 | 113.80 |
| 22 | 23S1 | 1665 | A | C5-C6-N6 | 10.63 | 132.21 | 123.70 |
| 22 | 23S1 | 415 | A | N3-C4-C5 | -10.63 | 119.36 | 126.80 |
| 22 | 23S1 | 1744 | A | N7-C8-N9 | -10.63 | 108.48 | 113.80 |
| 55 | PTR1 | 26 | A | C5-C6-N6 | 10.63 | 132.21 | 123.70 |
| 22 | 23S1 | 190 | A | N7-C8-N9 | -10.63 | 108.49 | 113.80 |
| 22 | 23S1 | 1142 | A | C5-C6-N6 | 10.63 | 132.20 | 123.70 |
| 1 | 16S1 | 1 | A | C5-C6-N6 | 10.63 | 132.20 | 123.70 |
| 22 | 23S1 | 1866 | A | N7-C8-N9 | -10.63 | 108.49 | 113.80 |
| 23 | 05S1 | 58 | A | N7-C8-N9 | -10.63 | 108.49 | 113.80 |
| 22 | 23S1 | 1321 | A | C5-C6-N6 | 10.63 | 132.20 | 123.70 |
| 22 | 23S1 | 2376 | A | C5-C6-N6 | 10.63 | 132.20 | 123.70 |
| 22 | 23S1 | 2448 | A | N7-C8-N9 | -10.62 | 108.49 | 113.80 |
| 1 | 16S1 | 430 | A | N7-C8-N9 | -10.62 | 108.49 | 113.80 |
| 22 | 23S1 | 217 | A | C5-C6-N6 | 10.62 | 132.20 | 123.70 |
| 22 | 23S1 | 453 | A | N7-C8-N9 | -10.62 | 108.49 | 113.80 |
| 22 | 23S1 | 2868 | A | N3-C4-C5 | -10.62 | 119.36 | 126.80 |
| 23 | 05S1 | 99 | A | N3-C4-C5 | -10.62 | 119.36 | 126.80 |
| 22 | 23S1 | 382 | A | N3-C4-C5 | -10.62 | 119.37 | 126.80 |
| 22 | 23S1 | 2600 | A | N7-C8-N9 | -10.62 | 108.49 | 113.80 |
| 22 | 23S1 | 1127 | A | C5-C6-N6 | 10.62 | 132.19 | 123.70 |
| 22 | 23S1 | 2241 | A | C5-C6-N6 | 10.62 | 132.19 | 123.70 |
| 1 | 16S1 | 167 | A | C5-C6-N6 | 10.61 | 132.19 | 123.70 |
| 1 | 16S1 | 1044 | A | N3-C4-C5 | -10.61 | 119.37 | 126.80 |
| 22 | 23S1 | 514 | A | C5-C6-N6 | 10.61 | 132.19 | 123.70 |
| 1 | 16S1 | 860 | A | N7-C8-N9 | -10.61 | 108.50 | 113.80 |
| 22 | 23S1 | 829 | A | C5-C6-N6 | 10.61 | 132.18 | 123.70 |
| 22 | 23S1 | 1050 | A | C5-C6-N6 | 10.61 | 132.19 | 123.70 |
| 22 | 23S1 | 1918 | A | N3-C4-C5 | -10.61 | 119.38 | 126.80 |
| 1 | 16S1 | 315 | A | C5-C6-N6 | 10.60 | 132.18 | 123.70 |
| 22 | 23S1 | 480 | A | C5-C6-N6 | 10.60 | 132.18 | 123.70 |
| 1 | 16S1 | 109 | A | C5-C6-N6 | 10.60 | 132.18 | 123.70 |
| 22 | 23S1 | 21 | A | N3-C4-C5 | -10.60 | 119.38 | 126.80 |
| 22 | 23S1 | 877 | A | N7-C8-N9 | -10.60 | 108.50 | 113.80 |
| 22 | 23S1 | 1213 | A | N3-C4-C5 | -10.60 | 119.38 | 126.80 |
| 22 | 23S1 | 1551 | A | N3-C4-C5 | -10.60 | 119.38 | 126.80 |
| 22 | 23S1 | 2071 | A | N7-C8-N9 | -10.60 | 108.50 | 113.80 |
| 1 | 16S1 | 1080 | A | C5-C6-N6 | 10.60 | 132.18 | 123.70 |
| 22 | 23S1 | 1189 | A | N3-C4-C5 | -10.60 | 119.38 | 126.80 |
| 22 | 23S1 | 1551 | A | C5-C6-N6 | 10.60 | 132.18 | 123.70 |
| 22 | 23S1 | 1616 | A | C5-C6-N6 | 10.60 | 132.18 | 123.70 |
| 22 | 23S1 | 1654 | A | N7-C8-N9 | -10.60 | 108.50 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 996 | A | C5-C6-N6 | 10.60 | 132.18 | 123.70 |
| 22 | 23S1 | 899 | A | N7-C8-N9 | -10.60 | 108.50 | 113.80 |
| 1 | 16S1 | 1492 | A | C5-C6-N6 | 10.59 | 132.17 | 123.70 |
| 1 | 16S1 | 1531 | A | C5-C6-N6 | 10.59 | 132.17 | 123.70 |
| 22 | 23S1 | 529 | A | N7-C8-N9 | -10.59 | 108.50 | 113.80 |
| 22 | 23S1 | 1819 | A | C5-C6-N6 | 10.59 | 132.17 | 123.70 |
| 22 | 23S1 | 2077 | A | N7-C8-N9 | -10.59 | 108.51 | 113.80 |
| 1 | 16S1 | 949 | A | C5-C6-N6 | 10.59 | 132.17 | 123.70 |
| 1 | 16S1 | 1111 | A | C5-C6-N6 | 10.59 | 132.17 | 123.70 |
| 22 | 23S1 | 74 | A | N3-C4-C5 | -10.59 | 119.39 | 126.80 |
| 22 | 23S1 | 1009 | A | N7-C8-N9 | -10.59 | 108.51 | 113.80 |
| 22 | 23S1 | 1020 | A | C5-C6-N6 | 10.59 | 132.17 | 123.70 |
| 22 | 23S1 | 1549 | A | C5-C6-N6 | 10.58 | 132.17 | 123.70 |
| 22 | 23S1 | 2054 | A | N3-C4-C5 | -10.58 | 119.39 | 126.80 |
| 22 | 23S1 | 820 | A | N3-C4-C5 | -10.58 | 119.39 | 126.80 |
| 22 | 23S1 | 347 | A | N3-C4-C5 | -10.58 | 119.39 | 126.80 |
| 22 | 23S1 | 849 | A | N7-C8-N9 | -10.58 | 108.51 | 113.80 |
| 22 | 23S1 | 1067 | A | C5-C6-N6 | 10.58 | 132.16 | 123.70 |
| 1 | 16S1 | 640 | A | C5-C6-N6 | 10.58 | 132.16 | 123.70 |
| 22 | 23S1 | 203 | A | C5-C6-N6 | 10.58 | 132.16 | 123.70 |
| 22 | 23S1 | 309 | A | N3-C4-C5 | -10.58 | 119.39 | 126.80 |
| 22 | 23S1 | 401 | A | C5-C6-N6 | 10.58 | 132.16 | 123.70 |
| 22 | 23S1 | 1029 | A | N3-C4-C5 | -10.58 | 119.39 | 126.80 |
| 1 | 16S1 | 149 | A | N7-C8-N9 | -10.57 | 108.51 | 113.80 |
| 1 | 16S1 | 681 | A | C5-C6-N6 | 10.57 | 132.16 | 123.70 |
| 22 | 23S1 | 2860 | A | N7-C8-N9 | -10.57 | 108.51 | 113.80 |
| 23 | 05S1 | 99 | A | N7-C8-N9 | -10.57 | 108.51 | 113.80 |
| 1 | 16S1 | 1324 | A | N3-C4-C5 | -10.57 | 119.40 | 126.80 |
| 1 | 16S1 | 539 | A | N7-C8-N9 | -10.57 | 108.52 | 113.80 |
| 22 | 23S1 | 415 | A | N7-C8-N9 | -10.57 | 108.52 | 113.80 |
| 1 | 16S1 | 1197 | A | C5-C6-N6 | 10.57 | 132.16 | 123.70 |
| 22 | 23S1 | 1000 | A | N3-C4-C5 | -10.57 | 119.40 | 126.80 |
| 23 | 05S1 | 104 | A | C5-C6-N6 | 10.57 | 132.16 | 123.70 |
| 1 | 16S1 | 509 | A | N3-C4-C5 | -10.57 | 119.40 | 126.80 |
| 22 | 23S1 | 13 | A | N7-C8-N9 | -10.57 | 108.52 | 113.80 |
| 22 | 23S1 | 71 | A | N3-C4-C5 | -10.57 | 119.40 | 126.80 |
| 22 | 23S1 | 1598 | A | N7-C8-N9 | -10.57 | 108.52 | 113.80 |
| 1 | 16S1 | 1476 | A | N3-C4-C5 | -10.56 | 119.41 | 126.80 |
| 22 | 23S1 | 789 | A | C5-C6-N6 | 10.56 | 132.15 | 123.70 |
| 22 | 23S1 | 1819 | A | N3-C4-C5 | -10.56 | 119.41 | 126.80 |
| 22 | 23S1 | 1889 | A | C5-C6-N6 | 10.56 | 132.15 | 123.70 |
| 22 | 23S1 | 2108 | A | N3-C4-C5 | -10.56 | 119.41 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 2654 | A | C5-C6-N6 | 10.56 | 132.15 | 123.70 |
| 22 | 23S1 | 2727 | A | N3-C4-C5 | -10.56 | 119.41 | 126.80 |
| 1 | 16S1 | 648 | A | N3-C4-C5 | -10.56 | 119.41 | 126.80 |
| 22 | 23S1 | 1641 | A | N7-C8-N9 | -10.56 | 108.52 | 113.80 |
| 22 | 23S1 | 1876 | A | C5-C6-N6 | 10.56 | 132.15 | 123.70 |
| 22 | 23S1 | 2080 | A | N3-C4-C5 | -10.56 | 119.41 | 126.80 |
| 22 | 23S1 | 2478 | A | C5-C6-N6 | 10.56 | 132.15 | 123.70 |
| 22 | 23S1 | 590 | A | N7-C8-N9 | -10.56 | 108.52 | 113.80 |
| 1 | 16S1 | 715 | A | C5-C6-N6 | 10.55 | 132.14 | 123.70 |
| 1 | 16S1 | 1269 | A | N3-C4-C5 | -10.55 | 119.41 | 126.80 |
| 22 | 23S1 | 191 | A | N7-C8-N9 | -10.55 | 108.52 | 113.80 |
| 22 | 23S1 | 1664 | A | C5-C6-N6 | 10.55 | 132.14 | 123.70 |
| 22 | 23S1 | 2366 | A | C5-C6-N6 | 10.56 | 132.15 | 123.70 |
| 22 | 23S1 | 1713 | A | C5-C6-N6 | 10.55 | 132.14 | 123.70 |
| 1 | 16S1 | 608 | A | N7-C8-N9 | -10.55 | 108.52 | 113.80 |
| 1 | 16S1 | 792 | A | C5-C6-N6 | 10.55 | 132.14 | 123.70 |
| 22 | 23S1 | 1247 | A | C5-C6-N6 | 10.55 | 132.14 | 123.70 |
| 22 | 23S1 | 1901 | A | N3-C4-C5 | -10.55 | 119.41 | 126.80 |
| 1 | 16S1 | 918 | A | N7-C8-N9 | -10.55 | 108.53 | 113.80 |
| 22 | 23S1 | 482 | A | N3-C4-C5 | -10.55 | 119.42 | 126.80 |
| 1 | 16S1 | 1092 | A | N7-C8-N9 | -10.55 | 108.53 | 113.80 |
| 22 | 23S1 | 1264 | A | N7-C8-N9 | -10.55 | 108.53 | 113.80 |
| 22 | 23S1 | 1535 | A | N3-C4-C5 | -10.55 | 119.42 | 126.80 |
| 1 | 16S1 | 182 | A | C5-C6-N6 | 10.55 | 132.14 | 123.70 |
| 1 | 16S1 | 448 | A | C5-C6-N6 | 10.55 | 132.14 | 123.70 |
| 22 | 23S1 | 244 | A | N3-C4-C5 | -10.54 | 119.42 | 126.80 |
| 22 | 23S1 | 1877 | A | N3-C4-C5 | -10.54 | 119.42 | 126.80 |
| 22 | 23S1 | 470 | A | N7-C8-N9 | -10.54 | 108.53 | 113.80 |
| 22 | 23S1 | 1749 | A | N3-C4-C5 | -10.54 | 119.42 | 126.80 |
| 1 | 16S1 | 228 | A | C5-C6-N6 | 10.54 | 132.13 | 123.70 |
| 1 | 16S1 | 640 | A | N3-C4-C5 | -10.54 | 119.42 | 126.80 |
| 22 | 23S1 | 959 | A | N3-C4-C5 | -10.54 | 119.42 | 126.80 |
| 22 | 23S1 | 1175 | A | N7-C8-N9 | -10.54 | 108.53 | 113.80 |
| 22 | 23S1 | 2809 | A | C5-C6-N6 | 10.54 | 132.13 | 123.70 |
| 23 | 05S1 | 52 | A | C5-C6-N6 | 10.54 | 132.13 | 123.70 |
| 1 | 16S1 | 1257 | A | C5-C6-N6 | 10.54 | 132.13 | 123.70 |
| 22 | 23S1 | 181 | A | N3-C4-C5 | -10.54 | 119.42 | 126.80 |
| 1 | 16S1 | 1508 | A | C5-C6-N6 | 10.54 | 132.13 | 123.70 |
| 22 | 23S1 | 1877 | A | C5-C6-N6 | 10.54 | 132.13 | 123.70 |
| 1 | 16S1 | 263 | A | N7-C8-N9 | -10.53 | 108.53 | 113.80 |
| 1 | 16S1 | 642 | A | C5-C6-N6 | 10.53 | 132.12 | 123.70 |
| 22 | 23S1 | 833 | A | C5-C6-N6 | 10.53 | 132.13 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 2482 | A | N7-C8-N9 | -10.53 | 108.53 | 113.80 |
| 1 | 16S1 | 1254 | A | N7-C8-N9 | -10.53 | 108.53 | 113.80 |
| 22 | 23S1 | 2003 | A | C5-C6-N6 | 10.53 | 132.12 | 123.70 |
| 1 | 16S1 | 496 | A | C5-C6-N6 | 10.53 | 132.12 | 123.70 |
| 22 | 23S1 | 244 | A | C5-C6-N6 | 10.53 | 132.12 | 123.70 |
| 22 | 23S1 | 753 | A | N3-C4-C5 | -10.53 | 119.43 | 126.80 |
| 22 | 23S1 | 1608 | A | N3-C4-C5 | -10.53 | 119.43 | 126.80 |
| 22 | 23S1 | 2432 | A | C5-C6-N6 | 10.53 | 132.12 | 123.70 |
| 22 | 23S1 | 64 | A | C5-C6-N6 | 10.53 | 132.12 | 123.70 |
| 22 | 23S1 | 654 | A | C5-C6-N6 | 10.53 | 132.12 | 123.70 |
| 22 | 23S1 | 1269 | A | N3-C4-C5 | -10.53 | 119.43 | 126.80 |
| 22 | 23S1 | 1927 | A | N3-C4-C5 | -10.53 | 119.43 | 126.80 |
| 23 | 05S1 | 39 | A | C5-C6-N6 | 10.53 | 132.12 | 123.70 |
| 1 | 16S1 | 918 | A | N3-C4-C5 | -10.52 | 119.43 | 126.80 |
| 22 | 23S1 | 2090 | A | N3-C4-C5 | -10.52 | 119.43 | 126.80 |
| 1 | 16S1 | 642 | A | N3-C4-C5 | -10.52 | 119.44 | 126.80 |
| 1 | 16S1 | 938 | A | N3-C4-C5 | -10.52 | 119.43 | 126.80 |
| 22 | 23S1 | 621 | A | N7-C8-N9 | -10.52 | 108.54 | 113.80 |
| 22 | 23S1 | 2266 | A | N3-C4-C5 | -10.52 | 119.44 | 126.80 |
| 22 | 23S1 | 2381 | A | C5-C6-N6 | 10.52 | 132.12 | 123.70 |
| 1 | 16S1 | 325 | A | N3-C4-C5 | -10.52 | 119.44 | 126.80 |
| 1 | 16S1 | 629 | A | N7-C8-N9 | -10.52 | 108.54 | 113.80 |
| 22 | 23S1 | 1754 | A | N7-C8-N9 | -10.52 | 108.54 | 113.80 |
| 1 | 16S1 | 908 | A | C5-C6-N6 | 10.52 | 132.11 | 123.70 |
| 1 | 16S1 | 28 | A | C5-C6-N6 | 10.52 | 132.11 | 123.70 |
| 22 | 23S1 | 160 | A | N3-C4-C5 | -10.52 | 119.44 | 126.80 |
| 23 | 05S1 | 119 | A | N3-C4-C5 | -10.51 | 119.44 | 126.80 |
| 22 | 23S1 | 42 | A | C5-C6-N6 | 10.51 | 132.11 | 123.70 |
| 22 | 23S1 | 909 | A | N7-C8-N9 | -10.51 | 108.54 | 113.80 |
| 22 | 23S1 | 943 | A | C5-C6-N6 | 10.51 | 132.11 | 123.70 |
| 1 | 16S1 | 139 | A | C5-C6-N6 | 10.51 | 132.10 | 123.70 |
| 22 | 23S1 | 666 | A | C5-C6-N6 | 10.51 | 132.11 | 123.70 |
| 22 | 23S1 | 845 | A | N7-C8-N9 | -10.51 | 108.55 | 113.80 |
| 1 | 16S1 | 1410 | A | C5-C6-N6 | 10.51 | 132.10 | 123.70 |
| 22 | 23S1 | 1276 | A | N3-C4-C5 | -10.51 | 119.45 | 126.80 |
| 22 | 23S1 | 2821 | A | C5-C6-N6 | 10.51 | 132.10 | 123.70 |
| 1 | 16S1 | 195 | A | C5-C6-N6 | 10.50 | 132.10 | 123.70 |
| 22 | 23S1 | 1938 | A | C5-C6-N6 | 10.50 | 132.10 | 123.70 |
| 22 | 23S1 | 2058 | A | N7-C8-N9 | -10.50 | 108.55 | 113.80 |
| 22 | 23S1 | 2298 | A | C5-C6-N6 | 10.50 | 132.10 | 123.70 |
| 1 | 16S1 | 373 | A | N3-C4-C5 | -10.50 | 119.45 | 126.80 |
| 22 | 23S1 | 2670 | A | N3-C4-C5 | -10.50 | 119.45 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 432 | A | N3-C4-C5 | -10.50 | 119.45 | 126.80 |
| 1 | 16S1 | 1441 | A | C5-C6-N6 | 10.50 | 132.10 | 123.70 |
| 22 | 23S1 | 975 | A | C5-C6-N6 | 10.50 | 132.10 | 123.70 |
| 22 | 23S1 | 2199 | A | C5-C6-N6 | 10.50 | 132.10 | 123.70 |
| 22 | 23S1 | 2727 | A | C5-C6-N6 | 10.50 | 132.10 | 123.70 |
| 1 | 16S1 | 10 | A | C5-C6-N6 | 10.49 | 132.10 | 123.70 |
| 1 | 16S1 | 181 | A | N3-C4-C5 | -10.49 | 119.45 | 126.80 |
| 1 | 16S1 | 1437 | A | C5-C6-N6 | 10.49 | 132.10 | 123.70 |
| 1 | 16S1 | 1191 | A | C5-C6-N6 | 10.49 | 132.09 | 123.70 |
| 22 | 23S1 | 983 | A | N7-C8-N9 | -10.49 | 108.55 | 113.80 |
| 22 | 23S1 | 1265 | A | N3-C4-C5 | -10.49 | 119.45 | 126.80 |
| 22 | 23S1 | 616 | A | C5-C6-N6 | 10.49 | 132.09 | 123.70 |
| 22 | 23S1 | 1111 | A | C5-C6-N6 | 10.49 | 132.09 | 123.70 |
| 22 | 23S1 | 1571 | A | N3-C4-C5 | -10.49 | 119.46 | 126.80 |
| 22 | 23S1 | 1596 | A | C5-C6-N6 | 10.49 | 132.09 | 123.70 |
| 22 | 23S1 | 1854 | A | N3-C4-C5 | -10.49 | 119.46 | 126.80 |
| 22 | 23S1 | 2327 | A | N3-C4-C5 | -10.49 | 119.46 | 126.80 |
| 22 | 23S1 | 127 | A | N7-C8-N9 | -10.49 | 108.56 | 113.80 |
| 22 | 23S1 | 503 | A | N7-C8-N9 | -10.49 | 108.56 | 113.80 |
| 23 | 05S1 | 94 | A | N7-C8-N9 | -10.49 | 108.56 | 113.80 |
| 22 | 23S1 | 1321 | A | N3-C4-C5 | -10.48 | 119.46 | 126.80 |
| 22 | 23S1 | 1373 | A | N7-C8-N9 | -10.48 | 108.56 | 113.80 |
| 55 | PTR1 | 42 | A | C5-C6-N6 | 10.48 | 132.09 | 123.70 |
| 1 | 16S1 | 946 | A | C5-C6-N6 | 10.48 | 132.09 | 123.70 |
| 22 | 23S1 | 2052 | A | C5-C6-N6 | 10.48 | 132.09 | 123.70 |
| 22 | 23S1 | 699 | A | N7-C8-N9 | -10.48 | 108.56 | 113.80 |
| 1 | 16S1 | 1170 | A | C4-C5-C6 | 10.48 | 122.24 | 117.00 |
| 22 | 23S1 | 2077 | A | N3-C4-C5 | -10.48 | 119.47 | 126.80 |
| 22 | 23S1 | 2740 | A | N3-C4-C5 | -10.48 | 119.47 | 126.80 |
| 1 | 16S1 | 865 | A | C5-C6-N6 | 10.47 | 132.08 | 123.70 |
| 1 | 16S1 | 520 | A | N3-C4-C5 | -10.47 | 119.47 | 126.80 |
| 22 | 23S1 | 1722 | A | N3-C4-C5 | -10.47 | 119.47 | 126.80 |
| 22 | 23S1 | 2042 | A | C5-C6-N6 | 10.47 | 132.08 | 123.70 |
| 22 | 23S1 | 514 | A | N7-C8-N9 | -10.47 | 108.56 | 113.80 |
| 22 | 23S1 | 1067 | A | N7-C8-N9 | -10.47 | 108.57 | 113.80 |
| 1 | 16S1 | 958 | A | C5-C6-N6 | 10.47 | 132.07 | 123.70 |
| 22 | 23S1 | 582 | A | N3-C4-C5 | -10.47 | 119.47 | 126.80 |
| 1 | 16S1 | 1081 | A | N3-C4-C5 | -10.46 | 119.47 | 126.80 |
| 22 | 23S1 | 2154 | A | N3-C4-C5 | -10.46 | 119.47 | 126.80 |
| 22 | 23S1 | 2333 | A | C5-C6-N6 | 10.46 | 132.07 | 123.70 |
| 22 | 23S1 | 2748 | A | C5-C6-N6 | 10.46 | 132.07 | 123.70 |
| 1 | 16S1 | 784 | A | C5-C6-N6 | 10.46 | 132.07 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 298 | A | C5-C6-N6 | 10.46 | 132.07 | 123.70 |
| 22 | 23S1 | 514 | A | N3-C4-C5 | -10.46 | 119.48 | 126.80 |
| 1 | 16S1 | 487 | A | N3-C4-C5 | -10.46 | 119.48 | 126.80 |
| 22 | 23S1 | 2679 | A | N3-C4-C5 | -10.46 | 119.48 | 126.80 |
| 22 | 23S1 | 255 | A | N7-C8-N9 | -10.46 | 108.57 | 113.80 |
| 22 | 23S1 | 342 | A | N3-C4-C5 | -10.46 | 119.48 | 126.80 |
| 22 | 23S1 | 1609 | A | C5-C6-N6 | 10.46 | 132.06 | 123.70 |
| 22 | 23S1 | 2513 | A | N7-C8-N9 | -10.46 | 108.57 | 113.80 |
| 23 | 05S1 | 78 | A | C5-C6-N6 | 10.45 | 132.06 | 123.70 |
| 22 | 23S1 | 404 | A | N7-C8-N9 | -10.45 | 108.58 | 113.80 |
| 22 | 23S1 | 1665 | A | N3-C4-C5 | -10.45 | 119.49 | 126.80 |
| 22 | 23S1 | 1912 | A | N3-C4-C5 | -10.45 | 119.49 | 126.80 |
| 1 | 16S1 | 282 | A | N7-C8-N9 | -10.45 | 108.58 | 113.80 |
| 1 | 16S1 | 728 | A | N7-C8-N9 | -10.45 | 108.58 | 113.80 |
| 22 | 23S1 | 1260 | A | N7-C8-N9 | -10.45 | 108.58 | 113.80 |
| 1 | 16S1 | 344 | A | C5-C6-N6 | 10.44 | 132.05 | 123.70 |
| 1 | 16S1 | 602 | A | C5-C6-N6 | 10.44 | 132.05 | 123.70 |
| 22 | 23S1 | 191 | A | N3-C4-C5 | -10.44 | 119.49 | 126.80 |
| 22 | 23S1 | 1810 | A | N1-C6-N6 | -10.44 | 112.33 | 118.60 |
| 1 | 16S1 | 968 | A | C5-C6-N6 | 10.44 | 132.05 | 123.70 |
| 1 | 16S1 | 466 | A | C5-C6-N6 | 10.44 | 132.05 | 123.70 |
| 1 | 16S1 | 532 | A | C5-C6-N6 | 10.44 | 132.05 | 123.70 |
| 22 | 23S1 | 2082 | A | N3-C4-C5 | -10.44 | 119.49 | 126.80 |
| 1 | 16S1 | 338 | A | C5-C6-N6 | 10.44 | 132.05 | 123.70 |
| 1 | 16S1 | 864 | A | C5-C6-N6 | 10.44 | 132.05 | 123.70 |
| 1 | 16S1 | 1465 | A | C5-C6-N6 | 10.44 | 132.05 | 123.70 |
| 22 | 23S1 | 1427 | A | N7-C8-N9 | -10.44 | 108.58 | 113.80 |
| 55 | PTR1 | 3 | A | C5-C6-N6 | 10.44 | 132.05 | 123.70 |
| 1 | 16S1 | 71 | A | C5-C6-N6 | 10.43 | 132.04 | 123.70 |
| 22 | 23S1 | 95 | A | C5-C6-N6 | 10.43 | 132.05 | 123.70 |
| 22 | 23S1 | 374 | A | C5-C6-N6 | 10.43 | 132.05 | 123.70 |
| 22 | 23S1 | 472 | A | N7-C8-N9 | -10.43 | 108.58 | 113.80 |
| 22 | 23S1 | 1307 | A | N3-C4-C5 | -10.43 | 119.50 | 126.80 |
| 23 | 05S1 | 58 | A | C5-C6-N6 | 10.43 | 132.05 | 123.70 |
| 1 | 16S1 | 860 | A | N3-C4-C5 | -10.43 | 119.50 | 126.80 |
| 22 | 23S1 | 104 | A | N3-C4-C5 | -10.43 | 119.50 | 126.80 |
| 22 | 23S1 | 21 | A | C5-C6-N6 | 10.43 | 132.04 | 123.70 |
| 22 | 23S1 | 2639 | A | N7-C8-N9 | -10.43 | 108.59 | 113.80 |
| 22 | 23S1 | 5 | A | C5-C6-N6 | 10.43 | 132.04 | 123.70 |
| 22 | 23S1 | 6 | A | N7-C8-N9 | -10.43 | 108.59 | 113.80 |
| 22 | 23S1 | 142 | A | N3-C4-C5 | -10.43 | 119.50 | 126.80 |
| 22 | 23S1 | 219 | A | N3-C4-C5 | -10.43 | 119.50 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 55 | PTR1 | 76 | A | C5-C6-N6 | 10.43 | 132.04 | 123.70 |
| 1 | 16S1 | 958 | A | N3-C4-C5 | -10.42 | 119.50 | 126.80 |
| 1 | 16S1 | 1410 | A | N3-C4-C5 | -10.42 | 119.50 | 126.80 |
| 22 | 23S1 | 739 | A | C5-C6-N6 | 10.42 | 132.04 | 123.70 |
| 1 | 16S1 | 907 | A | N3-C4-C5 | -10.42 | 119.50 | 126.80 |
| 1 | 16S1 | 1000 | A | N3-C4-C5 | -10.42 | 119.50 | 126.80 |
| 22 | 23S1 | 167 | A | C5-C6-N6 | 10.42 | 132.04 | 123.70 |
| 1 | 16S1 | 1252 | A | N3-C4-C5 | -10.42 | 119.51 | 126.80 |
| 1 | 16S1 | 1534 | A | C5-C6-N6 | 10.42 | 132.03 | 123.70 |
| 22 | 23S1 | 1689 | A | N3-C4-C5 | -10.42 | 119.51 | 126.80 |
| 22 | 23S1 | 2059 | A | N7-C8-N9 | -10.42 | 108.59 | 113.80 |
| 22 | 23S1 | 742 | A | N3-C4-C5 | -10.42 | 119.51 | 126.80 |
| 22 | 23S1 | 1927 | A | N7-C8-N9 | -10.42 | 108.59 | 113.80 |
| 22 | 23S1 | 2634 | A | N3-C4-C5 | -10.42 | 119.51 | 126.80 |
| 1 | 16S1 | 205 | A | N7-C8-N9 | -10.41 | 108.59 | 113.80 |
| 1 | 16S1 | 546 | A | C5-C6-N6 | 10.41 | 132.03 | 123.70 |
| 22 | 23S1 | 1749 | A | C5-C6-N6 | 10.41 | 132.03 | 123.70 |
| 22 | 23S1 | 2051 | A | C5-C6-N6 | 10.41 | 132.03 | 123.70 |
| 22 | 23S1 | 2097 | A | N3-C4-C5 | -10.41 | 119.51 | 126.80 |
| 22 | 23S1 | 2378 | A | C5-C6-N6 | 10.41 | 132.03 | 123.70 |
| 22 | 23S1 | 2482 | A | C5-C6-N6 | 10.41 | 132.03 | 123.70 |
| 22 | 23S1 | 2879 | A | N7-C8-N9 | -10.41 | 108.59 | 113.80 |
| 1 | 16S1 | 1046 | A | C5-C6-N6 | 10.41 | 132.03 | 123.70 |
| 22 | 23S1 | 429 | A | N7-C8-N9 | -10.41 | 108.59 | 113.80 |
| 1 | 16S1 | 579 | A | N3-C4-C5 | -10.41 | 119.51 | 126.80 |
| 22 | 23S1 | 1073 | A | N3-C4-C5 | -10.41 | 119.51 | 126.80 |
| 22 | 23S1 | 131 | A | N7-C8-N9 | -10.40 | 108.60 | 113.80 |
| 22 | 23S1 | 1111 | A | N3-C4-C5 | -10.40 | 119.52 | 126.80 |
| 22 | 23S1 | 1590 | A | N7-C8-N9 | -10.40 | 108.60 | 113.80 |
| 22 | 23S1 | 1773 | A | N3-C4-C5 | -10.40 | 119.52 | 126.80 |
| 1 | 16S1 | 223 | A | C5-C6-N6 | 10.40 | 132.02 | 123.70 |
| 1 | 16S1 | 130 | A | C5-C6-N6 | 10.40 | 132.02 | 123.70 |
| 22 | 23S1 | 2284 | A | C5-C6-N6 | 10.40 | 132.02 | 123.70 |
| 1 | 16S1 | 1151 | A | N3-C4-C5 | -10.40 | 119.52 | 126.80 |
| 1 | 16S1 | 1176 | A | N3-C4-C5 | -10.40 | 119.52 | 126.80 |
| 22 | 23S1 | 197 | A | N3-C4-C5 | -10.40 | 119.52 | 126.80 |
| 22 | 23S1 | 1301 | A | N7-C8-N9 | -10.40 | 108.60 | 113.80 |
| 22 | 23S1 | 172 | A | N3-C4-C5 | -10.40 | 119.52 | 126.80 |
| 22 | 23S1 | 979 | A | C5-C6-N6 | 10.40 | 132.02 | 123.70 |
| 22 | 23S1 | 2126 | A | N3-C4-C5 | -10.40 | 119.52 | 126.80 |
| 1 | 16S1 | 192 | A | N3-C4-C5 | -10.39 | 119.53 | 126.80 |
| 1 | 16S1 | 374 | A | C5-C6-N6 | 10.39 | 132.01 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 182 | A | N7-C8-N9 | -10.39 | 108.60 | 113.80 |
| 22 | 23S1 | 547 | A | C5-C6-N6 | 10.39 | 132.02 | 123.70 |
| 22 | 23S1 | 633 | A | N7-C8-N9 | -10.39 | 108.60 | 113.80 |
| 1 | 16S1 | 1274 | A | C5-C6-N6 | 10.39 | 132.01 | 123.70 |
| 1 | 16S1 | 622 | A | N7-C8-N9 | -10.39 | 108.61 | 113.80 |
| 22 | 23S1 | 155 | A | N3-C4-C5 | -10.39 | 119.53 | 126.80 |
| 22 | 23S1 | 1057 | A | C5-C6-N6 | 10.39 | 132.01 | 123.70 |
| 1 | 16S1 | 50 | A | C5-C6-N6 | 10.39 | 132.01 | 123.70 |
| 1 | 16S1 | 642 | A | N7-C8-N9 | -10.39 | 108.61 | 113.80 |
| 22 | 23S1 | 1014 | A | C5-C6-N6 | 10.39 | 132.01 | 123.70 |
| 22 | 23S1 | 227 | A | C5-C6-N6 | 10.39 | 132.01 | 123.70 |
| 22 | 23S1 | 1626 | A | C5-C6-N6 | 10.39 | 132.01 | 123.70 |
| 1 | 16S1 | 452 | A | N3-C4-C5 | -10.38 | 119.53 | 126.80 |
| 22 | 23S1 | 2725 | A | N3-C4-C5 | -10.38 | 119.53 | 126.80 |
| 22 | 23S1 | 2810 | A | N3-C4-C5 | -10.39 | 119.53 | 126.80 |
| 1 | 16S1 | 600 | A | N3-C4-C5 | -10.38 | 119.53 | 126.80 |
| 1 | 16S1 | 1431 | A | C5-C6-N6 | 10.38 | 132.00 | 123.70 |
| 22 | 23S1 | 2267 | A | C5-C6-N6 | 10.38 | 132.00 | 123.70 |
| 22 | 23S1 | 2267 | A | N7-C8-N9 | -10.38 | 108.61 | 113.80 |
| 1 | 16S1 | 1256 | A | C5-C6-N6 | 10.38 | 132.00 | 123.70 |
| 1 | 16S1 | 574 | A | N7-C8-N9 | -10.38 | 108.61 | 113.80 |
| 22 | 23S1 | 2497 | A | N3-C4-C5 | -10.38 | 119.54 | 126.80 |
| 22 | 23S1 | 2598 | A | N7-C8-N9 | -10.38 | 108.61 | 113.80 |
| 22 | 23S1 | 631 | A | N3-C4-C5 | -10.37 | 119.54 | 126.80 |
| 22 | 23S1 | 479 | A | C5-C6-N6 | 10.37 | 132.00 | 123.70 |
| 22 | 23S1 | 626 | A | N7-C8-N9 | -10.37 | 108.61 | 113.80 |
| 22 | 23S1 | 222 | A | C5-C6-N6 | 10.37 | 132.00 | 123.70 |
| 22 | 23S1 | 1151 | A | N3-C4-C5 | -10.37 | 119.54 | 126.80 |
| 22 | 23S1 | 2278 | A | C5-C6-N6 | 10.37 | 132.00 | 123.70 |
| 22 | 23S1 | 2411 | A | C5-C6-N6 | 10.37 | 132.00 | 123.70 |
| 1 | 16S1 | 655 | A | N7-C8-N9 | -10.37 | 108.62 | 113.80 |
| 1 | 16S1 | 747 | A | N3-C4-C5 | -10.37 | 119.54 | 126.80 |
| 1 | 16S1 | 1042 | A | C5-C6-N6 | 10.37 | 132.00 | 123.70 |
| 22 | 23S1 | 430 | A | N7-C8-N9 | -10.37 | 108.62 | 113.80 |
| 22 | 23S1 | 1784 | A | C5-C6-N6 | 10.37 | 132.00 | 123.70 |
| 22 | 23S1 | 2738 | A | N7-C8-N9 | -10.37 | 108.61 | 113.80 |
| 22 | 23S1 | 2809 | A | N7-C8-N9 | -10.37 | 108.61 | 113.80 |
| 22 | 23S1 | 19 | A | N3-C4-C5 | -10.37 | 119.54 | 126.80 |
| 22 | 23S1 | 1490 | A | N7-C8-N9 | -10.37 | 108.62 | 113.80 |
| 1 | 16S1 | 250 | A | C5-C6-N6 | 10.37 | 131.99 | 123.70 |
| 1 | 16S1 | 336 | A | N7-C8-N9 | -10.37 | 108.62 | 113.80 |
| 22 | 23S1 | 1913 | A | C5-C6-N6 | 10.36 | 131.99 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1046 | A | C5-C6-N6 | 10.36 | 131.99 | 123.70 |
| 22 | 23S1 | 1433 | A | N3-C4-C5 | -10.36 | 119.55 | 126.80 |
| 22 | 23S1 | 1528 | A | N7-C8-N9 | -10.36 | 108.62 | 113.80 |
| 22 | 23S1 | 1808 | A | C5-C6-N6 | 10.36 | 131.99 | 123.70 |
| 22 | 23S1 | 181 | A | C5-C6-N6 | 10.36 | 131.99 | 123.70 |
| 22 | 23S1 | 1916 | A | N3-C4-C5 | -10.36 | 119.55 | 126.80 |
| 23 | 05S1 | 94 | A | N3-C4-C5 | -10.36 | 119.55 | 126.80 |
| 1 | 16S1 | 1102 | A | N7-C8-N9 | -10.36 | 108.62 | 113.80 |
| 22 | 23S1 | 173 | A | N7-C8-N9 | -10.36 | 108.62 | 113.80 |
| 22 | 23S1 | 990 | A | N7-C8-N9 | -10.36 | 108.62 | 113.80 |
| 22 | 23S1 | 2088 | A | N3-C4-C5 | -10.36 | 119.55 | 126.80 |
| 23 | 05S1 | 50 | A | N3-C4-C5 | -10.36 | 119.55 | 126.80 |
| 22 | 23S1 | 782 | A | N7-C8-N9 | -10.36 | 108.62 | 113.80 |
| 1 | 16S1 | 1375 | A | N3-C4-C5 | -10.35 | 119.55 | 126.80 |
| 22 | 23S1 | 149 | A | C5-C6-N6 | 10.35 | 131.98 | 123.70 |
| 22 | 23S1 | 920 | A | C5-C6-N6 | 10.35 | 131.98 | 123.70 |
| 1 | 16S1 | 1398 | A | N7-C8-N9 | -10.35 | 108.62 | 113.80 |
| 22 | 23S1 | 794 | A | N7-C8-N9 | -10.35 | 108.62 | 113.80 |
| 1 | 16S1 | 80 | A | C5-C6-N6 | 10.35 | 131.98 | 123.70 |
| 1 | 16S1 | 681 | A | N3-C4-C5 | -10.35 | 119.56 | 126.80 |
| 22 | 23S1 | 2418 | A | N3-C4-C5 | -10.35 | 119.56 | 126.80 |
| 22 | 23S1 | 2700 | A | N3-C4-C5 | -10.35 | 119.56 | 126.80 |
| 22 | 23S1 | 804 | A | N3-C4-C5 | -10.35 | 119.56 | 126.80 |
| 1 | 16S1 | 496 | A | N3-C4-C5 | -10.35 | 119.56 | 126.80 |
| 1 | 16S1 | 1246 | A | N3-C4-C5 | -10.34 | 119.56 | 126.80 |
| 22 | 23S1 | 52 | A | C5-C6-N6 | 10.34 | 131.97 | 123.70 |
| 22 | 23S1 | 1744 | A | N3-C4-C5 | -10.34 | 119.56 | 126.80 |
| 22 | 23S1 | 2059 | A | N3-C4-C5 | -10.34 | 119.56 | 126.80 |
| 1 | 16S1 | 1503 | A | C5-C6-N6 | 10.34 | 131.97 | 123.70 |
| 22 | 23S1 | 756 | A | N3-C4-C5 | -10.34 | 119.56 | 126.80 |
| 22 | 23S1 | 83 | A | C5-C6-N6 | 10.34 | 131.97 | 123.70 |
| 22 | 23S1 | 1470 | A | C5-C6-N6 | 10.34 | 131.97 | 123.70 |
| 22 | 23S1 | 2082 | A | N7-C8-N9 | -10.34 | 108.63 | 113.80 |
| 22 | 23S1 | 2761 | A | N3-C4-C5 | -10.34 | 119.56 | 126.80 |
| 1 | 16S1 | 909 | A | N7-C8-N9 | -10.34 | 108.63 | 113.80 |
| 22 | 23S1 | 256 | A | C5-C6-N6 | 10.34 | 131.97 | 123.70 |
| 1 | 16S1 | 1163 | A | N3-C4-C5 | -10.34 | 119.57 | 126.80 |
| 22 | 23S1 | 1987 | A | C5-C6-N6 | 10.34 | 131.97 | 123.70 |
| 1 | 16S1 | 1318 | A | N7-C8-N9 | -10.33 | 108.63 | 113.80 |
| 22 | 23S1 | 2366 | A | N3-C4-C5 | -10.33 | 119.57 | 126.80 |
| 22 | 23S1 | 1966 | A | C5-C6-N6 | 10.33 | 131.97 | 123.70 |
| 22 | 23S1 | 2476 | A | N3-C4-C5 | -10.33 | 119.57 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 130 | A | N3-C4-C5 | -10.33 | 119.57 | 126.80 |
| 22 | 23S1 | 255 | A | C5-C6-N6 | 10.33 | 131.97 | 123.70 |
| 22 | 23S1 | 2660 | A | C5-C6-N6 | 10.33 | 131.97 | 123.70 |
| 1 | 16S1 | 303 | A | C5-C6-N6 | 10.33 | 131.96 | 123.70 |
| 1 | 16S1 | 1005 | A | C5-C6-N6 | 10.33 | 131.96 | 123.70 |
| 22 | 23S1 | 348 | A | N3-C4-C5 | -10.33 | 119.57 | 126.80 |
| 22 | 23S1 | 2799 | A | N3-C4-C5 | -10.33 | 119.57 | 126.80 |
| 1 | 16S1 | 1349 | A | C5-C6-N6 | 10.33 | 131.96 | 123.70 |
| 22 | 23S1 | 2108 | A | N7-C8-N9 | -10.33 | 108.64 | 113.80 |
| 1 | 16S1 | 431 | A | N7-C8-N9 | -10.33 | 108.64 | 113.80 |
| 22 | 23S1 | 753 | A | C5-C6-N6 | 10.33 | 131.96 | 123.70 |
| 1 | 16S1 | 1019 | A | C5-C6-N6 | 10.32 | 131.96 | 123.70 |
| 22 | 23S1 | 1598 | A | N3-C4-C5 | -10.32 | 119.57 | 126.80 |
| 22 | 23S1 | 1969 | A | C5-C6-N6 | 10.32 | 131.96 | 123.70 |
| 1 | 16S1 | 1374 | A | N3-C4-C5 | -10.32 | 119.58 | 126.80 |
| 22 | 23S1 | 1073 | A | C5-C6-N6 | 10.32 | 131.96 | 123.70 |
| 22 | 23S1 | 528 | A | N3-C4-C5 | -10.32 | 119.58 | 126.80 |
| 22 | 23S1 | 2740 | A | C5-C6-N6 | 10.32 | 131.96 | 123.70 |
| 23 | 05S1 | 59 | A | C5-C6-N1 | 10.32 | 122.86 | 117.70 |
| 23 | 05S1 | 119 | A | C5-C6-N6 | 10.32 | 131.96 | 123.70 |
| 22 | 23S1 | 233 | A | N3-C4-C5 | -10.32 | 119.58 | 126.80 |
| 22 | 23S1 | 300 | A | N7-C8-N9 | -10.32 | 108.64 | 113.80 |
| 22 | 23S1 | 861 | A | N3-C4-C5 | -10.32 | 119.58 | 126.80 |
| 22 | 23S1 | 2270 | A | N3-C4-C5 | -10.32 | 119.58 | 126.80 |
| 1 | 16S1 | 236 | A | N3-C4-C5 | -10.31 | 119.58 | 126.80 |
| 22 | 23S1 | 423 | A | N7-C8-N9 | -10.31 | 108.64 | 113.80 |
| 1 | 16S1 | 718 | A | N7-C8-N9 | -10.31 | 108.64 | 113.80 |
| 1 | 16S1 | 1311 | A | N3-C4-C5 | -10.31 | 119.58 | 126.80 |
| 22 | 23S1 | 2015 | A | N7-C8-N9 | -10.31 | 108.64 | 113.80 |
| 1 | 16S1 | 408 | A | N7-C8-N9 | -10.31 | 108.65 | 113.80 |
| 22 | 23S1 | 947 | A | N3-C4-C5 | -10.31 | 119.58 | 126.80 |
| 23 | 05S1 | 115 | A | C5-C6-N6 | 10.31 | 131.95 | 123.70 |
| 22 | 23S1 | 1496 | A | C5-C6-N6 | 10.31 | 131.95 | 123.70 |
| 1 | 16S1 | 753 | A | N3-C4-C5 | -10.31 | 119.58 | 126.80 |
| 1 | 16S1 | 1492 | A | N3-C4-C5 | -10.31 | 119.59 | 126.80 |
| 1 | 16S1 | 663 | A | N7-C8-N9 | -10.30 | 108.65 | 113.80 |
| 22 | 23S1 | 2725 | A | N7-C8-N9 | -10.30 | 108.65 | 113.80 |
| 22 | 23S1 | 996 | A | N3-C4-C5 | -10.30 | 119.59 | 126.80 |
| 22 | 23S1 | 2757 | A | N7-C8-N9 | -10.30 | 108.65 | 113.80 |
| 1 | 16S1 | 151 | A | N3-C4-C5 | -10.30 | 119.59 | 126.80 |
| 22 | 23S1 | 173 | A | N3-C4-C5 | -10.30 | 119.59 | 126.80 |
| 22 | 23S1 | 1028 | A | N3-C4-C5 | -10.30 | 119.59 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 2281 | A | N3-C4-C5 | -10.30 | 119.59 | 126.80 |
| 1 | 16S1 | 55 | A | C5-C6-N6 | 10.30 | 131.94 | 123.70 |
| 1 | 16S1 | 228 | A | N7-C8-N9 | -10.30 | 108.65 | 113.80 |
| 1 | 16S1 | 1499 | A | N3-C4-C5 | -10.29 | 119.59 | 126.80 |
| 22 | 23S1 | 563 | A | N3-C4-C5 | -10.29 | 119.59 | 126.80 |
| 22 | 23S1 | 1301 | A | C5-C6-N6 | 10.29 | 131.94 | 123.70 |
| 1 | 16S1 | 101 | A | N7-C8-N9 | -10.29 | 108.65 | 113.80 |
| 1 | 16S1 | 373 | A | C5-C6-N6 | 10.29 | 131.93 | 123.70 |
| 1 | 16S1 | 1158 | C | N1-C2-O2 | 10.29 | 125.08 | 118.90 |
| 1 | 16S1 | 1483 | A | C5-C6-N6 | 10.29 | 131.93 | 123.70 |
| 22 | 23S1 | 176 | A | C5-C6-N6 | 10.29 | 131.93 | 123.70 |
| 22 | 23S1 | 1175 | A | C5-C6-N6 | 10.29 | 131.93 | 123.70 |
| 22 | 23S1 | 2459 | A | N3-C4-C5 | -10.29 | 119.60 | 126.80 |
| 1 | 16S1 | 192 | A | C5-C6-N6 | 10.29 | 131.93 | 123.70 |
| 22 | 23S1 | 1365 | A | N3-C4-C5 | -10.29 | 119.60 | 126.80 |
| 1 | 16S1 | 1022 | A | C5-C6-N6 | 10.29 | 131.93 | 123.70 |
| 1 | 16S1 | 1434 | A | C5-C6-N6 | 10.29 | 131.93 | 123.70 |
| 22 | 23S1 | 1603 | A | N7-C8-N9 | -10.29 | 108.66 | 113.80 |
| 22 | 23S1 | 2134 | A | N7-C8-N9 | -10.29 | 108.66 | 113.80 |
| 22 | 23S1 | 1773 | A | N7-C8-N9 | -10.29 | 108.66 | 113.80 |
| 22 | 23S1 | 2471 | A | N3-C4-C5 | -10.29 | 119.60 | 126.80 |
| 1 | 16S1 | 482 | A | N3-C4-C5 | -10.28 | 119.60 | 126.80 |
| 1 | 16S1 | 919 | A | N7-C8-N9 | -10.29 | 108.66 | 113.80 |
| 22 | 23S1 | 447 | A | C5-C6-N6 | 10.29 | 131.93 | 123.70 |
| 22 | 23S1 | 1070 | A | N3-C4-C5 | -10.29 | 119.60 | 126.80 |
| 22 | 23S1 | 644 | A | C5-N7-C8 | 10.28 | 109.04 | 103.90 |
| 22 | 23S1 | 705 | A | N3-C4-C5 | -10.29 | 119.60 | 126.80 |
| 22 | 23S1 | 1593 | A | N3-C4-C5 | -10.29 | 119.60 | 126.80 |
| 22 | 23S1 | 1689 | A | N7-C8-N9 | -10.29 | 108.66 | 113.80 |
| 22 | 23S1 | 2003 | A | N3-C4-C5 | -10.29 | 119.60 | 126.80 |
| 22 | 23S1 | 574 | A | C5-C6-N6 | 10.28 | 131.93 | 123.70 |
| 22 | 23S1 | 1801 | A | N7-C8-N9 | -10.28 | 108.66 | 113.80 |
| 22 | 23S1 | 2799 | A | N7-C8-N9 | -10.28 | 108.66 | 113.80 |
| 1 | 16S1 | 313 | A | N3-C4-C5 | -10.28 | 119.61 | 126.80 |
| 1 | 16S1 | 1014 | A | N3-C4-C5 | -10.28 | 119.61 | 126.80 |
| 22 | 23S1 | 1126 | A | N3-C4-C5 | -10.28 | 119.61 | 126.80 |
| 22 | 23S1 | 2468 | A | C5-C6-N6 | 10.28 | 131.92 | 123.70 |
| 22 | 23S1 | 1147 | A | N3-C4-C5 | -10.27 | 119.61 | 126.80 |
| 22 | 23S1 | 1877 | A | N7-C8-N9 | -10.27 | 108.66 | 113.80 |
| 23 | 05S1 | 73 | A | N7-C8-N9 | -10.27 | 108.66 | 113.80 |
| 22 | 23S1 | 802 | A | N3-C4-C5 | -10.27 | 119.61 | 126.80 |
| 22 | 23S1 | 1268 | A | N7-C8-N9 | -10.27 | 108.66 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1762 | A | N7-C8-N9 | -10.27 | 108.66 | 113.80 |
| 22 | 23S1 | 218 | A | N3-C4-C5 | -10.27 | 119.61 | 126.80 |
| 22 | 23S1 | 689 | A | C5-C6-N6 | 10.27 | 131.91 | 123.70 |
| 22 | 23S1 | 1244 | A | C5-C6-N6 | 10.27 | 131.92 | 123.70 |
| 22 | 23S1 | 2670 | A | C5-C6-N6 | 10.27 | 131.92 | 123.70 |
| 22 | 23S1 | 1088 | A | C5-C6-N6 | 10.27 | 131.91 | 123.70 |
| 22 | 23S1 | 2114 | A | C5-C6-N6 | 10.27 | 131.91 | 123.70 |
| 1 | 16S1 | 190 | A | N1-C6-N6 | -10.27 | 112.44 | 118.60 |
| 1 | 16S1 | 729 | A | N3-C4-C5 | -10.27 | 119.61 | 126.80 |
| 22 | 23S1 | 2328 | A | C5-C6-N6 | 10.27 | 131.91 | 123.70 |
| 1 | 16S1 | 412 | A | N7-C8-N9 | -10.26 | 108.67 | 113.80 |
| 1 | 16S1 | 675 | A | C5-C6-N6 | 10.26 | 131.91 | 123.70 |
| 22 | 23S1 | 1532 | A | C5-C6-N6 | 10.26 | 131.91 | 123.70 |
| 22 | 23S1 | 1866 | A | N3-C4-C5 | -10.26 | 119.62 | 126.80 |
| 22 | 23S1 | 2386 | A | N3-C4-C5 | -10.26 | 119.62 | 126.80 |
| 22 | 23S1 | 2873 | A | N7-C8-N9 | -10.26 | 108.67 | 113.80 |
| 1 | 16S1 | 448 | A | N3-C4-C5 | -10.26 | 119.62 | 126.80 |
| 1 | 16S1 | 1093 | A | N3-C4-C5 | -10.26 | 119.62 | 126.80 |
| 1 | 16S1 | 1357 | A | N7-C8-N9 | -10.26 | 108.67 | 113.80 |
| 22 | 23S1 | 722 | A | N3-C4-C5 | -10.26 | 119.62 | 126.80 |
| 22 | 23S1 | 1952 | A | N3-C4-C5 | -10.26 | 119.62 | 126.80 |
| 1 | 16S1 | 974 | A | C5-C6-N6 | 10.26 | 131.91 | 123.70 |
| 1 | 16S1 | 946 | A | N3-C4-C5 | -10.26 | 119.62 | 126.80 |
| 22 | 23S1 | 1614 | A | C5-C6-N6 | 10.26 | 131.91 | 123.70 |
| 1 | 16S1 | 1318 | A | N3-C4-C5 | -10.26 | 119.62 | 126.80 |
| 1 | 16S1 | 1332 | A | N3-C4-C5 | -10.26 | 119.62 | 126.80 |
| 22 | 23S1 | 750 | A | C5-C6-N6 | 10.26 | 131.91 | 123.70 |
| 22 | 23S1 | 2037 | A | C5-C6-N6 | 10.26 | 131.90 | 123.70 |
| 1 | 16S1 | 959 | A | N3-C4-C5 | -10.25 | 119.62 | 126.80 |
| 22 | 23S1 | 2134 | A | N3-C4-C5 | -10.25 | 119.62 | 126.80 |
| 1 | 16S1 | 1418 | A | N3-C4-C5 | -10.25 | 119.63 | 126.80 |
| 22 | 23S1 | 480 | A | N7-C8-N9 | -10.25 | 108.67 | 113.80 |
| 22 | 23S1 | 1021 | A | N7-C8-N9 | -10.25 | 108.67 | 113.80 |
| 1 | 16S1 | 1246 | A | C5-C6-N6 | 10.25 | 131.90 | 123.70 |
| 22 | 23S1 | 1916 | A | N7-C8-N9 | -10.24 | 108.68 | 113.80 |
| 1 | 16S1 | 1229 | A | C5-C6-N6 | 10.24 | 131.89 | 123.70 |
| 1 | 16S1 | 412 | A | C5-C6-N6 | 10.24 | 131.89 | 123.70 |
| 1 | 16S1 | 1238 | A | N3-C4-C5 | -10.24 | 119.63 | 126.80 |
| 22 | 23S1 | 532 | A | N7-C8-N9 | -10.24 | 108.68 | 113.80 |
| 22 | 23S1 | 1676 | A | C5-C6-N6 | 10.24 | 131.89 | 123.70 |
| 22 | 23S1 | 730 | A | N7-C8-N9 | -10.24 | 108.68 | 113.80 |
| 22 | 23S1 | 756 | A | C5-C6-N6 | 10.24 | 131.89 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1373 | A | N3-C4-C5 | -10.24 | 119.64 | 126.80 |
| 22 | 23S1 | 1552 | A | C5-C6-N6 | 10.24 | 131.89 | 123.70 |
| 22 | 23S1 | 2376 | A | N3-C4-C5 | -10.23 | 119.64 | 126.80 |
| 22 | 23S1 | 2887 | A | C5-C6-N6 | 10.23 | 131.89 | 123.70 |
| 1 | 16S1 | 1155 | A | N3-C4-C5 | -10.23 | 119.64 | 126.80 |
| 22 | 23S1 | 471 | A | C5-C6-N6 | 10.23 | 131.88 | 123.70 |
| 22 | 23S1 | 1373 | A | C5-C6-N6 | 10.23 | 131.88 | 123.70 |
| 22 | 23S1 | 1591 | A | N3-C4-C5 | -10.23 | 119.64 | 126.80 |
| 1 | 16S1 | 33 | A | N3-C4-C5 | -10.23 | 119.64 | 126.80 |
| 1 | 16S1 | 81 | A | N3-C4-C5 | -10.23 | 119.64 | 126.80 |
| 1 | 16S1 | 1269 | A | N7-C8-N9 | -10.22 | 108.69 | 113.80 |
| 22 | 23S1 | 1226 | A | C5-C6-N6 | 10.22 | 131.88 | 123.70 |
| 22 | 23S1 | 1966 | A | N3-C4-C5 | -10.22 | 119.64 | 126.80 |
| 22 | 23S1 | 482 | A | N7-C8-N9 | -10.22 | 108.69 | 113.80 |
| 22 | 23S1 | 1889 | A | N3-C4-C5 | -10.22 | 119.65 | 126.80 |
| 55 | PTR1 | 42 | A | N3-C4-C5 | -10.22 | 119.64 | 126.80 |
| 1 | 16S1 | 478 | A | N7-C8-N9 | -10.22 | 108.69 | 113.80 |
| 22 | 23S1 | 428 | A | C5-C6-N6 | 10.22 | 131.87 | 123.70 |
| 22 | 23S1 | 739 | A | N7-C8-N9 | -10.22 | 108.69 | 113.80 |
| 22 | 23S1 | 984 | A | N7-C8-N9 | -10.22 | 108.69 | 113.80 |
| 22 | 23S1 | 1039 | A | C5-C6-N6 | 10.22 | 131.87 | 123.70 |
| 1 | 16S1 | 1468 | A | N7-C8-N9 | -10.21 | 108.69 | 113.80 |
| 1 | 16S1 | 371 | A | N3-C4-C5 | -10.21 | 119.65 | 126.80 |
| 1 | 16S1 | 743 | A | N3-C4-C5 | -10.21 | 119.65 | 126.80 |
| 22 | 23S1 | 466 | A | C5-C6-N6 | 10.21 | 131.87 | 123.70 |
| 22 | 23S1 | 1213 | A | N7-C8-N9 | -10.21 | 108.69 | 113.80 |
| 22 | 23S1 | 1711 | A | N3-C4-C5 | -10.21 | 119.65 | 126.80 |
| 22 | 23S1 | 2094 | A | N3-C4-C5 | -10.21 | 119.65 | 126.80 |
| 22 | 23S1 | 899 | A | N3-C4-C5 | -10.21 | 119.65 | 126.80 |
| 22 | 23S1 | 1054 | A | N3-C4-C5 | -10.21 | 119.65 | 126.80 |
| 22 | 23S1 | 1502 | A | N3-C4-C5 | -10.21 | 119.65 | 126.80 |
| 22 | 23S1 | 1847 | A | C5-C6-N6 | 10.21 | 131.87 | 123.70 |
| 1 | 16S1 | 10 | A | N3-C4-C5 | -10.21 | 119.65 | 126.80 |
| 1 | 16S1 | 1465 | A | N3-C4-C5 | -10.21 | 119.65 | 126.80 |
| 22 | 23S1 | 2225 | A | N3-C4-C5 | -10.21 | 119.65 | 126.80 |
| 22 | 23S1 | 1040 | A | C5-C6-N6 | 10.21 | 131.87 | 123.70 |
| 22 | 23S1 | 2886 | A | C5-C6-N6 | 10.21 | 131.87 | 123.70 |
| 1 | 16S1 | 609 | A | N7-C8-N9 | -10.21 | 108.70 | 113.80 |
| 1 | 16S1 | 1333 | A | N3-C4-C5 | -10.21 | 119.66 | 126.80 |
| 22 | 23S1 | 941 | A | N3-C4-C5 | -10.21 | 119.66 | 126.80 |
| 22 | 23S1 | 1050 | A | N3-C4-C5 | -10.21 | 119.66 | 126.80 |
| 22 | 23S1 | 1566 | A | C5-C6-N6 | 10.21 | 131.87 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 498 | A | N7-C8-N9 | -10.20 | 108.70 | 113.80 |
| 1 | 16S1 | 1288 | A | N7-C8-N9 | -10.20 | 108.70 | 113.80 |
| 22 | 23S1 | 2879 | A | N3-C4-C5 | -10.20 | 119.66 | 126.80 |
| 1 | 16S1 | 493 | A | N7-C8-N9 | -10.20 | 108.70 | 113.80 |
| 1 | 16S1 | 749 | A | C5-C6-N6 | 10.20 | 131.86 | 123.70 |
| 1 | 16S1 | 864 | A | N3-C4-C5 | -10.20 | 119.66 | 126.80 |
| 22 | 23S1 | 104 | A | C5-C6-N6 | 10.20 | 131.86 | 123.70 |
| 22 | 23S1 | 300 | A | N3-C4-C5 | -10.20 | 119.66 | 126.80 |
| 22 | 23S1 | 590 | A | N3-C4-C5 | -10.20 | 119.66 | 126.80 |
| 22 | 23S1 | 1260 | A | N3-C4-C5 | -10.20 | 119.66 | 126.80 |
| 1 | 16S1 | 59 | A | C5-C6-N6 | 10.20 | 131.86 | 123.70 |
| 1 | 16S1 | 65 | A | C5-C6-N6 | 10.20 | 131.86 | 123.70 |
| 1 | 16S1 | 747 | A | N7-C8-N9 | -10.19 | 108.70 | 113.80 |
| 22 | 23S1 | 945 | A | N3-C4-C5 | -10.19 | 119.66 | 126.80 |
| 22 | 23S1 | 2142 | A | N3-C4-C5 | -10.19 | 119.66 | 126.80 |
| 22 | 23S1 | 231 | A | C5-C6-N6 | 10.19 | 131.85 | 123.70 |
| 22 | 23S1 | 1490 | A | C5-C6-N6 | 10.19 | 131.85 | 123.70 |
| 22 | 23S1 | 2872 | A | C5-N7-C8 | 10.19 | 109.00 | 103.90 |
| 1 | 16S1 | 26 | A | N3-C4-C5 | -10.19 | 119.67 | 126.80 |
| 22 | 23S1 | 324 | A | N3-C4-C5 | -10.19 | 119.67 | 126.80 |
| 22 | 23S1 | 1347 | A | N3-C4-C5 | -10.19 | 119.67 | 126.80 |
| 22 | 23S1 | 2297 | A | N3-C4-C5 | -10.19 | 119.67 | 126.80 |
| 22 | 23S1 | 282 | A | C5-C6-N6 | 10.19 | 131.85 | 123.70 |
| 22 | 23S1 | 582 | A | C5-C6-N6 | 10.19 | 131.85 | 123.70 |
| 22 | 23S1 | 1133 | A | N7-C8-N9 | -10.19 | 108.71 | 113.80 |
| 22 | 23S1 | 1247 | A | N3-C4-C5 | -10.19 | 119.67 | 126.80 |
| 22 | 23S1 | 1664 | A | N7-C8-N9 | -10.19 | 108.71 | 113.80 |
| 1 | 16S1 | 1483 | A | N3-C4-C5 | -10.18 | 119.67 | 126.80 |
| 1 | 16S1 | 451 | A | C5-C6-N6 | 10.18 | 131.84 | 123.70 |
| 22 | 23S1 | 320 | A | C5-C6-N6 | 10.18 | 131.84 | 123.70 |
| 1 | 16S1 | 98 | A | C5-C6-N6 | 10.18 | 131.84 | 123.70 |
| 1 | 16S1 | 274 | A | C5-C6-N6 | 10.18 | 131.84 | 123.70 |
| 22 | 23S1 | 199 | A | N3-C4-C5 | -10.18 | 119.67 | 126.80 |
| 22 | 23S1 | 156 | A | N3-C4-C5 | -10.18 | 119.68 | 126.80 |
| 22 | 23S1 | 2757 | A | N3-C4-C5 | -10.18 | 119.67 | 126.80 |
| 1 | 16S1 | 205 | A | N3-C4-C5 | -10.18 | 119.68 | 126.80 |
| 1 | 16S1 | 665 | A | N7-C8-N9 | -10.18 | 108.71 | 113.80 |
| 1 | 16S1 | 815 | A | N3-C4-C5 | -10.18 | 119.68 | 126.80 |
| 1 | 16S1 | 819 | A | N3-C4-C5 | -10.18 | 119.68 | 126.80 |
| 22 | 23S1 | 346 | A | N3-C4-C5 | -10.18 | 119.68 | 126.80 |
| 22 | 23S1 | 1084 | A | N3-C4-C5 | -10.18 | 119.68 | 126.80 |
| 1 | 16S1 | 1155 | A | C5-C6-N6 | 10.18 | 131.84 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 63 | A | C5-C6-N6 | 10.18 | 131.84 | 123.70 |
| 22 | 23S1 | 1689 | A | C5-C6-N6 | 10.18 | 131.84 | 123.70 |
| 1 | 16S1 | 746 | A | C5-C6-N6 | 10.17 | 131.84 | 123.70 |
| 1 | 16S1 | 938 | A | C5-C6-N6 | 10.17 | 131.84 | 123.70 |
| 22 | 23S1 | 2015 | A | C5-C6-N6 | 10.17 | 131.84 | 123.70 |
| 1 | 16S1 | 1102 | A | N3-C4-C5 | -10.17 | 119.68 | 126.80 |
| 22 | 23S1 | 340 | A | N3-C4-C5 | -10.17 | 119.68 | 126.80 |
| 22 | 23S1 | 472 | A | C5-C6-N6 | 10.17 | 131.84 | 123.70 |
| 22 | 23S1 | 1603 | A | N3-C4-C5 | -10.17 | 119.68 | 126.80 |
| 22 | 23S1 | 73 | A | N7-C8-N9 | -10.17 | 108.72 | 113.80 |
| 22 | 23S1 | 1134 | A | C5-C6-N6 | 10.17 | 131.84 | 123.70 |
| 22 | 23S1 | 1641 | A | N3-C4-C5 | -10.17 | 119.68 | 126.80 |
| 55 | PTR1 | 9 | A | C5-C6-N6 | 10.17 | 131.84 | 123.70 |
| 22 | 23S1 | 793 | A | N3-C4-C5 | -10.17 | 119.68 | 126.80 |
| 22 | 23S1 | 2070 | A | N3-C4-C5 | -10.17 | 119.68 | 126.80 |
| 22 | 23S1 | 2268 | A | C5-C6-N6 | 10.17 | 131.83 | 123.70 |
| 22 | 23S1 | 2821 | A | N3-C4-C5 | -10.17 | 119.68 | 126.80 |
| 22 | 23S1 | 743 | A | C5-C6-N6 | 10.16 | 131.83 | 123.70 |
| 22 | 23S1 | 2352 | A | N7-C8-N9 | -10.16 | 108.72 | 113.80 |
| 22 | 23S1 | 149 | A | N3-C4-C5 | -10.16 | 119.69 | 126.80 |
| 22 | 23S1 | 2031 | A | N3-C4-C5 | -10.16 | 119.69 | 126.80 |
| 1 | 16S1 | 161 | A | N3-C4-C5 | -10.16 | 119.69 | 126.80 |
| 1 | 16S1 | 794 | A | N3-C4-C5 | -10.16 | 119.69 | 126.80 |
| 1 | 16S1 | 1169 | A | C5-C6-N6 | 10.16 | 131.83 | 123.70 |
| 22 | 23S1 | 311 | A | N3-C4-C5 | -10.16 | 119.69 | 126.80 |
| 1 | 16S1 | 499 | A | N3-C4-C5 | -10.16 | 119.69 | 126.80 |
| 1 | 16S1 | 459 | A | N7-C8-N9 | -10.16 | 108.72 | 113.80 |
| 22 | 23S1 | 1143 | A | N7-C8-N9 | -10.16 | 108.72 | 113.80 |
| 22 | 23S1 | 1553 | A | N3-C4-C5 | -10.16 | 119.69 | 126.80 |
| 22 | 23S1 | 2577 | A | N3-C4-C5 | -10.16 | 119.69 | 126.80 |
| 22 | 23S1 | 2765 | A | N7-C8-N9 | -10.16 | 108.72 | 113.80 |
| 22 | 23S1 | 430 | A | N3-C4-C5 | -10.15 | 119.69 | 126.80 |
| 22 | 23S1 | 646 | U | C5-C6-N1 | -10.15 | 117.62 | 122.70 |
| 22 | 23S1 | 1262 | A | N3-C4-C5 | -10.15 | 119.69 | 126.80 |
| 22 | 23S1 | 1268 | A | C5-C6-N6 | 10.15 | 131.82 | 123.70 |
| 1 | 16S1 | 460 | A | N3-C4-C5 | -10.15 | 119.70 | 126.80 |
| 1 | 16S1 | 1446 | A | C5-C6-N6 | 10.15 | 131.82 | 123.70 |
| 22 | 23S1 | 972 | A | N7-C8-N9 | -10.15 | 108.73 | 113.80 |
| 22 | 23S1 | 2135 | A | C5-C6-N6 | 10.15 | 131.82 | 123.70 |
| 22 | 23S1 | 2679 | A | C5-C6-N6 | 10.15 | 131.82 | 123.70 |
| 1 | 16S1 | 382 | A | C5-C6-N6 | 10.14 | 131.81 | 123.70 |
| 1 | 16S1 | 1012 | A | C5-C6-N6 | 10.14 | 131.81 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 1513 | A | C5-C6-N6 | 10.14 | 131.81 | 123.70 |
| 22 | 23S1 | 541 | A | N3-C4-C5 | -10.14 | 119.70 | 126.80 |
| 22 | 23S1 | 2314 | A | C5-C6-N6 | 10.14 | 131.81 | 123.70 |
| 22 | 23S1 | 1237 | A | C5-C6-N6 | 10.14 | 131.81 | 123.70 |
| 22 | 23S1 | 191 | A | C5-C6-N6 | 10.14 | 131.81 | 123.70 |
| 22 | 23S1 | 933 | A | C5-C6-N6 | 10.14 | 131.81 | 123.70 |
| 1 | 16S1 | 196 | A | N7-C8-N9 | -10.13 | 108.73 | 113.80 |
| 22 | 23S1 | 2482 | A | N3-C4-C5 | -10.14 | 119.70 | 126.80 |
| 22 | 23S1 | 2893 | A | C5-C6-N6 | 10.13 | 131.81 | 123.70 |
| 1 | 16S1 | 116 | A | N3-C4-C5 | -10.13 | 119.71 | 126.80 |
| 1 | 16S1 | 510 | A | C5-C6-N6 | 10.13 | 131.80 | 123.70 |
| 22 | 23S1 | 1572 | A | N7-C8-N9 | -10.13 | 108.73 | 113.80 |
| 22 | 23S1 | 2311 | A | N3-C4-C5 | -10.13 | 119.71 | 126.80 |
| 22 | 23S1 | 2531 | A | N3-C4-C5 | -10.13 | 119.71 | 126.80 |
| 22 | 23S1 | 670 | A | N3-C4-C5 | -10.12 | 119.71 | 126.80 |
| 22 | 23S1 | 1413 | A | N7-C8-N9 | -10.12 | 108.74 | 113.80 |
| 22 | 23S1 | 1745 | A | N7-C8-N9 | -10.12 | 108.74 | 113.80 |
| 22 | 23S1 | 2392 | A | N3-C4-C5 | -10.12 | 119.71 | 126.80 |
| 1 | 16S1 | 609 | A | C5-C6-N6 | 10.12 | 131.80 | 123.70 |
| 1 | 16S1 | 864 | A | N7-C8-N9 | -10.12 | 108.74 | 113.80 |
| 1 | 16S1 | 1275 | A | C5-C6-N6 | 10.12 | 131.80 | 123.70 |
| 22 | 23S1 | 1431 | A | N3-C4-C5 | -10.12 | 119.71 | 126.80 |
| 1 | 16S1 | 19 | A | N3-C4-C5 | -10.12 | 119.72 | 126.80 |
| 55 | PTR1 | 14 | A | C5-N7-C8 | 10.12 | 108.96 | 103.90 |
| 1 | 16S1 | 414 | A | N3-C4-C5 | -10.11 | 119.72 | 126.80 |
| 22 | 23S1 | 833 | A | N3-C4-C5 | -10.12 | 119.72 | 126.80 |
| 22 | 23S1 | 1637 | A | N3-C4-C5 | -10.12 | 119.72 | 126.80 |
| 22 | 23S1 | 2635 | A | N3-C4-C5 | -10.12 | 119.72 | 126.80 |
| 1 | 16S1 | 26 | A | N7-C8-N9 | -10.11 | 108.74 | 113.80 |
| 22 | 23S1 | 172 | A | C5-C6-N6 | 10.11 | 131.79 | 123.70 |
| 22 | 23S1 | 752 | A | N3-C4-C5 | -10.11 | 119.72 | 126.80 |
| 22 | 23S1 | 933 | A | N7-C8-N9 | -10.11 | 108.74 | 113.80 |
| 22 | 23S1 | 900 | A | N3-C4-C5 | -10.11 | 119.72 | 126.80 |
| 1 | 16S1 | 382 | A | N7-C8-N9 | -10.11 | 108.75 | 113.80 |
| 22 | 23S1 | 2135 | A | N3-C4-C5 | -10.11 | 119.72 | 126.80 |
| 22 | 23S1 | 2856 | A | C5-C6-N6 | 10.11 | 131.79 | 123.70 |
| 1 | 16S1 | 1197 | A | N3-C4-C5 | -10.11 | 119.72 | 126.80 |
| 22 | 23S1 | 2014 | A | C5-C6-N6 | 10.11 | 131.79 | 123.70 |
| 22 | 23S1 | 1307 | A | C5-C6-N6 | 10.10 | 131.78 | 123.70 |
| 1 | 16S1 | 1428 | A | N3-C4-C5 | -10.10 | 119.73 | 126.80 |
| 22 | 23S1 | 2212 | A | N3-C4-C5 | -10.10 | 119.73 | 126.80 |
| 22 | 23S1 | 2225 | A | C5-C6-N6 | 10.10 | 131.78 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 1552 | A | N3-C4-C5 | -10.10 | 119.73 | 126.80 |
| 1 | 16S1 | 1377 | A | N3-C4-C5 | -10.10 | 119.73 | 126.80 |
| 22 | 23S1 | 2541 | A | N3-C4-C5 | -10.10 | 119.73 | 126.80 |
| 1 | 16S1 | 807 | A | C5-C6-N6 | 10.09 | 131.78 | 123.70 |
| 1 | 16S1 | 1446 | A | N7-C8-N9 | -10.09 | 108.75 | 113.80 |
| 22 | 23S1 | 222 | A | N3-C4-C5 | -10.09 | 119.73 | 126.80 |
| 22 | 23S1 | 556 | A | N3-C4-C5 | -10.09 | 119.73 | 126.80 |
| 1 | 16S1 | 635 | A | N3-C4-C5 | -10.09 | 119.74 | 126.80 |
| 1 | 16S1 | 1036 | A | N7-C8-N9 | -10.09 | 108.75 | 113.80 |
| 1 | 16S1 | 1225 | A | N7-C8-N9 | -10.09 | 108.75 | 113.80 |
| 22 | 23S1 | 501 | A | N7-C8-N9 | -10.09 | 108.75 | 113.80 |
| 22 | 23S1 | 2873 | A | N3-C4-C5 | -10.09 | 119.74 | 126.80 |
| 1 | 16S1 | 1362 | A | C5-C6-N6 | 10.09 | 131.77 | 123.70 |
| 22 | 23S1 | 1739 | A | N3-C4-C5 | -10.09 | 119.74 | 126.80 |
| 1 | 16S1 | 1236 | A | C5-C6-N6 | 10.09 | 131.77 | 123.70 |
| 1 | 16S1 | 1534 | A | N3-C4-C5 | -10.09 | 119.74 | 126.80 |
| 22 | 23S1 | 918 | A | N7-C8-N9 | -10.09 | 108.76 | 113.80 |
| 1 | 16S1 | 288 | A | N3-C4-C5 | -10.08 | 119.74 | 126.80 |
| 22 | 23S1 | 2547 | A | N3-C4-C5 | -10.08 | 119.74 | 126.80 |
| 22 | 23S1 | 613 | A | C5-C6-N6 | 10.08 | 131.77 | 123.70 |
| 22 | 23S1 | 1590 | A | N3-C4-C5 | -10.08 | 119.74 | 126.80 |
| 1 | 16S1 | 451 | A | N3-C4-C5 | -10.08 | 119.74 | 126.80 |
| 1 | 16S1 | 729 | A | C5-C6-N6 | 10.08 | 131.76 | 123.70 |
| 22 | 23S1 | 330 | A | N7-C8-N9 | -10.08 | 108.76 | 113.80 |
| 22 | 23S1 | 6 | A | C5-C6-N6 | 10.08 | 131.76 | 123.70 |
| 22 | 23S1 | 1365 | A | N7-C8-N9 | -10.08 | 108.76 | 113.80 |
| 22 | 23S1 | 1668 | A | N3-C4-C5 | -10.08 | 119.74 | 126.80 |
| 1 | 16S1 | 975 | A | N7-C8-N9 | -10.08 | 108.76 | 113.80 |
| 1 | 16S1 | 1204 | A | N3-C4-C5 | -10.08 | 119.75 | 126.80 |
| 1 | 16S1 | 1329 | A | N3-C4-C5 | -10.08 | 119.75 | 126.80 |
| 22 | 23S1 | 1089 | A | N3-C4-C5 | -10.08 | 119.75 | 126.80 |
| 22 | 23S1 | 2241 | A | N7-C8-N9 | -10.08 | 108.76 | 113.80 |
| 1 | 16S1 | 1082 | A | N3-C4-C5 | -10.07 | 119.75 | 126.80 |
| 22 | 23S1 | 52 | A | N3-C4-C5 | -10.07 | 119.75 | 126.80 |
| 22 | 23S1 | 231 | A | N3-C4-C5 | -10.07 | 119.75 | 126.80 |
| 22 | 23S1 | 608 | A | C5-C6-N6 | 10.07 | 131.76 | 123.70 |
| 22 | 23S1 | 988 | A | N3-C4-C5 | -10.07 | 119.75 | 126.80 |
| 22 | 23S1 | 1014 | A | N3-C4-C5 | -10.07 | 119.75 | 126.80 |
| 22 | 23S1 | 2071 | A | N3-C4-C5 | -10.07 | 119.75 | 126.80 |
| 22 | 23S1 | 644 | A | C5-C6-N6 | 10.07 | 131.76 | 123.70 |
| 22 | 23S1 | 1735 | A | N3-C4-C5 | -10.07 | 119.75 | 126.80 |
| 22 | 23S1 | 1928 | A | N7-C8-N9 | -10.07 | 108.77 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 2184 | A | N3-C4-C5 | -10.07 | 119.75 | 126.80 |
| 1 | 16S1 | 78 | A | N3-C4-C5 | -10.07 | 119.75 | 126.80 |
| 1 | 16S1 | 1339 | A | N3-C4-C5 | -10.07 | 119.75 | 126.80 |
| 22 | 23S1 | 1654 | A | N3-C4-C5 | -10.07 | 119.75 | 126.80 |
| 1 | 16S1 | 430 | A | N3-C4-C5 | -10.06 | 119.75 | 126.80 |
| 22 | 23S1 | 715 | A | N3-C4-C5 | -10.06 | 119.75 | 126.80 |
| 22 | 23S1 | 820 | A | N7-C8-N9 | -10.06 | 108.77 | 113.80 |
| 1 | 16S1 | 559 | A | N7-C8-N9 | -10.06 | 108.77 | 113.80 |
| 1 | 16S1 | 621 | A | N7-C8-N9 | -10.06 | 108.77 | 113.80 |
| 1 | 16S1 | 338 | A | N7-C8-N9 | -10.06 | 108.77 | 113.80 |
| 1 | 16S1 | 784 | A | N3-C4-C5 | -10.06 | 119.76 | 126.80 |
| 22 | 23S1 | 1549 | A | N3-C4-C5 | -10.06 | 119.76 | 126.80 |
| 22 | 23S1 | 1593 | A | C5-C6-N6 | 10.06 | 131.75 | 123.70 |
| 23 | 05S1 | 108 | A | C5-C6-N6 | 10.06 | 131.75 | 123.70 |
| 22 | 23S1 | 64 | A | N3-C4-C5 | -10.06 | 119.76 | 126.80 |
| 22 | 23S1 | 218 | A | C5-C6-N6 | 10.06 | 131.75 | 123.70 |
| 22 | 23S1 | 1504 | A | C5-C6-N6 | 10.06 | 131.75 | 123.70 |
| 22 | 23S1 | 1978 | A | N7-C8-N9 | -10.06 | 108.77 | 113.80 |
| 1 | 16S1 | 53 | A | N3-C4-C5 | -10.06 | 119.76 | 126.80 |
| 22 | 23S1 | 1327 | A | C5-C6-N6 | 10.05 | 131.74 | 123.70 |
| 1 | 16S1 | 1349 | A | N3-C4-C5 | -10.05 | 119.76 | 126.80 |
| 22 | 23S1 | 207 | A | C5-C6-N6 | 10.05 | 131.74 | 123.70 |
| 1 | 16S1 | 189 | A | C5-C6-N6 | 10.05 | 131.74 | 123.70 |
| 1 | 16S1 | 1508 | A | N7-C8-N9 | -10.05 | 108.77 | 113.80 |
| 22 | 23S1 | 1572 | A | N3-C4-C5 | -10.05 | 119.76 | 126.80 |
| 22 | 23S1 | 1937 | A | C5-N7-C8 | 10.05 | 108.92 | 103.90 |
| 22 | 23S1 | 2268 | A | N7-C8-N9 | -10.05 | 108.78 | 113.80 |
| 23 | 05S1 | 34 | A | N3-C4-C5 | -10.05 | 119.76 | 126.80 |
| 23 | 05S1 | 101 | A | N3-C4-N9 | 10.05 | 135.44 | 127.40 |
| 23 | 05S1 | 109 | A | C5-C6-N6 | 10.05 | 131.74 | 123.70 |
| 1 | 16S1 | 845 | A | N3-C4-C5 | -10.05 | 119.77 | 126.80 |
| 1 | 16S1 | 560 | A | N3-C4-C5 | -10.05 | 119.77 | 126.80 |
| 22 | 23S1 | 1885 | A | C5-C6-N6 | 10.05 | 131.74 | 123.70 |
| 1 | 16S1 | 327 | A | C5-C6-N6 | 10.04 | 131.74 | 123.70 |
| 22 | 23S1 | 1080 | A | N3-C4-C5 | -10.04 | 119.77 | 126.80 |
| 23 | 05S1 | 34 | A | C5-C6-N6 | 10.04 | 131.74 | 123.70 |
| 23 | 05S1 | 101 | A | N7-C8-N9 | -10.04 | 108.78 | 113.80 |
| 22 | 23S1 | 1780 | A | N3-C4-C5 | -10.04 | 119.77 | 126.80 |
| 22 | 23S1 | 2778 | A | N3-C4-C5 | -10.04 | 119.77 | 126.80 |
| 1 | 16S1 | 466 | A | N3-C4-C5 | -10.04 | 119.77 | 126.80 |
| 1 | 16S1 | 1275 | A | N3-C4-C5 | -10.04 | 119.77 | 126.80 |
| 1 | 16S1 | 878 | A | N3-C4-C5 | -10.04 | 119.78 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 1357 | A | N3-C4-C5 | -10.03 | 119.78 | 126.80 |
| 55 | PTR1 | 14 | A | C5-C6-N6 | 10.04 | 131.73 | 123.70 |
| 1 | 16S1 | 1180 | A | N3-C4-C5 | -10.03 | 119.78 | 126.80 |
| 22 | 23S1 | 12 | U | N3-C2-O2 | -10.03 | 115.18 | 122.20 |
| 22 | 23S1 | 2317 | A | C5-C6-N6 | 10.03 | 131.72 | 123.70 |
| 22 | 23S1 | 1189 | A | C5-C6-N6 | 10.03 | 131.72 | 123.70 |
| 1 | 16S1 | 655 | A | C5-C6-N6 | 10.03 | 131.72 | 123.70 |
| 22 | 23S1 | 146 | A | C5-C6-N6 | 10.03 | 131.72 | 123.70 |
| 22 | 23S1 | 320 | A | N3-C4-C5 | -10.03 | 119.78 | 126.80 |
| 22 | 23S1 | 2665 | A | N3-C4-C5 | -10.03 | 119.78 | 126.80 |
| 22 | 23S1 | 2810 | A | N7-C8-N9 | -10.03 | 108.78 | 113.80 |
| 23 | 05S1 | 50 | A | C5-C6-N6 | 10.03 | 131.72 | 123.70 |
| 55 | PTR1 | 38 | A | N3-C4-C5 | -10.03 | 119.78 | 126.80 |
| 1 | 16S1 | 768 | A | N3-C4-C5 | -10.03 | 119.78 | 126.80 |
| 22 | 23S1 | 176 | A | N3-C4-C5 | -10.03 | 119.78 | 126.80 |
| 22 | 23S1 | 734 | A | N3-C4-C5 | -10.03 | 119.78 | 126.80 |
| 22 | 23S1 | 272 | A | N3-C4-C5 | -10.02 | 119.78 | 126.80 |
| 22 | 23S1 | 750 | A | N3-C4-C5 | -10.02 | 119.78 | 126.80 |
| 22 | 23S1 | 1039 | A | N3-C4-C5 | -10.02 | 119.78 | 126.80 |
| 22 | 23S1 | 2147 | A | C5-C6-N6 | 10.02 | 131.72 | 123.70 |
| 22 | 23S1 | 2189 | U | C5-C6-N1 | 10.02 | 127.71 | 122.70 |
| 22 | 23S1 | 928 | A | N7-C8-N9 | -10.02 | 108.79 | 113.80 |
| 22 | 23S1 | 936 | A | C5-C6-N6 | 10.02 | 131.72 | 123.70 |
| 22 | 23S1 | 1786 | A | N3-C4-C5 | -10.02 | 119.78 | 126.80 |
| 1 | 16S1 | 959 | A | C5-C6-N6 | 10.02 | 131.72 | 123.70 |
| 22 | 23S1 | 1655 | A | N3-C4-C5 | -10.02 | 119.79 | 126.80 |
| 1 | 16S1 | 1396 | A | N3-C4-C5 | -10.02 | 119.79 | 126.80 |
| 22 | 23S1 | 1978 | A | N3-C4-C5 | -10.02 | 119.79 | 126.80 |
| 22 | 23S1 | 2013 | A | N3-C4-C5 | -10.02 | 119.79 | 126.80 |
| 1 | 16S1 | 1105 | A | N3-C4-C5 | -10.02 | 119.79 | 126.80 |
| 22 | 23S1 | 1789 | A | N3-C4-C5 | -10.02 | 119.79 | 126.80 |
| 1 | 16S1 | 1157 | A | C5-C6-N6 | 10.01 | 131.71 | 123.70 |
| 22 | 23S1 | 1134 | A | N3-C4-C5 | -10.01 | 119.79 | 126.80 |
| 22 | 23S1 | 453 | A | N3-C4-C5 | -10.01 | 119.79 | 126.80 |
| 22 | 23S1 | 609 | A | N3-C4-C5 | -10.01 | 119.79 | 126.80 |
| 22 | 23S1 | 1805 | A | N3-C4-C5 | -10.01 | 119.79 | 126.80 |
| 55 | PTR1 | 23 | A | C5-C6-N6 | 10.01 | 131.71 | 123.70 |
| 22 | 23S1 | 348 | A | C5-C6-N6 | 10.01 | 131.71 | 123.70 |
| 22 | 23S1 | 1244 | A | N3-C4-C5 | -10.01 | 119.79 | 126.80 |
| 22 | 23S1 | 2425 | A | N3-C4-C5 | -10.01 | 119.79 | 126.80 |
| 22 | 23S1 | 2434 | A | N3-C4-C5 | -10.01 | 119.79 | 126.80 |
| 1 | 16S1 | 1429 | A | N3-C4-C5 | -10.01 | 119.79 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22 | 23S1 | 2792 | A | N3-C4-C5 | -10.01 | 119.79 | 126.80 |
| 1 | 16S1 | 189 | A | N3-C4-C5 | -10.01 | 119.79 | 126.80 |
| 22 | 23S1 | 936 | A | N3-C4-C5 | -10.01 | 119.79 | 126.80 |
| 1 | 16S1 | 629 | A | N3-C4-C5 | -10.01 | 119.80 | 126.80 |
| 1 | 16S1 | 873 | A | C5-C6-N6 | 10.01 | 131.70 | 123.70 |
| 1 | 16S1 | 1036 | A | N3-C4-C5 | -10.01 | 119.80 | 126.80 |
| 1 | 16S1 | 1306 | A | C5-C6-N6 | 10.01 | 131.71 | 123.70 |
| 1 | 16S1 | 1534 | A | N7-C8-N9 | -10.00 | 108.80 | 113.80 |
| 1 | 16S1 | 72 | A | N3-C4-C5 | -10.00 | 119.80 | 126.80 |
| 1 | 16S1 | 282 | A | N3-C4-C5 | -10.00 | 119.80 | 126.80 |
| 1 | 16S1 | 1102 | A | C5-C6-N6 | 10.00 | 131.70 | 123.70 |
| 22 | 23S1 | 1987 | A | N3-C4-C5 | -10.00 | 119.80 | 126.80 |
| 55 | PTR1 | 58 | A | N3-C4-C5 | -10.00 | 119.80 | 126.80 |
| 1 | 16S1 | 397 | A | N3-C4-N9 | 9.99 | 135.40 | 127.40 |
| 1 | 16S1 | 306 | A | N3-C4-C5 | -9.99 | 119.81 | 126.80 |
| 22 | 23S1 | 761 | A | N3-C4-C5 | -9.99 | 119.81 | 126.80 |
| 22 | 23S1 | 980 | A | N3-C4-C5 | -9.99 | 119.80 | 126.80 |
| 22 | 23S1 | 2837 | A | N3-C4-C5 | -9.99 | 119.81 | 126.80 |
| 1 | 16S1 | 435 | A | N3-C4-C5 | -9.99 | 119.81 | 126.80 |
| 1 | 16S1 | 892 | A | N3-C4-C5 | -9.99 | 119.81 | 126.80 |
| 1 | 16S1 | 1368 | A | N3-C4-C5 | -9.99 | 119.81 | 126.80 |
| 1 | 16S1 | 1418 | A | N7-C8-N9 | -9.99 | 108.81 | 113.80 |
| 22 | 23S1 | 56 | A | N3-C4-C5 | -9.99 | 119.81 | 126.80 |
| 22 | 23S1 | 2052 | A | N3-C4-C5 | -9.99 | 119.81 | 126.80 |
| 1 | 16S1 | 66 | A | N3-C4-C5 | -9.99 | 119.81 | 126.80 |
| 1 | 16S1 | 694 | A | N3-C4-C5 | -9.99 | 119.81 | 126.80 |
| 1 | 16S1 | 174 | A | C5-C6-N6 | 9.99 | 131.69 | 123.70 |
| 1 | 16S1 | 1014 | A | C5-C6-N6 | 9.99 | 131.69 | 123.70 |
| 22 | 23S1 | 428 | A | N3-C4-C5 | -9.99 | 119.81 | 126.80 |
| 22 | 23S1 | 718 | A | N3-C4-C5 | -9.99 | 119.81 | 126.80 |
| 22 | 23S1 | 1953 | A | N3-C4-C5 | -9.99 | 119.81 | 126.80 |
| 22 | 23S1 | 2407 | A | N7-C8-N9 | -9.99 | 108.81 | 113.80 |
| 1 | 16S1 | 1081 | A | N7-C8-N9 | -9.98 | 108.81 | 113.80 |
| 55 | PTR1 | 23 | A | N3-C4-C5 | -9.98 | 119.81 | 126.80 |
| 1 | 16S1 | 1306 | A | N3-C4-C5 | -9.98 | 119.81 | 126.80 |
| 1 | 16S1 | 602 | A | N3-C4-C5 | -9.98 | 119.81 | 126.80 |
| 1 | 16S1 | 792 | A | N3-C4-C5 | -9.98 | 119.81 | 126.80 |
| 22 | 23S1 | 466 | A | N7-C8-N9 | -9.98 | 108.81 | 113.80 |
| 22 | 23S1 | 1265 | A | N7-C8-N9 | -9.98 | 108.81 | 113.80 |
| 22 | 23S1 | 1420 | A | C5-C6-N6 | 9.98 | 131.69 | 123.70 |
| 1 | 16S1 | 1080 | A | N7-C8-N9 | -9.98 | 108.81 | 113.80 |
| 22 | 23S1 | 1127 | A | N3-C4-C5 | -9.98 | 119.81 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 943 | A | N3-C4-C5 | -9.98 | 119.82 | 126.80 |
| 1 | 16S1 | 468 | A | N3-C4-C5 | -9.97 | 119.82 | 126.80 |
| 22 | 23S1 | 477 | A | N3-C4-C5 | -9.97 | 119.82 | 126.80 |
| 22 | 23S1 | 103 | A | N3-C4-C5 | -9.97 | 119.82 | 126.80 |
| 22 | 23S1 | 661 | A | N3-C4-C5 | -9.97 | 119.82 | 126.80 |
| 22 | 23S1 | 1801 | A | C5-C6-N6 | 9.97 | 131.68 | 123.70 |
| 22 | 23S1 | 2433 | A | N3-C4-C5 | -9.97 | 119.82 | 126.80 |
| 22 | 23S1 | 344 | A | C5-C6-N6 | 9.97 | 131.68 | 123.70 |
| 22 | 23S1 | 1103 | A | C5-C6-N6 | 9.97 | 131.68 | 123.70 |
| 22 | 23S1 | 1960 | A | N3-C4-C5 | -9.97 | 119.82 | 126.80 |
| 1 | 16S1 | 608 | A | N3-C4-C5 | -9.97 | 119.82 | 126.80 |
| 22 | 23S1 | 101 | A | C5-C6-N6 | 9.97 | 131.68 | 123.70 |
| 1 | 16S1 | 1191 | A | N3-C4-C5 | -9.97 | 119.82 | 126.80 |
| 1 | 16S1 | 50 | A | N3-C4-C5 | -9.96 | 119.83 | 126.80 |
| 1 | 16S1 | 228 | A | N3-C4-C5 | -9.96 | 119.82 | 126.80 |
| 1 | 16S1 | 397 | A | N7-C8-N9 | -9.97 | 108.82 | 113.80 |
| 1 | 16S1 | 630 | A | N3-C4-C5 | -9.97 | 119.82 | 126.80 |
| 1 | 16S1 | 1251 | A | N3-C4-C5 | -9.97 | 119.82 | 126.80 |
| 1 | 16S1 | 546 | A | N3-C4-C5 | -9.96 | 119.83 | 126.80 |
| 1 | 16S1 | 1252 | A | N7-C8-N9 | -9.96 | 108.82 | 113.80 |
| 22 | 23S1 | 149 | A | N7-C8-N9 | -9.96 | 108.82 | 113.80 |
| 22 | 23S1 | 299 | A | N7-C8-N9 | -9.96 | 108.82 | 113.80 |
| 22 | 23S1 | 1268 | A | N3-C4-C5 | -9.97 | 119.82 | 126.80 |
| 22 | 23S1 | 1580 | A | N3-C4-C5 | -9.96 | 119.83 | 126.80 |
| 1 | 16S1 | 320 | A | N3-C4-C5 | -9.96 | 119.83 | 126.80 |
| 22 | 23S1 | 2835 | A | N3-C4-C5 | -9.96 | 119.83 | 126.80 |
| 22 | 23S1 | 626 | A | C5-C6-N6 | 9.96 | 131.67 | 123.70 |
| 1 | 16S1 | 120 | A | C5-C6-N6 | 9.96 | 131.66 | 123.70 |
| 1 | 16S1 | 790 | A | C5-C6-N6 | 9.96 | 131.67 | 123.70 |
| 1 | 16S1 | 1394 | A | C5-C6-N6 | 9.96 | 131.67 | 123.70 |
| 22 | 23S1 | 1433 | A | N7-C8-N9 | -9.96 | 108.82 | 113.80 |
| 22 | 23S1 | 2062 | A | N7-C8-N9 | -9.96 | 108.82 | 113.80 |
| 22 | 23S1 | 2170 | A | N3-C4-C5 | -9.96 | 119.83 | 126.80 |
| 22 | 23S1 | 2600 | A | N3-C4-C5 | -9.96 | 119.83 | 126.80 |
| 1 | 16S1 | 174 | A | N3-C4-C5 | -9.96 | 119.83 | 126.80 |
| 22 | 23S1 | 2823 | A | N3-C4-C5 | -9.95 | 119.83 | 126.80 |
| 1 | 16S1 | 329 | A | C5-C6-N6 | 9.95 | 131.66 | 123.70 |
| 1 | 16S1 | 600 | A | C5-C6-N6 | 9.95 | 131.66 | 123.70 |
| 1 | 16S1 | 1299 | A | N7-C8-N9 | -9.95 | 108.82 | 113.80 |
| 22 | 23S1 | 460 | A | C5-C6-N6 | 9.95 | 131.66 | 123.70 |
| 22 | 23S1 | 980 | A | N7-C8-N9 | -9.95 | 108.82 | 113.80 |
| 22 | 23S1 | 1151 | A | C5-C6-N6 | 9.95 | 131.66 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 2247 | A | N3-C4-C5 | -9.95 | 119.83 | 126.80 |
| 1 | 16S1 | 696 | A | N3-C4-C5 | -9.95 | 119.84 | 126.80 |
| 22 | 23S1 | 654 | A | N7-C8-N9 | -9.95 | 108.83 | 113.80 |
| 22 | 23S1 | 2450 | A | N7-C8-N9 | -9.95 | 108.83 | 113.80 |
| 22 | 23S1 | 199 | A | N7-C8-N9 | -9.95 | 108.83 | 113.80 |
| 23 | 05S1 | 59 | A | N3-C4-N9 | 9.95 | 135.36 | 127.40 |
| 1 | 16S1 | 706 | A | C5-C6-N6 | 9.94 | 131.65 | 123.70 |
| 22 | 23S1 | 279 | A | N3-C4-C5 | -9.94 | 119.84 | 126.80 |
| 22 | 23S1 | 2314 | A | N3-C4-C5 | -9.94 | 119.84 | 126.80 |
| 1 | 16S1 | 559 | A | N3-C4-C5 | -9.94 | 119.84 | 126.80 |
| 1 | 16S1 | 819 | A | N7-C8-N9 | -9.94 | 108.83 | 113.80 |
| 22 | 23S1 | 627 | A | N3-C4-C5 | -9.94 | 119.84 | 126.80 |
| 22 | 23S1 | 1328 | A | N3-C4-C5 | -9.94 | 119.84 | 126.80 |
| 22 | 23S1 | 1866 | A | C5-C6-N6 | 9.94 | 131.65 | 123.70 |
| 22 | 23S1 | 927 | A | N3-C4-C5 | -9.94 | 119.84 | 126.80 |
| 1 | 16S1 | 71 | A | N3-C4-C5 | -9.94 | 119.85 | 126.80 |
| 22 | 23S1 | 384 | A | N3-C4-C5 | -9.94 | 119.84 | 126.80 |
| 22 | 23S1 | 819 | A | N7-C8-N9 | -9.94 | 108.83 | 113.80 |
| 22 | 23S1 | 1937 | A | N3-C4-C5 | -9.94 | 119.84 | 126.80 |
| 22 | 23S1 | 2560 | A | C5-C6-N6 | 9.93 | 131.65 | 123.70 |
| 1 | 16S1 | 1236 | A | N3-C4-C5 | -9.93 | 119.85 | 126.80 |
| 22 | 23S1 | 282 | A | N3-C4-C5 | -9.93 | 119.85 | 126.80 |
| 1 | 16S1 | 815 | A | C5-N7-C8 | 9.93 | 108.86 | 103.90 |
| 22 | 23S1 | 216 | A | N3-C4-C5 | -9.93 | 119.85 | 126.80 |
| 1 | 16S1 | 694 | A | C5-N7-C8 | 9.93 | 108.86 | 103.90 |
| 22 | 23S1 | 182 | A | C5-C6-N6 | 9.93 | 131.64 | 123.70 |
| 22 | 23S1 | 19 | A | C5-C6-N6 | 9.92 | 131.64 | 123.70 |
| 22 | 23S1 | 478 | A | N7-C8-N9 | -9.92 | 108.84 | 113.80 |
| 22 | 23S1 | 429 | A | N3-C4-C5 | -9.92 | 119.86 | 126.80 |
| 22 | 23S1 | 1918 | A | N7-C8-N9 | -9.92 | 108.84 | 113.80 |
| 22 | 23S1 | 2765 | A | C5-C6-N6 | 9.92 | 131.64 | 123.70 |
| 1 | 16S1 | 199 | A | C5-C6-N6 | 9.92 | 131.64 | 123.70 |
| 1 | 16S1 | 983 | A | C5-C6-N6 | 9.92 | 131.64 | 123.70 |
| 22 | 23S1 | 432 | A | N3-C4-C5 | -9.92 | 119.86 | 126.80 |
| 22 | 23S1 | 909 | A | N3-C4-C5 | -9.92 | 119.86 | 126.80 |
| 22 | 23S1 | 1553 | A | C5-C6-N6 | 9.92 | 131.64 | 123.70 |
| 22 | 23S1 | 2154 | A | C5-C6-N6 | 9.92 | 131.63 | 123.70 |
| 22 | 23S1 | 2675 | A | N3-C4-C5 | -9.92 | 119.86 | 126.80 |
| 22 | 23S1 | 2748 | A | N3-C4-C5 | -9.92 | 119.86 | 126.80 |
| 22 | 23S1 | 2335 | A | N3-C4-C5 | -9.92 | 119.86 | 126.80 |
| 1 | 16S1 | 676 | A | N3-C4-C5 | -9.92 | 119.86 | 126.80 |
| 22 | 23S1 | 947 | A | C5-C6-N6 | 9.92 | 131.63 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 2534 | A | N3-C4-C5 | -9.92 | 119.86 | 126.80 |
| 1 | 16S1 | 539 | A | N3-C4-C5 | -9.91 | 119.86 | 126.80 |
| 1 | 16S1 | 167 | A | N3-C4-C5 | -9.91 | 119.86 | 126.80 |
| 1 | 16S1 | 1507 | A | N3-C4-C5 | -9.91 | 119.86 | 126.80 |
| 22 | 23S1 | 1226 | A | N7-C8-N9 | -9.91 | 108.84 | 113.80 |
| 22 | 23S1 | 2273 | A | N7-C8-N9 | -9.91 | 108.84 | 113.80 |
| 1 | 16S1 | 900 | A | N3-C4-C5 | -9.91 | 119.86 | 126.80 |
| 22 | 23S1 | 1597 | A | N3-C4-C5 | -9.91 | 119.86 | 126.80 |
| 22 | 23S1 | 2893 | A | N3-C4-C5 | -9.91 | 119.86 | 126.80 |
| 1 | 16S1 | 1081 | A | C5-C6-N6 | 9.91 | 131.62 | 123.70 |
| 22 | 23S1 | 508 | A | N3-C4-C5 | -9.91 | 119.87 | 126.80 |
| 22 | 23S1 | 945 | A | N7-C8-N9 | -9.91 | 108.85 | 113.80 |
| 22 | 23S1 | 2478 | A | N3-C4-C5 | -9.91 | 119.86 | 126.80 |
| 22 | 23S1 | 2632 | A | N3-C4-C5 | -9.91 | 119.87 | 126.80 |
| 1 | 16S1 | 777 | A | N3-C4-C5 | -9.90 | 119.87 | 126.80 |
| 22 | 23S1 | 251 | A | C4-C5-C6 | 9.90 | 121.95 | 117.00 |
| 22 | 23S1 | 1354 | A | N3-C4-C5 | -9.90 | 119.87 | 126.80 |
| 22 | 23S1 | 2900 | A | N3-C4-C5 | -9.90 | 119.87 | 126.80 |
| 1 | 16S1 | 523 | A | N3-C4-C5 | -9.90 | 119.87 | 126.80 |
| 1 | 16S1 | 44 | A | N3-C4-C5 | -9.90 | 119.87 | 126.80 |
| 1 | 16S1 | 149 | A | N3-C4-C5 | -9.90 | 119.87 | 126.80 |
| 22 | 23S1 | 1387 | A | N7-C8-N9 | -9.90 | 108.85 | 113.80 |
| 1 | 16S1 | 1055 | A | C5-C6-N6 | 9.89 | 131.62 | 123.70 |
| 22 | 23S1 | 627 | A | C5-C6-N6 | 9.89 | 131.62 | 123.70 |
| 22 | 23S1 | 1470 | A | N3-C4-C5 | -9.89 | 119.88 | 126.80 |
| 22 | 23S1 | 2278 | A | N3-C4-C5 | -9.89 | 119.87 | 126.80 |
| 1 | 16S1 | 539 | A | C5-C6-N6 | 9.89 | 131.61 | 123.70 |
| 1 | 16S1 | 1318 | A | C5-C6-N6 | 9.89 | 131.61 | 123.70 |
| 22 | 23S1 | 928 | A | C5-C6-N6 | 9.89 | 131.61 | 123.70 |
| 22 | 23S1 | 2711 | A | N3-C4-C5 | -9.89 | 119.88 | 126.80 |
| 22 | 23S1 | 1635 | A | N3-C4-C5 | -9.89 | 119.88 | 126.80 |
| 1 | 16S1 | 935 | A | N3-C4-C5 | -9.89 | 119.88 | 126.80 |
| 22 | 23S1 | 1579 | A | C5-C6-N6 | 9.89 | 131.61 | 123.70 |
| 1 | 16S1 | 171 | A | N3-C4-C5 | -9.88 | 119.88 | 126.80 |
| 1 | 16S1 | 315 | A | N3-C4-C5 | -9.89 | 119.88 | 126.80 |
| 1 | 16S1 | 873 | A | N3-C4-C5 | -9.88 | 119.88 | 126.80 |
| 22 | 23S1 | 1048 | A | N3-C4-C5 | -9.89 | 119.88 | 126.80 |
| 22 | 23S1 | 1413 | A | N3-C4-C5 | -9.88 | 119.88 | 126.80 |
| 1 | 16S1 | 759 | A | N3-C4-C5 | -9.88 | 119.88 | 126.80 |
| 22 | 23S1 | 661 | A | C5-C6-N6 | 9.88 | 131.61 | 123.70 |
| 22 | 23S1 | 1609 | A | N3-C4-C5 | -9.88 | 119.88 | 126.80 |
| 55 | PTR1 | 69 | A | N3-C4-C5 | -9.88 | 119.88 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 1067 | A | N3-C4-C5 | -9.88 | 119.88 | 126.80 |
| 22 | 23S1 | 2734 | A | C5-C6-N6 | 9.88 | 131.61 | 123.70 |
| 22 | 23S1 | 2534 | A | C5-C6-N6 | 9.88 | 131.60 | 123.70 |
| 1 | 16S1 | 2 | A | N7-C8-N9 | -9.88 | 108.86 | 113.80 |
| 1 | 16S1 | 609 | A | N3-C4-C5 | -9.88 | 119.89 | 126.80 |
| 1 | 16S1 | 1219 | A | N7-C8-N9 | -9.88 | 108.86 | 113.80 |
| 22 | 23S1 | 477 | A | N7-C8-N9 | -9.88 | 108.86 | 113.80 |
| 22 | 23S1 | 2205 | A | N3-C4-C5 | -9.88 | 119.89 | 126.80 |
| 1 | 16S1 | 55 | A | C5-N7-C8 | 9.88 | 108.84 | 103.90 |
| 1 | 16S1 | 161 | A | C5-C6-N6 | 9.88 | 131.60 | 123.70 |
| 1 | 16S1 | 1362 | A | N3-C4-C5 | -9.87 | 119.89 | 126.80 |
| 22 | 23S1 | 1169 | A | N3-C4-C5 | -9.88 | 119.89 | 126.80 |
| 23 | 05S1 | 45 | A | N3-C4-C5 | -9.88 | 119.89 | 126.80 |
| 1 | 16S1 | 649 | A | N3-C4-C5 | -9.87 | 119.89 | 126.80 |
| 1 | 16S1 | 1418 | A | C5-C6-N6 | 9.87 | 131.60 | 123.70 |
| 22 | 23S1 | 1791 | A | C5-C6-N6 | 9.87 | 131.59 | 123.70 |
| 22 | 23S1 | 2700 | A | C5-C6-N6 | 9.87 | 131.60 | 123.70 |
| 1 | 16S1 | 974 | A | N3-C4-C5 | -9.87 | 119.89 | 126.80 |
| 22 | 23S1 | 675 | A | N3-C4-C5 | -9.87 | 119.89 | 126.80 |
| 22 | 23S1 | 1876 | A | N3-C4-C5 | -9.87 | 119.89 | 126.80 |
| 1 | 16S1 | 329 | A | N3-C4-C5 | -9.87 | 119.89 | 126.80 |
| 1 | 16S1 | 336 | A | C5-C6-N6 | 9.87 | 131.59 | 123.70 |
| 22 | 23S1 | 74 | A | N7-C8-N9 | -9.87 | 108.87 | 113.80 |
| 22 | 23S1 | 1705 | A | N3-C4-C5 | -9.87 | 119.89 | 126.80 |
| 22 | 23S1 | 2530 | A | C5-C6-N6 | 9.87 | 131.59 | 123.70 |
| 23 | 05S1 | 66 | A | C5-C6-N6 | 9.87 | 131.59 | 123.70 |
| 22 | 23S1 | 203 | A | N3-C4-C5 | -9.86 | 119.90 | 126.80 |
| 22 | 23S1 | 371 | A | N3-C4-C5 | -9.86 | 119.90 | 126.80 |
| 22 | 23S1 | 2158 | A | C5-C6-N6 | 9.86 | 131.59 | 123.70 |
| 22 | 23S1 | 2721 | A | C5-C6-N6 | 9.86 | 131.59 | 123.70 |
| 22 | 23S1 | 1503 | A | N3-C4-C5 | -9.86 | 119.90 | 126.80 |
| 22 | 23S1 | 1717 | A | C5-C6-N6 | 9.86 | 131.59 | 123.70 |
| 1 | 16S1 | 179 | A | N3-C4-C5 | -9.86 | 119.90 | 126.80 |
| 1 | 16S1 | 712 | A | C5-C6-N6 | 9.86 | 131.58 | 123.70 |
| 22 | 23S1 | 788 | A | C5-C6-N6 | 9.86 | 131.58 | 123.70 |
| 22 | 23S1 | 1354 | A | C5-C6-N6 | 9.86 | 131.58 | 123.70 |
| 22 | 23S1 | 1505 | A | N3-C4-C5 | -9.86 | 119.90 | 126.80 |
| 22 | 23S1 | 911 | A | N3-C4-C5 | -9.85 | 119.90 | 126.80 |
| 22 | 23S1 | 2019 | A | N3-C4-C5 | -9.85 | 119.90 | 126.80 |
| 1 | 16S1 | 1374 | A | C5-C6-N6 | 9.85 | 131.58 | 123.70 |
| 22 | 23S1 | 1096 | A | N3-C4-C5 | -9.85 | 119.90 | 126.80 |
| 1 | 16S1 | 780 | A | N3-C4-C5 | -9.85 | 119.91 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 2298 | A | N3-C4-C5 | -9.85 | 119.91 | 126.80 |
| 22 | 23S1 | 1308 | A | N3-C4-C5 | -9.85 | 119.91 | 126.80 |
| 22 | 23S1 | 2080 | A | N7-C8-N9 | -9.85 | 108.88 | 113.80 |
| 22 | 23S1 | 1057 | A | N3-C4-C5 | -9.85 | 119.91 | 126.80 |
| 22 | 23S1 | 2781 | A | N7-C8-N9 | -9.84 | 108.88 | 113.80 |
| 1 | 16S1 | 19 | A | C5-N7-C8 | 9.84 | 108.82 | 103.90 |
| 1 | 16S1 | 816 | A | N3-C4-C5 | -9.84 | 119.91 | 126.80 |
| 1 | 16S1 | 901 | A | C4-C5-C6 | 9.84 | 121.92 | 117.00 |
| 22 | 23S1 | 632 | A | C5-C6-N6 | 9.84 | 131.57 | 123.70 |
| 1 | 16S1 | 1434 | A | N3-C4-C5 | -9.84 | 119.92 | 126.80 |
| 22 | 23S1 | 633 | A | C5-C6-N6 | 9.84 | 131.57 | 123.70 |
| 22 | 23S1 | 1095 | A | N3-C4-C5 | -9.84 | 119.92 | 126.80 |
| 22 | 23S1 | 1144 | A | C5-C6-N6 | 9.84 | 131.57 | 123.70 |
| 22 | 23S1 | 1431 | A | C5-C6-N6 | 9.84 | 131.57 | 123.70 |
| 22 | 23S1 | 2733 | A | N3-C4-C5 | -9.83 | 119.92 | 126.80 |
| 22 | 23S1 | 1791 | A | N3-C4-C5 | -9.83 | 119.92 | 126.80 |
| 1 | 16S1 | 1035 | A | N3-C4-C5 | -9.83 | 119.92 | 126.80 |
| 1 | 16S1 | 1357 | A | C5-C6-N6 | 9.83 | 131.56 | 123.70 |
| 22 | 23S1 | 2227 | A | N3-C4-C5 | -9.83 | 119.92 | 126.80 |
| 55 | PTR1 | 73 | A | C5-C6-N6 | 9.83 | 131.56 | 123.70 |
| 22 | 23S1 | 152 | A | N3-C4-C5 | -9.83 | 119.92 | 126.80 |
| 22 | 23S1 | 2058 | A | N3-C4-C5 | -9.83 | 119.92 | 126.80 |
| 1 | 16S1 | 155 | A | C5-C6-N6 | 9.82 | 131.56 | 123.70 |
| 1 | 16S1 | 1433 | A | N3-C4-C5 | -9.82 | 119.92 | 126.80 |
| 1 | 16S1 | 782 | A | N3-C4-C5 | -9.82 | 119.92 | 126.80 |
| 22 | 23S1 | 156 | A | C5-C6-N6 | 9.82 | 131.56 | 123.70 |
| 22 | 23S1 | 182 | A | N3-C4-C5 | -9.82 | 119.92 | 126.80 |
| 1 | 16S1 | 767 | A | C5-C6-N6 | 9.82 | 131.56 | 123.70 |
| 1 | 16S1 | 101 | A | C5-C6-N6 | 9.82 | 131.56 | 123.70 |
| 1 | 16S1 | 553 | A | N3-C4-C5 | -9.82 | 119.93 | 126.80 |
| 1 | 16S1 | 1254 | A | N3-C4-C5 | -9.82 | 119.93 | 126.80 |
| 22 | 23S1 | 1701 | A | N3-C4-C5 | -9.82 | 119.93 | 126.80 |
| 22 | 23S1 | 256 | A | N3-C4-C5 | -9.82 | 119.93 | 126.80 |
| 22 | 23S1 | 960 | A | C4-C5-C6 | 9.82 | 121.91 | 117.00 |
| 22 | 23S1 | 666 | A | N3-C4-C5 | -9.81 | 119.93 | 126.80 |
| 22 | 23S1 | 2071 | A | C5-C6-N6 | 9.81 | 131.55 | 123.70 |
| 1 | 16S1 | 533 | A | C5-N7-C8 | 9.81 | 108.81 | 103.90 |
| 1 | 16S1 | 596 | A | N3-C4-C5 | -9.81 | 119.93 | 126.80 |
| 22 | 23S1 | 412 | A | N3-C4-C5 | -9.81 | 119.93 | 126.80 |
| 22 | 23S1 | 1143 | A | C5-C6-N6 | 9.81 | 131.55 | 123.70 |
| 1 | 16S1 | 28 | A | N3-C4-C5 | -9.81 | 119.93 | 126.80 |
| 1 | 16S1 | 26 | A | C5-C6-N6 | 9.81 | 131.55 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 44 | A | C5-C6-N6 | 9.81 | 131.54 | 123.70 |
| 22 | 23S1 | 1508 | A | C5-C6-N6 | 9.80 | 131.54 | 123.70 |
| 22 | 23S1 | 1549 | A | N7-C8-N9 | -9.81 | 108.90 | 113.80 |
| 22 | 23S1 | 2082 | A | C5-C6-N6 | 9.81 | 131.54 | 123.70 |
| 22 | 23S1 | 2412 | A | N3-C4-C5 | -9.81 | 119.94 | 126.80 |
| 22 | 23S1 | 2705 | A | N7-C8-N9 | -9.80 | 108.90 | 113.80 |
| 1 | 16S1 | 349 | A | C5-C6-N6 | 9.80 | 131.54 | 123.70 |
| 1 | 16S1 | 937 | A | N3-C4-C5 | -9.80 | 119.94 | 126.80 |
| 1 | 16S1 | 430 | A | C5-C6-N6 | 9.80 | 131.54 | 123.70 |
| 1 | 16S1 | 595 | A | N3-C4-C5 | -9.80 | 119.94 | 126.80 |
| 22 | 23S1 | 1801 | A | N3-C4-C5 | -9.80 | 119.94 | 126.80 |
| 22 | 23S1 | 1705 | A | C5-C6-N6 | 9.80 | 131.54 | 123.70 |
| 22 | 23S1 | 218 | A | N7-C8-N9 | -9.80 | 108.90 | 113.80 |
| 22 | 23S1 | 2879 | A | C5-C6-N6 | 9.80 | 131.54 | 123.70 |
| 22 | 23S1 | 877 | A | N3-C4-C5 | -9.80 | 119.94 | 126.80 |
| 1 | 16S1 | 98 | A | N7-C8-N9 | -9.79 | 108.90 | 113.80 |
| 1 | 16S1 | 502 | A | N7-C8-N9 | -9.79 | 108.90 | 113.80 |
| 22 | 23S1 | 2392 | A | C5-C6-N6 | 9.79 | 131.53 | 123.70 |
| 1 | 16S1 | 262 | A | N3-C4-C5 | -9.79 | 119.95 | 126.80 |
| 22 | 23S1 | 94 | A | C5-C6-N6 | 9.79 | 131.53 | 123.70 |
| 1 | 16S1 | 459 | A | N3-C4-C5 | -9.79 | 119.95 | 126.80 |
| 1 | 16S1 | 1430 | A | N3-C4-C5 | -9.79 | 119.95 | 126.80 |
| 22 | 23S1 | 374 | A | N3-C4-C5 | -9.79 | 119.95 | 126.80 |
| 22 | 23S1 | 1522 | A | N3-C4-C5 | -9.79 | 119.95 | 126.80 |
| 22 | 23S1 | 1848 | A | C5-C6-N6 | 9.79 | 131.53 | 123.70 |
| 22 | 23S1 | 2015 | A | N3-C4-C5 | -9.79 | 119.95 | 126.80 |
| 22 | 23S1 | 2176 | A | N3-C4-C5 | -9.79 | 119.95 | 126.80 |
| 1 | 16S1 | 53 | A | C5-C6-N6 | 9.79 | 131.53 | 123.70 |
| 1 | 16S1 | 1005 | A | N3-C4-C5 | -9.79 | 119.95 | 126.80 |
| 22 | 23S1 | 196 | A | N7-C8-N9 | -9.79 | 108.91 | 113.80 |
| 22 | 23S1 | 2097 | A | C5-C6-N6 | 9.79 | 131.53 | 123.70 |
| 22 | 23S1 | 792 | A | N3-C4-C5 | -9.78 | 119.95 | 126.80 |
| 22 | 23S1 | 1214 | A | N3-C4-C5 | -9.78 | 119.95 | 126.80 |
| 23 | 05S1 | 15 | A | N3-C4-C5 | -9.78 | 119.95 | 126.80 |
| 1 | 16S1 | 263 | A | C5-C6-N6 | 9.78 | 131.52 | 123.70 |
| 1 | 16S1 | 279 | A | N7-C8-N9 | -9.78 | 108.91 | 113.80 |
| 22 | 23S1 | 454 | A | N3-C4-C5 | -9.78 | 119.95 | 126.80 |
| 22 | 23S1 | 1103 | A | N3-C4-C5 | -9.78 | 119.95 | 126.80 |
| 22 | 23S1 | 1383 | A | N3-C4-C5 | -9.78 | 119.95 | 126.80 |
| 1 | 16S1 | 236 | A | N7-C8-N9 | -9.78 | 108.91 | 113.80 |
| 22 | 23S1 | 1046 | A | N3-C4-C5 | -9.78 | 119.96 | 126.80 |
| 22 | 23S1 | 1194 | A | N3-C4-C5 | -9.78 | 119.96 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 16S1 | 1042 | A | N3-C4-C5 | -9.77 | 119.96 | 126.80 |
| 1 | 16S1 | 152 | A | N7-C8-N9 | -9.77 | 108.92 | 113.80 |
| 22 | 23S1 | 1525 | A | N3-C4-C5 | -9.77 | 119.96 | 126.80 |
| 22 | 23S1 | 2660 | A | N3-C4-C5 | -9.77 | 119.96 | 126.80 |
| 1 | 16S1 | 781 | A | N3-C4-C5 | -9.76 | 119.97 | 126.80 |
| 1 | 16S1 | 909 | A | N3-C4-C5 | -9.76 | 119.97 | 126.80 |
| 22 | 23S1 | 344 | A | N3-C4-C5 | -9.76 | 119.97 | 126.80 |
| 22 | 23S1 | 1650 | A | C5-C6-N6 | 9.76 | 131.51 | 123.70 |
| 22 | 23S1 | 845 | A | N3-C4-N9 | 9.76 | 135.21 | 127.40 |
| 1 | 16S1 | 794 | A | C5-N7-C8 | 9.76 | 108.78 | 103.90 |
| 22 | 23S1 | 2268 | A | N3-C4-C5 | -9.76 | 119.97 | 126.80 |
| 22 | 23S1 | 2476 | A | C5-C6-N6 | 9.76 | 131.51 | 123.70 |
| 1 | 16S1 | 441 | A | N3-C4-C5 | -9.76 | 119.97 | 126.80 |
| 22 | 23S1 | 602 | A | C5-C6-N6 | 9.76 | 131.50 | 123.70 |
| 22 | 23S1 | 1977 | A | C5-C6-N6 | 9.76 | 131.50 | 123.70 |
| 22 | 23S1 | 2516 | A | N3-C4-C5 | -9.76 | 119.97 | 126.80 |
| 22 | 23S1 | 2033 | A | N3-C4-C5 | -9.75 | 119.97 | 126.80 |
| 1 | 16S1 | 1495 | U | N3-C2-O2 | -9.75 | 115.37 | 122.20 |
| 22 | 23S1 | 42 | A | N3-C4-C5 | -9.75 | 119.97 | 126.80 |
| 22 | 23S1 | 101 | A | N7-C8-N9 | -9.75 | 108.93 | 113.80 |
| 1 | 16S1 | 908 | A | N3-C4-C5 | -9.75 | 119.98 | 126.80 |
| 22 | 23S1 | 217 | A | N3-C4-C5 | -9.75 | 119.98 | 126.80 |
| 22 | 23S1 | 1679 | A | N3-C4-C5 | -9.75 | 119.98 | 126.80 |
| 22 | 23S1 | 1496 | A | N3-C4-C5 | -9.74 | 119.98 | 126.80 |
| 22 | 23S1 | 1735 | A | C5-C6-N6 | 9.74 | 131.50 | 123.70 |
| 22 | 23S1 | 2042 | A | N3-C4-C5 | -9.74 | 119.98 | 126.80 |
| 22 | 23S1 | 2059 | A | C5-C6-N6 | 9.74 | 131.49 | 123.70 |
| 1 | 16S1 | 520 | A | C5-N7-C8 | 9.74 | 108.77 | 103.90 |
| 1 | 16S1 | 831 | A | N3-C4-C5 | -9.74 | 119.98 | 126.80 |
| 22 | 23S1 | 685 | A | N3-C4-C5 | -9.74 | 119.98 | 126.80 |
| 1 | 16S1 | 1021 | A | N3-C4-C5 | -9.74 | 119.98 | 126.80 |
| 1 | 16S1 | 1191 | A | N7-C8-N9 | -9.74 | 108.93 | 113.80 |
| 22 | 23S1 | 2054 | A | C5-C6-N6 | 9.74 | 131.49 | 123.70 |
| 1 | 16S1 | 1261 | A | C5-C6-N6 | 9.73 | 131.49 | 123.70 |
| 22 | 23S1 | 345 | A | N3-C4-C5 | -9.73 | 119.99 | 126.80 |
| 22 | 23S1 | 761 | A | N7-C8-N9 | -9.73 | 108.93 | 113.80 |
| 22 | 23S1 | 1392 | A | N7-C8-N9 | -9.73 | 108.93 | 113.80 |
| 22 | 23S1 | 2872 | A | C4-C5-N7 | -9.73 | 105.83 | 110.70 |
| 22 | 23S1 | 2381 | A | N3-C4-C5 | -9.73 | 119.99 | 126.80 |
| 22 | 23S1 | 699 | A | N3-C4-C5 | -9.73 | 119.99 | 126.80 |
| 22 | 23S1 | 972 | A | C5-C6-N6 | 9.73 | 131.48 | 123.70 |
| 1 | 16S1 | 906 | A | N3-C4-C5 | -9.73 | 119.99 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 1912 | A | C5-N7-C8 | 9.73 | 108.76 | 103.90 |
| 22 | 23S1 | 460 | A | N3-C4-C5 | -9.72 | 119.99 | 126.80 |
| 22 | 23S1 | 1603 | A | C5-C6-N6 | 9.72 | 131.48 | 123.70 |
| 22 | 23S1 | 1936 | A | C5-C6-N6 | 9.72 | 131.48 | 123.70 |
| 22 | 23S1 | 1027 | A | C5-C6-N6 | 9.72 | 131.48 | 123.70 |
| 22 | 23S1 | 602 | A | N3-C4-C5 | -9.72 | 120.00 | 126.80 |
| 22 | 23S1 | 2090 | A | C5-C6-N6 | 9.72 | 131.48 | 123.70 |
| 22 | 23S1 | 2317 | A | N3-C4-C5 | -9.72 | 120.00 | 126.80 |
| 1 | 16S1 | 383 | A | N3-C4-N9 | 9.72 | 135.18 | 127.40 |
| 22 | 23S1 | 1745 | A | C5-C6-N6 | 9.72 | 131.47 | 123.70 |
| 22 | 23S1 | 1287 | A | N3-C4-C5 | -9.72 | 120.00 | 126.80 |
| 22 | 23S1 | 2163 | A | N3-C4-C5 | -9.72 | 120.00 | 126.80 |
| 22 | 23S1 | 2430 | A | N1-C2-N3 | -9.72 | 124.44 | 129.30 |
| 22 | 23S1 | 1900 | A | N3-C4-C5 | -9.71 | 120.00 | 126.80 |
| 22 | 23S1 | 2333 | A | N3-C4-C5 | -9.71 | 120.00 | 126.80 |
| 22 | 23S1 | 1304 | A | N3-C4-C5 | -9.71 | 120.00 | 126.80 |
| 22 | 23S1 | 2820 | A | C5-C6-N6 | 9.71 | 131.47 | 123.70 |
| 22 | 23S1 | 592 | A | N3-C4-C5 | -9.71 | 120.00 | 126.80 |
| 22 | 23S1 | 2037 | A | N3-C4-C5 | -9.71 | 120.00 | 126.80 |
| 1 | 16S1 | 523 | A | C5-C6-N6 | 9.71 | 131.47 | 123.70 |
| 22 | 23S1 | 844 | A | N3-C4-C5 | -9.71 | 120.00 | 126.80 |
| 22 | 23S1 | 1650 | A | N3-C4-C5 | -9.71 | 120.00 | 126.80 |
| 22 | 23S1 | 2705 | A | N3-C4-C5 | -9.71 | 120.00 | 126.80 |
| 55 | PTR1 | 3 | A | N3-C4-C5 | -9.71 | 120.00 | 126.80 |
| 1 | 16S1 | 969 | A | N3-C4-C5 | -9.71 | 120.01 | 126.80 |
| 22 | 23S1 | 44 | A | N3-C4-C5 | -9.70 | 120.01 | 126.80 |
| 22 | 23S1 | 111 | A | N3-C4-C5 | -9.70 | 120.01 | 126.80 |
| 22 | 23S1 | 721 | A | N3-C4-C5 | -9.71 | 120.01 | 126.80 |
| 1 | 16S1 | 1271 | A | N3-C4-C5 | -9.70 | 120.01 | 126.80 |
| 22 | 23S1 | 1548 | A | C5-C6-N6 | 9.70 | 131.46 | 123.70 |
| 1 | 16S1 | 673 | A | C5-C6-N6 | 9.70 | 131.46 | 123.70 |
| 22 | 23S1 | 900 | A | C5-C6-N6 | 9.70 | 131.46 | 123.70 |
| 22 | 23S1 | 2346 | A | N3-C4-C5 | -9.70 | 120.01 | 126.80 |
| 22 | 23S1 | 501 | A | N3-C4-C5 | -9.69 | 120.02 | 126.80 |
| 1 | 16S1 | 780 | A | N7-C8-N9 | -9.69 | 108.96 | 113.80 |
| 22 | 23S1 | 1126 | A | N7-C8-N9 | -9.69 | 108.96 | 113.80 |
| 22 | 23S1 | 2530 | A | N3-C4-C5 | -9.69 | 120.02 | 126.80 |
| 22 | 23S1 | 2589 | A | N3-C4-C5 | -9.69 | 120.02 | 126.80 |
| 22 | 23S1 | 2826 | A | N3-C4-C5 | -9.69 | 120.02 | 126.80 |
| 1 | 16S1 | 635 | A | C5-C6-N6 | 9.69 | 131.45 | 123.70 |
| 22 | 23S1 | 1772 | A | N3-C4-C5 | -9.69 | 120.02 | 126.80 |
| 1 | 16S1 | 366 | A | N3-C4-C5 | -9.68 | 120.02 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 2176 | A | C5-C6-N6 | 9.68 | 131.44 | 123.70 |
| 22 | 23S1 | 1029 | A | C5-C6-N6 | 9.68 | 131.44 | 123.70 |
| 22 | 23S1 | 1169 | A | C5-C6-N6 | 9.68 | 131.44 | 123.70 |
| 23 | 05S1 | 104 | A | N3-C4-C5 | -9.68 | 120.03 | 126.80 |
| 22 | 23S1 | 207 | A | N3-C4-C5 | -9.67 | 120.03 | 126.80 |
| 22 | 23S1 | 632 | A | N3-C4-C5 | -9.67 | 120.03 | 126.80 |
| 22 | 23S1 | 1253 | A | N7-C8-N9 | -9.67 | 108.96 | 113.80 |
| 22 | 23S1 | 1901 | A | N7-C8-N9 | -9.67 | 108.96 | 113.80 |
| 22 | 23S1 | 2856 | A | N3-C4-C5 | -9.67 | 120.03 | 126.80 |
| 1 | 16S1 | 1531 | A | N3-C4-C5 | -9.67 | 120.03 | 126.80 |
| 22 | 23S1 | 1802 | A | C5-C6-N6 | 9.67 | 131.44 | 123.70 |
| 22 | 23S1 | 2080 | A | C5-C6-N6 | 9.67 | 131.43 | 123.70 |
| 22 | 23S1 | 706 | A | N3-C4-C5 | -9.66 | 120.03 | 126.80 |
| 22 | 23S1 | 2183 | A | N3-C4-C5 | -9.66 | 120.03 | 126.80 |
| 22 | 23S1 | 1453 | A | N3-C4-C5 | -9.66 | 120.04 | 126.80 |
| 22 | 23S1 | 2386 | A | C5-C6-N6 | 9.66 | 131.43 | 123.70 |
| 1 | 16S1 | 1480 | A | N3-C4-C5 | -9.66 | 120.04 | 126.80 |
| 1 | 16S1 | 1503 | A | N3-C4-C5 | -9.66 | 120.04 | 126.80 |
| 1 | 16S1 | 1044 | A | C5-C6-N6 | 9.66 | 131.43 | 123.70 |
| 1 | 16S1 | 1350 | A | N7-C8-N9 | -9.66 | 108.97 | 113.80 |
| 1 | 16S1 | 1437 | A | N3-C4-C5 | -9.66 | 120.04 | 126.80 |
| 1 | 16S1 | 608 | A | C5-C6-N6 | 9.65 | 131.42 | 123.70 |
| 22 | 23S1 | 466 | A | N3-C4-C5 | -9.65 | 120.04 | 126.80 |
| 22 | 23S1 | 633 | A | N3-C4-C5 | -9.65 | 120.04 | 126.80 |
| 22 | 23S1 | 1264 | A | N3-C4-C5 | -9.65 | 120.04 | 126.80 |
| 22 | 23S1 | 1679 | A | N7-C8-N9 | -9.65 | 108.97 | 113.80 |
| 22 | 23S1 | 1848 | A | N3-C4-C5 | -9.65 | 120.04 | 126.80 |
| 1 | 16S1 | 1014 | A | N7-C8-N9 | -9.65 | 108.97 | 113.80 |
| 1 | 16S1 | 1324 | A | N7-C8-N9 | -9.65 | 108.97 | 113.80 |
| 22 | 23S1 | 2101 | A | N3-C4-C5 | -9.65 | 120.05 | 126.80 |
| 22 | 23S1 | 2654 | A | N3-C4-C5 | -9.65 | 120.05 | 126.80 |
| 1 | 16S1 | 1151 | A | C5-C6-N6 | 9.65 | 131.42 | 123.70 |
| 22 | 23S1 | 1090 | A | N3-C4-C5 | -9.65 | 120.05 | 126.80 |
| 22 | 23S1 | 1571 | A | N7-C8-N9 | -9.64 | 108.98 | 113.80 |
| 22 | 23S1 | 1597 | A | C5-N7-C8 | 9.64 | 108.72 | 103.90 |
| 1 | 16S1 | 1339 | A | N7-C8-N9 | -9.64 | 108.98 | 113.80 |
| 1 | 16S1 | 533 | A | C5-C6-N6 | 9.63 | 131.41 | 123.70 |
| 1 | 16S1 | 1110 | A | N7-C8-N9 | -9.64 | 108.98 | 113.80 |
| 1 | 16S1 | 964 | A | C5-C6-N6 | 9.63 | 131.41 | 123.70 |
| 1 | 16S1 | 532 | A | N3-C4-C5 | -9.63 | 120.06 | 126.80 |
| 1 | 16S1 | 1274 | A | N3-C4-C5 | -9.63 | 120.06 | 126.80 |
| 22 | 23S1 | 439 | A | C5-C6-N6 | 9.63 | 131.40 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 1640 | A | N3-C4-C5 | -9.63 | 120.06 | 126.80 |
| 22 | 23S1 | 794 | A | C5-C6-N6 | 9.62 | 131.40 | 123.70 |
| 22 | 23S1 | 2392 | A | N7-C8-N9 | -9.62 | 108.99 | 113.80 |
| 22 | 23S1 | 2577 | A | C5-N7-C8 | 9.62 | 108.71 | 103.90 |
| 1 | 16S1 | 767 | A | N3-C4-C5 | -9.62 | 120.06 | 126.80 |
| 1 | 16S1 | 1110 | A | N3-C4-C5 | -9.62 | 120.06 | 126.80 |
| 22 | 23S1 | 422 | A | N7-C8-N9 | -9.62 | 108.99 | 113.80 |
| 22 | 23S1 | 905 | A | N3-C4-C5 | -9.62 | 120.06 | 126.80 |
| 55 | PTR1 | 21 | A | N3-C4-C5 | -9.62 | 120.06 | 126.80 |
| 1 | 16S1 | 1012 | A | N3-C4-C5 | -9.62 | 120.07 | 126.80 |
| 22 | 23S1 | 1672 | A | N3-C4-C5 | -9.62 | 120.07 | 126.80 |
| 22 | 23S1 | 126 | A | N3-C4-C5 | -9.62 | 120.07 | 126.80 |
| 22 | 23S1 | 861 | A | C5-C6-N6 | 9.62 | 131.39 | 123.70 |
| 22 | 23S1 | 1509 | A | N3-C4-C5 | -9.62 | 120.07 | 126.80 |
| 1 | 16S1 | 1447 | A | N3-C4-C5 | -9.61 | 120.07 | 126.80 |
| 22 | 23S1 | 1285 | A | N3-C4-C5 | -9.61 | 120.07 | 126.80 |
| 22 | 23S1 | 727 | A | C5-C6-N6 | 9.61 | 131.39 | 123.70 |
| 22 | 23S1 | 2800 | A | C5-C6-N6 | 9.61 | 131.39 | 123.70 |
| 1 | 16S1 | 1375 | A | C5-C6-N6 | 9.61 | 131.39 | 123.70 |
| 1 | 16S1 | 1456 | A | N3-C4-C5 | -9.61 | 120.08 | 126.80 |
| 22 | 23S1 | 2736 | A | N3-C4-C5 | -9.61 | 120.08 | 126.80 |
| 1 | 16S1 | 321 | A | N3-C4-C5 | -9.60 | 120.08 | 126.80 |
| 1 | 16S1 | 994 | A | C5-C6-N6 | 9.60 | 131.38 | 123.70 |
| 22 | 23S1 | 538 | A | N3-C4-C5 | -9.60 | 120.08 | 126.80 |
| 22 | 23S1 | 83 | A | N3-C4-C5 | -9.60 | 120.08 | 126.80 |
| 22 | 23S1 | 1155 | A | N3-C4-C5 | -9.60 | 120.08 | 126.80 |
| 1 | 16S1 | 338 | A | N3-C4-C5 | -9.60 | 120.08 | 126.80 |
| 1 | 16S1 | 1213 | A | N3-C4-C5 | -9.60 | 120.08 | 126.80 |
| 22 | 23S1 | 529 | A | N3-C4-C5 | -9.60 | 120.08 | 126.80 |
| 22 | 23S1 | 2587 | A | N3-C4-C5 | -9.59 | 120.08 | 126.80 |
| 22 | 23S1 | 1165 | A | N3-C4-C5 | -9.59 | 120.09 | 126.80 |
| 23 | 05S1 | 57 | A | N3-C4-C5 | -9.59 | 120.09 | 126.80 |
| 22 | 23S1 | 1274 | A | N3-C4-C5 | -9.59 | 120.09 | 126.80 |
| 22 | 23S1 | 1254 | A | N3-C4-C5 | -9.59 | 120.09 | 126.80 |
| 22 | 23S1 | 56 | A | C5-C6-N6 | 9.58 | 131.37 | 123.70 |
| 22 | 23S1 | 1276 | A | C5-C6-N6 | 9.58 | 131.37 | 123.70 |
| 22 | 23S1 | 2662 | A | C4-C5-C6 | 9.58 | 121.79 | 117.00 |
| 22 | 23S1 | 203 | A | N7-C8-N9 | -9.58 | 109.01 | 113.80 |
| 22 | 23S1 | 1469 | A | C5-C6-N6 | 9.58 | 131.36 | 123.70 |
| 1 | 16S1 | 1055 | A | N3-C4-C5 | -9.58 | 120.10 | 126.80 |
| 1 | 16S1 | 1196 | A | N3-C4-C5 | -9.58 | 120.10 | 126.80 |
| 22 | 23S1 | 2900 | A | C5-C6-N6 | 9.58 | 131.36 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 16S1 | 374 | A | N3-C4-C5 | -9.57 | 120.10 | 126.80 |
| 1 | 16S1 | 435 | A | C5-C6-N6 | 9.57 | 131.36 | 123.70 |
| 22 | 23S1 | 2634 | A | C5-C6-N6 | 9.57 | 131.36 | 123.70 |
| 1 | 16S1 | 1288 | A | N3-C4-C5 | -9.57 | 120.10 | 126.80 |
| 22 | 23S1 | 599 | A | C5-C6-N6 | 9.57 | 131.36 | 123.70 |
| 22 | 23S1 | 94 | A | N3-C4-C5 | -9.57 | 120.10 | 126.80 |
| 22 | 23S1 | 470 | A | C5-C6-N6 | 9.57 | 131.36 | 123.70 |
| 22 | 23S1 | 2322 | A | N3-C4-C5 | -9.57 | 120.10 | 126.80 |
| 22 | 23S1 | 616 | A | N3-C4-C5 | -9.57 | 120.10 | 126.80 |
| 22 | 23S1 | 368 | A | N3-C4-C5 | -9.56 | 120.11 | 126.80 |
| 22 | 23S1 | 2868 | A | N7-C8-N9 | -9.56 | 109.02 | 113.80 |
| 1 | 16S1 | 790 | A | N3-C4-C5 | -9.56 | 120.11 | 126.80 |
| 1 | 16S1 | 977 | A | N7-C8-N9 | -9.56 | 109.02 | 113.80 |
| 22 | 23S1 | 2340 | A | N3-C4-C5 | -9.56 | 120.11 | 126.80 |
| 22 | 23S1 | 415 | A | C5-C6-N6 | 9.56 | 131.35 | 123.70 |
| 22 | 23S1 | 742 | A | C5-C6-N6 | 9.56 | 131.35 | 123.70 |
| 22 | 23S1 | 2014 | A | N3-C4-C5 | -9.56 | 120.11 | 126.80 |
| 22 | 23S1 | 2288 | A | N3-C4-C5 | -9.56 | 120.11 | 126.80 |
| 1 | 16S1 | 1080 | A | N3-C4-C5 | -9.55 | 120.11 | 126.80 |
| 1 | 16S1 | 1513 | A | N3-C4-C5 | -9.56 | 120.11 | 126.80 |
| 22 | 23S1 | 990 | A | N3-C4-C5 | -9.56 | 120.11 | 126.80 |
| 22 | 23S1 | 572 | A | N7-C8-N9 | -9.55 | 109.02 | 113.80 |
| 1 | 16S1 | 1271 | A | C5-C6-N6 | 9.55 | 131.34 | 123.70 |
| 22 | 23S1 | 1532 | A | N3-C4-C5 | -9.55 | 120.11 | 126.80 |
| 22 | 23S1 | 1871 | A | N7-C8-N9 | -9.55 | 109.03 | 113.80 |
| 22 | 23S1 | 2734 | A | N3-C4-C5 | -9.55 | 120.11 | 126.80 |
| 1 | 16S1 | 1324 | A | C5-C6-N6 | 9.55 | 131.34 | 123.70 |
| 22 | 23S1 | 173 | A | C5-C6-N6 | 9.55 | 131.34 | 123.70 |
| 22 | 23S1 | 599 | A | N3-C4-C5 | -9.55 | 120.11 | 126.80 |
| 22 | 23S1 | 1032 | A | N3-C4-C5 | -9.55 | 120.12 | 126.80 |
| 22 | 23S1 | 155 | A | C5-C6-N6 | 9.55 | 131.34 | 123.70 |
| 1 | 16S1 | 1288 | A | C5-C6-N6 | 9.54 | 131.34 | 123.70 |
| 22 | 23S1 | 483 | A | N3-C4-C5 | -9.54 | 120.12 | 126.80 |
| 22 | 23S1 | 1586 | A | C5-C6-N6 | 9.54 | 131.34 | 123.70 |
| 22 | 23S1 | 2388 | A | N3-C4-C5 | -9.54 | 120.12 | 126.80 |
| 22 | 23S1 | 2432 | A | N3-C4-C5 | -9.54 | 120.12 | 126.80 |
| 22 | 23S1 | 272 | A | C5-C6-N6 | 9.54 | 131.33 | 123.70 |
| 22 | 23S1 | 2602 | A | N3-C4-C5 | -9.54 | 120.12 | 126.80 |
| 22 | 23S1 | 2829 | A | N3-C4-C5 | -9.54 | 120.12 | 126.80 |
| 22 | 23S1 | 2886 | A | N3-C4-C5 | -9.54 | 120.12 | 126.80 |
| 22 | 23S1 | 1133 | A | N3-C4-C5 | -9.53 | 120.13 | 126.80 |
| 22 | 23S1 | 1403 | A | C5-C6-N6 | 9.53 | 131.33 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 213 | A | N3-C4-C5 | -9.53 | 120.13 | 126.80 |
| 22 | 23S1 | 278 | A | N7-C8-N9 | -9.53 | 109.03 | 113.80 |
| 22 | 23S1 | 1040 | A | N3-C4-C5 | -9.53 | 120.13 | 126.80 |
| 22 | 23S1 | 721 | A | C5-C6-N6 | 9.53 | 131.32 | 123.70 |
| 22 | 23S1 | 2426 | A | N3-C4-C5 | -9.53 | 120.13 | 126.80 |
| 22 | 23S1 | 1269 | A | N7-C8-N9 | -9.53 | 109.03 | 113.80 |
| 22 | 23S1 | 1757 | A | N3-C4-C5 | -9.53 | 120.13 | 126.80 |
| 22 | 23S1 | 1634 | A | N3-C4-C5 | -9.53 | 120.13 | 126.80 |
| 22 | 23S1 | 2850 | A | N3-C4-C5 | -9.53 | 120.13 | 126.80 |
| 1 | 16S1 | 78 | A | N7-C8-N9 | -9.52 | 109.04 | 113.80 |
| 22 | 23S1 | 1098 | A | C5-C6-N6 | 9.52 | 131.32 | 123.70 |
| 1 | 16S1 | 364 | A | N3-C4-C5 | -9.52 | 120.14 | 126.80 |
| 22 | 23S1 | 125 | A | N3-C4-C5 | -9.52 | 120.14 | 126.80 |
| 22 | 23S1 | 1970 | A | N3-C4-C5 | -9.52 | 120.14 | 126.80 |
| 23 | 05S1 | 115 | A | N3-C4-C5 | -9.52 | 120.14 | 126.80 |
| 1 | 16S1 | 983 | A | N7-C8-N9 | -9.52 | 109.04 | 113.80 |
| 22 | 23S1 | 2461 | A | C5-C6-N6 | 9.52 | 131.32 | 123.70 |
| 22 | 23S1 | 505 | A | N3-C4-C5 | -9.52 | 120.14 | 126.80 |
| 22 | 23S1 | 505 | A | C5-C6-N6 | 9.52 | 131.31 | 123.70 |
| 22 | 23S1 | 2721 | A | N3-C4-C5 | -9.52 | 120.14 | 126.80 |
| 1 | 16S1 | 363 | A | N3-C4-C5 | -9.51 | 120.14 | 126.80 |
| 1 | 16S1 | 907 | A | C5-C6-N6 | 9.51 | 131.31 | 123.70 |
| 22 | 23S1 | 342 | A | C5-C6-N6 | 9.51 | 131.31 | 123.70 |
| 1 | 16S1 | 238 | A | N3-C4-C5 | -9.51 | 120.14 | 126.80 |
| 22 | 23S1 | 1366 | A | N3-C4-C5 | -9.51 | 120.14 | 126.80 |
| 22 | 23S1 | 1387 | A | C5-C6-N6 | 9.51 | 131.31 | 123.70 |
| 22 | 23S1 | 262 | A | N3-C4-C5 | -9.51 | 120.14 | 126.80 |
| 22 | 23S1 | 2468 | A | N3-C4-C5 | -9.51 | 120.14 | 126.80 |
| 22 | 23S1 | 2266 | A | N7-C8-N9 | -9.51 | 109.05 | 113.80 |
| 23 | 05S1 | 39 | A | N3-C4-C5 | -9.51 | 120.15 | 126.80 |
| 22 | 23S1 | 716 | A | N3-C4-C5 | -9.50 | 120.15 | 126.80 |
| 22 | 23S1 | 2814 | A | N3-C4-C5 | -9.50 | 120.15 | 126.80 |
| 1 | 16S1 | 996 | A | N3-C4-C5 | -9.50 | 120.15 | 126.80 |
| 1 | 16S1 | 1483 | A | N7-C8-N9 | -9.50 | 109.05 | 113.80 |
| 22 | 23S1 | 1241 | A | C5-C6-N6 | 9.50 | 131.30 | 123.70 |
| 1 | 16S1 | 270 | A | C5-C6-N6 | 9.49 | 131.30 | 123.70 |
| 22 | 23S1 | 614 | A | N3-C4-C5 | -9.49 | 120.16 | 126.80 |
| 22 | 23S1 | 1803 | A | N7-C8-N9 | -9.49 | 109.05 | 113.80 |
| 22 | 23S1 | 1848 | A | N7-C8-N9 | -9.49 | 109.05 | 113.80 |
| 22 | 23S1 | 1885 | A | N3-C4-C5 | -9.49 | 120.15 | 126.80 |
| 1 | 16S1 | 696 | A | N7-C8-N9 | -9.49 | 109.06 | 113.80 |
| 1 | 16S1 | 1093 | A | C5-C6-N6 | 9.49 | 131.29 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 152 | A | C5-C6-N6 | 9.49 | 131.29 | 123.70 |
| 22 | 23S1 | 1711 | A | C5-C6-N6 | 9.49 | 131.29 | 123.70 |
| 1 | 16S1 | 749 | A | N3-C4-C5 | -9.48 | 120.16 | 126.80 |
| 22 | 23S1 | 144 | A | C5-C6-N6 | 9.48 | 131.29 | 123.70 |
| 22 | 23S1 | 2749 | A | N3-C4-C5 | -9.48 | 120.16 | 126.80 |
| 23 | 05S1 | 109 | A | N3-C4-C5 | -9.48 | 120.16 | 126.80 |
| 22 | 23S1 | 294 | A | N3-C4-C5 | -9.48 | 120.16 | 126.80 |
| 1 | 16S1 | 389 | A | N7-C8-N9 | -9.48 | 109.06 | 113.80 |
| 22 | 23S1 | 53 | A | N3-C4-C5 | -9.48 | 120.17 | 126.80 |
| 22 | 23S1 | 1590 | A | C5-C6-N6 | 9.48 | 131.28 | 123.70 |
| 22 | 23S1 | 2851 | A | N3-C4-C5 | -9.47 | 120.17 | 126.80 |
| 23 | 05S1 | 108 | A | N3-C4-C5 | -9.47 | 120.17 | 126.80 |
| 1 | 16S1 | 120 | A | N3-C4-C5 | -9.47 | 120.17 | 126.80 |
| 1 | 16S1 | 431 | A | N9-C4-C5 | 9.47 | 109.59 | 105.80 |
| 1 | 16S1 | 825 | A | N3-C4-C5 | -9.47 | 120.17 | 126.80 |
| 22 | 23S1 | 1528 | A | C4-C5-C6 | 9.47 | 121.74 | 117.00 |
| 22 | 23S1 | 2813 | A | N3-C4-C5 | -9.47 | 120.17 | 126.80 |
| 22 | 23S1 | 131 | A | C5-C6-N6 | 9.47 | 131.27 | 123.70 |
| 22 | 23S1 | 866 | A | N3-C4-C5 | -9.47 | 120.17 | 126.80 |
| 22 | 23S1 | 1327 | A | N3-C4-C5 | -9.47 | 120.17 | 126.80 |
| 22 | 23S1 | 226 | A | N3-C4-C5 | -9.47 | 120.17 | 126.80 |
| 22 | 23S1 | 1596 | A | N3-C4-C5 | -9.47 | 120.17 | 126.80 |
| 22 | 23S1 | 2009 | A | N3-C4-C5 | -9.47 | 120.17 | 126.80 |
| 1 | 16S1 | 1261 | A | N3-C4-C5 | -9.46 | 120.17 | 126.80 |
| 23 | 05S1 | 59 | A | C5-N7-C8 | 9.46 | 108.63 | 103.90 |
| 1 | 16S1 | 1171 | A | C5-C6-N6 | 9.46 | 131.27 | 123.70 |
| 22 | 23S1 | 1336 | A | C5-C6-N6 | 9.46 | 131.27 | 123.70 |
| 22 | 23S1 | 89 | A | C5-C6-N6 | 9.46 | 131.27 | 123.70 |
| 22 | 23S1 | 401 | A | N3-C4-C5 | -9.46 | 120.18 | 126.80 |
| 22 | 23S1 | 1626 | A | N3-C4-C5 | -9.46 | 120.18 | 126.80 |
| 1 | 16S1 | 298 | A | N3-C4-C5 | -9.46 | 120.18 | 126.80 |
| 1 | 16S1 | 465 | A | C5-C6-N6 | 9.46 | 131.27 | 123.70 |
| 22 | 23S1 | 1302 | A | N3-C4-C5 | -9.46 | 120.18 | 126.80 |
| 22 | 23S1 | 764 | A | N3-C4-C5 | -9.46 | 120.18 | 126.80 |
| 1 | 16S1 | 78 | A | C5-C6-N6 | 9.45 | 131.26 | 123.70 |
| 1 | 16S1 | 695 | A | N7-C8-N9 | -9.46 | 109.07 | 113.80 |
| 22 | 23S1 | 2119 | A | N3-C4-C5 | -9.46 | 120.18 | 126.80 |
| 1 | 16S1 | 139 | A | N3-C4-C5 | -9.45 | 120.18 | 126.80 |
| 1 | 16S1 | 1256 | A | N3-C4-C5 | -9.45 | 120.18 | 126.80 |
| 22 | 23S1 | 878 | A | N3-C4-C5 | -9.45 | 120.18 | 126.80 |
| 22 | 23S1 | 2358 | A | N3-C4-C5 | -9.45 | 120.18 | 126.80 |
| 22 | 23S1 | 1420 | A | N3-C4-C5 | -9.45 | 120.19 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 2497 | A | N7-C8-N9 | -9.45 | 109.08 | 113.80 |
| 22 | 23S1 | 1745 | A | N3-C4-C5 | -9.44 | 120.19 | 126.80 |
| 22 | 23S1 | 668 | A | N3-C4-C5 | -9.44 | 120.19 | 126.80 |
| 22 | 23S1 | 1579 | A | N3-C4-C5 | -9.44 | 120.19 | 126.80 |
| 22 | 23S1 | 2163 | A | O5'-P-OP1 | -9.44 | 97.20 | 105.70 |
| 1 | 16S1 | 1257 | A | N3-C4-C5 | -9.44 | 120.19 | 126.80 |
| 22 | 23S1 | 2614 | A | C5-C6-N6 | 9.44 | 131.25 | 123.70 |
| 22 | 23S1 | 443 | A | N3-C4-C5 | -9.44 | 120.19 | 126.80 |
| 22 | 23S1 | 911 | A | C5-C6-N6 | 9.44 | 131.25 | 123.70 |
| 22 | 23S1 | 1969 | A | N3-C4-C5 | -9.44 | 120.19 | 126.80 |
| 55 | PTR1 | 9 | A | N3-C4-C5 | -9.44 | 120.19 | 126.80 |
| 22 | 23S1 | 2516 | A | C5-C6-N6 | 9.44 | 131.25 | 123.70 |
| 22 | 23S1 | 2750 | A | N3-C4-C5 | -9.43 | 120.20 | 126.80 |
| 1 | 16S1 | 1158 | C | C2-N1-C1' | 9.43 | 129.17 | 118.80 |
| 1 | 16S1 | 1179 | A | N3-C4-C5 | -9.43 | 120.20 | 126.80 |
| 22 | 23S1 | 1054 | A | C5-C6-N6 | 9.43 | 131.24 | 123.70 |
| 22 | 23S1 | 1608 | A | N7-C8-N9 | -9.43 | 109.08 | 113.80 |
| 22 | 23S1 | 1027 | A | N3-C4-C5 | -9.43 | 120.20 | 126.80 |
| 1 | 16S1 | 1394 | A | N3-C4-C5 | -9.43 | 120.20 | 126.80 |
| 22 | 23S1 | 1069 | A | N3-C4-C5 | -9.43 | 120.20 | 126.80 |
| 22 | 23S1 | 764 | A | N7-C8-N9 | -9.42 | 109.09 | 113.80 |
| 1 | 16S1 | 119 | A | N3-C4-C5 | -9.42 | 120.21 | 126.80 |
| 1 | 16S1 | 535 | A | N3-C4-C5 | -9.42 | 120.21 | 126.80 |
| 1 | 16S1 | 787 | A | N3-C4-C5 | -9.42 | 120.21 | 126.80 |
| 1 | 16S1 | 510 | A | N3-C4-C5 | -9.41 | 120.21 | 126.80 |
| 22 | 23S1 | 502 | A | N3-C4-C5 | -9.41 | 120.21 | 126.80 |
| 22 | 23S1 | 2837 | A | C5-C6-N6 | 9.41 | 131.23 | 123.70 |
| 22 | 23S1 | 471 | A | N3-C4-C5 | -9.41 | 120.21 | 126.80 |
| 22 | 23S1 | 1698 | A | N3-C4-C5 | -9.41 | 120.21 | 126.80 |
| 1 | 16S1 | 327 | A | N3-C4-C5 | -9.41 | 120.21 | 126.80 |
| 22 | 23S1 | 655 | A | N3-C4-C5 | -9.41 | 120.21 | 126.80 |
| 22 | 23S1 | 1393 | A | N7-C8-N9 | -9.41 | 109.09 | 113.80 |
| 22 | 23S1 | 1439 | A | N3-C4-C5 | -9.41 | 120.21 | 126.80 |
| 22 | 23S1 | 1803 | A | N3-C4-C5 | -9.41 | 120.21 | 126.80 |
| 1 | 16S1 | 456 | A | N3-C4-C5 | -9.41 | 120.21 | 126.80 |
| 22 | 23S1 | 2435 | A | N3-C4-C5 | -9.41 | 120.22 | 126.80 |
| 22 | 23S1 | 1434 | A | C5-N7-C8 | 9.40 | 108.60 | 103.90 |
| 22 | 23S1 | 1630 | A | C5-N7-C8 | 9.40 | 108.60 | 103.90 |
| 22 | 23S1 | 2031 | A | C5-N7-C8 | 9.40 | 108.60 | 103.90 |
| 22 | 23S1 | 2147 | A | N3-C4-C5 | -9.40 | 120.22 | 126.80 |
| 1 | 16S1 | 495 | A | N3-C4-C5 | -9.40 | 120.22 | 126.80 |
| 22 | 23S1 | 1919 | A | N7-C8-N9 | -9.40 | 109.10 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 16S1 | 274 | A | N3-C4-C5 | -9.40 | 120.22 | 126.80 |
| 1 | 16S1 | 1227 | A | N3-C4-C5 | -9.39 | 120.22 | 126.80 |
| 22 | 23S1 | 2281 | A | C5-C6-N6 | 9.39 | 131.22 | 123.70 |
| 22 | 23S1 | 233 | A | C5-C6-N6 | 9.39 | 131.22 | 123.70 |
| 1 | 16S1 | 356 | A | C5-C6-N6 | 9.39 | 131.21 | 123.70 |
| 22 | 23S1 | 975 | A | N3-C4-C5 | -9.39 | 120.23 | 126.80 |
| 22 | 23S1 | 1286 | A | N3-C4-C5 | -9.39 | 120.23 | 126.80 |
| 22 | 23S1 | 1545 | A | N3-C4-C5 | -9.39 | 120.23 | 126.80 |
| 22 | 23S1 | 1676 | A | N3-C4-C5 | -9.39 | 120.23 | 126.80 |
| 22 | 23S1 | 1919 | A | N3-C4-C5 | -9.39 | 120.23 | 126.80 |
| 22 | 23S1 | 2378 | A | N3-C4-C5 | -9.39 | 120.23 | 126.80 |
| 22 | 23S1 | 2434 | A | N7-C8-N9 | -9.39 | 109.11 | 113.80 |
| 1 | 16S1 | 129 | A | N3-C4-C5 | -9.38 | 120.23 | 126.80 |
| 1 | 16S1 | 160 | A | N3-C4-C5 | -9.38 | 120.23 | 126.80 |
| 22 | 23S1 | 845 | A | C5-C6-N6 | 9.39 | 131.21 | 123.70 |
| 1 | 16S1 | 498 | A | N3-C4-N9 | 9.38 | 134.91 | 127.40 |
| 1 | 16S1 | 1431 | A | N3-C4-C5 | -9.38 | 120.23 | 126.80 |
| 22 | 23S1 | 14 | A | N3-C4-C5 | -9.38 | 120.23 | 126.80 |
| 22 | 23S1 | 752 | A | C5-N7-C8 | 9.38 | 108.59 | 103.90 |
| 22 | 23S1 | 1385 | A | N3-C4-C5 | -9.38 | 120.23 | 126.80 |
| 22 | 23S1 | 1010 | A | N3-C4-C5 | -9.38 | 120.24 | 126.80 |
| 1 | 16S1 | 60 | A | N3-C4-C5 | -9.37 | 120.24 | 126.80 |
| 55 | PTR1 | 21 | A | N7-C8-N9 | -9.37 | 109.11 | 113.80 |
| 22 | 23S1 | 920 | A | N3-C4-C5 | -9.37 | 120.24 | 126.80 |
| 22 | 23S1 | 2899 | A | N3-C4-C5 | -9.37 | 120.24 | 126.80 |
| 22 | 23S1 | 983 | A | N3-C4-C5 | -9.37 | 120.24 | 126.80 |
| 22 | 23S1 | 788 | A | N3-C4-C5 | -9.37 | 120.25 | 126.80 |
| 22 | 23S1 | 1717 | A | N3-C4-C5 | -9.36 | 120.25 | 126.80 |
| 22 | 23S1 | 2765 | A | N3-C4-N9 | 9.36 | 134.89 | 127.40 |
| 22 | 23S1 | 789 | A | N3-C4-C5 | -9.36 | 120.25 | 126.80 |
| 22 | 23S1 | 1785 | A | N7-C8-N9 | -9.36 | 109.12 | 113.80 |
| 1 | 16S1 | 116 | A | C5-C6-N6 | 9.36 | 131.19 | 123.70 |
| 22 | 23S1 | 1700 | A | N3-C4-C5 | -9.36 | 120.25 | 126.80 |
| 22 | 23S1 | 2882 | A | N3-C4-C5 | -9.36 | 120.25 | 126.80 |
| 22 | 23S1 | 2407 | A | C5-C6-N6 | 9.36 | 131.19 | 123.70 |
| 1 | 16S1 | 1287 | A | N3-C4-C5 | -9.36 | 120.25 | 126.80 |
| 22 | 23S1 | 2675 | A | C5-C6-N6 | 9.35 | 131.18 | 123.70 |
| 22 | 23S1 | 167 | A | N3-C4-C5 | -9.35 | 120.26 | 126.80 |
| 22 | 23S1 | 626 | A | N3-C4-C5 | -9.35 | 120.26 | 126.80 |
| 1 | 16S1 | 466 | A | N7-C8-N9 | -9.34 | 109.13 | 113.80 |
| 22 | 23S1 | 979 | A | N3-C4-C5 | -9.34 | 120.26 | 126.80 |
| 1 | 16S1 | 51 | A | N3-C4-C5 | -9.34 | 120.26 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 16S1 | 411 | A | N3-C4-C5 | -9.34 | 120.26 | 126.80 |
| 1 | 16S1 | 968 | A | N3-C4-C5 | -9.34 | 120.26 | 126.80 |
| 22 | 23S1 | 2377 | A | N3-C4-C5 | -9.34 | 120.26 | 126.80 |
| 1 | 16S1 | 309 | A | N3-C4-C5 | -9.34 | 120.27 | 126.80 |
| 22 | 23S1 | 833 | A | N7-C8-N9 | -9.34 | 109.13 | 113.80 |
| 22 | 23S1 | 1932 | A | N3-C4-C5 | -9.33 | 120.27 | 126.80 |
| 1 | 16S1 | 109 | A | N3-C4-C5 | -9.33 | 120.27 | 126.80 |
| 1 | 16S1 | 1111 | A | N3-C4-C5 | -9.33 | 120.27 | 126.80 |
| 1 | 16S1 | 1169 | A | N3-C4-C5 | -9.33 | 120.27 | 126.80 |
| 22 | 23S1 | 783 | A | N3-C4-N9 | 9.32 | 134.86 | 127.40 |
| 1 | 16S1 | 1130 | A | N3-C4-C5 | -9.32 | 120.28 | 126.80 |
| 1 | 16S1 | 1441 | A | N3-C4-C5 | -9.32 | 120.28 | 126.80 |
| 22 | 23S1 | 735 | A | N3-C4-C5 | -9.32 | 120.27 | 126.80 |
| 22 | 23S1 | 1384 | A | N3-C4-C5 | -9.32 | 120.28 | 126.80 |
| 22 | 23S1 | 1156 | A | N3-C4-C5 | -9.32 | 120.28 | 126.80 |
| 1 | 16S1 | 663 | A | C5-C6-N6 | 9.32 | 131.15 | 123.70 |
| 1 | 16S1 | 253 | A | N3-C4-C5 | -9.32 | 120.28 | 126.80 |
| 22 | 23S1 | 1085 | A | C5-N7-C8 | 9.32 | 108.56 | 103.90 |
| 22 | 23S1 | 2753 | A | N3-C4-C5 | -9.31 | 120.28 | 126.80 |
| 1 | 16S1 | 195 | A | N7-C8-N9 | -9.31 | 109.14 | 113.80 |
| 22 | 23S1 | 2158 | A | N3-C4-C5 | -9.31 | 120.28 | 126.80 |
| 22 | 23S1 | 2639 | A | N3-C4-C5 | -9.31 | 120.28 | 126.80 |
| 22 | 23S1 | 1928 | A | N3-C4-C5 | -9.31 | 120.28 | 126.80 |
| 1 | 16S1 | 1101 | A | N3-C4-C5 | -9.30 | 120.29 | 126.80 |
| 1 | 16S1 | 1150 | A | N3-C4-C5 | -9.30 | 120.29 | 126.80 |
| 22 | 23S1 | 1477 | A | N3-C4-C5 | -9.30 | 120.29 | 126.80 |
| 1 | 16S1 | 1398 | A | N3-C4-C5 | -9.30 | 120.29 | 126.80 |
| 22 | 23S1 | 63 | A | N3-C4-C5 | -9.30 | 120.29 | 126.80 |
| 22 | 23S1 | 1755 | A | N3-C4-C5 | -9.30 | 120.29 | 126.80 |
| 22 | 23S1 | 2614 | A | N7-C8-N9 | -9.30 | 109.15 | 113.80 |
| 22 | 23S1 | 2792 | A | C5-C6-N6 | 9.30 | 131.14 | 123.70 |
| 1 | 16S1 | 16 | A | C5-N7-C8 | 9.30 | 108.55 | 103.90 |
| 23 | 05S1 | 52 | A | N3-C4-C5 | -9.29 | 120.29 | 126.80 |
| 1 | 16S1 | 1019 | A | N3-C4-C5 | -9.29 | 120.30 | 126.80 |
| 22 | 23S1 | 1213 | A | C5-C6-N6 | 9.29 | 131.13 | 123.70 |
| 22 | 23S1 | 2411 | A | N3-C4-C5 | -9.29 | 120.30 | 126.80 |
| 22 | 23S1 | 1378 | A | N3-C4-C5 | -9.29 | 120.30 | 126.80 |
| 1 | 16S1 | 72 | A | C5-C6-N6 | 9.29 | 131.13 | 123.70 |
| 1 | 16S1 | 77 | A | N7-C8-N9 | -9.29 | 109.16 | 113.80 |
| 22 | 23S1 | 477 | A | C5-C6-N6 | 9.29 | 131.13 | 123.70 |
| 22 | 23S1 | 265 | A | N3-C4-C5 | -9.29 | 120.30 | 126.80 |
| 22 | 23S1 | 1086 | A | C5-N7-C8 | 9.29 | 108.54 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 89 | A | N3-C4-C5 | -9.28 | 120.30 | 126.80 |
| 22 | 23S1 | 1129 | A | N3-C4-C5 | -9.28 | 120.30 | 126.80 |
| 55 | PTR1 | 59 | A | N3-C4-C5 | -9.28 | 120.30 | 126.80 |
| 22 | 23S1 | 1028 | A | C5-C6-N6 | 9.28 | 131.12 | 123.70 |
| 22 | 23S1 | 472 | A | N3-C4-C5 | -9.27 | 120.31 | 126.80 |
| 1 | 16S1 | 131 | A | N3-C4-C5 | -9.27 | 120.31 | 126.80 |
| 22 | 23S1 | 1566 | A | N3-C4-C5 | -9.27 | 120.31 | 126.80 |
| 1 | 16S1 | 1092 | A | N3-C4-C5 | -9.27 | 120.31 | 126.80 |
| 1 | 16S1 | 1413 | A | N3-C4-C5 | -9.27 | 120.31 | 126.80 |
| 22 | 23S1 | 1580 | A | C5-C6-N6 | 9.27 | 131.12 | 123.70 |
| 22 | 23S1 | 95 | A | N3-C4-C5 | -9.27 | 120.31 | 126.80 |
| 1 | 16S1 | 66 | A | N7-C8-N9 | -9.27 | 109.17 | 113.80 |
| 22 | 23S1 | 1977 | A | N3-C4-C5 | -9.26 | 120.31 | 126.80 |
| 22 | 23S1 | 2336 | A | N3-C4-C5 | -9.26 | 120.32 | 126.80 |
| 1 | 16S1 | 336 | A | N3-C4-C5 | -9.26 | 120.32 | 126.80 |
| 22 | 23S1 | 1080 | A | C5-C6-N6 | 9.26 | 131.11 | 123.70 |
| 1 | 16S1 | 547 | A | N3-C4-C5 | -9.25 | 120.32 | 126.80 |
| 22 | 23S1 | 1630 | A | N3-C4-C5 | -9.25 | 120.32 | 126.80 |
| 22 | 23S1 | 1713 | A | N3-C4-C5 | -9.25 | 120.32 | 126.80 |
| 22 | 23S1 | 1427 | A | N3-C4-C5 | -9.25 | 120.33 | 126.80 |
| 22 | 23S1 | 1677 | A | N3-C4-C5 | -9.25 | 120.33 | 126.80 |
| 1 | 16S1 | 461 | A | N3-C4-C5 | -9.24 | 120.33 | 126.80 |
| 1 | 16S1 | 860 | A | C5-N7-C8 | 9.24 | 108.52 | 103.90 |
| 22 | 23S1 | 1393 | A | N3-C4-C5 | -9.24 | 120.33 | 126.80 |
| 1 | 16S1 | 498 | A | C5-C6-N6 | 9.24 | 131.09 | 123.70 |
| 22 | 23S1 | 1367 | A | N3-C4-C5 | -9.24 | 120.33 | 126.80 |
| 1 | 16S1 | 81 | A | N7-C8-N9 | -9.24 | 109.18 | 113.80 |
| 22 | 23S1 | 447 | A | N3-C4-C5 | -9.24 | 120.33 | 126.80 |
| 22 | 23S1 | 492 | A | N7-C8-N9 | -9.24 | 109.18 | 113.80 |
| 1 | 16S1 | 964 | A | N7-C8-N9 | -9.23 | 109.18 | 113.80 |
| 22 | 23S1 | 1815 | A | N7-C8-N9 | -9.23 | 109.18 | 113.80 |
| 22 | 23S1 | 1544 | A | N7-C8-N9 | -9.23 | 109.18 | 113.80 |
| 22 | 23S1 | 423 | A | N3-C4-C5 | -9.23 | 120.34 | 126.80 |
| 22 | 23S1 | 918 | A | N3-C4-C5 | -9.23 | 120.34 | 126.80 |
| 1 | 16S1 | 743 | A | C5-C6-N6 | 9.22 | 131.08 | 123.70 |
| 22 | 23S1 | 1936 | A | N7-C8-N9 | -9.22 | 109.19 | 113.80 |
| 1 | 16S1 | 7 | A | N3-C4-C5 | -9.22 | 120.34 | 126.80 |
| 22 | 23S1 | 522 | A | C5-C6-N6 | 9.22 | 131.08 | 123.70 |
| 23 | 05S1 | 101 | A | C4-C5-C6 | 9.22 | 121.61 | 117.00 |
| 1 | 16S1 | 520 | A | N9-C4-C5 | 9.21 | 109.49 | 105.80 |
| 1 | 16S1 | 1067 | A | N3-C4-C5 | -9.21 | 120.35 | 126.80 |
| 22 | 23S1 | 165 | A | N3-C4-C5 | -9.22 | 120.35 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 53 | A | C5-C6-N6 | 9.21 | 131.07 | 123.70 |
| 1 | 16S1 | 1213 | A | C5-N7-C8 | 9.21 | 108.51 | 103.90 |
| 22 | 23S1 | 28 | A | N3-C4-C5 | -9.21 | 120.35 | 126.80 |
| 22 | 23S1 | 492 | A | C5-C6-N6 | 9.21 | 131.07 | 123.70 |
| 22 | 23S1 | 1722 | A | C4-C5-C6 | 9.21 | 121.61 | 117.00 |
| 1 | 16S1 | 452 | A | C5-C6-N6 | 9.21 | 131.07 | 123.70 |
| 1 | 16S1 | 554 | A | C5-N7-C8 | 9.21 | 108.50 | 103.90 |
| 22 | 23S1 | 574 | A | N3-C4-C5 | -9.21 | 120.36 | 126.80 |
| 1 | 16S1 | 935 | A | C5-C6-N6 | 9.21 | 131.06 | 123.70 |
| 1 | 16S1 | 1248 | A | N3-C4-C5 | -9.20 | 120.36 | 126.80 |
| 1 | 16S1 | 411 | A | C5-C6-N6 | 9.20 | 131.06 | 123.70 |
| 1 | 16S1 | 901 | A | N7-C8-N9 | -9.20 | 109.20 | 113.80 |
| 22 | 23S1 | 575 | A | N3-C4-C5 | -9.19 | 120.36 | 126.80 |
| 22 | 23S1 | 2758 | A | N3-C4-C5 | -9.19 | 120.36 | 126.80 |
| 1 | 16S1 | 33 | A | C5-C6-N6 | 9.19 | 131.05 | 123.70 |
| 22 | 23S1 | 526 | A | N3-C4-C5 | -9.19 | 120.36 | 126.80 |
| 1 | 16S1 | 915 | A | N3-C4-C5 | -9.19 | 120.37 | 126.80 |
| 22 | 23S1 | 829 | A | N3-C4-C5 | -9.19 | 120.37 | 126.80 |
| 22 | 23S1 | 1308 | A | C5-N7-C8 | 9.19 | 108.49 | 103.90 |
| 22 | 23S1 | 1815 | A | N3-C4-C5 | -9.19 | 120.37 | 126.80 |
| 1 | 16S1 | 77 | A | C5-C6-N6 | 9.18 | 131.05 | 123.70 |
| 22 | 23S1 | 1050 | A | C5-N7-C8 | 9.18 | 108.49 | 103.90 |
| 1 | 16S1 | 533 | A | C4-C5-C6 | 9.18 | 121.59 | 117.00 |
| 22 | 23S1 | 1998 | A | C5-N7-C8 | 9.18 | 108.49 | 103.90 |
| 55 | PTR1 | 17 | U | C5-C6-N1 | -9.18 | 118.11 | 122.70 |
| 22 | 23S1 | 310 | A | N3-C4-C5 | -9.18 | 120.38 | 126.80 |
| 22 | 23S1 | 1495 | A | N3-C4-C5 | -9.18 | 120.38 | 126.80 |
| 22 | 23S1 | 1913 | A | N3-C4-C5 | -9.18 | 120.38 | 126.80 |
| 23 | 05S1 | 59 | A | C4-C5-C6 | 9.18 | 121.59 | 117.00 |
| 1 | 16S1 | 1531 | A | N7-C8-N9 | -9.18 | 109.21 | 113.80 |
| 22 | 23S1 | 1204 | A | N3-C4-C5 | -9.18 | 120.38 | 126.80 |
| 22 | 23S1 | 2469 | A | C5-C6-N6 | 9.17 | 131.04 | 123.70 |
| 1 | 16S1 | 574 | A | N3-C4-C5 | -9.17 | 120.38 | 126.80 |
| 1 | 16S1 | 1022 | A | N7-C8-N9 | -9.17 | 109.22 | 113.80 |
| 1 | 16S1 | 1152 | A | C5-C6-N6 | 9.17 | 131.04 | 123.70 |
| 1 | 16S1 | 1250 | A | N3-C4-C5 | -9.17 | 120.38 | 126.80 |
| 1 | 16S1 | 865 | A | N7-C8-N9 | -9.17 | 109.22 | 113.80 |
| 1 | 16S1 | 1340 | A | N3-C4-C5 | -9.17 | 120.38 | 126.80 |
| 22 | 23S1 | 1669 | A | N7-C8-N9 | -9.17 | 109.22 | 113.80 |
| 1 | 16S1 | 162 | A | N3-C4-N9 | 9.16 | 134.73 | 127.40 |
| 22 | 23S1 | 544 | C | N1-C2-O2 | 9.16 | 124.40 | 118.90 |
| 22 | 23S1 | 2451 | A | N3-C4-C5 | -9.16 | 120.39 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 2706 | A | C5-C6-N6 | 9.16 | 131.03 | 123.70 |
| 22 | 23S1 | 637 | A | N3-C4-C5 | -9.16 | 120.39 | 126.80 |
| 22 | 23S1 | 1785 | A | N3-C4-C5 | -9.16 | 120.39 | 126.80 |
| 22 | 23S1 | 2088 | A | C5-C6-N6 | 9.16 | 131.03 | 123.70 |
| 22 | 23S1 | 2726 | A | N3-C4-C5 | -9.16 | 120.39 | 126.80 |
| 1 | 16S1 | 978 | A | N3-C4-C5 | -9.15 | 120.39 | 126.80 |
| 22 | 23S1 | 1494 | A | N3-C4-C5 | -9.15 | 120.39 | 126.80 |
| 22 | 23S1 | 515 | A | N3-C4-C5 | -9.15 | 120.39 | 126.80 |
| 1 | 16S1 | 182 | A | N3-C4-C5 | -9.15 | 120.39 | 126.80 |
| 1 | 16S1 | 344 | A | N3-C4-C5 | -9.15 | 120.39 | 126.80 |
| 22 | 23S1 | 1739 | A | N7-C8-N9 | -9.14 | 109.23 | 113.80 |
| 1 | 16S1 | 1285 | A | N3-C4-C5 | -9.14 | 120.40 | 126.80 |
| 22 | 23S1 | 1787 | A | N7-C8-N9 | -9.14 | 109.23 | 113.80 |
| 22 | 23S1 | 1890 | A | N3-C4-C5 | -9.14 | 120.40 | 126.80 |
| 1 | 16S1 | 1 | A | N3-C4-C5 | -9.14 | 120.40 | 126.80 |
| 1 | 16S1 | 675 | A | N3-C4-C5 | -9.13 | 120.41 | 126.80 |
| 22 | 23S1 | 497 | A | N3-C4-C5 | -9.13 | 120.41 | 126.80 |
| 22 | 23S1 | 2171 | A | N3-C4-C5 | -9.13 | 120.41 | 126.80 |
| 22 | 23S1 | 482 | A | C4-C5-C6 | 9.13 | 121.56 | 117.00 |
| 1 | 16S1 | 349 | A | N3-C4-C5 | -9.13 | 120.41 | 126.80 |
| 22 | 23S1 | 751 | A | N3-C4-C5 | -9.13 | 120.41 | 126.80 |
| 22 | 23S1 | 2439 | A | N3-C4-C5 | -9.13 | 120.41 | 126.80 |
| 22 | 23S1 | 1690 | A | N3-C4-C5 | -9.12 | 120.41 | 126.80 |
| 1 | 16S1 | 8 | A | N3-C4-C5 | -9.12 | 120.42 | 126.80 |
| 22 | 23S1 | 1504 | A | N3-C4-C5 | -9.12 | 120.42 | 126.80 |
| 22 | 23S1 | 1783 | A | N3-C4-C5 | -9.12 | 120.42 | 126.80 |
| 1 | 16S1 | 1167 | A | N3-C4-C5 | -9.11 | 120.42 | 126.80 |
| 1 | 16S1 | 1493 | A | N3-C4-C5 | -9.11 | 120.42 | 126.80 |
| 1 | 16S1 | 303 | A | N3-C4-C5 | -9.11 | 120.42 | 126.80 |
| 22 | 23S1 | 1938 | A | N3-C4-C5 | -9.11 | 120.43 | 126.80 |
| 1 | 16S1 | 1408 | A | N3-C4-C5 | -9.10 | 120.43 | 126.80 |
| 22 | 23S1 | 603 | A | N3-C4-C5 | -9.10 | 120.43 | 126.80 |
| 22 | 23S1 | 2899 | A | C5-C6-N6 | 9.10 | 130.98 | 123.70 |
| 22 | 23S1 | 503 | A | C5-C6-N6 | 9.09 | 130.97 | 123.70 |
| 1 | 16S1 | 489 | C | C2-N1-C1' | 9.09 | 128.80 | 118.80 |
| 22 | 23S1 | 1583 | A | N3-C4-C5 | -9.09 | 120.44 | 126.80 |
| 22 | 23S1 | 213 | A | C5-C6-N6 | 9.09 | 130.97 | 123.70 |
| 22 | 23S1 | 479 | A | N3-C4-C5 | -9.09 | 120.44 | 126.80 |
| 22 | 23S1 | 2198 | A | N3-C4-C5 | -9.09 | 120.44 | 126.80 |
| 22 | 23S1 | 727 | A | N3-C4-C5 | -9.09 | 120.44 | 126.80 |
| 22 | 23S1 | 1029 | A | N7-C8-N9 | -9.09 | 109.26 | 113.80 |
| 1 | 16S1 | 461 | A | C5-C6-N6 | 9.08 | 130.97 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 896 | A | N3-C4-C5 | -9.08 | 120.44 | 126.80 |
| 22 | 23S1 | 2711 | A | C5-N7-C8 | 9.08 | 108.44 | 103.90 |
| 55 | PTR1 | 69 | A | C5-C6-N6 | 9.08 | 130.97 | 123.70 |
| 22 | 23S1 | 270 | A | N3-C4-C5 | -9.08 | 120.44 | 126.80 |
| 22 | 23S1 | 1616 | A | N3-C4-C5 | -9.08 | 120.44 | 126.80 |
| 22 | 23S1 | 1853 | A | N3-C4-C5 | -9.07 | 120.45 | 126.80 |
| 22 | 23S1 | 2706 | A | N7-C8-N9 | -9.07 | 109.26 | 113.80 |
| 23 | 05S1 | 66 | A | N3-C4-C5 | -9.07 | 120.45 | 126.80 |
| 1 | 16S1 | 687 | A | N3-C4-C5 | -9.07 | 120.45 | 126.80 |
| 22 | 23S1 | 1313 | U | C2-N1-C1' | 9.07 | 128.58 | 117.70 |
| 1 | 16S1 | 949 | A | C5-N7-C8 | 9.06 | 108.43 | 103.90 |
| 1 | 16S1 | 1016 | A | N3-C4-C5 | -9.06 | 120.46 | 126.80 |
| 22 | 23S1 | 1700 | A | C5-N7-C8 | 9.06 | 108.43 | 103.90 |
| 1 | 16S1 | 1201 | A | C5-C6-N1 | 9.06 | 122.23 | 117.70 |
| 22 | 23S1 | 2297 | A | C5-N7-C8 | 9.06 | 108.43 | 103.90 |
| 29 | L091 | 122 | LEU | CA-CB-CG | 9.06 | 136.13 | 115.30 |
| 1 | 16S1 | 250 | A | N3-C4-C5 | -9.06 | 120.46 | 126.80 |
| 22 | 23S1 | 2005 | A | N3-C4-C5 | -9.05 | 120.46 | 126.80 |
| 1 | 16S1 | 1188 | A | N3-C4-C5 | -9.05 | 120.47 | 126.80 |
| 1 | 16S1 | 246 | A | N3-C4-C5 | -9.05 | 120.47 | 126.80 |
| 22 | 23S1 | 2453 | A | C5-N7-C8 | 9.05 | 108.42 | 103.90 |
| 22 | 23S1 | 2632 | A | C5-N7-C8 | 9.05 | 108.42 | 103.90 |
| 23 | 05S1 | 78 | A | N3-C4-C5 | -9.04 | 120.47 | 126.80 |
| 23 | 05S1 | 94 | A | C5-C6-N6 | 9.05 | 130.94 | 123.70 |
| 22 | 23S1 | 1008 | A | N3-C4-C5 | -9.04 | 120.47 | 126.80 |
| 22 | 23S1 | 2682 | A | N3-C4-C5 | -9.04 | 120.47 | 126.80 |
| 22 | 23S1 | 2820 | A | N3-C4-C5 | -9.04 | 120.47 | 126.80 |
| 22 | 23S1 | 800 | A | N3-C4-C5 | -9.04 | 120.47 | 126.80 |
| 22 | 23S1 | 1434 | A | N9-C4-C5 | 9.03 | 109.41 | 105.80 |
| 22 | 23S1 | 1872 | A | C5-C6-N6 | 9.03 | 130.93 | 123.70 |
| 1 | 16S1 | 1000 | A | C5-C6-N6 | 9.03 | 130.92 | 123.70 |
| 22 | 23S1 | 449 | A | C5-N7-C8 | 9.03 | 108.41 | 103.90 |
| 22 | 23S1 | 2564 | A | N3-C4-C5 | -9.03 | 120.48 | 126.80 |
| 22 | 23S1 | 676 | A | N3-C4-C5 | -9.03 | 120.48 | 126.80 |
| 55 | PTR1 | 51 | A | N3-C4-C5 | -9.03 | 120.48 | 126.80 |
| 1 | 16S1 | 554 | A | N9-C4-C5 | 9.02 | 109.41 | 105.80 |
| 22 | 23S1 | 1284 | A | N3-C4-C5 | -9.02 | 120.48 | 126.80 |
| 22 | 23S1 | 1854 | A | N7-C8-N9 | -9.02 | 109.29 | 113.80 |
| 1 | 16S1 | 496 | A | N7-C8-N9 | -9.02 | 109.29 | 113.80 |
| 1 | 16S1 | 1500 | A | N3-C4-C5 | -9.02 | 120.49 | 126.80 |
| 22 | 23S1 | 1143 | A | N3-C4-C5 | -9.02 | 120.49 | 126.80 |
| 1 | 16S1 | 889 | A | N3-C4-C5 | -9.02 | 120.49 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 1021 | A | N3-C4-N9 | 9.02 | 134.61 | 127.40 |
| 22 | 23S1 | 1937 | A | N9-C4-C5 | 9.02 | 109.41 | 105.80 |
| 22 | 23S1 | 49 | A | C5-N7-C8 | 9.01 | 108.41 | 103.90 |
| 55 | PTR1 | 58 | A | C5-N7-C8 | 9.01 | 108.40 | 103.90 |
| 22 | 23S1 | 730 | A | C5-C6-N6 | 9.00 | 130.90 | 123.70 |
| 22 | 23S1 | 2274 | A | N3-C4-C5 | -9.00 | 120.50 | 126.80 |
| 1 | 16S1 | 300 | A | N3-C4-N9 | 9.00 | 134.60 | 127.40 |
| 22 | 23S1 | 1434 | A | N3-C4-C5 | -9.00 | 120.50 | 126.80 |
| 1 | 16S1 | 802 | A | N3-C4-C5 | -9.00 | 120.50 | 126.80 |
| 22 | 23S1 | 1088 | A | C5-N7-C8 | 9.00 | 108.40 | 103.90 |
| 1 | 16S1 | 715 | A | N3-C4-C5 | -8.99 | 120.50 | 126.80 |
| 22 | 23S1 | 118 | A | N3-C4-C5 | -8.99 | 120.50 | 126.80 |
| 22 | 23S1 | 973 | A | N3-C4-C5 | -8.99 | 120.50 | 126.80 |
| 22 | 23S1 | 643 | A | N3-C4-C5 | -8.99 | 120.51 | 126.80 |
| 22 | 23S1 | 2725 | A | C5-C6-N6 | 8.99 | 130.89 | 123.70 |
| 23 | 05S1 | 53 | A | N3-C4-C5 | -8.99 | 120.51 | 126.80 |
| 22 | 23S1 | 2077 | A | C5-C6-N6 | 8.98 | 130.89 | 123.70 |
| 23 | 05S1 | 75 | G | C6-N1-C2 | -8.98 | 119.71 | 125.10 |
| 1 | 16S1 | 1219 | A | C5-C6-N6 | 8.97 | 130.88 | 123.70 |
| 1 | 16S1 | 300 | A | N1-C6-N6 | -8.97 | 113.22 | 118.60 |
| 22 | 23S1 | 322 | A | N3-C4-C5 | -8.97 | 120.52 | 126.80 |
| 1 | 16S1 | 190 | A | N3-C4-N9 | 8.96 | 134.57 | 127.40 |
| 22 | 23S1 | 1655 | A | C5-N7-C8 | 8.96 | 108.38 | 103.90 |
| 22 | 23S1 | 2298 | A | C5-N7-C8 | 8.96 | 108.38 | 103.90 |
| 22 | 23S1 | 2766 | A | N3-C4-N9 | 8.96 | 134.56 | 127.40 |
| 1 | 16S1 | 1227 | A | C5-C6-N6 | 8.96 | 130.86 | 123.70 |
| 22 | 23S1 | 820 | A | C5-C6-N6 | 8.96 | 130.87 | 123.70 |
| 22 | 23S1 | 1395 | A | N3-C4-C5 | -8.96 | 120.53 | 126.80 |
| 22 | 23S1 | 2764 | A | N3-C4-C5 | -8.96 | 120.53 | 126.80 |
| 22 | 23S1 | 2369 | A | C5-C6-N6 | 8.95 | 130.86 | 123.70 |
| 22 | 23S1 | 2572 | A | N3-C4-C5 | -8.95 | 120.53 | 126.80 |
| 1 | 16S1 | 704 | A | N3-C4-C5 | -8.95 | 120.54 | 126.80 |
| 22 | 23S1 | 1678 | A | N3-C4-C5 | -8.95 | 120.54 | 126.80 |
| 22 | 23S1 | 1572 | A | C5-C6-N6 | 8.95 | 130.86 | 123.70 |
| 22 | 23S1 | 1821 | A | N3-C4-C5 | -8.95 | 120.54 | 126.80 |
| 1 | 16S1 | 1339 | A | C5-C6-N6 | 8.94 | 130.85 | 123.70 |
| 1 | 16S1 | 152 | A | N3-C4-C5 | -8.93 | 120.55 | 126.80 |
| 22 | 23S1 | 960 | A | N7-C8-N9 | -8.93 | 109.34 | 113.80 |
| 22 | 23S1 | 1676 | A | N7-C8-N9 | -8.93 | 109.33 | 113.80 |
| 22 | 23S1 | 2602 | A | C5-N7-C8 | 8.93 | 108.36 | 103.90 |
| 1 | 16S1 | 1363 | A | C5-N7-C8 | 8.93 | 108.36 | 103.90 |
| 22 | 23S1 | 547 | A | N3-C4-C5 | -8.93 | 120.55 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 101 | A | N3-C4-N9 | 8.92 | 134.53 | 127.40 |
| 22 | 23S1 | 1570 | A | N3-C4-C5 | -8.92 | 120.56 | 126.80 |
| 22 | 23S1 | 2590 | A | C5-N7-C8 | 8.92 | 108.36 | 103.90 |
| 22 | 23S1 | 340 | A | C5-N7-C8 | 8.91 | 108.36 | 103.90 |
| 22 | 23S1 | 2887 | A | N3-C4-C5 | -8.91 | 120.56 | 126.80 |
| 22 | 23S1 | 586 | A | N7-C8-N9 | -8.91 | 109.35 | 113.80 |
| 22 | 23S1 | 2598 | A | N3-C4-C5 | -8.91 | 120.57 | 126.80 |
| 1 | 16S1 | 365 | U | C5-C4-O4 | 8.90 | 131.24 | 125.90 |
| 1 | 16S1 | 197 | A | N3-C4-C5 | -8.90 | 120.57 | 126.80 |
| 1 | 16S1 | 432 | A | C5-N7-C8 | 8.90 | 108.35 | 103.90 |
| 22 | 23S1 | 270 | A | C5-N7-C8 | 8.90 | 108.35 | 103.90 |
| 1 | 16S1 | 460 | A | C5-C6-N6 | 8.90 | 130.82 | 123.70 |
| 22 | 23S1 | 2309 | A | N3-C4-C5 | -8.90 | 120.57 | 126.80 |
| 1 | 16S1 | 563 | A | N3-C4-N9 | 8.89 | 134.51 | 127.40 |
| 1 | 16S1 | 1503 | A | C5-N7-C8 | 8.89 | 108.34 | 103.90 |
| 22 | 23S1 | 2311 | A | C5-N7-C8 | 8.89 | 108.34 | 103.90 |
| 22 | 23S1 | 2388 | A | C5-N7-C8 | 8.89 | 108.34 | 103.90 |
| 22 | 23S1 | 2406 | A | N3-C4-C5 | -8.89 | 120.58 | 126.80 |
| 22 | 23S1 | 2430 | A | C4-C5-C6 | 8.89 | 121.44 | 117.00 |
| 1 | 16S1 | 572 | A | C5-N7-C8 | 8.88 | 108.34 | 103.90 |
| 1 | 16S1 | 1441 | A | C5-N7-C8 | 8.88 | 108.34 | 103.90 |
| 22 | 23S1 | 1970 | A | C5-C6-N6 | 8.88 | 130.81 | 123.70 |
| 55 | PTR1 | 73 | A | N3-C4-C5 | -8.88 | 120.58 | 126.80 |
| 23 | 05S1 | 46 | A | N3-C4-C5 | -8.88 | 120.59 | 126.80 |
| 22 | 23S1 | 1077 | A | N3-C4-C5 | -8.87 | 120.59 | 126.80 |
| 1 | 16S1 | 533 | A | N3-C4-N9 | 8.87 | 134.50 | 127.40 |
| 22 | 23S1 | 844 | A | C5-C6-N6 | 8.87 | 130.80 | 123.70 |
| 22 | 23S1 | 2095 | A | N3-C4-C5 | -8.87 | 120.59 | 126.80 |
| 1 | 16S1 | 16 | A | N3-C4-C5 | -8.87 | 120.59 | 126.80 |
| 1 | 16S1 | 161 | A | N7-C8-N9 | -8.86 | 109.37 | 113.80 |
| 22 | 23S1 | 673 | C | C2-N3-C4 | -8.86 | 115.47 | 119.90 |
| 22 | 23S1 | 2837 | A | C5-N7-C8 | 8.86 | 108.33 | 103.90 |
| 1 | 16S1 | 1004 | A | C4-C5-N7 | -8.86 | 106.27 | 110.70 |
| 22 | 23S1 | 2426 | A | C5-C6-N6 | 8.86 | 130.79 | 123.70 |
| 1 | 16S1 | 1502 | A | N3-C4-C5 | -8.86 | 120.60 | 126.80 |
| 55 | PTR1 | 14 | A | C4-C5-C6 | 8.86 | 121.43 | 117.00 |
| 22 | 23S1 | 621 | A | N3-C4-C5 | -8.85 | 120.60 | 126.80 |
| 22 | 23S1 | 2114 | A | N3-C4-N9 | 8.85 | 134.48 | 127.40 |
| 1 | 16S1 | 923 | A | N7-C8-N9 | -8.85 | 109.38 | 113.80 |
| 22 | 23S1 | 1791 | A | N7-C8-N9 | -8.84 | 109.38 | 113.80 |
| 22 | 23S1 | 2741 | A | N3-C4-C5 | -8.84 | 120.61 | 126.80 |
| 1 | 16S1 | 1332 | A | N7-C8-N9 | -8.84 | 109.38 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 23 | 05S1 | 119 | A | C5-N7-C8 | 8.84 | 108.32 | 103.90 |
| 22 | 23S1 | 693 | A | C5-C6-N6 | 8.84 | 130.77 | 123.70 |
| 22 | 23S1 | 2227 | A | C5-N7-C8 | 8.84 | 108.32 | 103.90 |
| 22 | 23S1 | 863 | A | C5-C6-N6 | 8.83 | 130.77 | 123.70 |
| 1 | 16S1 | 44 | A | C5-N7-C8 | 8.83 | 108.31 | 103.90 |
| 22 | 23S1 | 910 | A | C5-N7-C8 | 8.83 | 108.31 | 103.90 |
| 22 | 23S1 | 1569 | A | N3-C4-C5 | -8.83 | 120.62 | 126.80 |
| 22 | 23S1 | 1237 | A | N3-C4-C5 | -8.83 | 120.62 | 126.80 |
| 22 | 23S1 | 2435 | A | C5-N7-C8 | 8.83 | 108.31 | 103.90 |
| 1 | 16S1 | 130 | A | C5-N7-C8 | 8.82 | 108.31 | 103.90 |
| 22 | 23S1 | 749 | A | N3-C4-C5 | -8.82 | 120.62 | 126.80 |
| 22 | 23S1 | 2572 | A | C5-N7-C8 | 8.81 | 108.31 | 103.90 |
| 1 | 16S1 | 545 | C | C6-N1-C2 | -8.81 | 116.78 | 120.30 |
| 1 | 16S1 | 3 | A | N3-C4-C5 | -8.81 | 120.63 | 126.80 |
| 1 | 16S1 | 243 | A | N3-C4-C5 | -8.81 | 120.64 | 126.80 |
| 1 | 16S1 | 1170 | A | C5-N7-C8 | 8.81 | 108.30 | 103.90 |
| 22 | 23S1 | 1580 | A | C5-N7-C8 | 8.81 | 108.30 | 103.90 |
| 23 | 05S1 | 101 | A | C5-N7-C8 | 8.81 | 108.30 | 103.90 |
| 55 | PTR1 | 26 | A | N3-C4-C5 | -8.81 | 120.63 | 126.80 |
| 1 | 16S1 | 596 | A | C5-N7-C8 | 8.80 | 108.30 | 103.90 |
| 22 | 23S1 | 2340 | A | C5-C6-N6 | 8.81 | 130.75 | 123.70 |
| 22 | 23S1 | 38 | A | C5-N7-C8 | 8.80 | 108.30 | 103.90 |
| 22 | 23S1 | 371 | A | C5-N7-C8 | 8.80 | 108.30 | 103.90 |
| 22 | 23S1 | 1342 | A | N3-C4-C5 | -8.80 | 120.64 | 126.80 |
| 22 | 23S1 | 1508 | A | N3-C4-C5 | -8.80 | 120.64 | 126.80 |
| 1 | 16S1 | 583 | A | N3-C4-C5 | -8.80 | 120.64 | 126.80 |
| 1 | 16S1 | 1413 | A | C5-N7-C8 | 8.79 | 108.30 | 103.90 |
| 22 | 23S1 | 1322 | A | N3-C4-C5 | -8.79 | 120.64 | 126.80 |
| 22 | 23S1 | 2094 | A | C5-C6-N6 | 8.79 | 130.74 | 123.70 |
| 22 | 23S1 | 227 | A | N3-C4-C5 | -8.79 | 120.64 | 126.80 |
| 1 | 16S1 | 1117 | A | N3-C4-C5 | -8.79 | 120.65 | 126.80 |
| 22 | 23S1 | 2766 | A | C5-C6-N6 | 8.79 | 130.73 | 123.70 |
| 22 | 23S1 | 1226 | A | N3-C4-C5 | -8.79 | 120.65 | 126.80 |
| 22 | 23S1 | 1614 | A | N3-C4-C5 | -8.79 | 120.65 | 126.80 |
| 22 | 23S1 | 332 | A | N3-C4-C5 | -8.78 | 120.65 | 126.80 |
| 1 | 16S1 | 179 | A | C5-N7-C8 | 8.78 | 108.29 | 103.90 |
| 22 | 23S1 | 1304 | A | C5-N7-C8 | 8.78 | 108.29 | 103.90 |
| 22 | 23S1 | 2169 | A | C5-N7-C8 | 8.78 | 108.29 | 103.90 |
| 1 | 16S1 | 353 | A | N3-C4-C5 | -8.78 | 120.66 | 126.80 |
| 22 | 23S1 | 1652 | A | C5-N7-C8 | 8.77 | 108.28 | 103.90 |
| 22 | 23S1 | 223 | A | N3-C4-C5 | -8.76 | 120.67 | 126.80 |
| 1 | 16S1 | 49 | U | C5-C4-O4 | 8.76 | 131.16 | 125.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 16S1 | 1507 | A | C5-C6-N6 | 8.76 | 130.71 | 123.70 |
| 22 | 23S1 | 1469 | A | C5-N7-C8 | 8.76 | 108.28 | 103.90 |
| 22 | 23S1 | 1829 | A | C5-N7-C8 | 8.76 | 108.28 | 103.90 |
| 22 | 23S1 | 1111 | A | C5-N7-C8 | 8.75 | 108.28 | 103.90 |
| 22 | 23S1 | 1359 | A | N3-C4-C5 | -8.75 | 120.67 | 126.80 |
| 22 | 23S1 | 1241 | A | C4-C5-C6 | 8.75 | 121.38 | 117.00 |
| 1 | 16S1 | 1289 | A | N3-C4-C5 | -8.75 | 120.67 | 126.80 |
| 22 | 23S1 | 825 | A | C5-N7-C8 | 8.75 | 108.27 | 103.90 |
| 1 | 16S1 | 468 | A | C5-N7-C8 | 8.74 | 108.27 | 103.90 |
| 1 | 16S1 | 554 | A | N3-C4-C5 | -8.74 | 120.68 | 126.80 |
| 1 | 16S1 | 782 | A | C5-N7-C8 | 8.74 | 108.27 | 103.90 |
| 1 | 16S1 | 1239 | A | N3-C4-C5 | -8.74 | 120.68 | 126.80 |
| 22 | 23S1 | 2430 | A | N3-C4-C5 | -8.74 | 120.68 | 126.80 |
| 22 | 23S1 | 2850 | A | C5-N7-C8 | 8.74 | 108.27 | 103.90 |
| 1 | 16S1 | 143 | A | N3-C4-C5 | -8.74 | 120.68 | 126.80 |
| 1 | 16S1 | 279 | A | N3-C4-C5 | -8.74 | 120.68 | 126.80 |
| 22 | 23S1 | 362 | A | N3-C4-N9 | 8.74 | 134.39 | 127.40 |
| 1 | 16S1 | 946 | A | C5-N7-C8 | 8.73 | 108.27 | 103.90 |
| 22 | 23S1 | 2469 | A | N3-C4-C5 | -8.73 | 120.69 | 126.80 |
| 22 | 23S1 | 1147 | A | C5-N7-C8 | 8.73 | 108.27 | 103.90 |
| 22 | 23S1 | 2101 | A | C5-N7-C8 | 8.73 | 108.27 | 103.90 |
| 22 | 23S1 | 2738 | A | N3-C4-C5 | -8.73 | 120.69 | 126.80 |
| 22 | 23S1 | 2590 | A | N3-C4-C5 | -8.73 | 120.69 | 126.80 |
| 22 | 23S1 | 2565 | A | N3-C4-C5 | -8.72 | 120.69 | 126.80 |
| 1 | 16S1 | 665 | A | N3-C4-C5 | -8.72 | 120.70 | 126.80 |
| 1 | 16S1 | 1499 | A | C5-N7-C8 | 8.72 | 108.26 | 103.90 |
| 55 | PTR1 | 17 | U | N1-C2-O2 | 8.72 | 128.90 | 122.80 |
| 22 | 23S1 | 402 | A | N3-C4-C5 | -8.72 | 120.70 | 126.80 |
| 1 | 16S1 | 459 | A | C5-C6-N6 | 8.71 | 130.67 | 123.70 |
| 22 | 23S1 | 1244 | A | C5-N7-C8 | 8.71 | 108.26 | 103.90 |
| 22 | 23S1 | 2270 | A | C5-N7-C8 | 8.71 | 108.26 | 103.90 |
| 1 | 16S1 | 274 | A | C5-N7-C8 | 8.71 | 108.26 | 103.90 |
| 22 | 23S1 | 586 | A | N3-C4-C5 | -8.71 | 120.70 | 126.80 |
| 22 | 23S1 | 1730 | C | C2-N1-C1' | 8.71 | 128.38 | 118.80 |
| 1 | 16S1 | 246 | A | C5-N7-C8 | 8.70 | 108.25 | 103.90 |
| 1 | 16S1 | 415 | A | C5-N7-C8 | 8.70 | 108.25 | 103.90 |
| 22 | 23S1 | 1652 | A | N3-C4-C5 | -8.70 | 120.71 | 126.80 |
| 22 | 23S1 | 2736 | A | C5-N7-C8 | 8.70 | 108.25 | 103.90 |
| 1 | 16S1 | 321 | A | C5-N7-C8 | 8.70 | 108.25 | 103.90 |
| 22 | 23S1 | 614 | A | C5-N7-C8 | 8.69 | 108.25 | 103.90 |
| 22 | 23S1 | 2542 | A | N3-C4-C5 | -8.69 | 120.72 | 126.80 |
| 22 | 23S1 | 2781 | A | N3-C4-C5 | -8.69 | 120.72 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22 | 23S1 | 981 | A | N3-C4-C5 | -8.69 | 120.72 | 126.80 |
| 1 | 16S1 | 65 | A | N3-C4-C5 | -8.69 | 120.72 | 126.80 |
| 22 | 23S1 | 1805 | A | C5-N7-C8 | 8.69 | 108.24 | 103.90 |
| 22 | 23S1 | 1669 | A | N3-C4-N9 | 8.68 | 134.34 | 127.40 |
| 22 | 23S1 | 1784 | A | N3-C4-C5 | -8.68 | 120.73 | 126.80 |
| 22 | 23S1 | 1872 | A | N3-C4-N9 | 8.68 | 134.34 | 127.40 |
| 1 | 16S1 | 502 | A | C5-C6-N6 | 8.67 | 130.64 | 123.70 |
| 1 | 16S1 | 1152 | A | N7-C8-N9 | -8.67 | 109.47 | 113.80 |
| 22 | 23S1 | 2013 | A | C5-N7-C8 | 8.66 | 108.23 | 103.90 |
| 1 | 16S1 | 309 | A | C5-N7-C8 | 8.66 | 108.23 | 103.90 |
| 22 | 23S1 | 819 | A | C5-C6-N6 | 8.66 | 130.63 | 123.70 |
| 22 | 23S1 | 1241 | A | C5-N7-C8 | 8.66 | 108.23 | 103.90 |
| 22 | 23S1 | 2660 | A | C5-N7-C8 | 8.66 | 108.23 | 103.90 |
| 22 | 23S1 | 1515 | A | N3-C4-C5 | -8.65 | 120.74 | 126.80 |
| 22 | 23S1 | 204 | A | N3-C4-C5 | -8.65 | 120.75 | 126.80 |
| 22 | 23S1 | 743 | A | N7-C8-N9 | -8.65 | 109.47 | 113.80 |
| 1 | 16S1 | 1329 | A | C5-N7-C8 | 8.65 | 108.22 | 103.90 |
| 22 | 23S1 | 10 | A | N3-C4-C5 | -8.65 | 120.75 | 126.80 |
| 22 | 23S1 | 2872 | A | N3-C4-C5 | -8.65 | 120.75 | 126.80 |
| 22 | 23S1 | 2566 | A | C5-N7-C8 | 8.65 | 108.22 | 103.90 |
| 23 | 05S1 | 29 | A | C5-N7-C8 | 8.65 | 108.22 | 103.90 |
| 22 | 23S1 | 646 | U | O4'-C1'-N1 | 8.64 | 115.12 | 108.20 |
| 22 | 23S1 | 1230 | A | C5-N7-C8 | 8.64 | 108.22 | 103.90 |
| 1 | 16S1 | 356 | A | C5-N7-C8 | 8.64 | 108.22 | 103.90 |
| 1 | 16S1 | 1311 | A | C5-N7-C8 | 8.64 | 108.22 | 103.90 |
| 23 | 05S1 | 34 | A | C5-N7-C8 | 8.64 | 108.22 | 103.90 |
| 1 | 16S1 | 383 | A | N1-C6-N6 | -8.64 | 113.42 | 118.60 |
| 1 | 16S1 | 681 | A | C5-N7-C8 | 8.64 | 108.22 | 103.90 |
| 22 | 23S1 | 73 | A | N3-C4-C5 | -8.64 | 120.75 | 126.80 |
| 1 | 16S1 | 431 | A | N3-C4-C5 | -8.64 | 120.75 | 126.80 |
| 1 | 16S1 | 563 | A | C5-C6-N6 | 8.64 | 130.61 | 123.70 |
| 1 | 16S1 | 1105 | A | C5-N7-C8 | 8.64 | 108.22 | 103.90 |
| 22 | 23S1 | 2191 | A | N7-C8-N9 | -8.64 | 109.48 | 113.80 |
| 22 | 23S1 | 2821 | A | C5-N7-C8 | 8.64 | 108.22 | 103.90 |
| 23 | 05S1 | 52 | A | C5-N7-C8 | 8.64 | 108.22 | 103.90 |
| 22 | 23S1 | 892 | A | C5-N7-C8 | 8.63 | 108.22 | 103.90 |
| 22 | 23S1 | 2211 | A | N3-C4-C5 | -8.64 | 120.75 | 126.80 |
| 1 | 16S1 | 1158 | C | N3-C2-O2 | -8.63 | 115.86 | 121.90 |
| 1 | 16S1 | 702 | A | N3-C4-C5 | -8.62 | 120.76 | 126.80 |
| 1 | 16S1 | 95 | C | N1-C2-O2 | 8.62 | 124.07 | 118.90 |
| 22 | 23S1 | 2003 | A | C5-N7-C8 | 8.62 | 108.21 | 103.90 |
| 22 | 23S1 | 2126 | A | C5-N7-C8 | 8.62 | 108.21 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 2247 | A | C5-N7-C8 | 8.62 | 108.21 | 103.90 |
| 22 | 23S1 | 352 | A | N3-C4-C5 | -8.62 | 120.77 | 126.80 |
| 22 | 23S1 | 722 | A | C5-C6-N6 | 8.62 | 130.59 | 123.70 |
| 1 | 16S1 | 448 | A | C5-N7-C8 | 8.61 | 108.21 | 103.90 |
| 22 | 23S1 | 807 | U | C2-N3-C4 | -8.61 | 121.83 | 127.00 |
| 1 | 16S1 | 983 | A | N3-C4-N9 | 8.61 | 134.29 | 127.40 |
| 22 | 23S1 | 1021 | A | C5-N7-C8 | 8.61 | 108.21 | 103.90 |
| 22 | 23S1 | 1730 | C | N3-C2-O2 | -8.61 | 115.87 | 121.90 |
| 1 | 16S1 | 1360 | A | C5-N7-C8 | 8.61 | 108.20 | 103.90 |
| 22 | 23S1 | 1347 | A | C5-N7-C8 | 8.61 | 108.20 | 103.90 |
| 22 | 23S1 | 2471 | A | C5-N7-C8 | 8.61 | 108.20 | 103.90 |
| 22 | 23S1 | 278 | A | N3-C4-N9 | 8.60 | 134.28 | 127.40 |
| 22 | 23S1 | 101 | A | C4-C5-C6 | 8.60 | 121.30 | 117.00 |
| 22 | 23S1 | 513 | A | C4-C5-C6 | 8.60 | 121.30 | 117.00 |
| 1 | 16S1 | 441 | A | C5-C6-N6 | 8.60 | 130.58 | 123.70 |
| 1 | 16S1 | 696 | A | C5-C6-N6 | 8.60 | 130.58 | 123.70 |
| 22 | 23S1 | 167 | A | C5-N7-C8 | 8.59 | 108.20 | 103.90 |
| 22 | 23S1 | 5 | A | C5-N7-C8 | 8.59 | 108.19 | 103.90 |
| 22 | 23S1 | 2682 | A | C5-N7-C8 | 8.59 | 108.19 | 103.90 |
| 22 | 23S1 | 1953 | A | C5-N7-C8 | 8.59 | 108.19 | 103.90 |
| 22 | 23S1 | 241 | A | N3-C4-C5 | -8.59 | 120.79 | 126.80 |
| 22 | 23S1 | 324 | A | C5-C6-N6 | 8.59 | 130.57 | 123.70 |
| 22 | 23S1 | 2274 | A | N7-C8-N9 | -8.59 | 109.51 | 113.80 |
| 1 | 16S1 | 768 | A | C5-N7-C8 | 8.58 | 108.19 | 103.90 |
| 22 | 23S1 | 111 | A | C5-N7-C8 | 8.58 | 108.19 | 103.90 |
| 22 | 23S1 | 1665 | A | C5-N7-C8 | 8.58 | 108.19 | 103.90 |
| 22 | 23S1 | 2020 | A | N3-C4-C5 | -8.58 | 120.80 | 126.80 |
| 1 | 16S1 | 1046 | A | C5-N7-C8 | 8.58 | 108.19 | 103.90 |
| 22 | 23S1 | 2860 | A | N3-C4-C5 | -8.58 | 120.80 | 126.80 |
| 22 | 23S1 | 2753 | A | C5-N7-C8 | 8.57 | 108.19 | 103.90 |
| 22 | 23S1 | 1420 | A | C5-N7-C8 | 8.57 | 108.18 | 103.90 |
| 22 | 23S1 | 1586 | A | N7-C8-N9 | -8.57 | 109.52 | 113.80 |
| 1 | 16S1 | 520 | A | C4-C5-N7 | -8.56 | 106.42 | 110.70 |
| 22 | 23S1 | 454 | A | C5-N7-C8 | 8.56 | 108.18 | 103.90 |
| 22 | 23S1 | 119 | A | N3-C4-C5 | -8.56 | 120.81 | 126.80 |
| 22 | 23S1 | 1246 | A | C5-N7-C8 | 8.56 | 108.18 | 103.90 |
| 22 | 23S1 | 984 | A | C5-N7-C8 | 8.56 | 108.18 | 103.90 |
| 22 | 23S1 | 2726 | A | C5-N7-C8 | 8.56 | 108.18 | 103.90 |
| 22 | 23S1 | 513 | A | N7-C8-N9 | -8.55 | 109.52 | 113.80 |
| 22 | 23S1 | 718 | A | C5-N7-C8 | 8.55 | 108.17 | 103.90 |
| 22 | 23S1 | 1635 | A | C5-N7-C8 | 8.55 | 108.17 | 103.90 |
| 22 | 23S1 | 2776 | A | C5-N7-C8 | 8.55 | 108.17 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 783 | A | N7-C8-N9 | -8.55 | 109.53 | 113.80 |
| 22 | 23S1 | 91 | A | N3-C4-C5 | -8.55 | 120.82 | 126.80 |
| 22 | 23S1 | 1610 | A | N3-C4-C5 | -8.54 | 120.82 | 126.80 |
| 55 | PTR1 | 51 | A | C5-N7-C8 | 8.54 | 108.17 | 103.90 |
| 22 | 23S1 | 804 | A | C5-N7-C8 | 8.54 | 108.17 | 103.90 |
| 1 | 16S1 | 996 | A | C5-N7-C8 | 8.54 | 108.17 | 103.90 |
| 1 | 16S1 | 1145 | A | N3-C4-C5 | -8.54 | 120.82 | 126.80 |
| 1 | 16S1 | 792 | A | C5-N7-C8 | 8.54 | 108.17 | 103.90 |
| 22 | 23S1 | 2119 | A | C8-N9-C4 | 8.54 | 109.22 | 105.80 |
| 1 | 16S1 | 1319 | A | N3-C4-C5 | -8.54 | 120.82 | 126.80 |
| 22 | 23S1 | 2451 | A | C5-C6-N1 | 8.54 | 121.97 | 117.70 |
| 1 | 16S1 | 754 | C | N1-C2-O2 | 8.53 | 124.02 | 118.90 |
| 22 | 23S1 | 716 | A | C5-N7-C8 | 8.53 | 108.17 | 103.90 |
| 22 | 23S1 | 1247 | A | C5-N7-C8 | 8.53 | 108.16 | 103.90 |
| 22 | 23S1 | 2147 | A | N7-C8-N9 | -8.53 | 109.53 | 113.80 |
| 22 | 23S1 | 1920 | C | C6-N1-C2 | -8.53 | 116.89 | 120.30 |
| 1 | 16S1 | 553 | A | C5-N7-C8 | 8.52 | 108.16 | 103.90 |
| 22 | 23S1 | 1276 | A | C5-N7-C8 | 8.52 | 108.16 | 103.90 |
| 22 | 23S1 | 1057 | A | C5-N7-C8 | 8.52 | 108.16 | 103.90 |
| 22 | 23S1 | 2278 | A | C5-N7-C8 | 8.52 | 108.16 | 103.90 |
| 1 | 16S1 | 766 | A | N3-C4-C5 | -8.52 | 120.84 | 126.80 |
| 22 | 23S1 | 2560 | A | C5-N7-C8 | 8.52 | 108.16 | 103.90 |
| 1 | 16S1 | 969 | A | C5-N7-C8 | 8.52 | 108.16 | 103.90 |
| 1 | 16S1 | 572 | A | N3-C4-C5 | -8.52 | 120.84 | 126.80 |
| 1 | 16S1 | 1101 | A | C5-N7-C8 | 8.52 | 108.16 | 103.90 |
| 22 | 23S1 | 2406 | A | C5-N7-C8 | 8.51 | 108.16 | 103.90 |
| 1 | 16S1 | 412 | A | N3-C4-C5 | -8.51 | 120.84 | 126.80 |
| 22 | 23S1 | 155 | A | C5-N7-C8 | 8.51 | 108.16 | 103.90 |
| 22 | 23S1 | 2284 | A | C5-N7-C8 | 8.51 | 108.16 | 103.90 |
| 22 | 23S1 | 1189 | A | C5-N7-C8 | 8.51 | 108.15 | 103.90 |
| 22 | 23S1 | 2183 | A | C5-N7-C8 | 8.51 | 108.15 | 103.90 |
| 1 | 16S1 | 831 | A | C5-N7-C8 | 8.51 | 108.15 | 103.90 |
| 1 | 16S1 | 1216 | A | N3-C4-C5 | -8.50 | 120.85 | 126.80 |
| 22 | 23S1 | 181 | A | C5-N7-C8 | 8.50 | 108.15 | 103.90 |
| 1 | 16S1 | 919 | A | N3-C4-C5 | -8.50 | 120.85 | 126.80 |
| 1 | 16S1 | 1201 | A | N3-C4-N9 | 8.50 | 134.20 | 127.40 |
| 22 | 23S1 | 2327 | A | C5-N7-C8 | 8.50 | 108.15 | 103.90 |
| 1 | 16S1 | 431 | A | C5-N7-C8 | 8.49 | 108.15 | 103.90 |
| 22 | 23S1 | 1551 | A | C5-N7-C8 | 8.49 | 108.15 | 103.90 |
| 22 | 23S1 | 925 | A | C5-N7-C8 | 8.49 | 108.15 | 103.90 |
| 1 | 16S1 | 199 | A | C5-N7-C8 | 8.49 | 108.14 | 103.90 |
| 22 | 23S1 | 492 | A | C4-C5-C6 | 8.49 | 121.24 | 117.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 538 | A | C5-N7-C8 | 8.49 | 108.14 | 103.90 |
| 22 | 23S1 | 693 | A | C5-N7-C8 | 8.49 | 108.14 | 103.90 |
| 1 | 16S1 | 371 | A | C5-N7-C8 | 8.48 | 108.14 | 103.90 |
| 1 | 16S1 | 1252 | A | C5-C6-N6 | 8.48 | 130.49 | 123.70 |
| 1 | 16S1 | 1476 | A | C5-N7-C8 | 8.48 | 108.14 | 103.90 |
| 1 | 16S1 | 32 | A | C5-C6-N6 | 8.48 | 130.48 | 123.70 |
| 22 | 23S1 | 1073 | A | C5-N7-C8 | 8.47 | 108.14 | 103.90 |
| 1 | 16S1 | 1468 | A | N3-C4-N9 | 8.47 | 134.18 | 127.40 |
| 1 | 16S1 | 74 | A | N3-C4-C5 | -8.47 | 120.87 | 126.80 |
| 1 | 16S1 | 977 | A | N3-C4-N9 | 8.47 | 134.17 | 127.40 |
| 22 | 23S1 | 1000 | A | C5-N7-C8 | 8.47 | 108.13 | 103.90 |
| 22 | 23S1 | 2450 | A | N3-C4-C5 | -8.47 | 120.87 | 126.80 |
| 1 | 16S1 | 1201 | A | C5-N7-C8 | 8.46 | 108.13 | 103.90 |
| 22 | 23S1 | 1090 | A | C5-N7-C8 | 8.46 | 108.13 | 103.90 |
| 22 | 23S1 | 1754 | A | N3-C4-C5 | -8.46 | 120.88 | 126.80 |
| 22 | 23S1 | 127 | A | N3-C4-C5 | -8.46 | 120.88 | 126.80 |
| 22 | 23S1 | 2835 | A | C5-N7-C8 | 8.46 | 108.13 | 103.90 |
| 55 | PTR1 | 76 | A | N3-C4-C5 | -8.46 | 120.88 | 126.80 |
| 22 | 23S1 | 196 | A | C5-N7-C8 | 8.46 | 108.13 | 103.90 |
| 22 | 23S1 | 1439 | A | C5-N7-C8 | 8.46 | 108.13 | 103.90 |
| 22 | 23S1 | 2451 | A | N9-C4-C5 | 8.45 | 109.18 | 105.80 |
| 22 | 23S1 | 2565 | A | C5-N7-C8 | 8.45 | 108.13 | 103.90 |
| 22 | 23S1 | 2635 | A | C5-N7-C8 | 8.45 | 108.13 | 103.90 |
| 22 | 23S1 | 2662 | A | C5-C6-N6 | 8.45 | 130.46 | 123.70 |
| 22 | 23S1 | 1014 | A | C5-N7-C8 | 8.45 | 108.12 | 103.90 |
| 22 | 23S1 | 354 | A | N3-C4-C5 | -8.45 | 120.89 | 126.80 |
| 1 | 16S1 | 499 | A | C5-N7-C8 | 8.44 | 108.12 | 103.90 |
| 1 | 16S1 | 781 | A | C5-N7-C8 | 8.44 | 108.12 | 103.90 |
| 22 | 23S1 | 1532 | A | C5-N7-C8 | 8.44 | 108.12 | 103.90 |
| 22 | 23S1 | 2448 | A | N3-C4-C5 | -8.44 | 120.89 | 126.80 |
| 1 | 16S1 | 1213 | A | N9-C4-C5 | 8.43 | 109.17 | 105.80 |
| 22 | 23S1 | 2614 | A | C5-N7-C8 | 8.43 | 108.12 | 103.90 |
| 1 | 16S1 | 1163 | A | C5-C6-N6 | 8.43 | 130.45 | 123.70 |
| 1 | 16S1 | 155 | A | C5-N7-C8 | 8.43 | 108.11 | 103.90 |
| 22 | 23S1 | 347 | A | C5-N7-C8 | 8.43 | 108.11 | 103.90 |
| 1 | 16S1 | 172 | A | N3-C4-C5 | -8.42 | 120.90 | 126.80 |
| 22 | 23S1 | 2776 | A | N3-C4-C5 | -8.42 | 120.91 | 126.80 |
| 22 | 23S1 | 1069 | A | C5-N7-C8 | 8.42 | 108.11 | 103.90 |
| 22 | 23S1 | 1275 | A | N3-C4-C5 | -8.42 | 120.91 | 126.80 |
| 1 | 16S1 | 196 | A | N3-C4-C5 | -8.41 | 120.91 | 126.80 |
| 22 | 23S1 | 705 | A | C5-C6-N6 | 8.41 | 130.43 | 123.70 |
| 22 | 23S1 | 1490 | A | N3-C4-N9 | 8.41 | 134.13 | 127.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 29 | L091 | 68 | ARG | NE-CZ-NH1 | 8.41 | 124.50 | 120.30 |
| 22 | 23S1 | 197 | A | C5-N7-C8 | 8.41 | 108.10 | 103.90 |
| 22 | 23S1 | 2679 | A | C5-N7-C8 | 8.41 | 108.10 | 103.90 |
| 22 | 23S1 | 706 | A | C5-N7-C8 | 8.40 | 108.10 | 103.90 |
| 1 | 16S1 | 451 | A | C5-N7-C8 | 8.40 | 108.10 | 103.90 |
| 22 | 23S1 | 677 | A | C5-C6-N6 | 8.40 | 130.42 | 123.70 |
| 1 | 16S1 | 1280 | A | N3-C4-C5 | -8.39 | 120.92 | 126.80 |
| 22 | 23S1 | 1739 | A | C5-C6-N6 | 8.39 | 130.41 | 123.70 |
| 23 | 05S1 | 45 | A | C5-C6-N6 | 8.39 | 130.41 | 123.70 |
| 1 | 16S1 | 509 | A | C5-N7-C8 | 8.39 | 108.09 | 103.90 |
| 1 | 16S1 | 1428 | A | C5-N7-C8 | 8.39 | 108.10 | 103.90 |
| 22 | 23S1 | 412 | A | C5-N7-C8 | 8.39 | 108.09 | 103.90 |
| 1 | 16S1 | 1204 | A | C5-N7-C8 | 8.39 | 108.09 | 103.90 |
| 22 | 23S1 | 2740 | A | C5-N7-C8 | 8.39 | 108.09 | 103.90 |
| 22 | 23S1 | 1780 | A | C5-N7-C8 | 8.39 | 108.09 | 103.90 |
| 1 | 16S1 | 1005 | A | C5-N7-C8 | 8.38 | 108.09 | 103.90 |
| 1 | 16S1 | 195 | A | N3-C4-C5 | -8.38 | 120.93 | 126.80 |
| 22 | 23S1 | 1129 | A | C5-N7-C8 | 8.38 | 108.09 | 103.90 |
| 22 | 23S1 | 344 | A | C5-N7-C8 | 8.38 | 108.09 | 103.90 |
| 1 | 16S1 | 373 | A | C5-N7-C8 | 8.38 | 108.09 | 103.90 |
| 1 | 16S1 | 1229 | A | C5-N7-C8 | 8.37 | 108.09 | 103.90 |
| 22 | 23S1 | 1772 | A | C5-N7-C8 | 8.37 | 108.09 | 103.90 |
| 1 | 16S1 | 1299 | A | N3-C4-N9 | 8.37 | 134.10 | 127.40 |
| 22 | 23S1 | 12 | U | C2-N1-C1' | 8.37 | 127.75 | 117.70 |
| 22 | 23S1 | 432 | A | C5-N7-C8 | 8.37 | 108.08 | 103.90 |
| 22 | 23S1 | 195 | A | N3-C4-C5 | -8.37 | 120.94 | 126.80 |
| 22 | 23S1 | 1937 | A | C4-C5-N7 | -8.37 | 106.52 | 110.70 |
| 22 | 23S1 | 2328 | A | N7-C8-N9 | -8.36 | 109.62 | 113.80 |
| 22 | 23S1 | 1755 | A | C5-N7-C8 | 8.36 | 108.08 | 103.90 |
| 22 | 23S1 | 522 | A | C5-N7-C8 | 8.36 | 108.08 | 103.90 |
| 22 | 23S1 | 1819 | A | C5-N7-C8 | 8.36 | 108.08 | 103.90 |
| 1 | 16S1 | 320 | A | C5-N7-C8 | 8.35 | 108.08 | 103.90 |
| 22 | 23S1 | 480 | A | C5-N7-C8 | 8.35 | 108.08 | 103.90 |
| 22 | 23S1 | 2459 | A | C5-C6-N6 | 8.35 | 130.38 | 123.70 |
| 1 | 16S1 | 602 | A | C5-N7-C8 | 8.35 | 108.08 | 103.90 |
| 22 | 23S1 | 792 | A | C5-N7-C8 | 8.35 | 108.08 | 103.90 |
| 1 | 16S1 | 649 | A | C5-N7-C8 | 8.35 | 108.07 | 103.90 |
| 1 | 16S1 | 51 | A | C5-N7-C8 | 8.35 | 108.07 | 103.90 |
| 22 | 23S1 | 2412 | A | C5-N7-C8 | 8.34 | 108.07 | 103.90 |
| 1 | 16S1 | 8 | A | C5-N7-C8 | 8.34 | 108.07 | 103.90 |
| 22 | 23S1 | 1591 | A | C5-C6-N6 | 8.34 | 130.37 | 123.70 |
| 22 | 23S1 | 878 | A | C5-N7-C8 | 8.34 | 108.07 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22 | 23S1 | 512 | G | O4'-C1'-N9 | 8.34 | 114.87 | 108.20 |
| 22 | 23S1 | 960 | A | C5-C6-N6 | 8.34 | 130.37 | 123.70 |
| 22 | 23S1 | 422 | A | C5-C6-N6 | 8.34 | 130.37 | 123.70 |
| 22 | 23S1 | 532 | A | C5-N7-C8 | 8.34 | 108.07 | 103.90 |
| 22 | 23S1 | 2800 | A | N3-C4-C5 | -8.34 | 120.97 | 126.80 |
| 1 | 16S1 | 1170 | A | N3-C4-N9 | 8.33 | 134.07 | 127.40 |
| 1 | 16S1 | 1500 | A | C5-N7-C8 | 8.33 | 108.07 | 103.90 |
| 22 | 23S1 | 927 | A | C5-N7-C8 | 8.33 | 108.07 | 103.90 |
| 1 | 16S1 | 1340 | A | C5-N7-C8 | 8.32 | 108.06 | 103.90 |
| 1 | 16S1 | 545 | C | C5-C6-N1 | 8.31 | 125.16 | 121.00 |
| 1 | 16S1 | 923 | A | C5-C6-N6 | 8.31 | 130.35 | 123.70 |
| 22 | 23S1 | 2882 | A | C5-N7-C8 | 8.31 | 108.06 | 103.90 |
| 22 | 23S1 | 382 | A | C5-N7-C8 | 8.31 | 108.06 | 103.90 |
| 22 | 23S1 | 1328 | A | C5-N7-C8 | 8.31 | 108.06 | 103.90 |
| 22 | 23S1 | 2352 | A | C5-N7-C8 | 8.31 | 108.06 | 103.90 |
| 1 | 16S1 | 1275 | A | C5-N7-C8 | 8.31 | 108.05 | 103.90 |
| 1 | 16S1 | 1503 | A | C8-N9-C4 | 8.31 | 109.12 | 105.80 |
| 22 | 23S1 | 734 | A | C5-N7-C8 | 8.31 | 108.05 | 103.90 |
| 22 | 23S1 | 2205 | A | C5-N7-C8 | 8.31 | 108.05 | 103.90 |
| 1 | 16S1 | 915 | A | C5-N7-C8 | 8.30 | 108.05 | 103.90 |
| 1 | 16S1 | 1157 | A | C5-N7-C8 | 8.30 | 108.05 | 103.90 |
| 1 | 16S1 | 728 | A | C5-N7-C8 | 8.30 | 108.05 | 103.90 |
| 1 | 16S1 | 1042 | A | C5-N7-C8 | 8.30 | 108.05 | 103.90 |
| 1 | 16S1 | 487 | A | C5-N7-C8 | 8.30 | 108.05 | 103.90 |
| 22 | 23S1 | 925 | A | C5-C6-N6 | 8.30 | 130.34 | 123.70 |
| 22 | 23S1 | 2589 | A | C5-N7-C8 | 8.30 | 108.05 | 103.90 |
| 22 | 23S1 | 52 | A | C5-N7-C8 | 8.30 | 108.05 | 103.90 |
| 22 | 23S1 | 1794 | A | C5-N7-C8 | 8.30 | 108.05 | 103.90 |
| 22 | 23S1 | 677 | A | N3-C4-N9 | 8.30 | 134.04 | 127.40 |
| 22 | 23S1 | 2019 | A | C5-N7-C8 | 8.30 | 108.05 | 103.90 |
| 1 | 16S1 | 607 | A | N3-C4-C5 | -8.30 | 120.99 | 126.80 |
| 1 | 16S1 | 364 | A | C5-N7-C8 | 8.29 | 108.05 | 103.90 |
| 22 | 23S1 | 756 | A | C5-N7-C8 | 8.29 | 108.05 | 103.90 |
| 22 | 23S1 | 1084 | A | C5-N7-C8 | 8.29 | 108.05 | 103.90 |
| 22 | 23S1 | 1808 | A | N3-C4-C5 | -8.29 | 121.00 | 126.80 |
| 1 | 16S1 | 1250 | A | C5-N7-C8 | 8.28 | 108.04 | 103.90 |
| 22 | 23S1 | 563 | A | C5-N7-C8 | 8.28 | 108.04 | 103.90 |
| 22 | 23S1 | 1134 | A | C5-N7-C8 | 8.28 | 108.04 | 103.90 |
| 22 | 23S1 | 1889 | A | C5-N7-C8 | 8.28 | 108.04 | 103.90 |
| 22 | 23S1 | 1253 | A | N3-C4-C5 | -8.28 | 121.01 | 126.80 |
| 22 | 23S1 | 348 | A | C5-N7-C8 | 8.28 | 108.04 | 103.90 |
| 22 | 23S1 | 1535 | A | C5-N7-C8 | 8.28 | 108.04 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 391 | A | C5-N7-C8 | 8.27 | 108.04 | 103.90 |
| 22 | 23S1 | 829 | A | C5-N7-C8 | 8.27 | 108.04 | 103.90 |
| 22 | 23S1 | 1650 | A | C5-N7-C8 | 8.27 | 108.04 | 103.90 |
| 22 | 23S1 | 165 | A | C5-N7-C8 | 8.27 | 108.03 | 103.90 |
| 22 | 23S1 | 1810 | A | N3-C4-N9 | 8.27 | 134.01 | 127.40 |
| 22 | 23S1 | 1070 | A | C5-N7-C8 | 8.26 | 108.03 | 103.90 |
| 22 | 23S1 | 1783 | A | C5-N7-C8 | 8.26 | 108.03 | 103.90 |
| 1 | 16S1 | 1346 | A | N3-C4-C5 | -8.26 | 121.02 | 126.80 |
| 1 | 16S1 | 1447 | A | C5-N7-C8 | 8.26 | 108.03 | 103.90 |
| 22 | 23S1 | 256 | A | C5-N7-C8 | 8.26 | 108.03 | 103.90 |
| 22 | 23S1 | 2184 | A | C5-N7-C8 | 8.26 | 108.03 | 103.90 |
| 1 | 16S1 | 498 | A | C5-N7-C8 | 8.25 | 108.03 | 103.90 |
| 22 | 23S1 | 2469 | A | C8-N9-C4 | 8.25 | 109.10 | 105.80 |
| 1 | 16S1 | 1227 | A | C4-C5-C6 | 8.25 | 121.12 | 117.00 |
| 1 | 16S1 | 1396 | A | C5-C6-N6 | 8.25 | 130.30 | 123.70 |
| 22 | 23S1 | 457 | A | C5-N7-C8 | 8.25 | 108.02 | 103.90 |
| 22 | 23S1 | 2051 | A | N7-C8-N9 | -8.25 | 109.67 | 113.80 |
| 22 | 23S1 | 2171 | A | C8-N9-C4 | 8.24 | 109.10 | 105.80 |
| 22 | 23S1 | 689 | A | C5-N7-C8 | 8.24 | 108.02 | 103.90 |
| 1 | 16S1 | 706 | A | C5-N7-C8 | 8.23 | 108.02 | 103.90 |
| 1 | 16S1 | 489 | C | N1-C2-O2 | 8.23 | 123.84 | 118.90 |
| 1 | 16S1 | 807 | A | C5-N7-C8 | 8.23 | 108.02 | 103.90 |
| 22 | 23S1 | 849 | A | C5-N7-C8 | 8.23 | 108.02 | 103.90 |
| 13 | S131 | 79 | ARG | NE-CZ-NH2 | 8.23 | 124.41 | 120.30 |
| 22 | 23S1 | 1048 | A | C5-N7-C8 | 8.23 | 108.01 | 103.90 |
| 1 | 16S1 | 1225 | A | C5-N7-C8 | 8.22 | 108.01 | 103.90 |
| 22 | 23S1 | 172 | A | C5-N7-C8 | 8.22 | 108.01 | 103.90 |
| 22 | 23S1 | 2060 | A | C5-N7-C8 | 8.22 | 108.01 | 103.90 |
| 22 | 23S1 | 644 | A | N3-C4-N9 | 8.22 | 133.98 | 127.40 |
| 22 | 23S1 | 2173 | A | C5-N7-C8 | 8.22 | 108.01 | 103.90 |
| 55 | PTR1 | 59 | A | C5-N7-C8 | 8.22 | 108.01 | 103.90 |
| 22 | 23S1 | 262 | A | C5-N7-C8 | 8.22 | 108.01 | 103.90 |
| 22 | 23S1 | 783 | A | C5-N7-C8 | 8.21 | 108.01 | 103.90 |
| 22 | 23S1 | 1098 | A | C5-N7-C8 | 8.21 | 108.01 | 103.90 |
| 22 | 23S1 | 1504 | A | C5-N7-C8 | 8.21 | 108.01 | 103.90 |
| 1 | 16S1 | 80 | A | N7-C8-N9 | -8.21 | 109.69 | 113.80 |
| 22 | 23S1 | 911 | A | N7-C8-N9 | -8.21 | 109.69 | 113.80 |
| 22 | 23S1 | 2199 | A | C5-N7-C8 | 8.21 | 108.01 | 103.90 |
| 22 | 23S1 | 354 | A | C5-N7-C8 | 8.21 | 108.00 | 103.90 |
| 23 | 05S1 | 59 | A | C5-C6-N6 | 8.21 | 130.27 | 123.70 |
| 22 | 23S1 | 219 | A | C5-N7-C8 | 8.20 | 108.00 | 103.90 |
| 22 | 23S1 | 582 | A | C5-N7-C8 | 8.21 | 108.00 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 1583 | A | C5-N7-C8 | 8.21 | 108.00 | 103.90 |
| 22 | 23S1 | 2587 | A | C5-N7-C8 | 8.21 | 108.00 | 103.90 |
| 22 | 23S1 | 2883 | A | N3-C4-C5 | -8.21 | 121.06 | 126.80 |
| 1 | 16S1 | 412 | A | C5-C6-N1 | 8.20 | 121.80 | 117.70 |
| 1 | 16S1 | 493 | A | N3-C4-C5 | -8.20 | 121.06 | 126.80 |
| 1 | 16S1 | 975 | A | N3-C4-C5 | -8.20 | 121.06 | 126.80 |
| 1 | 16S1 | 411 | A | C5-N7-C8 | 8.20 | 108.00 | 103.90 |
| 22 | 23S1 | 1722 | A | C5-C6-N6 | 8.20 | 130.26 | 123.70 |
| 1 | 16S1 | 535 | A | C5-N7-C8 | 8.20 | 108.00 | 103.90 |
| 22 | 23S1 | 996 | A | C5-N7-C8 | 8.20 | 108.00 | 103.90 |
| 1 | 16S1 | 1257 | A | C5-N7-C8 | 8.19 | 108.00 | 103.90 |
| 22 | 23S1 | 231 | A | C5-N7-C8 | 8.19 | 108.00 | 103.90 |
| 22 | 23S1 | 1641 | A | C5-N7-C8 | 8.19 | 107.99 | 103.90 |
| 55 | PTR1 | 38 | A | C5-C6-N6 | 8.19 | 130.25 | 123.70 |
| 22 | 23S1 | 1175 | A | N3-C4-N9 | 8.19 | 133.95 | 127.40 |
| 22 | 23S1 | 279 | A | C5-N7-C8 | 8.18 | 107.99 | 103.90 |
| 22 | 23S1 | 905 | A | C5-N7-C8 | 8.18 | 107.99 | 103.90 |
| 1 | 16S1 | 151 | A | C5-N7-C8 | 8.18 | 107.99 | 103.90 |
| 1 | 16S1 | 784 | A | C5-N7-C8 | 8.18 | 107.99 | 103.90 |
| 22 | 23S1 | 63 | A | C5-N7-C8 | 8.18 | 107.99 | 103.90 |
| 22 | 23S1 | 195 | A | N9-C4-C5 | 8.17 | 109.07 | 105.80 |
| 22 | 23S1 | 1876 | A | C5-N7-C8 | 8.17 | 107.99 | 103.90 |
| 1 | 16S1 | 547 | A | C5-N7-C8 | 8.17 | 107.98 | 103.90 |
| 1 | 16S1 | 1239 | A | C5-N7-C8 | 8.17 | 107.99 | 103.90 |
| 22 | 23S1 | 1336 | A | C5-N7-C8 | 8.17 | 107.99 | 103.90 |
| 22 | 23S1 | 2176 | A | N7-C8-N9 | -8.17 | 109.72 | 113.80 |
| 1 | 16S1 | 1333 | A | C5-N7-C8 | 8.16 | 107.98 | 103.90 |
| 22 | 23S1 | 1272 | A | N3-C4-C5 | -8.16 | 121.09 | 126.80 |
| 22 | 23S1 | 1434 | A | C4-C5-N7 | -8.16 | 106.62 | 110.70 |
| 22 | 23S1 | 2425 | A | C5-N7-C8 | 8.16 | 107.98 | 103.90 |
| 1 | 16S1 | 223 | A | C5-N7-C8 | 8.16 | 107.98 | 103.90 |
| 1 | 16S1 | 411 | A | C8-N9-C4 | 8.16 | 109.06 | 105.80 |
| 1 | 16S1 | 845 | A | C5-N7-C8 | 8.16 | 107.98 | 103.90 |
| 22 | 23S1 | 917 | A | C5-N7-C8 | 8.16 | 107.98 | 103.90 |
| 22 | 23S1 | 1342 | A | C5-N7-C8 | 8.16 | 107.98 | 103.90 |
| 22 | 23S1 | 644 | A | C4-C5-C6 | 8.16 | 121.08 | 117.00 |
| 1 | 16S1 | 1465 | A | C5-N7-C8 | 8.15 | 107.98 | 103.90 |
| 22 | 23S1 | 685 | A | C5-N7-C8 | 8.15 | 107.98 | 103.90 |
| 22 | 23S1 | 863 | A | C5-N7-C8 | 8.15 | 107.98 | 103.90 |
| 1 | 16S1 | 918 | A | C5-N7-C8 | 8.15 | 107.97 | 103.90 |
| 22 | 23S1 | 71 | A | C5-N7-C8 | 8.15 | 107.97 | 103.90 |
| 22 | 23S1 | 1847 | A | N7-C8-N9 | -8.15 | 109.73 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 142 | A | N7-C8-N9 | -8.14 | 109.73 | 113.80 |
| 22 | 23S1 | 2014 | A | C5-N7-C8 | 8.14 | 107.97 | 103.90 |
| 1 | 16S1 | 313 | A | C5-N7-C8 | 8.14 | 107.97 | 103.90 |
| 1 | 16S1 | 1021 | A | C5-N7-C8 | 8.14 | 107.97 | 103.90 |
| 22 | 23S1 | 1670 | C | O5'-P-OP2 | -8.14 | 98.37 | 105.70 |
| 22 | 23S1 | 1809 | A | C5-N7-C8 | 8.14 | 107.97 | 103.90 |
| 1 | 16S1 | 959 | A | N7-C8-N9 | -8.14 | 109.73 | 113.80 |
| 22 | 23S1 | 866 | A | C5-N7-C8 | 8.14 | 107.97 | 103.90 |
| 22 | 23S1 | 1502 | A | C5-N7-C8 | 8.14 | 107.97 | 103.90 |
| 22 | 23S1 | 176 | A | C5-N7-C8 | 8.13 | 107.97 | 103.90 |
| 22 | 23S1 | 2433 | A | C5-N7-C8 | 8.14 | 107.97 | 103.90 |
| 1 | 16S1 | 1236 | A | C5-N7-C8 | 8.13 | 107.97 | 103.90 |
| 1 | 16S1 | 901 | A | N3-C4-N9 | 8.13 | 133.90 | 127.40 |
| 22 | 23S1 | 362 | A | C4-C5-C6 | 8.13 | 121.07 | 117.00 |
| 22 | 23S1 | 608 | A | C5-N7-C8 | 8.13 | 107.97 | 103.90 |
| 22 | 23S1 | 2095 | A | C5-N7-C8 | 8.13 | 107.97 | 103.90 |
| 22 | 23S1 | 2170 | A | C5-N7-C8 | 8.13 | 107.97 | 103.90 |
| 22 | 23S1 | 1095 | A | C5-N7-C8 | 8.13 | 107.96 | 103.90 |
| 22 | 23S1 | 1155 | A | C5-N7-C8 | 8.13 | 107.96 | 103.90 |
| 23 | 05S1 | 53 | A | C5-N7-C8 | 8.13 | 107.96 | 103.90 |
| 1 | 16S1 | 1408 | A | C5-N7-C8 | 8.13 | 107.96 | 103.90 |
| 22 | 23S1 | 2108 | A | C5-N7-C8 | 8.13 | 107.96 | 103.90 |
| 1 | 16S1 | 465 | A | N3-C4-N9 | 8.12 | 133.90 | 127.40 |
| 1 | 16S1 | 315 | A | C5-N7-C8 | 8.12 | 107.96 | 103.90 |
| 22 | 23S1 | 2135 | A | C5-N7-C8 | 8.12 | 107.96 | 103.90 |
| 22 | 23S1 | 2634 | A | C5-N7-C8 | 8.12 | 107.96 | 103.90 |
| 22 | 23S1 | 1570 | A | C5-N7-C8 | 8.12 | 107.96 | 103.90 |
| 1 | 16S1 | 182 | A | C5-N7-C8 | 8.12 | 107.96 | 103.90 |
| 22 | 23S1 | 2314 | A | C5-N7-C8 | 8.12 | 107.96 | 103.90 |
| 22 | 23S1 | 528 | A | C5-N7-C8 | 8.12 | 107.96 | 103.90 |
| 22 | 23S1 | 1966 | A | C5-N7-C8 | 8.12 | 107.96 | 103.90 |
| 22 | 23S1 | 2432 | A | C5-N7-C8 | 8.11 | 107.96 | 103.90 |
| 21 | S211 | 16 | LEU | CA-CB-CG | 8.11 | 133.96 | 115.30 |
| 22 | 23S1 | 311 | A | C5-N7-C8 | 8.11 | 107.96 | 103.90 |
| 22 | 23S1 | 1899 | A | C4-C5-C6 | 8.11 | 121.06 | 117.00 |
| 23 | 05S1 | 109 | A | C5-N7-C8 | 8.11 | 107.96 | 103.90 |
| 22 | 23S1 | 1525 | A | C5-N7-C8 | 8.11 | 107.95 | 103.90 |
| 22 | 23S1 | 1029 | A | C4-C5-C6 | 8.11 | 121.05 | 117.00 |
| 1 | 16S1 | 151 | A | N9-C4-C5 | 8.11 | 109.04 | 105.80 |
| 10 | S101 | 92 | LEU | CB-CG-CD1 | -8.11 | 97.22 | 111.00 |
| 22 | 23S1 | 668 | A | C5-N7-C8 | 8.11 | 107.95 | 103.90 |
| 22 | 23S1 | 933 | A | N3-C4-N9 | 8.11 | 133.88 | 127.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 984 | A | N3-C4-N9 | 8.11 | 133.88 | 127.40 |
| 22 | 23S1 | 1096 | A | C5-N7-C8 | 8.11 | 107.95 | 103.90 |
| 1 | 16S1 | 181 | A | C5-C6-N6 | 8.10 | 130.18 | 123.70 |
| 1 | 16S1 | 648 | A | C5-N7-C8 | 8.10 | 107.95 | 103.90 |
| 22 | 23S1 | 161 | A | N3-C4-C5 | -8.10 | 121.13 | 126.80 |
| 22 | 23S1 | 2518 | A | N3-C4-N9 | 8.10 | 133.88 | 127.40 |
| 22 | 23S1 | 2447 | G | C6-N1-C2 | -8.10 | 120.24 | 125.10 |
| 22 | 23S1 | 821 | A | C5-N7-C8 | 8.10 | 107.95 | 103.90 |
| 22 | 23S1 | 2101 | A | N9-C4-C5 | 8.09 | 109.04 | 105.80 |
| 22 | 23S1 | 2287 | A | C5-N7-C8 | 8.09 | 107.94 | 103.90 |
| 1 | 16S1 | 1306 | A | C5-N7-C8 | 8.09 | 107.94 | 103.90 |
| 22 | 23S1 | 144 | A | C5-N7-C8 | 8.09 | 107.94 | 103.90 |
| 22 | 23S1 | 2513 | A | C5-N7-C8 | 8.09 | 107.94 | 103.90 |
| 22 | 23S1 | 2657 | A | N3-C4-C5 | -8.09 | 121.14 | 126.80 |
| 1 | 16S1 | 28 | A | C5-N7-C8 | 8.08 | 107.94 | 103.90 |
| 22 | 23S1 | 505 | A | C5-N7-C8 | 8.08 | 107.94 | 103.90 |
| 22 | 23S1 | 1571 | A | C5-C6-N6 | 8.08 | 130.16 | 123.70 |
| 22 | 23S1 | 2516 | A | C5-N7-C8 | 8.08 | 107.94 | 103.90 |
| 22 | 23S1 | 936 | A | C5-N7-C8 | 8.08 | 107.94 | 103.90 |
| 22 | 23S1 | 2212 | A | C5-N7-C8 | 8.08 | 107.94 | 103.90 |
| 22 | 23S1 | 1040 | A | C5-N7-C8 | 8.07 | 107.94 | 103.90 |
| 22 | 23S1 | 637 | A | C5-N7-C8 | 8.07 | 107.94 | 103.90 |
| 22 | 23S1 | 2542 | A | C5-N7-C8 | 8.07 | 107.94 | 103.90 |
| 1 | 16S1 | 1176 | A | C5-N7-C8 | 8.07 | 107.94 | 103.90 |
| 22 | 23S1 | 522 | A | C4-C5-C6 | 8.07 | 121.03 | 117.00 |
| 22 | 23S1 | 1127 | A | C5-N7-C8 | 8.07 | 107.94 | 103.90 |
| 22 | 23S1 | 1786 | A | C5-N7-C8 | 8.07 | 107.94 | 103.90 |
| 1 | 16S1 | 1410 | A | C5-N7-C8 | 8.07 | 107.93 | 103.90 |
| 22 | 23S1 | 1165 | A | C5-N7-C8 | 8.07 | 107.93 | 103.90 |
| 22 | 23S1 | 1858 | A | C5-N7-C8 | 8.07 | 107.93 | 103.90 |
| 22 | 23S1 | 322 | A | C5-N7-C8 | 8.06 | 107.93 | 103.90 |
| 1 | 16S1 | 60 | A | C5-N7-C8 | 8.06 | 107.93 | 103.90 |
| 1 | 16S1 | 560 | A | C5-N7-C8 | 8.06 | 107.93 | 103.90 |
| 22 | 23S1 | 346 | A | C5-N7-C8 | 8.06 | 107.93 | 103.90 |
| 22 | 23S1 | 2154 | A | C5-N7-C8 | 8.06 | 107.93 | 103.90 |
| 22 | 23S1 | 160 | A | C5-N7-C8 | 8.06 | 107.93 | 103.90 |
| 22 | 23S1 | 547 | A | C5-N7-C8 | 8.06 | 107.93 | 103.90 |
| 22 | 23S1 | 513 | A | N3-C4-N9 | 8.06 | 133.85 | 127.40 |
| 1 | 16S1 | 435 | A | C5-N7-C8 | 8.06 | 107.93 | 103.90 |
| 1 | 16S1 | 499 | A | C5-C6-N6 | 8.06 | 130.15 | 123.70 |
| 22 | 23S1 | 374 | A | C5-N7-C8 | 8.06 | 107.93 | 103.90 |
| 1 | 16S1 | 1246 | A | C5-N7-C8 | 8.06 | 107.93 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 125 | A | C5-N7-C8 | 8.06 | 107.93 | 103.90 |
| 1 | 16S1 | 579 | A | C5-N7-C8 | 8.05 | 107.93 | 103.90 |
| 22 | 23S1 | 781 | A | C5-N7-C8 | 8.05 | 107.93 | 103.90 |
| 22 | 23S1 | 782 | A | C5-N7-C8 | 8.06 | 107.93 | 103.90 |
| 22 | 23S1 | 2142 | A | C5-N7-C8 | 8.05 | 107.93 | 103.90 |
| 22 | 23S1 | 1802 | A | C5-N7-C8 | 8.05 | 107.93 | 103.90 |
| 22 | 23S1 | 233 | A | C5-N7-C8 | 8.05 | 107.92 | 103.90 |
| 1 | 16S1 | 499 | A | C8-N9-C4 | 8.05 | 109.02 | 105.80 |
| 1 | 16S1 | 629 | A | C5-N7-C8 | 8.05 | 107.92 | 103.90 |
| 1 | 16S1 | 1374 | A | C5-N7-C8 | 8.05 | 107.92 | 103.90 |
| 22 | 23S1 | 1669 | A | C5-N7-C8 | 8.05 | 107.92 | 103.90 |
| 22 | 23S1 | 541 | A | C5-N7-C8 | 8.04 | 107.92 | 103.90 |
| 22 | 23S1 | 1098 | A | C4-C5-C6 | 8.04 | 121.02 | 117.00 |
| 22 | 23S1 | 278 | A | C4-C5-C6 | 8.04 | 121.02 | 117.00 |
| 1 | 16S1 | 270 | A | C5-N7-C8 | 8.04 | 107.92 | 103.90 |
| 1 | 16S1 | 1067 | A | C5-N7-C8 | 8.04 | 107.92 | 103.90 |
| 22 | 23S1 | 661 | A | C5-N7-C8 | 8.04 | 107.92 | 103.90 |
| 22 | 23S1 | 2381 | A | C5-N7-C8 | 8.04 | 107.92 | 103.90 |
| 22 | 23S1 | 2829 | A | C5-N7-C8 | 8.04 | 107.92 | 103.90 |
| 22 | 23S1 | 1970 | A | C8-N9-C4 | 8.03 | 109.01 | 105.80 |
| 1 | 16S1 | 706 | A | C4-C5-C6 | 8.03 | 121.02 | 117.00 |
| 1 | 16S1 | 1346 | A | C5-N7-C8 | 8.03 | 107.92 | 103.90 |
| 22 | 23S1 | 402 | A | C5-N7-C8 | 8.03 | 107.92 | 103.90 |
| 1 | 16S1 | 908 | A | C5-N7-C8 | 8.03 | 107.92 | 103.90 |
| 22 | 23S1 | 753 | A | C5-N7-C8 | 8.03 | 107.91 | 103.90 |
| 1 | 16S1 | 143 | A | C5-N7-C8 | 8.03 | 107.91 | 103.90 |
| 22 | 23S1 | 1713 | A | C5-N7-C8 | 8.03 | 107.91 | 103.90 |
| 22 | 23S1 | 2418 | A | C5-N7-C8 | 8.03 | 107.91 | 103.90 |
| 1 | 16S1 | 383 | A | N7-C8-N9 | -8.02 | 109.79 | 113.80 |
| 22 | 23S1 | 1144 | A | C5-N7-C8 | 8.02 | 107.91 | 103.90 |
| 21 | S211 | 16 | LEU | CB-CG-CD1 | -8.02 | 97.36 | 111.00 |
| 22 | 23S1 | 2665 | A | C5-N7-C8 | 8.02 | 107.91 | 103.90 |
| 22 | 23S1 | 19 | A | C5-N7-C8 | 8.02 | 107.91 | 103.90 |
| 22 | 23S1 | 670 | A | C5-N7-C8 | 8.02 | 107.91 | 103.90 |
| 22 | 23S1 | 345 | A | C5-N7-C8 | 8.02 | 107.91 | 103.90 |
| 22 | 23S1 | 1789 | A | C5-N7-C8 | 8.02 | 107.91 | 103.90 |
| 1 | 16S1 | 190 | A | N7-C8-N9 | -8.02 | 109.79 | 113.80 |
| 1 | 16S1 | 197 | A | C5-N7-C8 | 8.02 | 107.91 | 103.90 |
| 22 | 23S1 | 819 | A | C4-C5-C6 | 8.01 | 121.01 | 117.00 |
| 23 | 05S1 | 101 | A | C5-C6-N6 | 8.01 | 130.11 | 123.70 |
| 1 | 16S1 | 563 | A | C5-N7-C8 | 8.01 | 107.91 | 103.90 |
| 22 | 23S1 | 190 | A | C5-N7-C8 | 8.01 | 107.91 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 1020 | A | C8-N9-C4 | 8.01 | 109.00 | 105.80 |
| 22 | 23S1 | 1353 | A | C5-N7-C8 | 8.01 | 107.91 | 103.90 |
| 22 | 23S1 | 2376 | A | C5-N7-C8 | 8.01 | 107.91 | 103.90 |
| 22 | 23S1 | 1854 | A | C5-C6-N6 | 8.01 | 130.11 | 123.70 |
| 23 | 05S1 | 15 | A | C5-N7-C8 | 8.01 | 107.91 | 103.90 |
| 1 | 16S1 | 478 | A | C5-N7-C8 | 8.01 | 107.90 | 103.90 |
| 1 | 16S1 | 1117 | A | C5-N7-C8 | 8.01 | 107.90 | 103.90 |
| 22 | 23S1 | 64 | A | C5-N7-C8 | 8.01 | 107.90 | 103.90 |
| 22 | 23S1 | 227 | A | C5-N7-C8 | 8.01 | 107.90 | 103.90 |
| 22 | 23S1 | 457 | A | N3-C4-C5 | -8.01 | 121.20 | 126.80 |
| 22 | 23S1 | 1548 | A | C5-N7-C8 | 8.00 | 107.90 | 103.90 |
| 22 | 23S1 | 1596 | A | C5-N7-C8 | 8.00 | 107.90 | 103.90 |
| 1 | 16S1 | 621 | A | C5-N7-C8 | 8.00 | 107.90 | 103.90 |
| 55 | PTR1 | 17 | U | N3-C4-C5 | 8.00 | 119.40 | 114.60 |
| 22 | 23S1 | 735 | A | C5-N7-C8 | 8.00 | 107.90 | 103.90 |
| 22 | 23S1 | 800 | A | C5-N7-C8 | 8.00 | 107.90 | 103.90 |
| 22 | 23S1 | 1088 | A | C4-C5-C6 | 8.00 | 121.00 | 117.00 |
| 55 | PTR1 | 76 | A | C8-N9-C4 | 8.00 | 109.00 | 105.80 |
| 1 | 16S1 | 1493 | A | C5-N7-C8 | 7.99 | 107.90 | 103.90 |
| 22 | 23S1 | 1668 | A | C5-N7-C8 | 7.99 | 107.90 | 103.90 |
| 1 | 16S1 | 502 | A | C4-C5-C6 | 7.99 | 121.00 | 117.00 |
| 1 | 16S1 | 746 | A | C5-N7-C8 | 7.99 | 107.89 | 103.90 |
| 22 | 23S1 | 213 | A | C5-N7-C8 | 7.99 | 107.89 | 103.90 |
| 22 | 23S1 | 513 | A | C5-C6-N6 | 7.99 | 130.09 | 123.70 |
| 22 | 23S1 | 1981 | A | N3-C4-C5 | -7.99 | 121.21 | 126.80 |
| 1 | 16S1 | 640 | A | C5-N7-C8 | 7.99 | 107.89 | 103.90 |
| 22 | 23S1 | 2317 | A | C5-N7-C8 | 7.99 | 107.89 | 103.90 |
| 22 | 23S1 | 1528 | A | C5-N7-C8 | 7.99 | 107.89 | 103.90 |
| 22 | 23S1 | 2826 | A | C5-N7-C8 | 7.99 | 107.89 | 103.90 |
| 22 | 23S1 | 21 | A | C5-N7-C8 | 7.99 | 107.89 | 103.90 |
| 1 | 16S1 | 167 | A | C5-N7-C8 | 7.98 | 107.89 | 103.90 |
| 1 | 16S1 | 1429 | A | C5-N7-C8 | 7.98 | 107.89 | 103.90 |
| 22 | 23S1 | 191 | A | C5-N7-C8 | 7.98 | 107.89 | 103.90 |
| 22 | 23S1 | 103 | A | C5-N7-C8 | 7.98 | 107.89 | 103.90 |
| 22 | 23S1 | 142 | A | C4-C5-C6 | 7.98 | 120.99 | 117.00 |
| 22 | 23S1 | 2288 | A | C5-N7-C8 | 7.98 | 107.89 | 103.90 |
| 22 | 23S1 | 959 | A | C5-N7-C8 | 7.97 | 107.89 | 103.90 |
| 22 | 23S1 | 1802 | A | C4-C5-C6 | 7.97 | 120.99 | 117.00 |
| 22 | 23S1 | 2054 | A | C5-N7-C8 | 7.97 | 107.89 | 103.90 |
| 22 | 23S1 | 616 | A | C5-N7-C8 | 7.97 | 107.89 | 103.90 |
| 22 | 23S1 | 655 | A | C5-N7-C8 | 7.97 | 107.89 | 103.90 |
| 22 | 23S1 | 2070 | A | C5-N7-C8 | 7.97 | 107.89 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 16S1 | 393 | A | C5-N7-C8 | 7.97 | 107.88 | 103.90 |
| 1 | 16S1 | 814 | A | C5-N7-C8 | 7.97 | 107.88 | 103.90 |
| 22 | 23S1 | 1205 | A | N3-C4-C5 | -7.97 | 121.22 | 126.80 |
| 22 | 23S1 | 404 | A | N3-C4-C5 | -7.97 | 121.22 | 126.80 |
| 22 | 23S1 | 2267 | A | N3-C4-N9 | 7.96 | 133.77 | 127.40 |
| 22 | 23S1 | 2476 | A | C5-N7-C8 | 7.96 | 107.88 | 103.90 |
| 22 | 23S1 | 294 | A | C5-N7-C8 | 7.96 | 107.88 | 103.90 |
| 22 | 23S1 | 1571 | A | C4-C5-C6 | 7.96 | 120.98 | 117.00 |
| 22 | 23S1 | 2750 | A | C5-N7-C8 | 7.96 | 107.88 | 103.90 |
| 23 | 05S1 | 104 | A | C5-N7-C8 | 7.96 | 107.88 | 103.90 |
| 22 | 23S1 | 13 | A | C5-N7-C8 | 7.96 | 107.88 | 103.90 |
| 22 | 23S1 | 1383 | A | C5-N7-C8 | 7.96 | 107.88 | 103.90 |
| 22 | 23S1 | 1156 | A | C5-N7-C8 | 7.96 | 107.88 | 103.90 |
| 22 | 23S1 | 677 | A | C5-N7-C8 | 7.95 | 107.88 | 103.90 |
| 22 | 23S1 | 1419 | A | N3-C4-C5 | -7.95 | 121.23 | 126.80 |
| 22 | 23S1 | 979 | A | C5-N7-C8 | 7.95 | 107.87 | 103.90 |
| 22 | 23S1 | 1021 | A | C4-C5-C6 | 7.95 | 120.97 | 117.00 |
| 22 | 23S1 | 2366 | A | C5-N7-C8 | 7.95 | 107.87 | 103.90 |
| 1 | 16S1 | 923 | A | N3-C4-N9 | 7.94 | 133.75 | 127.40 |
| 1 | 16S1 | 958 | A | C5-N7-C8 | 7.94 | 107.87 | 103.90 |
| 22 | 23S1 | 544 | C | C2-N1-C1' | 7.94 | 127.54 | 118.80 |
| 22 | 23S1 | 794 | A | N3-C4-N9 | 7.94 | 133.75 | 127.40 |
| 22 | 23S1 | 2005 | A | C5-N7-C8 | 7.94 | 107.87 | 103.90 |
| 22 | 23S1 | 2094 | A | C5-N7-C8 | 7.94 | 107.87 | 103.90 |
| 1 | 16S1 | 162 | A | N7-C8-N9 | -7.94 | 109.83 | 113.80 |
| 22 | 23S1 | 2117 | A | C5-N7-C8 | 7.94 | 107.87 | 103.90 |
| 1 | 16S1 | 1280 | A | C5-N7-C8 | 7.94 | 107.87 | 103.90 |
| 22 | 23S1 | 819 | A | N3-C4-N9 | 7.94 | 133.75 | 127.40 |
| 22 | 23S1 | 1302 | A | C5-N7-C8 | 7.94 | 107.87 | 103.90 |
| 23 | 05S1 | 58 | A | C5-N7-C8 | 7.94 | 107.87 | 103.90 |
| 1 | 16S1 | 288 | A | C5-N7-C8 | 7.93 | 107.87 | 103.90 |
| 1 | 16S1 | 1238 | A | C5-N7-C8 | 7.93 | 107.87 | 103.90 |
| 22 | 23S1 | 947 | A | C5-N7-C8 | 7.93 | 107.87 | 103.90 |
| 22 | 23S1 | 1453 | A | C5-N7-C8 | 7.93 | 107.86 | 103.90 |
| 22 | 23S1 | 900 | A | C5-N7-C8 | 7.93 | 107.86 | 103.90 |
| 1 | 16S1 | 171 | A | C5-N7-C8 | 7.92 | 107.86 | 103.90 |
| 1 | 16S1 | 363 | A | C5-N7-C8 | 7.92 | 107.86 | 103.90 |
| 22 | 23S1 | 613 | A | C5-N7-C8 | 7.92 | 107.86 | 103.90 |
| 22 | 23S1 | 532 | A | N3-C4-N9 | 7.92 | 133.74 | 127.40 |
| 1 | 16S1 | 892 | A | C5-N7-C8 | 7.92 | 107.86 | 103.90 |
| 22 | 23S1 | 1039 | A | C5-N7-C8 | 7.92 | 107.86 | 103.90 |
| 22 | 23S1 | 1046 | A | C5-N7-C8 | 7.92 | 107.86 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 1509 | A | C5-N7-C8 | 7.92 | 107.86 | 103.90 |
| 22 | 23S1 | 1913 | A | C5-N7-C8 | 7.92 | 107.86 | 103.90 |
| 22 | 23S1 | 2346 | A | C5-N7-C8 | 7.92 | 107.86 | 103.90 |
| 1 | 16S1 | 32 | A | N3-C4-N9 | 7.92 | 133.73 | 127.40 |
| 22 | 23S1 | 146 | A | C5-N7-C8 | 7.92 | 107.86 | 103.90 |
| 22 | 23S1 | 56 | A | C5-N7-C8 | 7.91 | 107.86 | 103.90 |
| 1 | 16S1 | 994 | A | N3-C4-N9 | 7.91 | 133.73 | 127.40 |
| 1 | 16S1 | 1480 | A | C5-N7-C8 | 7.91 | 107.86 | 103.90 |
| 22 | 23S1 | 1746 | A | C5-N7-C8 | 7.91 | 107.86 | 103.90 |
| 22 | 23S1 | 2309 | A | C5-N7-C8 | 7.91 | 107.86 | 103.90 |
| 22 | 23S1 | 1001 | A | N3-C4-C5 | -7.91 | 121.26 | 126.80 |
| 22 | 23S1 | 2856 | A | C5-N7-C8 | 7.91 | 107.85 | 103.90 |
| 22 | 23S1 | 1274 | A | C5-N7-C8 | 7.91 | 107.85 | 103.90 |
| 1 | 16S1 | 1418 | A | C4-C5-C6 | 7.91 | 120.95 | 117.00 |
| 1 | 16S1 | 1225 | A | N3-C4-N9 | 7.90 | 133.72 | 127.40 |
| 22 | 23S1 | 216 | A | C5-N7-C8 | 7.90 | 107.85 | 103.90 |
| 22 | 23S1 | 590 | A | C5-N7-C8 | 7.90 | 107.85 | 103.90 |
| 22 | 23S1 | 1088 | A | N3-C4-N9 | 7.90 | 133.72 | 127.40 |
| 1 | 16S1 | 74 | A | C5-N7-C8 | 7.90 | 107.85 | 103.90 |
| 1 | 16S1 | 253 | A | C5-N7-C8 | 7.90 | 107.85 | 103.90 |
| 22 | 23S1 | 2799 | A | N3-C4-N9 | 7.90 | 133.72 | 127.40 |
| 1 | 16S1 | 1146 | A | C5-N7-C8 | 7.90 | 107.85 | 103.90 |
| 1 | 16S1 | 1151 | A | C5-N7-C8 | 7.90 | 107.85 | 103.90 |
| 22 | 23S1 | 255 | A | C5-N7-C8 | 7.90 | 107.85 | 103.90 |
| 22 | 23S1 | 613 | A | N3-C4-N9 | 7.90 | 133.72 | 127.40 |
| 22 | 23S1 | 2531 | A | C5-N7-C8 | 7.90 | 107.85 | 103.90 |
| 1 | 16S1 | 1035 | A | C5-N7-C8 | 7.90 | 107.85 | 103.90 |
| 1 | 16S1 | 2 | A | C5-N7-C8 | 7.89 | 107.85 | 103.90 |
| 22 | 23S1 | 309 | A | C5-N7-C8 | 7.89 | 107.85 | 103.90 |
| 22 | 23S1 | 1927 | A | C5-N7-C8 | 7.89 | 107.85 | 103.90 |
| 22 | 23S1 | 2614 | A | C5-C6-N1 | 7.89 | 121.65 | 117.70 |
| 22 | 23S1 | 2766 | A | N7-C8-N9 | -7.89 | 109.85 | 113.80 |
| 22 | 23S1 | 631 | A | C5-N7-C8 | 7.89 | 107.85 | 103.90 |
| 1 | 16S1 | 635 | A | C5-N7-C8 | 7.89 | 107.84 | 103.90 |
| 22 | 23S1 | 204 | A | C5-N7-C8 | 7.89 | 107.84 | 103.90 |
| 22 | 23S1 | 1403 | A | C5-N7-C8 | 7.89 | 107.84 | 103.90 |
| 22 | 23S1 | 2449 | U | N3-C2-O2 | -7.89 | 116.68 | 122.20 |
| 22 | 23S1 | 428 | A | C5-N7-C8 | 7.89 | 107.84 | 103.90 |
| 22 | 23S1 | 278 | A | C5-N7-C8 | 7.88 | 107.84 | 103.90 |
| 22 | 23S1 | 1591 | A | C5-N7-C8 | 7.88 | 107.84 | 103.90 |
| 22 | 23S1 | 794 | A | C5-N7-C8 | 7.88 | 107.84 | 103.90 |
| 22 | 23S1 | 1503 | A | C5-N7-C8 | 7.88 | 107.84 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 1552 | A | C5-N7-C8 | 7.88 | 107.84 | 103.90 |
| 1 | 16S1 | 478 | A | N3-C4-N9 | 7.88 | 133.71 | 127.40 |
| 1 | 16S1 | 1375 | A | C5-N7-C8 | 7.88 | 107.84 | 103.90 |
| 22 | 23S1 | 251 | A | C5-C6-N6 | 7.88 | 130.00 | 123.70 |
| 22 | 23S1 | 988 | A | C5-N7-C8 | 7.88 | 107.84 | 103.90 |
| 22 | 23S1 | 1194 | A | C5-N7-C8 | 7.87 | 107.84 | 103.90 |
| 22 | 23S1 | 1669 | A | C4-C5-C6 | 7.87 | 120.94 | 117.00 |
| 22 | 23S1 | 1762 | A | C5-N7-C8 | 7.87 | 107.84 | 103.90 |
| 22 | 23S1 | 1871 | A | C5-N7-C8 | 7.87 | 107.84 | 103.90 |
| 23 | 05S1 | 115 | A | C5-N7-C8 | 7.87 | 107.84 | 103.90 |
| 55 | PTR1 | 3 | A | C5-N7-C8 | 7.87 | 107.84 | 103.90 |
| 1 | 16S1 | 389 | A | C5-N7-C8 | 7.87 | 107.83 | 103.90 |
| 22 | 23S1 | 1086 | A | N3-C4-N9 | 7.87 | 133.70 | 127.40 |
| 22 | 23S1 | 821 | A | N3-C4-C5 | -7.87 | 121.29 | 126.80 |
| 22 | 23S1 | 1528 | A | C5-C6-N6 | 7.87 | 130.00 | 123.70 |
| 22 | 23S1 | 2614 | A | N9-C4-C5 | 7.87 | 108.95 | 105.80 |
| 1 | 16S1 | 687 | A | C5-N7-C8 | 7.87 | 107.83 | 103.90 |
| 1 | 16S1 | 306 | A | C5-N7-C8 | 7.87 | 107.83 | 103.90 |
| 22 | 23S1 | 483 | A | C5-N7-C8 | 7.86 | 107.83 | 103.90 |
| 22 | 23S1 | 715 | A | C5-N7-C8 | 7.86 | 107.83 | 103.90 |
| 22 | 23S1 | 1272 | A | C8-N9-C4 | 7.86 | 108.94 | 105.80 |
| 22 | 23S1 | 2333 | A | C5-N7-C8 | 7.86 | 107.83 | 103.90 |
| 22 | 23S1 | 783 | A | C4-C5-C6 | 7.86 | 120.93 | 117.00 |
| 1 | 16S1 | 327 | A | C5-N7-C8 | 7.86 | 107.83 | 103.90 |
| 1 | 16S1 | 729 | A | C5-N7-C8 | 7.86 | 107.83 | 103.90 |
| 1 | 16S1 | 825 | A | C5-N7-C8 | 7.86 | 107.83 | 103.90 |
| 1 | 16S1 | 1299 | A | C4-C5-C6 | 7.86 | 120.93 | 117.00 |
| 22 | 23S1 | 1773 | A | C5-N7-C8 | 7.86 | 107.83 | 103.90 |
| 22 | 23S1 | 2335 | A | C5-N7-C8 | 7.86 | 107.83 | 103.90 |
| 1 | 16S1 | 365 | U | N3-C2-O2 | -7.86 | 116.70 | 122.20 |
| 22 | 23S1 | 2173 | A | N3-C4-N9 | 7.86 | 133.69 | 127.40 |
| 22 | 23S1 | 342 | A | C5-N7-C8 | 7.86 | 107.83 | 103.90 |
| 22 | 23S1 | 196 | A | N3-C4-N9 | 7.85 | 133.68 | 127.40 |
| 1 | 16S1 | 397 | A | C4-C5-C6 | 7.85 | 120.93 | 117.00 |
| 22 | 23S1 | 507 | A | N3-C4-C5 | -7.85 | 121.30 | 126.80 |
| 22 | 23S1 | 1089 | A | C5-N7-C8 | 7.85 | 107.83 | 103.90 |
| 22 | 23S1 | 845 | A | C5-N7-C8 | 7.85 | 107.83 | 103.90 |
| 55 | PTR1 | 38 | A | C5-N7-C8 | 7.85 | 107.83 | 103.90 |
| 1 | 16S1 | 53 | A | C5-N7-C8 | 7.85 | 107.82 | 103.90 |
| 1 | 16S1 | 1188 | A | C5-N7-C8 | 7.85 | 107.82 | 103.90 |
| 22 | 23S1 | 1960 | A | C5-N7-C8 | 7.85 | 107.82 | 103.90 |
| 22 | 23S1 | 2518 | A | C5-N7-C8 | 7.85 | 107.82 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 16S1 | 754 | C | N3-C2-O2 | -7.84 | 116.41 | 121.90 |
| 22 | 23S1 | 627 | A | C5-N7-C8 | 7.84 | 107.82 | 103.90 |
| 22 | 23S1 | 1321 | A | C5-N7-C8 | 7.84 | 107.82 | 103.90 |
| 22 | 23S1 | 1853 | A | C5-N7-C8 | 7.84 | 107.82 | 103.90 |
| 22 | 23S1 | 2117 | A | C8-N9-C4 | 7.84 | 108.94 | 105.80 |
| 22 | 23S1 | 222 | A | C5-N7-C8 | 7.83 | 107.82 | 103.90 |
| 22 | 23S1 | 332 | A | C5-N7-C8 | 7.83 | 107.82 | 103.90 |
| 22 | 23S1 | 2778 | A | C5-N7-C8 | 7.83 | 107.82 | 103.90 |
| 22 | 23S1 | 126 | A | C5-N7-C8 | 7.83 | 107.81 | 103.90 |
| 22 | 23S1 | 1711 | A | C5-N7-C8 | 7.83 | 107.81 | 103.90 |
| 1 | 16S1 | 1299 | A | C5-N7-C8 | 7.83 | 107.81 | 103.90 |
| 1 | 16S1 | 1456 | A | C5-N7-C8 | 7.83 | 107.81 | 103.90 |
| 22 | 23S1 | 482 | A | N3-C4-N9 | 7.83 | 133.66 | 127.40 |
| 22 | 23S1 | 443 | A | C5-N7-C8 | 7.83 | 107.81 | 103.90 |
| 55 | PTR1 | 14 | A | N3-C4-N9 | 7.83 | 133.66 | 127.40 |
| 1 | 16S1 | 1179 | A | C5-N7-C8 | 7.82 | 107.81 | 103.90 |
| 22 | 23S1 | 352 | A | C5-N7-C8 | 7.82 | 107.81 | 103.90 |
| 22 | 23S1 | 1640 | A | C5-N7-C8 | 7.82 | 107.81 | 103.90 |
| 1 | 16S1 | 174 | A | C5-N7-C8 | 7.82 | 107.81 | 103.90 |
| 1 | 16S1 | 974 | A | C5-N7-C8 | 7.82 | 107.81 | 103.90 |
| 22 | 23S1 | 2088 | A | C5-N7-C8 | 7.82 | 107.81 | 103.90 |
| 22 | 23S1 | 1722 | A | C5-N7-C8 | 7.82 | 107.81 | 103.90 |
| 1 | 16S1 | 1269 | A | C5-N7-C8 | 7.82 | 107.81 | 103.90 |
| 22 | 23S1 | 789 | A | C5-N7-C8 | 7.82 | 107.81 | 103.90 |
| 1 | 16S1 | 1167 | A | C5-N7-C8 | 7.81 | 107.81 | 103.90 |
| 1 | 16S1 | 33 | A | C5-N7-C8 | 7.81 | 107.81 | 103.90 |
| 1 | 16S1 | 655 | A | C5-N7-C8 | 7.81 | 107.81 | 103.90 |
| 22 | 23S1 | 1632 | A | C5-N7-C8 | 7.81 | 107.81 | 103.90 |
| 22 | 23S1 | 2411 | A | C5-N7-C8 | 7.81 | 107.81 | 103.90 |
| 1 | 16S1 | 10 | A | C5-N7-C8 | 7.81 | 107.81 | 103.90 |
| 22 | 23S1 | 1672 | A | C5-N7-C8 | 7.81 | 107.81 | 103.90 |
| 1 | 16S1 | 914 | A | N3-C4-C5 | -7.81 | 121.33 | 126.80 |
| 22 | 23S1 | 272 | A | C5-N7-C8 | 7.81 | 107.81 | 103.90 |
| 22 | 23S1 | 1847 | A | C4-C5-C6 | 7.81 | 120.91 | 117.00 |
| 1 | 16S1 | 189 | A | C5-N7-C8 | 7.81 | 107.80 | 103.90 |
| 1 | 16S1 | 498 | A | C4-C5-C6 | 7.81 | 120.90 | 117.00 |
| 22 | 23S1 | 705 | A | C5-N7-C8 | 7.81 | 107.80 | 103.90 |
| 22 | 23S1 | 2727 | A | C5-N7-C8 | 7.81 | 107.80 | 103.90 |
| 22 | 23S1 | 1032 | A | C5-N7-C8 | 7.81 | 107.80 | 103.90 |
| 1 | 16S1 | 129 | A | C5-N7-C8 | 7.80 | 107.80 | 103.90 |
| 22 | 23S1 | 1505 | A | C5-N7-C8 | 7.80 | 107.80 | 103.90 |
| 1 | 16S1 | 408 | A | C5-N7-C8 | 7.80 | 107.80 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 16S1 | 675 | A | C5-N7-C8 | 7.80 | 107.80 | 103.90 |
| 1 | 16S1 | 715 | A | C5-N7-C8 | 7.80 | 107.80 | 103.90 |
| 22 | 23S1 | 2033 | A | C5-N7-C8 | 7.80 | 107.80 | 103.90 |
| 22 | 23S1 | 1098 | A | N3-C4-N9 | 7.80 | 133.64 | 127.40 |
| 22 | 23S1 | 429 | A | C5-N7-C8 | 7.80 | 107.80 | 103.90 |
| 22 | 23S1 | 1287 | A | C5-N7-C8 | 7.80 | 107.80 | 103.90 |
| 22 | 23S1 | 2530 | A | C5-N7-C8 | 7.80 | 107.80 | 103.90 |
| 1 | 16S1 | 482 | A | C5-N7-C8 | 7.79 | 107.80 | 103.90 |
| 1 | 16S1 | 1492 | A | C5-N7-C8 | 7.79 | 107.80 | 103.90 |
| 22 | 23S1 | 1821 | A | C5-N7-C8 | 7.79 | 107.80 | 103.90 |
| 1 | 16S1 | 1171 | A | N3-C4-N9 | 7.79 | 133.63 | 127.40 |
| 22 | 23S1 | 497 | A | C5-N7-C8 | 7.79 | 107.80 | 103.90 |
| 1 | 16S1 | 978 | A | C5-N7-C8 | 7.79 | 107.79 | 103.90 |
| 22 | 23S1 | 439 | A | C5-N7-C8 | 7.79 | 107.80 | 103.90 |
| 22 | 23S1 | 602 | A | C5-N7-C8 | 7.79 | 107.80 | 103.90 |
| 1 | 16S1 | 50 | A | C5-N7-C8 | 7.79 | 107.79 | 103.90 |
| 22 | 23S1 | 1009 | A | C5-N7-C8 | 7.79 | 107.79 | 103.90 |
| 22 | 23S1 | 1175 | A | C5-N7-C8 | 7.79 | 107.79 | 103.90 |
| 22 | 23S1 | 1866 | A | C5-N7-C8 | 7.79 | 107.79 | 103.90 |
| 23 | 05S1 | 50 | A | C5-N7-C8 | 7.78 | 107.79 | 103.90 |
| 1 | 16S1 | 554 | A | C4-C5-N7 | -7.78 | 106.81 | 110.70 |
| 1 | 16S1 | 777 | A | C5-N7-C8 | 7.78 | 107.79 | 103.90 |
| 22 | 23S1 | 101 | A | C5-N7-C8 | 7.78 | 107.79 | 103.90 |
| 22 | 23S1 | 2873 | A | C5-N7-C8 | 7.78 | 107.79 | 103.90 |
| 1 | 16S1 | 1197 | A | C5-N7-C8 | 7.78 | 107.79 | 103.90 |
| 22 | 23S1 | 2225 | A | C5-N7-C8 | 7.78 | 107.79 | 103.90 |
| 22 | 23S1 | 920 | A | C5-N7-C8 | 7.77 | 107.79 | 103.90 |
| 1 | 16S1 | 192 | A | C5-N7-C8 | 7.77 | 107.78 | 103.90 |
| 22 | 23S1 | 207 | A | C5-N7-C8 | 7.77 | 107.78 | 103.90 |
| 23 | 05S1 | 39 | A | C5-N7-C8 | 7.77 | 107.78 | 103.90 |
| 1 | 16S1 | 503 | C | N1-C2-O2 | 7.77 | 123.56 | 118.90 |
| 1 | 16S1 | 1044 | A | C5-N7-C8 | 7.77 | 107.78 | 103.90 |
| 23 | 05S1 | 108 | A | C5-N7-C8 | 7.77 | 107.78 | 103.90 |
| 1 | 16S1 | 499 | A | N3-C4-N9 | 7.77 | 133.61 | 127.40 |
| 1 | 16S1 | 673 | A | C5-N7-C8 | 7.76 | 107.78 | 103.90 |
| 22 | 23S1 | 2060 | A | N3-C4-C5 | -7.76 | 121.36 | 126.80 |
| 22 | 23S1 | 1981 | A | C5-N7-C8 | 7.76 | 107.78 | 103.90 |
| 22 | 23S1 | 2077 | A | C4-C5-C6 | 7.76 | 120.88 | 117.00 |
| 1 | 16S1 | 1251 | A | C5-N7-C8 | 7.76 | 107.78 | 103.90 |
| 22 | 23S1 | 2009 | A | C5-N7-C8 | 7.76 | 107.78 | 103.90 |
| 1 | 16S1 | 263 | A | C5-N7-C8 | 7.76 | 107.78 | 103.90 |
| 1 | 16S1 | 1055 | A | C5-N7-C8 | 7.76 | 107.78 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 1285 | A | C5-N7-C8 | 7.76 | 107.78 | 103.90 |
| 1 | 16S1 | 1377 | A | C5-N7-C8 | 7.76 | 107.78 | 103.90 |
| 22 | 23S1 | 118 | A | C5-N7-C8 | 7.76 | 107.78 | 103.90 |
| 1 | 16S1 | 353 | A | C5-N7-C8 | 7.75 | 107.78 | 103.90 |
| 22 | 23S1 | 320 | A | C5-N7-C8 | 7.75 | 107.78 | 103.90 |
| 22 | 23S1 | 2322 | A | C5-N7-C8 | 7.75 | 107.78 | 103.90 |
| 48 | L321 | 40 | ARG | NE-CZ-NH1 | 7.75 | 124.18 | 120.30 |
| 1 | 16S1 | 630 | A | C5-N7-C8 | 7.75 | 107.78 | 103.90 |
| 22 | 23S1 | 739 | A | C5-N7-C8 | 7.75 | 107.78 | 103.90 |
| 22 | 23S1 | 1890 | A | C5-N7-C8 | 7.75 | 107.78 | 103.90 |
| 22 | 23S1 | 2090 | A | C5-N7-C8 | 7.75 | 107.78 | 103.90 |
| 1 | 16S1 | 712 | A | C5-N7-C8 | 7.75 | 107.77 | 103.90 |
| 22 | 23S1 | 845 | A | C5-C6-N1 | 7.75 | 121.57 | 117.70 |
| 22 | 23S1 | 1705 | A | C5-N7-C8 | 7.75 | 107.77 | 103.90 |
| 1 | 16S1 | 923 | A | C4-C5-C6 | 7.75 | 120.87 | 117.00 |
| 1 | 16S1 | 1000 | A | C5-N7-C8 | 7.75 | 107.77 | 103.90 |
| 1 | 16S1 | 1093 | A | C5-N7-C8 | 7.75 | 107.77 | 103.90 |
| 22 | 23S1 | 2273 | A | C5-N7-C8 | 7.75 | 107.77 | 103.90 |
| 22 | 23S1 | 44 | A | C5-N7-C8 | 7.74 | 107.77 | 103.90 |
| 22 | 23S1 | 1262 | A | C5-N7-C8 | 7.74 | 107.77 | 103.90 |
| 1 | 16S1 | 754 | C | C2-N1-C1' | 7.74 | 127.31 | 118.80 |
| 22 | 23S1 | 751 | A | C5-N7-C8 | 7.74 | 107.77 | 103.90 |
| 22 | 23S1 | 430 | A | C5-N7-C8 | 7.74 | 107.77 | 103.90 |
| 22 | 23S1 | 925 | A | N3-C4-N9 | 7.74 | 133.59 | 127.40 |
| 22 | 23S1 | 2117 | A | N3-C4-C5 | -7.74 | 121.38 | 126.80 |
| 23 | 05S1 | 46 | A | C5-N7-C8 | 7.74 | 107.77 | 103.90 |
| 1 | 16S1 | 753 | A | C5-N7-C8 | 7.74 | 107.77 | 103.90 |
| 22 | 23S1 | 2042 | A | C5-N7-C8 | 7.74 | 107.77 | 103.90 |
| 23 | 05S1 | 45 | A | C5-C6-N1 | 7.74 | 121.57 | 117.70 |
| 1 | 16S1 | 865 | A | C4-C5-C6 | 7.73 | 120.86 | 117.00 |
| 22 | 23S1 | 861 | A | C5-N7-C8 | 7.73 | 107.76 | 103.90 |
| 22 | 23S1 | 1654 | A | C5-N7-C8 | 7.73 | 107.76 | 103.90 |
| 1 | 16S1 | 873 | A | C5-N7-C8 | 7.72 | 107.76 | 103.90 |
| 1 | 16S1 | 1016 | A | C5-N7-C8 | 7.72 | 107.76 | 103.90 |
| 1 | 16S1 | 250 | A | C5-N7-C8 | 7.72 | 107.76 | 103.90 |
| 1 | 16S1 | 1082 | A | C5-N7-C8 | 7.72 | 107.76 | 103.90 |
| 22 | 23S1 | 251 | A | N3-C4-N9 | 7.72 | 133.58 | 127.40 |
| 22 | 23S1 | 705 | A | C4-C5-C6 | 7.72 | 120.86 | 117.00 |
| 22 | 23S1 | 213 | A | C8-N9-C4 | 7.72 | 108.89 | 105.80 |
| 22 | 23S1 | 1313 | U | N1-C2-O2 | 7.72 | 128.21 | 122.80 |
| 22 | 23S1 | 2449 | U | N3-C4-C5 | 7.72 | 119.23 | 114.60 |
| 1 | 16S1 | 1213 | A | C4-C5-N7 | -7.72 | 106.84 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 1142 | A | C5-N7-C8 | 7.72 | 107.76 | 103.90 |
| 22 | 23S1 | 2352 | A | C4-C5-C6 | 7.72 | 120.86 | 117.00 |
| 22 | 23S1 | 2799 | A | C5-C6-N6 | 7.72 | 129.88 | 123.70 |
| 1 | 16S1 | 978 | A | N9-C4-C5 | 7.72 | 108.89 | 105.80 |
| 1 | 16S1 | 1437 | A | C5-N7-C8 | 7.72 | 107.76 | 103.90 |
| 22 | 23S1 | 1854 | A | C4-C5-C6 | 7.72 | 120.86 | 117.00 |
| 1 | 16S1 | 889 | A | C5-N7-C8 | 7.72 | 107.76 | 103.90 |
| 22 | 23S1 | 1010 | A | C5-N7-C8 | 7.72 | 107.76 | 103.90 |
| 22 | 23S1 | 1085 | A | C4-C5-C6 | 7.72 | 120.86 | 117.00 |
| 22 | 23S1 | 1237 | A | C5-N7-C8 | 7.72 | 107.76 | 103.90 |
| 22 | 23S1 | 2547 | A | C5-N7-C8 | 7.72 | 107.76 | 103.90 |
| 1 | 16S1 | 595 | A | C5-N7-C8 | 7.71 | 107.76 | 103.90 |
| 22 | 23S1 | 522 | A | N3-C4-N9 | 7.71 | 133.57 | 127.40 |
| 22 | 23S1 | 2813 | A | C5-N7-C8 | 7.71 | 107.76 | 103.90 |
| 22 | 23S1 | 1689 | A | C5-N7-C8 | 7.71 | 107.76 | 103.90 |
| 22 | 23S1 | 1213 | A | C4-C5-C6 | 7.71 | 120.86 | 117.00 |
| 22 | 23S1 | 1469 | A | C4-C5-C6 | 7.71 | 120.86 | 117.00 |
| 22 | 23S1 | 1759 | A | C5-N7-C8 | 7.71 | 107.76 | 103.90 |
| 1 | 16S1 | 913 | A | N3-C4-C5 | -7.71 | 121.40 | 126.80 |
| 1 | 16S1 | 1022 | A | C4-C5-C6 | 7.71 | 120.86 | 117.00 |
| 22 | 23S1 | 1241 | A | N3-C4-N9 | 7.71 | 133.57 | 127.40 |
| 1 | 16S1 | 1508 | A | C5-N7-C8 | 7.71 | 107.75 | 103.90 |
| 23 | 05S1 | 73 | A | N3-C4-N9 | 7.71 | 133.57 | 127.40 |
| 1 | 16S1 | 1196 | A | C5-N7-C8 | 7.71 | 107.75 | 103.90 |
| 22 | 23S1 | 244 | A | C5-N7-C8 | 7.71 | 107.75 | 103.90 |
| 22 | 23S1 | 2887 | A | C5-N7-C8 | 7.71 | 107.75 | 103.90 |
| 22 | 23S1 | 1378 | A | C5-N7-C8 | 7.70 | 107.75 | 103.90 |
| 1 | 16S1 | 243 | A | C5-N7-C8 | 7.70 | 107.75 | 103.90 |
| 1 | 16S1 | 860 | A | C4-C5-C6 | 7.70 | 120.85 | 117.00 |
| 22 | 23S1 | 1664 | A | C5-N7-C8 | 7.70 | 107.75 | 103.90 |
| 22 | 23S1 | 2765 | A | C5-N7-C8 | 7.70 | 107.75 | 103.90 |
| 1 | 16S1 | 1256 | A | C5-N7-C8 | 7.70 | 107.75 | 103.90 |
| 22 | 23S1 | 2369 | A | N7-C8-N9 | -7.70 | 109.95 | 113.80 |
| 1 | 16S1 | 59 | A | C5-N7-C8 | 7.69 | 107.75 | 103.90 |
| 22 | 23S1 | 1899 | A | N7-C8-N9 | -7.69 | 109.95 | 113.80 |
| 1 | 16S1 | 696 | A | C4-C5-C6 | 7.69 | 120.85 | 117.00 |
| 22 | 23S1 | 104 | A | C5-N7-C8 | 7.69 | 107.75 | 103.90 |
| 22 | 23S1 | 1151 | A | C5-N7-C8 | 7.69 | 107.75 | 103.90 |
| 22 | 23S1 | 2468 | A | C5-N7-C8 | 7.69 | 107.75 | 103.90 |
| 22 | 23S1 | 2764 | A | C5-N7-C8 | 7.69 | 107.75 | 103.90 |
| 22 | 23S1 | 1494 | A | C5-N7-C8 | 7.69 | 107.75 | 103.90 |
| 22 | 23S1 | 2082 | A | C5-N7-C8 | 7.69 | 107.75 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 16S1 | 397 | A | C5-C6-N1 | 7.69 | 121.55 | 117.70 |
| 22 | 23S1 | 422 | A | N3-C4-N9 | 7.69 | 133.55 | 127.40 |
| 22 | 23S1 | 2052 | A | C5-N7-C8 | 7.69 | 107.74 | 103.90 |
| 22 | 23S1 | 556 | A | C5-N7-C8 | 7.69 | 107.74 | 103.90 |
| 22 | 23S1 | 1392 | A | C5-N7-C8 | 7.68 | 107.74 | 103.90 |
| 22 | 23S1 | 2566 | A | C8-N9-C4 | 7.68 | 108.87 | 105.80 |
| 1 | 16S1 | 389 | A | N3-C4-N9 | 7.68 | 133.54 | 127.40 |
| 22 | 23S1 | 1367 | A | C5-N7-C8 | 7.68 | 107.74 | 103.90 |
| 22 | 23S1 | 156 | A | C5-N7-C8 | 7.68 | 107.74 | 103.90 |
| 22 | 23S1 | 1286 | A | C5-N7-C8 | 7.68 | 107.74 | 103.90 |
| 1 | 16S1 | 71 | A | C5-N7-C8 | 7.68 | 107.74 | 103.90 |
| 1 | 16S1 | 1271 | A | C5-N7-C8 | 7.68 | 107.74 | 103.90 |
| 22 | 23S1 | 52 | A | C4-C5-C6 | 7.68 | 120.84 | 117.00 |
| 22 | 23S1 | 226 | A | C5-N7-C8 | 7.68 | 107.74 | 103.90 |
| 22 | 23S1 | 152 | A | C5-N7-C8 | 7.67 | 107.74 | 103.90 |
| 22 | 23S1 | 960 | A | N3-C4-N9 | 7.67 | 133.53 | 127.40 |
| 22 | 23S1 | 609 | A | C5-N7-C8 | 7.67 | 107.73 | 103.90 |
| 22 | 23S1 | 1936 | A | N3-C4-N9 | 7.67 | 133.53 | 127.40 |
| 23 | 05S1 | 99 | A | C5-N7-C8 | 7.67 | 107.73 | 103.90 |
| 22 | 23S1 | 1080 | A | C5-N7-C8 | 7.67 | 107.73 | 103.90 |
| 22 | 23S1 | 1313 | U | N3-C2-O2 | -7.67 | 116.83 | 122.20 |
| 22 | 23S1 | 675 | A | C5-N7-C8 | 7.66 | 107.73 | 103.90 |
| 55 | PTR1 | 42 | A | C5-N7-C8 | 7.66 | 107.73 | 103.90 |
| 1 | 16S1 | 1111 | A | C5-N7-C8 | 7.66 | 107.73 | 103.90 |
| 22 | 23S1 | 42 | A | C5-N7-C8 | 7.66 | 107.73 | 103.90 |
| 22 | 23S1 | 1637 | A | C5-N7-C8 | 7.66 | 107.73 | 103.90 |
| 23 | 05S1 | 78 | A | C5-N7-C8 | 7.66 | 107.73 | 103.90 |
| 1 | 16S1 | 51 | A | C4-C5-C6 | 7.66 | 120.83 | 117.00 |
| 22 | 23S1 | 1103 | A | C5-N7-C8 | 7.66 | 107.73 | 103.90 |
| 22 | 23S1 | 2459 | A | N3-C4-N9 | 7.66 | 133.52 | 127.40 |
| 22 | 23S1 | 1470 | A | C5-N7-C8 | 7.65 | 107.73 | 103.90 |
| 22 | 23S1 | 265 | A | C5-N7-C8 | 7.65 | 107.72 | 103.90 |
| 22 | 23S1 | 941 | A | C5-N7-C8 | 7.65 | 107.72 | 103.90 |
| 22 | 23S1 | 330 | A | C5-N7-C8 | 7.65 | 107.72 | 103.90 |
| 1 | 16S1 | 238 | A | C5-N7-C8 | 7.65 | 107.72 | 103.90 |
| 1 | 16S1 | 298 | A | C5-N7-C8 | 7.65 | 107.72 | 103.90 |
| 1 | 16S1 | 477 | C | N1-C2-O2 | 7.65 | 123.49 | 118.90 |
| 1 | 16S1 | 914 | A | C5-N7-C8 | 7.65 | 107.72 | 103.90 |
| 1 | 16S1 | 98 | A | C4-C5-C6 | 7.65 | 120.82 | 117.00 |
| 22 | 23S1 | 1634 | A | C5-N7-C8 | 7.64 | 107.72 | 103.90 |
| 1 | 16S1 | 900 | A | C5-N7-C8 | 7.64 | 107.72 | 103.90 |
| 22 | 23S1 | 863 | A | N3-C4-N9 | 7.64 | 133.51 | 127.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 83 | A | C5-N7-C8 | 7.64 | 107.72 | 103.90 |
| 22 | 23S1 | 1354 | A | C5-N7-C8 | 7.64 | 107.72 | 103.90 |
| 22 | 23S1 | 2646 | C | C6-N1-C2 | -7.64 | 117.25 | 120.30 |
| 22 | 23S1 | 1938 | A | C5-N7-C8 | 7.63 | 107.72 | 103.90 |
| 1 | 16S1 | 787 | A | C5-N7-C8 | 7.63 | 107.72 | 103.90 |
| 22 | 23S1 | 972 | A | C5-N7-C8 | 7.63 | 107.72 | 103.90 |
| 22 | 23S1 | 2461 | A | C5-N7-C8 | 7.63 | 107.71 | 103.90 |
| 1 | 16S1 | 935 | A | C5-N7-C8 | 7.62 | 107.71 | 103.90 |
| 1 | 16S1 | 1368 | A | C5-N7-C8 | 7.62 | 107.71 | 103.90 |
| 22 | 23S1 | 1205 | A | C5-N7-C8 | 7.62 | 107.71 | 103.90 |
| 1 | 16S1 | 139 | A | C5-N7-C8 | 7.62 | 107.71 | 103.90 |
| 22 | 23S1 | 1871 | A | C4-C5-C6 | 7.62 | 120.81 | 117.00 |
| 22 | 23S1 | 2733 | A | C5-N7-C8 | 7.62 | 107.71 | 103.90 |
| 1 | 16S1 | 1036 | A | C5-N7-C8 | 7.62 | 107.71 | 103.90 |
| 22 | 23S1 | 1314 | C | C6-N1-C2 | -7.62 | 117.25 | 120.30 |
| 1 | 16S1 | 1285 | A | C5-N7-C8 | 7.62 | 107.71 | 103.90 |
| 22 | 23S1 | 666 | A | C5-N7-C8 | 7.62 | 107.71 | 103.90 |
| 22 | 23S1 | 2378 | A | C5-N7-C8 | 7.62 | 107.71 | 103.90 |
| 1 | 16S1 | 149 | A | C5-N7-C8 | 7.62 | 107.71 | 103.90 |
| 22 | 23S1 | 1169 | A | C5-N7-C8 | 7.62 | 107.71 | 103.90 |
| 1 | 16S1 | 1534 | A | C5-N7-C8 | 7.61 | 107.71 | 103.90 |
| 22 | 23S1 | 457 | A | C8-N9-C4 | 7.61 | 108.85 | 105.80 |
| 22 | 23S1 | 2114 | A | C4-C5-C6 | 7.61 | 120.81 | 117.00 |
| 22 | 23S1 | 2800 | A | C8-N9-C4 | 7.61 | 108.84 | 105.80 |
| 22 | 23S1 | 12 | U | N1-C2-O2 | 7.61 | 128.13 | 122.80 |
| 22 | 23S1 | 1385 | A | C5-N7-C8 | 7.61 | 107.71 | 103.90 |
| 1 | 16S1 | 325 | A | C5-N7-C8 | 7.61 | 107.70 | 103.90 |
| 1 | 16S1 | 523 | A | C5-N7-C8 | 7.61 | 107.70 | 103.90 |
| 22 | 23S1 | 1373 | A | C5-N7-C8 | 7.61 | 107.70 | 103.90 |
| 22 | 23S1 | 1544 | A | N9-C4-C5 | 7.61 | 108.84 | 105.80 |
| 22 | 23S1 | 1322 | A | C5-N7-C8 | 7.61 | 107.70 | 103.90 |
| 22 | 23S1 | 2189 | U | C6-N1-C2 | -7.61 | 116.44 | 121.00 |
| 22 | 23S1 | 1111 | A | C4-C5-C6 | 7.61 | 120.80 | 117.00 |
| 22 | 23S1 | 1987 | A | C5-N7-C8 | 7.61 | 107.70 | 103.90 |
| 1 | 16S1 | 1274 | A | C5-N7-C8 | 7.60 | 107.70 | 103.90 |
| 22 | 23S1 | 1054 | A | C5-N7-C8 | 7.60 | 107.70 | 103.90 |
| 22 | 23S1 | 1431 | A | C5-N7-C8 | 7.60 | 107.70 | 103.90 |
| 1 | 16S1 | 1019 | A | C5-N7-C8 | 7.60 | 107.70 | 103.90 |
| 22 | 23S1 | 160 | A | N9-C4-C5 | 7.60 | 108.84 | 105.80 |
| 1 | 16S1 | 858 | G | N1-C6-O6 | -7.60 | 115.34 | 119.90 |
| 1 | 16S1 | 938 | A | C5-N7-C8 | 7.60 | 107.70 | 103.90 |
| 22 | 23S1 | 1307 | A | C5-N7-C8 | 7.60 | 107.70 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 16S1 | 489 | C | N3-C2-O2 | -7.60 | 116.58 | 121.90 |
| 1 | 16S1 | 1201 | A | C4-C5-C6 | 7.60 | 120.80 | 117.00 |
| 1 | 16S1 | 1434 | A | C5-N7-C8 | 7.60 | 107.70 | 103.90 |
| 22 | 23S1 | 793 | A | C5-N7-C8 | 7.60 | 107.70 | 103.90 |
| 22 | 23S1 | 1614 | A | C5-N7-C8 | 7.60 | 107.70 | 103.90 |
| 22 | 23S1 | 1970 | A | C5-N7-C8 | 7.60 | 107.70 | 103.90 |
| 22 | 23S1 | 2077 | A | C5-N7-C8 | 7.60 | 107.70 | 103.90 |
| 1 | 16S1 | 510 | A | C5-N7-C8 | 7.59 | 107.70 | 103.90 |
| 1 | 16S1 | 431 | A | C4-C5-N7 | -7.59 | 106.90 | 110.70 |
| 22 | 23S1 | 2469 | A | C5-N7-C8 | 7.59 | 107.69 | 103.90 |
| 22 | 23S1 | 1757 | A | C5-N7-C8 | 7.59 | 107.69 | 103.90 |
| 1 | 16S1 | 600 | A | C5-N7-C8 | 7.59 | 107.69 | 103.90 |
| 1 | 16S1 | 743 | A | C5-N7-C8 | 7.59 | 107.69 | 103.90 |
| 22 | 23S1 | 1384 | A | C5-N7-C8 | 7.59 | 107.69 | 103.90 |
| 22 | 23S1 | 1490 | A | C5-N7-C8 | 7.59 | 107.69 | 103.90 |
| 22 | 23S1 | 1545 | A | C5-N7-C8 | 7.59 | 107.69 | 103.90 |
| 22 | 23S1 | 2541 | A | C5-N7-C8 | 7.59 | 107.69 | 103.90 |
| 1 | 16S1 | 349 | A | C5-N7-C8 | 7.58 | 107.69 | 103.90 |
| 1 | 16S1 | 937 | A | C5-N7-C8 | 7.58 | 107.69 | 103.90 |
| 1 | 16S1 | 181 | A | N3-C4-N9 | 7.58 | 133.47 | 127.40 |
| 1 | 16S1 | 262 | A | C5-N7-C8 | 7.58 | 107.69 | 103.90 |
| 22 | 23S1 | 223 | A | C5-N7-C8 | 7.58 | 107.69 | 103.90 |
| 22 | 23S1 | 503 | A | C5-N7-C8 | 7.58 | 107.69 | 103.90 |
| 22 | 23S1 | 1365 | A | C5-N7-C8 | 7.58 | 107.69 | 103.90 |
| 22 | 23S1 | 2281 | A | C5-N7-C8 | 7.58 | 107.69 | 103.90 |
| 22 | 23S1 | 1952 | A | C5-N7-C8 | 7.58 | 107.69 | 103.90 |
| 22 | 23S1 | 2058 | A | C5-N7-C8 | 7.58 | 107.69 | 103.90 |
| 1 | 16S1 | 1004 | A | N9-C4-C5 | 7.58 | 108.83 | 105.80 |
| 1 | 16S1 | 1170 | A | C5-C6-N6 | 7.58 | 129.76 | 123.70 |
| 22 | 23S1 | 91 | A | C5-N7-C8 | 7.58 | 107.69 | 103.90 |
| 22 | 23S1 | 1260 | A | C5-N7-C8 | 7.58 | 107.69 | 103.90 |
| 22 | 23S1 | 1735 | A | C5-N7-C8 | 7.58 | 107.69 | 103.90 |
| 1 | 16S1 | 160 | A | C5-N7-C8 | 7.57 | 107.69 | 103.90 |
| 22 | 23S1 | 2158 | A | C5-N7-C8 | 7.57 | 107.68 | 103.90 |
| 1 | 16S1 | 414 | A | C5-N7-C8 | 7.57 | 107.68 | 103.90 |
| 1 | 16S1 | 532 | A | C5-N7-C8 | 7.56 | 107.68 | 103.90 |
| 1 | 16S1 | 1152 | A | C4-C5-C6 | 7.56 | 120.78 | 117.00 |
| 22 | 23S1 | 1269 | A | C5-N7-C8 | 7.56 | 107.68 | 103.90 |
| 1 | 16S1 | 906 | A | C5-N7-C8 | 7.56 | 107.68 | 103.90 |
| 22 | 23S1 | 84 | A | N3-C4-C5 | -7.56 | 121.51 | 126.80 |
| 22 | 23S1 | 1566 | A | C5-N7-C8 | 7.56 | 107.68 | 103.90 |
| 22 | 23S1 | 899 | A | C5-N7-C8 | 7.56 | 107.68 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 453 | A | C5-N7-C8 | 7.56 | 107.68 | 103.90 |
| 22 | 23S1 | 191 | A | C4-C5-C6 | 7.56 | 120.78 | 117.00 |
| 22 | 23S1 | 1301 | A | C5-N7-C8 | 7.55 | 107.68 | 103.90 |
| 22 | 23S1 | 2020 | A | C5-N7-C8 | 7.55 | 107.68 | 103.90 |
| 1 | 16S1 | 461 | A | C5-N7-C8 | 7.55 | 107.68 | 103.90 |
| 1 | 16S1 | 901 | A | C5-C6-N6 | 7.55 | 129.74 | 123.70 |
| 22 | 23S1 | 2748 | A | C5-N7-C8 | 7.55 | 107.68 | 103.90 |
| 1 | 16S1 | 1216 | A | C5-N7-C8 | 7.55 | 107.67 | 103.90 |
| 22 | 23S1 | 492 | A | N3-C4-N9 | 7.55 | 133.44 | 127.40 |
| 22 | 23S1 | 943 | A | C5-N7-C8 | 7.55 | 107.67 | 103.90 |
| 22 | 23S1 | 603 | A | C5-N7-C8 | 7.55 | 107.67 | 103.90 |
| 22 | 23S1 | 2071 | A | C5-N7-C8 | 7.55 | 107.67 | 103.90 |
| 1 | 16S1 | 759 | A | C5-N7-C8 | 7.54 | 107.67 | 103.90 |
| 22 | 23S1 | 415 | A | C5-N7-C8 | 7.54 | 107.67 | 103.90 |
| 22 | 23S1 | 1387 | A | C5-N7-C8 | 7.54 | 107.67 | 103.90 |
| 1 | 16S1 | 98 | A | C5-N7-C8 | 7.54 | 107.67 | 103.90 |
| 22 | 23S1 | 1866 | A | C4-C5-C6 | 7.54 | 120.77 | 117.00 |
| 55 | PTR1 | 76 | A | C5-N7-C8 | 7.54 | 107.67 | 103.90 |
| 1 | 16S1 | 143 | A | C8-N9-C4 | 7.54 | 108.82 | 105.80 |
| 1 | 16S1 | 1289 | A | C5-N7-C8 | 7.54 | 107.67 | 103.90 |
| 22 | 23S1 | 384 | A | C5-N7-C8 | 7.54 | 107.67 | 103.90 |
| 22 | 23S1 | 574 | A | C8-N9-C4 | 7.54 | 108.82 | 105.80 |
| 22 | 23S1 | 2328 | A | C4-C5-C6 | 7.54 | 120.77 | 117.00 |
| 22 | 23S1 | 2386 | A | C5-N7-C8 | 7.54 | 107.67 | 103.90 |
| 1 | 16S1 | 573 | A | C5-N7-C8 | 7.53 | 107.67 | 103.90 |
| 1 | 16S1 | 878 | A | C5-N7-C8 | 7.53 | 107.67 | 103.90 |
| 1 | 16S1 | 1180 | A | C5-N7-C8 | 7.53 | 107.67 | 103.90 |
| 22 | 23S1 | 1077 | A | C5-N7-C8 | 7.53 | 107.67 | 103.90 |
| 22 | 23S1 | 2163 | A | C5-N7-C8 | 7.53 | 107.67 | 103.90 |
| 1 | 16S1 | 1363 | A | N3-C4-N9 | 7.53 | 133.42 | 127.40 |
| 22 | 23S1 | 2893 | A | C5-N7-C8 | 7.53 | 107.66 | 103.90 |
| 1 | 16S1 | 3 | A | C5-N7-C8 | 7.53 | 107.66 | 103.90 |
| 22 | 23S1 | 515 | A | C5-N7-C8 | 7.53 | 107.66 | 103.90 |
| 22 | 23S1 | 401 | A | C5-N7-C8 | 7.52 | 107.66 | 103.90 |
| 1 | 16S1 | 300 | A | C6-C5-N7 | -7.52 | 127.03 | 132.30 |
| 1 | 16S1 | 1145 | A | C5-N7-C8 | 7.52 | 107.66 | 103.90 |
| 1 | 16S1 | 1046 | A | C4-C5-C6 | 7.52 | 120.76 | 117.00 |
| 1 | 16S1 | 873 | A | C4-C5-C6 | 7.52 | 120.76 | 117.00 |
| 22 | 23S1 | 14 | A | C5-N7-C8 | 7.52 | 107.66 | 103.90 |
| 22 | 23S1 | 960 | A | C5-N7-C8 | 7.52 | 107.66 | 103.90 |
| 22 | 23S1 | 819 | A | C5-N7-C8 | 7.52 | 107.66 | 103.90 |
| 22 | 23S1 | 1802 | A | N3-C4-N9 | 7.52 | 133.41 | 127.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 16S1 | 205 | A | C5-N7-C8 | 7.52 | 107.66 | 103.90 |
| 1 | 16S1 | 1430 | A | C5-N7-C8 | 7.51 | 107.66 | 103.90 |
| 22 | 23S1 | 802 | A | C5-N7-C8 | 7.51 | 107.66 | 103.90 |
| 22 | 23S1 | 2883 | A | C5-N7-C8 | 7.51 | 107.66 | 103.90 |
| 22 | 23S1 | 1609 | A | C5-N7-C8 | 7.51 | 107.65 | 103.90 |
| 22 | 23S1 | 1916 | A | C5-N7-C8 | 7.51 | 107.66 | 103.90 |
| 22 | 23S1 | 2600 | A | C5-N7-C8 | 7.51 | 107.65 | 103.90 |
| 1 | 16S1 | 88 | U | N3-C2-O2 | -7.51 | 116.94 | 122.20 |
| 1 | 16S1 | 1150 | A | C5-N7-C8 | 7.51 | 107.65 | 103.90 |
| 1 | 16S1 | 1394 | A | C5-N7-C8 | 7.51 | 107.65 | 103.90 |
| 22 | 23S1 | 877 | A | C5-N7-C8 | 7.51 | 107.65 | 103.90 |
| 22 | 23S1 | 1739 | A | C4-C5-C6 | 7.51 | 120.75 | 117.00 |
| 22 | 23S1 | 2191 | A | C4-C5-C6 | 7.51 | 120.75 | 117.00 |
| 22 | 23S1 | 2700 | A | C5-N7-C8 | 7.51 | 107.65 | 103.90 |
| 1 | 16S1 | 441 | A | C5-N7-C8 | 7.50 | 107.65 | 103.90 |
| 1 | 16S1 | 502 | A | N3-C4-N9 | 7.50 | 133.40 | 127.40 |
| 22 | 23S1 | 1969 | A | C5-N7-C8 | 7.50 | 107.65 | 103.90 |
| 22 | 23S1 | 2134 | A | C5-N7-C8 | 7.50 | 107.65 | 103.90 |
| 22 | 23S1 | 195 | A | N7-C8-N9 | -7.50 | 110.05 | 113.80 |
| 22 | 23S1 | 2241 | A | C5-N7-C8 | 7.50 | 107.65 | 103.90 |
| 1 | 16S1 | 8 | A | C8-N9-C4 | 7.50 | 108.80 | 105.80 |
| 1 | 16S1 | 1349 | A | C5-N7-C8 | 7.50 | 107.65 | 103.90 |
| 22 | 23S1 | 470 | A | C5-N7-C8 | 7.49 | 107.65 | 103.90 |
| 22 | 23S1 | 572 | A | C5-N7-C8 | 7.49 | 107.65 | 103.90 |
| 22 | 23S1 | 1553 | A | C5-N7-C8 | 7.49 | 107.65 | 103.90 |
| 22 | 23S1 | 2023 | C | C6-N1-C2 | -7.49 | 117.30 | 120.30 |
| 22 | 23S1 | 820 | A | C4-C5-C6 | 7.49 | 120.74 | 117.00 |
| 22 | 23S1 | 1722 | A | N3-C4-N9 | 7.49 | 133.39 | 127.40 |
| 22 | 23S1 | 2734 | A | C5-N7-C8 | 7.49 | 107.64 | 103.90 |
| 22 | 23S1 | 1928 | A | C5-N7-C8 | 7.49 | 107.64 | 103.90 |
| 22 | 23S1 | 2675 | A | C5-N7-C8 | 7.49 | 107.64 | 103.90 |
| 1 | 16S1 | 1287 | A | C5-N7-C8 | 7.48 | 107.64 | 103.90 |
| 22 | 23S1 | 1028 | A | C5-N7-C8 | 7.48 | 107.64 | 103.90 |
| 22 | 23S1 | 1312 | U | C5-C4-O4 | 7.48 | 130.39 | 125.90 |
| 1 | 16S1 | 131 | A | C5-N7-C8 | 7.48 | 107.64 | 103.90 |
| 22 | 23S1 | 2037 | A | C5-N7-C8 | 7.48 | 107.64 | 103.90 |
| 1 | 16S1 | 1441 | A | C8-N9-C4 | 7.48 | 108.79 | 105.80 |
| 22 | 23S1 | 1366 | A | C5-N7-C8 | 7.48 | 107.64 | 103.90 |
| 22 | 23S1 | 572 | A | C4-C5-C6 | 7.47 | 120.74 | 117.00 |
| 22 | 23S1 | 2198 | A | C5-N7-C8 | 7.47 | 107.64 | 103.90 |
| 1 | 16S1 | 303 | A | C5-N7-C8 | 7.47 | 107.64 | 103.90 |
| 1 | 16S1 | 374 | A | C5-N7-C8 | 7.47 | 107.64 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 1 | 16S1 | 749 | A | C5-N7-C8 | 7.47 | 107.64 | 103.90 |
| 1 | 16S1 | 706 | A | N3-C4-N9 | 7.47 | 133.38 | 127.40 |
| 22 | 23S1 | 1001 | A | C5-N7-C8 | 7.47 | 107.64 | 103.90 |
| 22 | 23S1 | 1598 | A | C5-N7-C8 | 7.47 | 107.63 | 103.90 |
| 1 | 16S1 | 465 | A | C5-N7-C8 | 7.46 | 107.63 | 103.90 |
| 22 | 23S1 | 2453 | A | N9-C4-C5 | 7.46 | 108.78 | 105.80 |
| 22 | 23S1 | 892 | A | N3-C4-N9 | 7.46 | 133.37 | 127.40 |
| 22 | 23S1 | 221 | A | C8-N9-C4 | 7.46 | 108.78 | 105.80 |
| 22 | 23S1 | 1528 | A | N3-C4-N9 | 7.46 | 133.37 | 127.40 |
| 22 | 23S1 | 2287 | A | N3-C4-N9 | 7.46 | 133.37 | 127.40 |
| 1 | 16S1 | 1362 | A | C5-N7-C8 | 7.46 | 107.63 | 103.90 |
| 1 | 16S1 | 1433 | A | C5-N7-C8 | 7.45 | 107.63 | 103.90 |
| 1 | 16S1 | 116 | A | C5-N7-C8 | 7.45 | 107.63 | 103.90 |
| 1 | 16S1 | 994 | A | C5-N7-C8 | 7.45 | 107.63 | 103.90 |
| 1 | 16S1 | 495 | A | C5-N7-C8 | 7.45 | 107.62 | 103.90 |
| 1 | 16S1 | 77 | A | N3-C4-N9 | 7.45 | 133.36 | 127.40 |
| 22 | 23S1 | 1272 | A | C5-N7-C8 | 7.45 | 107.62 | 103.90 |
| 22 | 23S1 | 2809 | A | C5-N7-C8 | 7.45 | 107.62 | 103.90 |
| 22 | 23S1 | 470 | A | N3-C4-N9 | 7.44 | 133.35 | 127.40 |
| 22 | 23S1 | 2572 | A | C8-N9-C4 | 7.44 | 108.78 | 105.80 |
| 22 | 23S1 | 2851 | A | C5-N7-C8 | 7.44 | 107.62 | 103.90 |
| 1 | 16S1 | 676 | A | C5-N7-C8 | 7.44 | 107.62 | 103.90 |
| 22 | 23S1 | 479 | A | C5-N7-C8 | 7.44 | 107.62 | 103.90 |
| 22 | 23S1 | 896 | A | C5-N7-C8 | 7.44 | 107.62 | 103.90 |
| 22 | 23S1 | 1626 | A | C5-N7-C8 | 7.44 | 107.62 | 103.90 |
| 22 | 23S1 | 2741 | A | C5-N7-C8 | 7.44 | 107.62 | 103.90 |
| 22 | 23S1 | 2823 | A | C5-N7-C8 | 7.44 | 107.62 | 103.90 |
| 1 | 16S1 | 32 | A | C5-N7-C8 | 7.44 | 107.62 | 103.90 |
| 1 | 16S1 | 865 | A | C5-N7-C8 | 7.44 | 107.62 | 103.90 |
| 1 | 16S1 | 802 | A | C5-N7-C8 | 7.44 | 107.62 | 103.90 |
| 1 | 16S1 | 1130 | A | C5-N7-C8 | 7.44 | 107.62 | 103.90 |
| 22 | 23S1 | 654 | A | C5-N7-C8 | 7.44 | 107.62 | 103.90 |
| 22 | 23S1 | 2267 | A | C5-N7-C8 | 7.44 | 107.62 | 103.90 |
| 22 | 23S1 | 131 | A | N3-C4-N9 | 7.43 | 133.35 | 127.40 |
| 22 | 23S1 | 310 | A | C5-N7-C8 | 7.43 | 107.62 | 103.90 |
| 22 | 23S1 | 2879 | A | C5-N7-C8 | 7.43 | 107.62 | 103.90 |
| 22 | 23S1 | 933 | A | C5-N7-C8 | 7.43 | 107.62 | 103.90 |
| 22 | 23S1 | 2358 | A | C5-N7-C8 | 7.43 | 107.61 | 103.90 |
| 1 | 16S1 | 1163 | A | C5-N7-C8 | 7.43 | 107.61 | 103.90 |
| 22 | 23S1 | 2377 | A | C5-N7-C8 | 7.43 | 107.61 | 103.90 |
| 1 | 16S1 | 1483 | A | C4-C5-C6 | 7.42 | 120.71 | 117.00 |
| 22 | 23S1 | 2461 | A | C5-C6-N1 | 7.42 | 121.41 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 2051 | A | N3-C4-N9 | 7.42 | 133.34 | 127.40 |
| 22 | 23S1 | 592 | A | C5-N7-C8 | 7.42 | 107.61 | 103.90 |
| 22 | 23S1 | 2369 | A | C4-C5-C6 | 7.42 | 120.71 | 117.00 |
| 42 | L241 | 52 | LEU | CA-CB-CG | 7.42 | 132.37 | 115.30 |
| 1 | 16S1 | 747 | A | C5-N7-C8 | 7.42 | 107.61 | 103.90 |
| 1 | 16S1 | 1014 | A | C5-N7-C8 | 7.42 | 107.61 | 103.90 |
| 1 | 16S1 | 1248 | A | C5-N7-C8 | 7.42 | 107.61 | 103.90 |
| 22 | 23S1 | 1953 | A | C4-C5-C6 | 7.42 | 120.71 | 117.00 |
| 22 | 23S1 | 1677 | A | C5-N7-C8 | 7.41 | 107.61 | 103.90 |
| 22 | 23S1 | 471 | A | C5-N7-C8 | 7.41 | 107.61 | 103.90 |
| 22 | 23S1 | 1254 | A | C5-N7-C8 | 7.41 | 107.61 | 103.90 |
| 22 | 23S1 | 742 | A | C5-N7-C8 | 7.41 | 107.60 | 103.90 |
| 22 | 23S1 | 2706 | A | N3-C4-N9 | 7.41 | 133.33 | 127.40 |
| 22 | 23S1 | 227 | A | C8-N9-C4 | 7.41 | 108.76 | 105.80 |
| 22 | 23S1 | 167 | A | C8-N9-C4 | 7.41 | 108.76 | 105.80 |
| 22 | 23S1 | 1496 | A | C5-N7-C8 | 7.41 | 107.60 | 103.90 |
| 1 | 16S1 | 608 | A | C5-N7-C8 | 7.40 | 107.60 | 103.90 |
| 22 | 23S1 | 2082 | A | C4-C5-C6 | 7.40 | 120.70 | 117.00 |
| 22 | 23S1 | 574 | A | C5-N7-C8 | 7.40 | 107.60 | 103.90 |
| 22 | 23S1 | 2407 | A | N3-C4-N9 | 7.40 | 133.32 | 127.40 |
| 22 | 23S1 | 984 | A | C4-C5-C6 | 7.40 | 120.70 | 117.00 |
| 22 | 23S1 | 1495 | A | C5-N7-C8 | 7.40 | 107.60 | 103.90 |
| 1 | 16S1 | 32 | A | C4-C5-C6 | 7.40 | 120.70 | 117.00 |
| 1 | 16S1 | 872 | A | N7-C8-N9 | -7.39 | 110.10 | 113.80 |
| 22 | 23S1 | 2478 | A | C5-N7-C8 | 7.39 | 107.60 | 103.90 |
| 22 | 23S1 | 973 | A | N7-C8-N9 | -7.39 | 110.10 | 113.80 |
| 22 | 23S1 | 1314 | C | C2-N1-C1' | 7.39 | 126.93 | 118.80 |
| 1 | 16S1 | 452 | A | C5-N7-C8 | 7.39 | 107.59 | 103.90 |
| 22 | 23S1 | 255 | A | C4-C5-C6 | 7.39 | 120.69 | 117.00 |
| 22 | 23S1 | 654 | A | N3-C4-N9 | 7.39 | 133.31 | 127.40 |
| 1 | 16S1 | 246 | A | C8-N9-C4 | 7.38 | 108.75 | 105.80 |
| 1 | 16S1 | 642 | A | C5-N7-C8 | 7.38 | 107.59 | 103.90 |
| 1 | 16S1 | 1398 | A | C5-N7-C8 | 7.38 | 107.59 | 103.90 |
| 22 | 23S1 | 482 | A | C5-C6-N6 | 7.38 | 129.61 | 123.70 |
| 55 | PTR1 | 23 | A | C5-N7-C8 | 7.38 | 107.59 | 103.90 |
| 1 | 16S1 | 546 | A | C5-N7-C8 | 7.38 | 107.59 | 103.90 |
| 22 | 23S1 | 2564 | A | C5-N7-C8 | 7.38 | 107.59 | 103.90 |
| 1 | 16S1 | 451 | A | C4-C5-C6 | 7.38 | 120.69 | 117.00 |
| 22 | 23S1 | 1701 | A | C5-N7-C8 | 7.38 | 107.59 | 103.90 |
| 22 | 23S1 | 1970 | A | N3-C4-N9 | 7.38 | 133.30 | 127.40 |
| 22 | 23S1 | 1284 | A | C5-N7-C8 | 7.38 | 107.59 | 103.90 |
| 22 | 23S1 | 1142 | A | N3-C4-N9 | 7.38 | 133.30 | 127.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 22 | 23S1 | 460 | A | C5-N7-C8 | 7.37 | 107.59 | 103.90 |
| 22 | 23S1 | 2189 | U | N1-C2-O2 | 7.37 | 127.96 | 122.80 |
| 1 | 16S1 | 949 | A | C4-C5-C6 | 7.37 | 120.69 | 117.00 |
| 22 | 23S1 | 28 | A | C5-N7-C8 | 7.37 | 107.58 | 103.90 |
| 22 | 23S1 | 599 | A | C5-N7-C8 | 7.37 | 107.58 | 103.90 |
| 1 | 16S1 | 663 | A | C5-N7-C8 | 7.37 | 107.58 | 103.90 |
| 1 | 16S1 | 702 | A | C5-N7-C8 | 7.37 | 107.58 | 103.90 |
| 1 | 16S1 | 901 | A | C5-N7-C8 | 7.37 | 107.58 | 103.90 |
| 22 | 23S1 | 1314 | C | N1-C2-O2 | 7.37 | 123.32 | 118.90 |
| 22 | 23S1 | 2820 | A | C5-N7-C8 | 7.37 | 107.58 | 103.90 |
| 1 | 16S1 | 907 | A | C5-N7-C8 | 7.37 | 107.58 | 103.90 |
| 22 | 23S1 | 1808 | A | C5-N7-C8 | 7.37 | 107.58 | 103.90 |
| 22 | 23S1 | 727 | A | C8-N9-C4 | 7.37 | 108.75 | 105.80 |
| 22 | 23S1 | 49 | A | C4-C5-C6 | 7.36 | 120.68 | 117.00 |
| 22 | 23S1 | 1998 | A | C4-C5-C6 | 7.36 | 120.68 | 117.00 |
| 22 | 23S1 | 721 | A | C5-N7-C8 | 7.36 | 107.58 | 103.90 |
| 1 | 16S1 | 55 | A | C4-C5-C6 | 7.36 | 120.68 | 117.00 |
| 22 | 23S1 | 1689 | A | C4-C5-C6 | 7.36 | 120.68 | 117.00 |
| 22 | 23S1 | 1877 | A | C5-N7-C8 | 7.36 | 107.58 | 103.90 |
| 1 | 16S1 | 7 | A | C5-N7-C8 | 7.36 | 107.58 | 103.90 |
| 1 | 16S1 | 1102 | A | C5-N7-C8 | 7.36 | 107.58 | 103.90 |
| 23 | 05S1 | 73 | A | C5-N7-C8 | 7.36 | 107.58 | 103.90 |
| 1 | 16S1 | 80 | A | C4-C5-C6 | 7.36 | 120.68 | 117.00 |
| 22 | 23S1 | 196 | A | C4-C5-C6 | 7.36 | 120.68 | 117.00 |
| 1 | 16S1 | 1468 | A | C5-C6-N6 | 7.36 | 129.58 | 123.70 |
| 22 | 23S1 | 632 | A | C5-N7-C8 | 7.35 | 107.58 | 103.90 |
| 22 | 23S1 | 1028 | A | C5-C6-N1 | 7.35 | 121.38 | 117.70 |
| 22 | 23S1 | 2749 | A | C5-N7-C8 | 7.35 | 107.58 | 103.90 |
| 1 | 16S1 | 430 | A | C4-C5-C6 | 7.35 | 120.68 | 117.00 |
| 22 | 23S1 | 1469 | A | N3-C4-N9 | 7.35 | 133.28 | 127.40 |
| 22 | 23S1 | 2199 | A | N3-C4-N9 | 7.35 | 133.28 | 127.40 |
| 22 | 23S1 | 1854 | A | N3-C4-N9 | 7.35 | 133.28 | 127.40 |
| 22 | 23S1 | 572 | A | N3-C4-N9 | 7.35 | 133.28 | 127.40 |
| 22 | 23S1 | 6 | A | C5-N7-C8 | 7.34 | 107.57 | 103.90 |
| 22 | 23S1 | 750 | A | C5-N7-C8 | 7.34 | 107.57 | 103.90 |
| 22 | 23S1 | 1593 | A | C5-N7-C8 | 7.34 | 107.57 | 103.90 |
| 1 | 16S1 | 1468 | A | C4-C5-C6 | 7.34 | 120.67 | 117.00 |
| 22 | 23S1 | 324 | A | C5-N7-C8 | 7.34 | 107.57 | 103.90 |
| 22 | 23S1 | 730 | A | C5-N7-C8 | 7.34 | 107.57 | 103.90 |
| 22 | 23S1 | 928 | A | C5-N7-C8 | 7.34 | 107.57 | 103.90 |
| 22 | 23S1 | 502 | A | C5-N7-C8 | 7.34 | 107.57 | 103.90 |
| 22 | 23S1 | 749 | A | C5-N7-C8 | 7.34 | 107.57 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 1579 | A | C5-N7-C8 | 7.34 | 107.57 | 103.90 |
| 22 | 23S1 | 221 | A | N3-C4-C5 | -7.33 | 121.67 | 126.80 |
| 22 | 23S1 | 820 | A | C5-N7-C8 | 7.33 | 107.57 | 103.90 |
| 1 | 16S1 | 673 | A | N3-C4-N9 | 7.33 | 133.26 | 127.40 |
| 1 | 16S1 | 790 | A | C5-N7-C8 | 7.33 | 107.56 | 103.90 |
| 1 | 16S1 | 1257 | A | C8-N9-C4 | 7.33 | 108.73 | 105.80 |
| 1 | 16S1 | 1269 | A | C4-C5-C6 | 7.33 | 120.67 | 117.00 |
| 1 | 16S1 | 1319 | A | C5-N7-C8 | 7.33 | 107.56 | 103.90 |
| 1 | 16S1 | 1483 | A | C5-N7-C8 | 7.33 | 107.56 | 103.90 |
| 22 | 23S1 | 1264 | A | C5-N7-C8 | 7.32 | 107.56 | 103.90 |
| 22 | 23S1 | 2439 | A | C5-N7-C8 | 7.32 | 107.56 | 103.90 |
| 22 | 23S1 | 2757 | A | C5-N7-C8 | 7.32 | 107.56 | 103.90 |
| 22 | 23S1 | 1387 | A | N3-C4-N9 | 7.32 | 133.26 | 127.40 |
| 1 | 16S1 | 767 | A | C5-N7-C8 | 7.32 | 107.56 | 103.90 |
| 22 | 23S1 | 241 | A | C5-N7-C8 | 7.32 | 107.56 | 103.90 |
| 22 | 23S1 | 2670 | A | C5-N7-C8 | 7.32 | 107.56 | 103.90 |
| 22 | 23S1 | 2451 | A | N7-C8-N9 | -7.32 | 110.14 | 113.80 |
| 22 | 23S1 | 2761 | A | C5-N7-C8 | 7.32 | 107.56 | 103.90 |
| 22 | 23S1 | 2886 | A | C5-N7-C8 | 7.32 | 107.56 | 103.90 |
| 22 | 23S1 | 2900 | A | C5-N7-C8 | 7.31 | 107.56 | 103.90 |
| 1 | 16S1 | 816 | A | C5-N7-C8 | 7.31 | 107.56 | 103.90 |
| 22 | 23S1 | 575 | A | C5-N7-C8 | 7.31 | 107.56 | 103.90 |
| 22 | 23S1 | 1678 | A | C5-N7-C8 | 7.31 | 107.56 | 103.90 |
| 22 | 23S1 | 677 | A | C5-C6-N1 | 7.31 | 121.35 | 117.70 |
| 1 | 16S1 | 101 | A | C5-N7-C8 | 7.31 | 107.55 | 103.90 |
| 22 | 23S1 | 699 | A | C5-N7-C8 | 7.30 | 107.55 | 103.90 |
| 22 | 23S1 | 2336 | A | C5-N7-C8 | 7.30 | 107.55 | 103.90 |
| 22 | 23S1 | 2097 | A | C5-N7-C8 | 7.30 | 107.55 | 103.90 |
| 1 | 16S1 | 1254 | A | C5-N7-C8 | 7.30 | 107.55 | 103.90 |
| 22 | 23S1 | 199 | A | C5-N7-C8 | 7.30 | 107.55 | 103.90 |
| 22 | 23S1 | 217 | A | C5-N7-C8 | 7.30 | 107.55 | 103.90 |
| 22 | 23S1 | 693 | A | N3-C4-N9 | 7.30 | 133.24 | 127.40 |
| 22 | 23S1 | 2800 | A | C5-N7-C8 | 7.30 | 107.55 | 103.90 |
| 1 | 16S1 | 907 | A | N3-C4-N9 | 7.30 | 133.24 | 127.40 |
| 22 | 23S1 | 820 | A | N3-C4-N9 | 7.30 | 133.24 | 127.40 |
| 22 | 23S1 | 1133 | A | C5-N7-C8 | 7.30 | 107.55 | 103.90 |
| 22 | 23S1 | 1433 | A | C5-N7-C8 | 7.30 | 107.55 | 103.90 |
| 22 | 23S1 | 1591 | A | N3-C4-N9 | 7.30 | 133.24 | 127.40 |
| 22 | 23S1 | 2566 | A | N3-C4-C5 | -7.30 | 121.69 | 126.80 |
| 22 | 23S1 | 2706 | A | C4-C5-C6 | 7.30 | 120.65 | 117.00 |
| 1 | 16S1 | 1046 | A | N3-C4-N9 | 7.29 | 133.23 | 127.40 |
| 1 | 16S1 | 1375 | A | C4-C5-C6 | 7.29 | 120.65 | 117.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|------|-------------|----------|
| 22 | 23S1 | 705 | A | N3-C4-N9 | 7.29 | 133.23 | 127.40 |
| 1 | 16S1 | 429 | U | O4'-C1'-N1 | 7.29 | 114.03 | 108.20 |
| 1 | 16S1 | 98 | A | N3-C4-N9 | 7.29 | 133.23 | 127.40 |
| 7 | S071 | 23 | LEU | CA-CB-CG | 7.28 | 132.05 | 115.30 |
| 22 | 23S1 | 2632 | A | C8-N9-C4 | 7.28 | 108.71 | 105.80 |
| 22 | 23S1 | 2814 | A | C5-N7-C8 | 7.28 | 107.54 | 103.90 |
| 1 | 16S1 | 499 | A | C4-C5-C6 | 7.28 | 120.64 | 117.00 |
| 22 | 23S1 | 466 | A | C4-C5-C6 | 7.28 | 120.64 | 117.00 |
| 22 | 23S1 | 1569 | A | C5-N7-C8 | 7.28 | 107.54 | 103.90 |
| 22 | 23S1 | 2448 | A | N9-C4-C5 | 7.28 | 108.71 | 105.80 |
| 22 | 23S1 | 2765 | A | C4-C5-C6 | 7.28 | 120.64 | 117.00 |
| 1 | 16S1 | 1157 | A | N3-C4-N9 | 7.28 | 133.22 | 127.40 |
| 22 | 23S1 | 1918 | A | C5-N7-C8 | 7.28 | 107.54 | 103.90 |
| 22 | 23S1 | 2758 | A | C5-N7-C8 | 7.28 | 107.54 | 103.90 |
| 22 | 23S1 | 2542 | A | N9-C4-C5 | 7.27 | 108.71 | 105.80 |
| 22 | 23S1 | 415 | A | N3-C4-N9 | 7.27 | 133.22 | 127.40 |
| 22 | 23S1 | 2426 | A | C5-N7-C8 | 7.27 | 107.53 | 103.90 |
| 22 | 23S1 | 10 | A | C5-N7-C8 | 7.27 | 107.53 | 103.90 |
| 22 | 23S1 | 422 | A | C4-C5-C6 | 7.27 | 120.64 | 117.00 |
| 22 | 23S1 | 2654 | A | C5-N7-C8 | 7.27 | 107.53 | 103.90 |
| 1 | 16S1 | 996 | A | C8-N9-C4 | 7.26 | 108.71 | 105.80 |
| 1 | 16S1 | 1171 | A | C5-N7-C8 | 7.26 | 107.53 | 103.90 |
| 22 | 23S1 | 727 | A | C5-N7-C8 | 7.26 | 107.53 | 103.90 |
| 22 | 23S1 | 1214 | A | C5-N7-C8 | 7.26 | 107.53 | 103.90 |
| 22 | 23S1 | 2211 | A | C5-N7-C8 | 7.26 | 107.53 | 103.90 |
| 1 | 16S1 | 282 | A | C5-N7-C8 | 7.26 | 107.53 | 103.90 |
| 22 | 23S1 | 368 | A | C5-N7-C8 | 7.26 | 107.53 | 103.90 |
| 22 | 23S1 | 1586 | A | C4-C5-C6 | 7.26 | 120.63 | 117.00 |
| 22 | 23S1 | 131 | A | C5-N7-C8 | 7.26 | 107.53 | 103.90 |
| 22 | 23S1 | 2051 | A | C4-C5-C6 | 7.26 | 120.63 | 117.00 |
| 22 | 23S1 | 1204 | A | C5-N7-C8 | 7.26 | 107.53 | 103.90 |
| 1 | 16S1 | 607 | A | C5-N7-C8 | 7.25 | 107.53 | 103.90 |
| 22 | 23S1 | 282 | A | C5-N7-C8 | 7.25 | 107.53 | 103.90 |
| 22 | 23S1 | 1275 | A | C5-N7-C8 | 7.25 | 107.53 | 103.90 |
| 22 | 23S1 | 1359 | A | C5-N7-C8 | 7.25 | 107.53 | 103.90 |
| 22 | 23S1 | 1936 | A | C4-C5-C6 | 7.25 | 120.63 | 117.00 |
| 22 | 23S1 | 2407 | A | C5-N7-C8 | 7.25 | 107.53 | 103.90 |
| 1 | 16S1 | 72 | A | N3-C4-N9 | 7.25 | 133.20 | 127.40 |
| 22 | 23S1 | 1616 | A | C5-N7-C8 | 7.25 | 107.53 | 103.90 |
| 22 | 23S1 | 2657 | A | C5-N7-C8 | 7.25 | 107.53 | 103.90 |
| 1 | 16S1 | 572 | A | C8-N9-C4 | 7.25 | 108.70 | 105.80 |
| 1 | 16S1 | 1513 | A | C5-N7-C8 | 7.25 | 107.52 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 480 | A | C4-C5-C6 | 7.25 | 120.62 | 117.00 |
| 22 | 23S1 | 1265 | A | C5-N7-C8 | 7.25 | 107.52 | 103.90 |
| 55 | PTR1 | 26 | A | C5-N7-C8 | 7.25 | 107.52 | 103.90 |
| 22 | 23S1 | 677 | A | C4-C5-C6 | 7.25 | 120.62 | 117.00 |
| 22 | 23S1 | 2810 | A | C5-N7-C8 | 7.25 | 107.52 | 103.90 |
| 22 | 23S1 | 507 | A | N7-C8-N9 | -7.24 | 110.18 | 113.80 |
| 1 | 16S1 | 622 | A | N3-C4-C5 | -7.24 | 121.73 | 126.80 |
| 1 | 16S1 | 864 | A | C5-N7-C8 | 7.24 | 107.52 | 103.90 |
| 1 | 16S1 | 55 | A | N3-C4-N9 | 7.24 | 133.19 | 127.40 |
| 22 | 23S1 | 1069 | A | C8-N9-C4 | 7.24 | 108.70 | 105.80 |
| 22 | 23S1 | 2534 | A | C5-N7-C8 | 7.24 | 107.52 | 103.90 |
| 1 | 16S1 | 1092 | A | C5-N7-C8 | 7.24 | 107.52 | 103.90 |
| 1 | 16S1 | 1155 | A | C5-N7-C8 | 7.24 | 107.52 | 103.90 |
| 1 | 16S1 | 1280 | A | C8-N9-C4 | 7.24 | 108.69 | 105.80 |
| 55 | PTR1 | 73 | A | C5-N7-C8 | 7.24 | 107.52 | 103.90 |
| 22 | 23S1 | 2662 | A | N3-C4-N9 | 7.24 | 133.19 | 127.40 |
| 1 | 16S1 | 431 | A | C6-N1-C2 | 7.23 | 122.94 | 118.60 |
| 22 | 23S1 | 1522 | A | C5-N7-C8 | 7.23 | 107.52 | 103.90 |
| 22 | 23S1 | 2062 | A | N3-C4-N9 | 7.23 | 133.19 | 127.40 |
| 1 | 16S1 | 59 | A | N3-C4-N9 | 7.23 | 133.19 | 127.40 |
| 1 | 16S1 | 389 | A | C5-C6-N1 | 7.23 | 121.31 | 117.70 |
| 22 | 23S1 | 94 | A | C5-N7-C8 | 7.23 | 107.51 | 103.90 |
| 1 | 16S1 | 373 | A | N3-C4-N9 | 7.23 | 133.18 | 127.40 |
| 22 | 23S1 | 470 | A | C4-C5-C6 | 7.22 | 120.61 | 117.00 |
| 22 | 23S1 | 1276 | A | N3-C4-N9 | 7.22 | 133.18 | 127.40 |
| 22 | 23S1 | 1420 | A | C8-N9-C4 | 7.22 | 108.69 | 105.80 |
| 1 | 16S1 | 1032 | G | C2-N3-C4 | 7.22 | 115.51 | 111.90 |
| 22 | 23S1 | 627 | A | C8-N9-C4 | 7.22 | 108.69 | 105.80 |
| 1 | 16S1 | 65 | A | C5-N7-C8 | 7.22 | 107.51 | 103.90 |
| 22 | 23S1 | 84 | A | C5-N7-C8 | 7.22 | 107.51 | 103.90 |
| 22 | 23S1 | 844 | A | C5-N7-C8 | 7.22 | 107.51 | 103.90 |
| 22 | 23S1 | 2114 | A | N7-C8-N9 | -7.22 | 110.19 | 113.80 |
| 22 | 23S1 | 2142 | A | N3-C4-N9 | 7.22 | 133.18 | 127.40 |
| 22 | 23S1 | 947 | A | N3-C4-N9 | 7.22 | 133.18 | 127.40 |
| 22 | 23S1 | 2868 | A | C5-N7-C8 | 7.22 | 107.51 | 103.90 |
| 1 | 16S1 | 397 | A | C5-C6-N6 | 7.22 | 129.47 | 123.70 |
| 1 | 16S1 | 1508 | A | C4-C5-C6 | 7.22 | 120.61 | 117.00 |
| 22 | 23S1 | 1978 | A | C5-N7-C8 | 7.22 | 107.51 | 103.90 |
| 22 | 23S1 | 2614 | A | C4-C5-C6 | 7.22 | 120.61 | 117.00 |
| 23 | 05S1 | 57 | A | C5-N7-C8 | 7.22 | 107.51 | 103.90 |
| 55 | PTR1 | 9 | A | C5-N7-C8 | 7.22 | 107.51 | 103.90 |
| 1 | 16S1 | 913 | A | C5-N7-C8 | 7.21 | 107.51 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 16S1 | 1446 | A | C5-N7-C8 | 7.21 | 107.51 | 103.90 |
| 1 | 16S1 | 349 | A | C8-N9-C4 | 7.21 | 108.68 | 105.80 |
| 22 | 23S1 | 300 | A | C5-N7-C8 | 7.21 | 107.50 | 103.90 |
| 22 | 23S1 | 983 | A | C5-N7-C8 | 7.21 | 107.50 | 103.90 |
| 1 | 16S1 | 430 | A | C5-N7-C8 | 7.20 | 107.50 | 103.90 |
| 22 | 23S1 | 1477 | A | C5-N7-C8 | 7.20 | 107.50 | 103.90 |
| 1 | 16S1 | 860 | A | C4-C5-N7 | -7.20 | 107.10 | 110.70 |
| 22 | 23S1 | 2461 | A | N3-C4-N9 | 7.20 | 133.16 | 127.40 |
| 22 | 23S1 | 2426 | A | C8-N9-C4 | 7.20 | 108.68 | 105.80 |
| 22 | 23S1 | 613 | A | C4-C5-C6 | 7.20 | 120.60 | 117.00 |
| 22 | 23S1 | 788 | A | C5-N7-C8 | 7.20 | 107.50 | 103.90 |
| 22 | 23S1 | 2062 | A | C5-N7-C8 | 7.20 | 107.50 | 103.90 |
| 1 | 16S1 | 1339 | A | C4-C5-C6 | 7.20 | 120.60 | 117.00 |
| 22 | 23S1 | 477 | A | C4-C5-C6 | 7.20 | 120.60 | 117.00 |
| 1 | 16S1 | 860 | A | N9-C4-C5 | 7.20 | 108.68 | 105.80 |
| 1 | 16S1 | 1418 | A | C5-N7-C8 | 7.20 | 107.50 | 103.90 |
| 22 | 23S1 | 2101 | A | C4-C5-N7 | -7.19 | 107.10 | 110.70 |
| 1 | 16S1 | 460 | A | C5-N7-C8 | 7.19 | 107.50 | 103.90 |
| 1 | 16S1 | 968 | A | C5-N7-C8 | 7.19 | 107.50 | 103.90 |
| 22 | 23S1 | 730 | A | N3-C4-N9 | 7.19 | 133.16 | 127.40 |
| 22 | 23S1 | 119 | A | C5-N7-C8 | 7.19 | 107.50 | 103.90 |
| 22 | 23S1 | 2059 | A | N3-C4-N9 | 7.19 | 133.15 | 127.40 |
| 22 | 23S1 | 2721 | A | C5-N7-C8 | 7.19 | 107.50 | 103.90 |
| 22 | 23S1 | 508 | A | C5-N7-C8 | 7.19 | 107.49 | 103.90 |
| 22 | 23S1 | 752 | A | N9-C4-C5 | 7.19 | 108.67 | 105.80 |
| 22 | 23S1 | 503 | A | C4-C5-C6 | 7.18 | 120.59 | 117.00 |
| 22 | 23S1 | 2111 | U | N1-C2-O2 | 7.18 | 127.83 | 122.80 |
| 22 | 23S1 | 1029 | A | C5-N7-C8 | 7.18 | 107.49 | 103.90 |
| 22 | 23S1 | 89 | A | C5-N7-C8 | 7.18 | 107.49 | 103.90 |
| 1 | 16S1 | 502 | A | C5-N7-C8 | 7.18 | 107.49 | 103.90 |
| 1 | 16S1 | 1014 | A | C4-C5-C6 | 7.18 | 120.59 | 117.00 |
| 22 | 23S1 | 330 | A | N3-C4-N9 | 7.18 | 133.14 | 127.40 |
| 1 | 16S1 | 329 | A | C4-C5-C6 | 7.18 | 120.59 | 117.00 |
| 1 | 16S1 | 1022 | A | C5-N7-C8 | 7.18 | 107.49 | 103.90 |
| 22 | 23S1 | 1301 | A | N3-C4-N9 | 7.18 | 133.14 | 127.40 |
| 22 | 23S1 | 2792 | A | C5-N7-C8 | 7.18 | 107.49 | 103.90 |
| 22 | 23S1 | 1029 | A | N3-C4-N9 | 7.17 | 133.14 | 127.40 |
| 22 | 23S1 | 1213 | A | C5-N7-C8 | 7.17 | 107.49 | 103.90 |
| 22 | 23S1 | 2119 | A | C4-C5-N7 | -7.17 | 107.11 | 110.70 |
| 22 | 23S1 | 1387 | A | C4-C5-C6 | 7.17 | 120.59 | 117.00 |
| 1 | 16S1 | 718 | A | C5-N7-C8 | 7.17 | 107.48 | 103.90 |
| 1 | 16S1 | 977 | A | C5-N7-C8 | 7.17 | 107.48 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 16S1 | 1502 | A | C5-N7-C8 | 7.17 | 107.48 | 103.90 |
| 1 | 16S1 | 344 | A | C5-N7-C8 | 7.17 | 107.48 | 103.90 |
| 1 | 16S1 | 865 | A | N3-C4-N9 | 7.17 | 133.13 | 127.40 |
| 1 | 16S1 | 1158 | C | C6-N1-C2 | -7.17 | 117.43 | 120.30 |
| 22 | 23S1 | 1754 | A | C5-N7-C8 | 7.17 | 107.48 | 103.90 |
| 1 | 16S1 | 1169 | A | C5-N7-C8 | 7.16 | 107.48 | 103.90 |
| 22 | 23S1 | 449 | A | N3-C4-N9 | 7.16 | 133.13 | 127.40 |
| 22 | 23S1 | 1848 | A | C4-C5-C6 | 7.16 | 120.58 | 117.00 |
| 1 | 16S1 | 533 | A | C5-C6-N1 | 7.16 | 121.28 | 117.70 |
| 22 | 23S1 | 482 | A | C5-N7-C8 | 7.16 | 107.48 | 103.90 |
| 1 | 16S1 | 663 | A | N3-C4-N9 | 7.16 | 133.13 | 127.40 |
| 1 | 16S1 | 1431 | A | C5-N7-C8 | 7.16 | 107.48 | 103.90 |
| 22 | 23S1 | 2426 | A | N3-C4-N9 | 7.16 | 133.13 | 127.40 |
| 1 | 16S1 | 1318 | A | C5-N7-C8 | 7.16 | 107.48 | 103.90 |
| 1 | 16S1 | 1333 | A | N9-C4-C5 | 7.16 | 108.66 | 105.80 |
| 1 | 16S1 | 356 | A | N3-C4-N9 | 7.15 | 133.12 | 127.40 |
| 22 | 23S1 | 1977 | A | C5-N7-C8 | 7.15 | 107.48 | 103.90 |
| 22 | 23S1 | 2340 | A | C5-N7-C8 | 7.15 | 107.48 | 103.90 |
| 22 | 23S1 | 1175 | A | C4-C5-C6 | 7.15 | 120.58 | 117.00 |
| 22 | 23S1 | 1690 | A | C5-N7-C8 | 7.15 | 107.47 | 103.90 |
| 1 | 16S1 | 95 | C | N3-C2-O2 | -7.15 | 116.90 | 121.90 |
| 1 | 16S1 | 365 | U | N1-C2-O2 | 7.15 | 127.80 | 122.80 |
| 22 | 23S1 | 1336 | A | N3-C4-N9 | 7.15 | 133.12 | 127.40 |
| 22 | 23S1 | 1749 | A | C5-N7-C8 | 7.15 | 107.47 | 103.90 |
| 22 | 23S1 | 1067 | A | C5-N7-C8 | 7.14 | 107.47 | 103.90 |
| 1 | 16S1 | 456 | A | C5-N7-C8 | 7.14 | 107.47 | 103.90 |
| 22 | 23S1 | 2425 | A | C4-C5-C6 | 7.14 | 120.57 | 117.00 |
| 1 | 16S1 | 263 | A | C4-C5-C6 | 7.14 | 120.57 | 117.00 |
| 1 | 16S1 | 694 | A | C4-C5-C6 | 7.14 | 120.57 | 117.00 |
| 22 | 23S1 | 504 | A | C5-N7-C8 | 7.14 | 107.47 | 103.90 |
| 22 | 23S1 | 2169 | A | C4-C5-C6 | 7.14 | 120.57 | 117.00 |
| 1 | 16S1 | 189 | A | C4-C5-C6 | 7.14 | 120.57 | 117.00 |
| 1 | 16S1 | 919 | A | C5-N7-C8 | 7.14 | 107.47 | 103.90 |
| 22 | 23S1 | 1086 | A | C4-C5-C6 | 7.13 | 120.57 | 117.00 |
| 1 | 16S1 | 181 | A | C5-N7-C8 | 7.13 | 107.47 | 103.90 |
| 22 | 23S1 | 529 | A | C5-N7-C8 | 7.13 | 107.47 | 103.90 |
| 1 | 16S1 | 77 | A | C4-C5-C6 | 7.13 | 120.56 | 117.00 |
| 22 | 23S1 | 221 | A | C5-N7-C8 | 7.13 | 107.46 | 103.90 |
| 22 | 23S1 | 1808 | A | C8-N9-C4 | 7.13 | 108.65 | 105.80 |
| 22 | 23S1 | 2111 | U | C2-N1-C1' | 7.13 | 126.25 | 117.70 |
| 22 | 23S1 | 2433 | A | C4-C5-C6 | 7.13 | 120.56 | 117.00 |
| 22 | 23S1 | 1571 | A | N3-C4-N9 | 7.12 | 133.10 | 127.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 975 | A | C5-N7-C8 | 7.12 | 107.46 | 103.90 |
| 1 | 16S1 | 199 | A | N3-C4-N9 | 7.12 | 133.09 | 127.40 |
| 22 | 23S1 | 1784 | A | C8-N9-C4 | 7.12 | 108.65 | 105.80 |
| 1 | 16S1 | 119 | A | C5-N7-C8 | 7.12 | 107.46 | 103.90 |
| 1 | 16S1 | 1163 | A | N3-C4-N9 | 7.11 | 133.09 | 127.40 |
| 22 | 23S1 | 925 | A | C4-C5-C6 | 7.11 | 120.56 | 117.00 |
| 55 | PTR1 | 20 | U | N3-C2-O2 | -7.11 | 117.22 | 122.20 |
| 1 | 16S1 | 72 | A | C5-C6-N1 | 7.11 | 121.26 | 117.70 |
| 1 | 16S1 | 263 | A | N3-C4-N9 | 7.11 | 133.09 | 127.40 |
| 22 | 23S1 | 1269 | A | C4-C5-C6 | 7.11 | 120.56 | 117.00 |
| 23 | 05S1 | 75 | G | N3-C4-C5 | -7.11 | 125.05 | 128.60 |
| 22 | 23S1 | 676 | A | C5-N7-C8 | 7.11 | 107.45 | 103.90 |
| 22 | 23S1 | 722 | A | N3-C4-N9 | 7.11 | 133.09 | 127.40 |
| 22 | 23S1 | 2088 | A | N3-C4-N9 | 7.11 | 133.09 | 127.40 |
| 1 | 16S1 | 914 | A | C8-N9-C4 | 7.11 | 108.64 | 105.80 |
| 22 | 23S1 | 1570 | A | N9-C4-C5 | 7.11 | 108.64 | 105.80 |
| 22 | 23S1 | 2054 | A | N3-C4-N9 | 7.11 | 133.09 | 127.40 |
| 22 | 23S1 | 2883 | A | C8-N9-C4 | 7.11 | 108.64 | 105.80 |
| 1 | 16S1 | 1374 | A | N3-C4-N9 | 7.10 | 133.08 | 127.40 |
| 22 | 23S1 | 255 | A | N3-C4-N9 | 7.10 | 133.08 | 127.40 |
| 22 | 23S1 | 503 | A | N3-C4-N9 | 7.10 | 133.08 | 127.40 |
| 22 | 23S1 | 2077 | A | N3-C4-N9 | 7.10 | 133.08 | 127.40 |
| 22 | 23S1 | 2191 | A | N3-C4-N9 | 7.10 | 133.08 | 127.40 |
| 22 | 23S1 | 2566 | A | N9-C4-C5 | 7.10 | 108.64 | 105.80 |
| 22 | 23S1 | 2879 | A | N3-C4-N9 | 7.10 | 133.08 | 127.40 |
| 1 | 16S1 | 236 | A | C5-N7-C8 | 7.10 | 107.45 | 103.90 |
| 22 | 23S1 | 1932 | A | C5-N7-C8 | 7.10 | 107.45 | 103.90 |
| 22 | 23S1 | 1413 | A | C5-N7-C8 | 7.10 | 107.45 | 103.90 |
| 22 | 23S1 | 2142 | A | C5-C6-N6 | 7.10 | 129.38 | 123.70 |
| 1 | 16S1 | 65 | A | C8-N9-C4 | 7.10 | 108.64 | 105.80 |
| 22 | 23S1 | 1787 | A | N3-C4-N9 | 7.10 | 133.08 | 127.40 |
| 1 | 16S1 | 1219 | A | N3-C4-N9 | 7.09 | 133.07 | 127.40 |
| 1 | 16S1 | 695 | A | C4-C5-C6 | 7.09 | 120.55 | 117.00 |
| 1 | 16S1 | 109 | A | C5-N7-C8 | 7.09 | 107.45 | 103.90 |
| 1 | 16S1 | 1375 | A | N3-C4-N9 | 7.09 | 133.07 | 127.40 |
| 22 | 23S1 | 1730 | C | C6-N1-C2 | -7.09 | 117.46 | 120.30 |
| 22 | 23S1 | 2766 | A | C4-C5-C6 | 7.09 | 120.55 | 117.00 |
| 22 | 23S1 | 2094 | A | C8-N9-C4 | 7.09 | 108.64 | 105.80 |
| 1 | 16S1 | 329 | A | C5-N7-C8 | 7.09 | 107.44 | 103.90 |
| 1 | 16S1 | 432 | A | C4-C5-C6 | 7.09 | 120.54 | 117.00 |
| 22 | 23S1 | 972 | A | N3-C4-N9 | 7.09 | 133.07 | 127.40 |
| 22 | 23S1 | 2142 | A | C8-N9-C4 | 7.08 | 108.63 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 16S1 | 466 | A | C5-N7-C8 | 7.08 | 107.44 | 103.90 |
| 22 | 23S1 | 2879 | A | C4-C5-C6 | 7.08 | 120.54 | 117.00 |
| 1 | 16S1 | 478 | A | C4-C5-C6 | 7.08 | 120.54 | 117.00 |
| 22 | 23S1 | 730 | A | C4-C5-C6 | 7.08 | 120.54 | 117.00 |
| 1 | 16S1 | 814 | A | N3-C4-N9 | 7.08 | 133.06 | 127.40 |
| 1 | 16S1 | 655 | A | C4-C5-C6 | 7.08 | 120.54 | 117.00 |
| 22 | 23S1 | 909 | A | C5-N7-C8 | 7.08 | 107.44 | 103.90 |
| 55 | PTR1 | 51 | A | N9-C4-C5 | 7.07 | 108.63 | 105.80 |
| 22 | 23S1 | 655 | A | C8-N9-C4 | 7.07 | 108.63 | 105.80 |
| 22 | 23S1 | 1276 | A | C4-C5-C6 | 7.07 | 120.53 | 117.00 |
| 22 | 23S1 | 990 | A | C5-N7-C8 | 7.07 | 107.43 | 103.90 |
| 22 | 23S1 | 2268 | A | C5-N7-C8 | 7.07 | 107.43 | 103.90 |
| 22 | 23S1 | 2497 | A | C5-N7-C8 | 7.07 | 107.43 | 103.90 |
| 22 | 23S1 | 2094 | A | N3-C4-N9 | 7.06 | 133.05 | 127.40 |
| 22 | 23S1 | 2321 | U | N3-C2-O2 | -7.06 | 117.26 | 122.20 |
| 1 | 16S1 | 959 | A | C4-C5-C6 | 7.06 | 120.53 | 117.00 |
| 22 | 23S1 | 119 | A | N9-C4-C5 | 7.06 | 108.62 | 105.80 |
| 1 | 16S1 | 1346 | A | C8-N9-C4 | 7.06 | 108.62 | 105.80 |
| 1 | 16S1 | 949 | A | N3-C4-N9 | 7.06 | 133.04 | 127.40 |
| 22 | 23S1 | 2171 | A | N3-C4-N9 | 7.05 | 133.04 | 127.40 |
| 22 | 23S1 | 391 | A | N3-C4-N9 | 7.05 | 133.04 | 127.40 |
| 22 | 23S1 | 478 | A | C5-N7-C8 | 7.05 | 107.43 | 103.90 |
| 1 | 16S1 | 1 | A | C5-N7-C8 | 7.05 | 107.43 | 103.90 |
| 1 | 16S1 | 1188 | A | C8-N9-C4 | 7.05 | 108.62 | 105.80 |
| 22 | 23S1 | 1504 | A | C8-N9-C4 | 7.05 | 108.62 | 105.80 |
| 1 | 16S1 | 1004 | A | N3-C4-N9 | 7.05 | 133.04 | 127.40 |
| 22 | 23S1 | 466 | A | C5-N7-C8 | 7.04 | 107.42 | 103.90 |
| 1 | 16S1 | 1046 | A | C5-C6-N1 | 7.04 | 121.22 | 117.70 |
| 22 | 23S1 | 1189 | A | C4-C5-C6 | 7.04 | 120.52 | 117.00 |
| 22 | 23S1 | 1544 | A | C5-N7-C8 | 7.04 | 107.42 | 103.90 |
| 1 | 16S1 | 1146 | A | N3-C4-N9 | 7.04 | 133.03 | 127.40 |
| 22 | 23S1 | 945 | A | C5-N7-C8 | 7.04 | 107.42 | 103.90 |
| 22 | 23S1 | 2662 | A | N7-C8-N9 | -7.04 | 110.28 | 113.80 |
| 1 | 16S1 | 451 | A | N3-C4-N9 | 7.04 | 133.03 | 127.40 |
| 22 | 23S1 | 2284 | A | C4-C5-C6 | 7.04 | 120.52 | 117.00 |
| 1 | 16S1 | 1201 | A | C5-C6-N6 | 7.04 | 129.33 | 123.70 |
| 22 | 23S1 | 2598 | A | C5-N7-C8 | 7.04 | 107.42 | 103.90 |
| 1 | 16S1 | 161 | A | C4-C5-C6 | 7.03 | 120.52 | 117.00 |
| 1 | 16S1 | 609 | A | C5-N7-C8 | 7.03 | 107.42 | 103.90 |
| 22 | 23S1 | 1553 | A | N3-C4-N9 | 7.03 | 133.03 | 127.40 |
| 1 | 16S1 | 621 | A | N3-C4-N9 | 7.03 | 133.03 | 127.40 |
| 22 | 23S1 | 2059 | A | C5-N7-C8 | 7.03 | 107.42 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 415 | A | C4-C5-C6 | 7.03 | 120.52 | 117.00 |
| 22 | 23S1 | 1819 | A | N3-C4-N9 | 7.03 | 133.02 | 127.40 |
| 22 | 23S1 | 2407 | A | C4-C5-C6 | 7.03 | 120.52 | 117.00 |
| 55 | PTR1 | 20 | U | N3-C4-C5 | 7.03 | 118.82 | 114.60 |
| 1 | 16S1 | 120 | A | C5-N7-C8 | 7.03 | 107.41 | 103.90 |
| 1 | 16S1 | 116 | A | N3-C4-N9 | 7.03 | 133.02 | 127.40 |
| 1 | 16S1 | 1055 | A | C4-C5-C6 | 7.03 | 120.51 | 117.00 |
| 1 | 16S1 | 1152 | A | N3-C4-N9 | 7.03 | 133.02 | 127.40 |
| 22 | 23S1 | 643 | A | C5-N7-C8 | 7.03 | 107.41 | 103.90 |
| 22 | 23S1 | 1353 | A | N9-C4-C5 | 7.03 | 108.61 | 105.80 |
| 22 | 23S1 | 2482 | A | C5-N7-C8 | 7.03 | 107.41 | 103.90 |
| 1 | 16S1 | 663 | A | C4-C5-C6 | 7.02 | 120.51 | 117.00 |
| 1 | 16S1 | 869 | G | N1-C6-O6 | -7.02 | 115.69 | 119.90 |
| 22 | 23S1 | 74 | A | C5-N7-C8 | 7.02 | 107.41 | 103.90 |
| 22 | 23S1 | 804 | A | N9-C4-C5 | 7.02 | 108.61 | 105.80 |
| 1 | 16S1 | 208 | U | C5-C4-O4 | 7.02 | 130.11 | 125.90 |
| 1 | 16S1 | 746 | A | N3-C4-N9 | 7.02 | 133.02 | 127.40 |
| 22 | 23S1 | 146 | A | C4-C5-C6 | 7.02 | 120.51 | 117.00 |
| 22 | 23S1 | 1713 | A | C8-N9-C4 | 7.02 | 108.61 | 105.80 |
| 22 | 23S1 | 2080 | A | N3-C4-N9 | 7.02 | 133.02 | 127.40 |
| 1 | 16S1 | 704 | A | C5-N7-C8 | 7.02 | 107.41 | 103.90 |
| 1 | 16S1 | 807 | A | N3-C4-N9 | 7.02 | 133.01 | 127.40 |
| 1 | 16S1 | 964 | A | N3-C4-N9 | 7.02 | 133.01 | 127.40 |
| 1 | 16S1 | 1172 | C | N1-C2-O2 | 7.02 | 123.11 | 118.90 |
| 22 | 23S1 | 1664 | A | C4-C5-C6 | 7.02 | 120.51 | 117.00 |
| 22 | 23S1 | 1969 | A | C8-N9-C4 | 7.02 | 108.61 | 105.80 |
| 1 | 16S1 | 393 | A | N3-C4-N9 | 7.01 | 133.01 | 127.40 |
| 22 | 23S1 | 1580 | A | C4-C5-C6 | 7.01 | 120.51 | 117.00 |
| 1 | 16S1 | 356 | A | C4-C5-C6 | 7.01 | 120.51 | 117.00 |
| 22 | 23S1 | 2434 | A | C5-N7-C8 | 7.01 | 107.41 | 103.90 |
| 1 | 16S1 | 2 | A | N3-C4-N9 | 7.01 | 133.01 | 127.40 |
| 1 | 16S1 | 415 | A | C4-C5-C6 | 7.01 | 120.50 | 117.00 |
| 22 | 23S1 | 182 | A | C5-N7-C8 | 7.01 | 107.41 | 103.90 |
| 1 | 16S1 | 642 | A | C4-C5-C6 | 7.01 | 120.50 | 117.00 |
| 1 | 16S1 | 383 | A | C6-C5-N7 | -7.01 | 127.39 | 132.30 |
| 1 | 16S1 | 80 | A | N3-C4-N9 | 7.00 | 133.00 | 127.40 |
| 1 | 16S1 | 81 | A | C5-N7-C8 | 7.00 | 107.40 | 103.90 |
| 1 | 16S1 | 746 | A | C5-C6-N1 | 7.00 | 121.20 | 117.70 |
| 22 | 23S1 | 1885 | A | C5-N7-C8 | 7.00 | 107.40 | 103.90 |
| 22 | 23S1 | 1189 | A | N3-C4-N9 | 7.00 | 133.00 | 127.40 |
| 22 | 23S1 | 1871 | A | N9-C4-C5 | 7.00 | 108.60 | 105.80 |
| 22 | 23S1 | 423 | A | C5-N7-C8 | 7.00 | 107.40 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 492 | A | C5-N7-C8 | 7.00 | 107.40 | 103.90 |
| 22 | 23S1 | 627 | A | N3-C4-N9 | 7.00 | 133.00 | 127.40 |
| 1 | 16S1 | 1508 | A | N3-C4-N9 | 7.00 | 133.00 | 127.40 |
| 22 | 23S1 | 95 | A | C5-N7-C8 | 7.00 | 107.40 | 103.90 |
| 22 | 23S1 | 514 | A | C5-N7-C8 | 7.00 | 107.40 | 103.90 |
| 22 | 23S1 | 2328 | A | N3-C4-N9 | 7.00 | 133.00 | 127.40 |
| 1 | 16S1 | 635 | A | C4-C5-C6 | 6.99 | 120.50 | 117.00 |
| 22 | 23S1 | 161 | A | C5-N7-C8 | 6.99 | 107.40 | 103.90 |
| 22 | 23S1 | 1744 | A | C5-N7-C8 | 6.99 | 107.40 | 103.90 |
| 22 | 23S1 | 2590 | A | C8-N9-C4 | 6.99 | 108.60 | 105.80 |
| 23 | 05S1 | 45 | A | N3-C4-N9 | 6.99 | 132.99 | 127.40 |
| 22 | 23S1 | 1336 | A | C4-C5-C6 | 6.99 | 120.50 | 117.00 |
| 1 | 16S1 | 71 | A | C4-C5-C6 | 6.99 | 120.49 | 117.00 |
| 1 | 16S1 | 655 | A | N3-C4-N9 | 6.99 | 132.99 | 127.40 |
| 22 | 23S1 | 1126 | A | C5-N7-C8 | 6.99 | 107.39 | 103.90 |
| 22 | 23S1 | 1899 | A | N9-C4-C5 | 6.99 | 108.59 | 105.80 |
| 23 | 05S1 | 29 | A | N9-C4-C5 | 6.98 | 108.59 | 105.80 |
| 23 | 05S1 | 109 | A | C8-N9-C4 | 6.98 | 108.59 | 105.80 |
| 1 | 16S1 | 448 | A | N3-C4-N9 | 6.98 | 132.99 | 127.40 |
| 22 | 23S1 | 1809 | A | N3-C4-N9 | 6.98 | 132.98 | 127.40 |
| 22 | 23S1 | 2284 | A | N3-C4-N9 | 6.98 | 132.98 | 127.40 |
| 1 | 16S1 | 72 | A | C5-N7-C8 | 6.98 | 107.39 | 103.90 |
| 22 | 23S1 | 794 | A | C4-C5-C6 | 6.98 | 120.49 | 117.00 |
| 1 | 16S1 | 780 | A | C5-N7-C8 | 6.97 | 107.39 | 103.90 |
| 1 | 16S1 | 716 | A | C5-N7-C8 | 6.97 | 107.39 | 103.90 |
| 1 | 16S1 | 819 | A | C5-N7-C8 | 6.97 | 107.39 | 103.90 |
| 22 | 23S1 | 5 | A | N3-C4-N9 | 6.97 | 132.98 | 127.40 |
| 22 | 23S1 | 2776 | A | C8-N9-C4 | 6.97 | 108.59 | 105.80 |
| 22 | 23S1 | 299 | A | C5-N7-C8 | 6.97 | 107.39 | 103.90 |
| 22 | 23S1 | 2459 | A | C5-N7-C8 | 6.97 | 107.39 | 103.90 |
| 22 | 23S1 | 1572 | A | N3-C4-N9 | 6.97 | 132.98 | 127.40 |
| 1 | 16S1 | 1360 | A | N9-C4-C5 | 6.97 | 108.59 | 105.80 |
| 1 | 16S1 | 695 | A | C5-N7-C8 | 6.97 | 107.38 | 103.90 |
| 1 | 16S1 | 16 | A | C8-N9-C4 | 6.96 | 108.59 | 105.80 |
| 1 | 16S1 | 382 | A | C5-N7-C8 | 6.96 | 107.38 | 103.90 |
| 1 | 16S1 | 1340 | A | C8-N9-C4 | 6.96 | 108.59 | 105.80 |
| 22 | 23S1 | 447 | A | C5-N7-C8 | 6.96 | 107.38 | 103.90 |
| 22 | 23S1 | 1027 | A | C5-N7-C8 | 6.96 | 107.38 | 103.90 |
| 22 | 23S1 | 1127 | A | C4-C5-C6 | 6.96 | 120.48 | 117.00 |
| 22 | 23S1 | 1591 | A | C8-N9-C4 | 6.96 | 108.59 | 105.80 |
| 22 | 23S1 | 1597 | A | C4-C5-N7 | -6.96 | 107.22 | 110.70 |
| 22 | 23S1 | 2169 | A | N3-C4-N9 | 6.96 | 132.97 | 127.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 22 | 23S1 | 2412 | A | C4-C5-C6 | 6.96 | 120.48 | 117.00 |
| 1 | 16S1 | 642 | A | N3-C4-N9 | 6.96 | 132.97 | 127.40 |
| 1 | 16S1 | 228 | A | C5-N7-C8 | 6.96 | 107.38 | 103.90 |
| 1 | 16S1 | 1081 | A | C5-N7-C8 | 6.96 | 107.38 | 103.90 |
| 22 | 23S1 | 1392 | A | N3-C4-N9 | 6.96 | 132.97 | 127.40 |
| 22 | 23S1 | 2369 | A | N3-C4-N9 | 6.96 | 132.97 | 127.40 |
| 22 | 23S1 | 2287 | A | C4-C5-C6 | 6.96 | 120.48 | 117.00 |
| 55 | PTR1 | 69 | A | C5-N7-C8 | 6.96 | 107.38 | 103.90 |
| 1 | 16S1 | 19 | A | C8-N9-C4 | 6.96 | 108.58 | 105.80 |
| 22 | 23S1 | 1603 | A | C5-N7-C8 | 6.96 | 107.38 | 103.90 |
| 22 | 23S1 | 1717 | A | C5-N7-C8 | 6.96 | 107.38 | 103.90 |
| 1 | 16S1 | 452 | A | N3-C4-N9 | 6.95 | 132.96 | 127.40 |
| 1 | 16S1 | 994 | A | C4-C5-C6 | 6.95 | 120.48 | 117.00 |
| 22 | 23S1 | 1664 | A | N3-C4-N9 | 6.95 | 132.96 | 127.40 |
| 22 | 23S1 | 2015 | A | C5-N7-C8 | 6.95 | 107.38 | 103.90 |
| 22 | 23S1 | 2453 | A | C4-C5-C6 | 6.95 | 120.48 | 117.00 |
| 1 | 16S1 | 579 | A | N3-C4-N9 | 6.95 | 132.96 | 127.40 |
| 1 | 16S1 | 1000 | A | N3-C4-N9 | 6.95 | 132.96 | 127.40 |
| 22 | 23S1 | 2899 | A | C5-N7-C8 | 6.95 | 107.38 | 103.90 |
| 1 | 16S1 | 496 | A | N3-C4-N9 | 6.95 | 132.96 | 127.40 |
| 1 | 16S1 | 539 | A | C5-N7-C8 | 6.95 | 107.37 | 103.90 |
| 1 | 16S1 | 1145 | A | C8-N9-C4 | 6.95 | 108.58 | 105.80 |
| 1 | 16S1 | 1252 | A | C5-N7-C8 | 6.95 | 107.37 | 103.90 |
| 22 | 23S1 | 203 | A | C5-N7-C8 | 6.95 | 107.37 | 103.90 |
| 22 | 23S1 | 2142 | A | C5-C6-N1 | 6.95 | 121.17 | 117.70 |
| 1 | 16S1 | 1080 | A | C5-N7-C8 | 6.95 | 107.37 | 103.90 |
| 22 | 23S1 | 1571 | A | C5-N7-C8 | 6.95 | 107.37 | 103.90 |
| 22 | 23S1 | 1616 | A | C8-N9-C4 | 6.95 | 108.58 | 105.80 |
| 23 | 05S1 | 94 | A | C5-N7-C8 | 6.95 | 107.37 | 103.90 |
| 55 | PTR1 | 38 | A | N3-C4-N9 | 6.95 | 132.96 | 127.40 |
| 1 | 16S1 | 466 | A | C4-C5-C6 | 6.94 | 120.47 | 117.00 |
| 1 | 16S1 | 766 | A | C5-N7-C8 | 6.94 | 107.37 | 103.90 |
| 22 | 23S1 | 342 | A | N3-C4-N9 | 6.94 | 132.96 | 127.40 |
| 1 | 16S1 | 729 | A | C4-C5-C6 | 6.94 | 120.47 | 117.00 |
| 1 | 16S1 | 1167 | A | C8-N9-C4 | 6.94 | 108.58 | 105.80 |
| 1 | 16S1 | 1357 | A | C5-N7-C8 | 6.94 | 107.37 | 103.90 |
| 1 | 16S1 | 33 | A | N3-C4-N9 | 6.94 | 132.95 | 127.40 |
| 1 | 16S1 | 1012 | A | C5-N7-C8 | 6.94 | 107.37 | 103.90 |
| 22 | 23S1 | 2434 | A | N9-C4-C5 | 6.94 | 108.58 | 105.80 |
| 22 | 23S1 | 104 | A | N3-C4-N9 | 6.94 | 132.95 | 127.40 |
| 22 | 23S1 | 1548 | A | N3-C4-N9 | 6.94 | 132.95 | 127.40 |
| 22 | 23S1 | 1679 | A | C5-N7-C8 | 6.94 | 107.37 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 16S1 | 162 | A | C5-N7-C8 | 6.93 | 107.37 | 103.90 |
| 1 | 16S1 | 1396 | A | N3-C4-N9 | 6.93 | 132.95 | 127.40 |
| 22 | 23S1 | 198 | C | C6-N1-C2 | -6.93 | 117.53 | 120.30 |
| 1 | 16S1 | 441 | A | N3-C4-N9 | 6.93 | 132.95 | 127.40 |
| 22 | 23S1 | 218 | A | C5-N7-C8 | 6.93 | 107.37 | 103.90 |
| 22 | 23S1 | 1583 | A | C8-N9-C4 | 6.93 | 108.57 | 105.80 |
| 22 | 23S1 | 144 | A | N3-C4-N9 | 6.93 | 132.94 | 127.40 |
| 22 | 23S1 | 608 | A | N3-C4-N9 | 6.93 | 132.94 | 127.40 |
| 1 | 16S1 | 366 | A | C5-N7-C8 | 6.93 | 107.36 | 103.90 |
| 22 | 23S1 | 1548 | A | C4-C5-C6 | 6.93 | 120.46 | 117.00 |
| 22 | 23S1 | 2560 | A | N3-C4-N9 | 6.93 | 132.94 | 127.40 |
| 1 | 16S1 | 397 | A | C5-N7-C8 | 6.92 | 107.36 | 103.90 |
| 1 | 16S1 | 964 | A | C4-C5-C6 | 6.92 | 120.46 | 117.00 |
| 22 | 23S1 | 2448 | A | C5-N7-C8 | 6.92 | 107.36 | 103.90 |
| 1 | 16S1 | 563 | A | C4-C5-C6 | 6.92 | 120.46 | 117.00 |
| 1 | 16S1 | 574 | A | C5-N7-C8 | 6.92 | 107.36 | 103.90 |
| 1 | 16S1 | 718 | A | N3-C4-N9 | 6.92 | 132.93 | 127.40 |
| 22 | 23S1 | 146 | A | N3-C4-N9 | 6.92 | 132.93 | 127.40 |
| 22 | 23S1 | 781 | A | N3-C4-N9 | 6.92 | 132.93 | 127.40 |
| 22 | 23S1 | 2108 | A | C4-C5-C6 | 6.92 | 120.46 | 117.00 |
| 22 | 23S1 | 2171 | A | C5-C6-N6 | 6.92 | 129.23 | 123.70 |
| 22 | 23S1 | 2270 | A | C4-C5-C6 | 6.92 | 120.46 | 117.00 |
| 22 | 23S1 | 1008 | A | C5-N7-C8 | 6.92 | 107.36 | 103.90 |
| 22 | 23S1 | 2135 | A | C4-C5-C6 | 6.92 | 120.46 | 117.00 |
| 22 | 23S1 | 2614 | A | N3-C4-N9 | 6.91 | 132.93 | 127.40 |
| 1 | 16S1 | 864 | A | C4-C5-C6 | 6.91 | 120.45 | 117.00 |
| 1 | 16S1 | 1022 | A | N3-C4-N9 | 6.91 | 132.93 | 127.40 |
| 22 | 23S1 | 1759 | A | N3-C4-N9 | 6.91 | 132.93 | 127.40 |
| 1 | 16S1 | 696 | A | N3-C4-N9 | 6.91 | 132.93 | 127.40 |
| 22 | 23S1 | 1700 | A | C8-N9-C4 | 6.91 | 108.56 | 105.80 |
| 22 | 23S1 | 1920 | C | C5-C6-N1 | 6.91 | 124.45 | 121.00 |
| 22 | 23S1 | 2727 | A | N3-C4-N9 | 6.91 | 132.93 | 127.40 |
| 1 | 16S1 | 152 | A | N9-C4-C5 | 6.90 | 108.56 | 105.80 |
| 22 | 23S1 | 1085 | A | N3-C4-N9 | 6.90 | 132.92 | 127.40 |
| 22 | 23S1 | 53 | A | C5-N7-C8 | 6.90 | 107.35 | 103.90 |
| 1 | 16S1 | 373 | A | C4-C5-C6 | 6.90 | 120.45 | 117.00 |
| 22 | 23S1 | 479 | A | C8-N9-C4 | 6.90 | 108.56 | 105.80 |
| 1 | 16S1 | 695 | A | N3-C4-N9 | 6.89 | 132.92 | 127.40 |
| 1 | 16S1 | 1318 | A | N3-C4-N9 | 6.89 | 132.91 | 127.40 |
| 22 | 23S1 | 845 | A | C4-C5-C6 | 6.89 | 120.45 | 117.00 |
| 22 | 23S1 | 722 | A | C5-N7-C8 | 6.89 | 107.34 | 103.90 |
| 1 | 16S1 | 1261 | A | C5-N7-C8 | 6.89 | 107.34 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 6 | A | C4-C5-C6 | 6.89 | 120.44 | 117.00 |
| 22 | 23S1 | 1787 | A | C5-N7-C8 | 6.89 | 107.34 | 103.90 |
| 22 | 23S1 | 2430 | A | N9-C4-C5 | 6.89 | 108.56 | 105.80 |
| 22 | 23S1 | 2518 | A | C4-C5-C6 | 6.89 | 120.44 | 117.00 |
| 1 | 16S1 | 873 | A | N3-C4-N9 | 6.89 | 132.91 | 127.40 |
| 22 | 23S1 | 1237 | A | C8-N9-C4 | 6.89 | 108.56 | 105.80 |
| 1 | 16S1 | 49 | U | N3-C4-O4 | -6.89 | 114.58 | 119.40 |
| 22 | 23S1 | 2241 | A | N3-C4-N9 | 6.89 | 132.91 | 127.40 |
| 22 | 23S1 | 1050 | A | C8-N9-C4 | 6.88 | 108.55 | 105.80 |
| 22 | 23S1 | 439 | A | N3-C4-N9 | 6.88 | 132.91 | 127.40 |
| 23 | 05S1 | 94 | A | N3-C4-N9 | 6.88 | 132.91 | 127.40 |
| 22 | 23S1 | 2577 | A | C4-C5-C6 | 6.88 | 120.44 | 117.00 |
| 22 | 23S1 | 2799 | A | C4-C5-C6 | 6.88 | 120.44 | 117.00 |
| 22 | 23S1 | 1739 | A | N3-C4-N9 | 6.88 | 132.90 | 127.40 |
| 22 | 23S1 | 2809 | A | N3-C4-N9 | 6.88 | 132.90 | 127.40 |
| 1 | 16S1 | 250 | A | C8-N9-C4 | 6.88 | 108.55 | 105.80 |
| 22 | 23S1 | 1490 | A | C4-C5-C6 | 6.88 | 120.44 | 117.00 |
| 22 | 23S1 | 1698 | A | C5-N7-C8 | 6.88 | 107.34 | 103.90 |
| 22 | 23S1 | 528 | A | N3-C4-N9 | 6.88 | 132.90 | 127.40 |
| 22 | 23S1 | 149 | A | C5-N7-C8 | 6.87 | 107.34 | 103.90 |
| 22 | 23S1 | 1246 | A | C5-C6-N1 | 6.87 | 121.14 | 117.70 |
| 22 | 23S1 | 2893 | A | N3-C4-N9 | 6.87 | 132.90 | 127.40 |
| 22 | 23S1 | 391 | A | C4-C5-C6 | 6.87 | 120.43 | 117.00 |
| 22 | 23S1 | 981 | A | C5-N7-C8 | 6.87 | 107.33 | 103.90 |
| 23 | 05S1 | 99 | A | N3-C4-N9 | 6.87 | 132.89 | 127.40 |
| 1 | 16S1 | 728 | A | N9-C4-C5 | 6.87 | 108.55 | 105.80 |
| 22 | 23S1 | 84 | A | C8-N9-C4 | 6.87 | 108.55 | 105.80 |
| 1 | 16S1 | 1093 | A | N3-C4-N9 | 6.86 | 132.89 | 127.40 |
| 1 | 16S1 | 1151 | A | C5-C6-N1 | 6.86 | 121.13 | 117.70 |
| 22 | 23S1 | 972 | A | C4-C5-C6 | 6.86 | 120.43 | 117.00 |
| 22 | 23S1 | 1787 | A | C4-C5-C6 | 6.86 | 120.43 | 117.00 |
| 22 | 23S1 | 2090 | A | N3-C4-N9 | 6.86 | 132.89 | 127.40 |
| 22 | 23S1 | 1912 | A | N3-C4-N9 | 6.86 | 132.89 | 127.40 |
| 22 | 23S1 | 2392 | A | C4-C5-C6 | 6.86 | 120.43 | 117.00 |
| 1 | 16S1 | 673 | A | C4-C5-C6 | 6.86 | 120.43 | 117.00 |
| 22 | 23S1 | 514 | A | C5-C6-N1 | 6.86 | 121.13 | 117.70 |
| 22 | 23S1 | 1608 | A | C4-C5-C6 | 6.86 | 120.43 | 117.00 |
| 55 | PTR1 | 38 | A | C8-N9-C4 | 6.86 | 108.54 | 105.80 |
| 1 | 16S1 | 977 | A | C4-C5-C6 | 6.85 | 120.43 | 117.00 |
| 22 | 23S1 | 2266 | A | N3-C4-N9 | 6.85 | 132.88 | 127.40 |
| 22 | 23S1 | 1603 | A | N3-C4-N9 | 6.85 | 132.88 | 127.40 |
| 23 | 05S1 | 108 | A | C8-N9-C4 | 6.85 | 108.54 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 1073 | A | C4-C5-C6 | 6.85 | 120.42 | 117.00 |
| 1 | 16S1 | 81 | A | C4-C5-C6 | 6.85 | 120.42 | 117.00 |
| 1 | 16S1 | 182 | A | C8-N9-C4 | 6.85 | 108.54 | 105.80 |
| 1 | 16S1 | 1171 | A | C4-C5-C6 | 6.85 | 120.42 | 117.00 |
| 22 | 23S1 | 878 | A | C8-N9-C4 | 6.85 | 108.54 | 105.80 |
| 22 | 23S1 | 1307 | A | N3-C4-N9 | 6.85 | 132.88 | 127.40 |
| 22 | 23S1 | 1321 | A | N3-C4-N9 | 6.85 | 132.88 | 127.40 |
| 22 | 23S1 | 2060 | A | C8-N9-C4 | 6.85 | 108.54 | 105.80 |
| 22 | 23S1 | 547 | A | C8-N9-C4 | 6.85 | 108.54 | 105.80 |
| 22 | 23S1 | 2837 | A | C8-N9-C4 | 6.85 | 108.54 | 105.80 |
| 1 | 16S1 | 983 | A | C5-N7-C8 | 6.85 | 107.32 | 103.90 |
| 1 | 16S1 | 908 | A | C4-C5-C6 | 6.84 | 120.42 | 117.00 |
| 1 | 16S1 | 1534 | A | C4-C5-C6 | 6.84 | 120.42 | 117.00 |
| 22 | 23S1 | 10 | A | C5-C6-N1 | 6.84 | 121.12 | 117.70 |
| 22 | 23S1 | 752 | A | C4-C5-N7 | -6.84 | 107.28 | 110.70 |
| 22 | 23S1 | 2657 | A | C8-N9-C4 | 6.84 | 108.54 | 105.80 |
| 1 | 16S1 | 746 | A | C4-C5-C6 | 6.84 | 120.42 | 117.00 |
| 1 | 16S1 | 66 | A | C4-C5-C6 | 6.84 | 120.42 | 117.00 |
| 1 | 16S1 | 559 | A | C5-N7-C8 | 6.84 | 107.32 | 103.90 |
| 1 | 16S1 | 1252 | A | C4-C5-C6 | 6.84 | 120.42 | 117.00 |
| 22 | 23S1 | 1392 | A | C5-C6-N1 | 6.84 | 121.12 | 117.70 |
| 22 | 23S1 | 2126 | A | C4-C5-C6 | 6.84 | 120.42 | 117.00 |
| 22 | 23S1 | 2837 | A | N3-C4-N9 | 6.84 | 132.87 | 127.40 |
| 22 | 23S1 | 739 | A | N3-C4-N9 | 6.84 | 132.87 | 127.40 |
| 1 | 16S1 | 415 | A | N3-C4-N9 | 6.84 | 132.87 | 127.40 |
| 22 | 23S1 | 204 | A | C8-N9-C4 | 6.84 | 108.53 | 105.80 |
| 29 | L091 | 71 | LYS | CD-CE-NZ | 6.84 | 127.42 | 111.70 |
| 1 | 16S1 | 712 | A | C5-C6-N1 | 6.83 | 121.12 | 117.70 |
| 22 | 23S1 | 197 | A | N3-C4-N9 | 6.83 | 132.87 | 127.40 |
| 22 | 23S1 | 218 | A | C4-C5-C6 | 6.83 | 120.42 | 117.00 |
| 1 | 16S1 | 1418 | A | N3-C4-N9 | 6.83 | 132.87 | 127.40 |
| 1 | 16S1 | 382 | A | N3-C4-N9 | 6.83 | 132.87 | 127.40 |
| 1 | 16S1 | 712 | A | N3-C4-N9 | 6.83 | 132.86 | 127.40 |
| 22 | 23S1 | 2887 | A | C8-N9-C4 | 6.83 | 108.53 | 105.80 |
| 1 | 16S1 | 101 | A | N3-C4-N9 | 6.83 | 132.86 | 127.40 |
| 22 | 23S1 | 917 | A | N3-C4-N9 | 6.83 | 132.86 | 127.40 |
| 22 | 23S1 | 1268 | A | C5-N7-C8 | 6.83 | 107.31 | 103.90 |
| 1 | 16S1 | 274 | A | C8-N9-C4 | 6.83 | 108.53 | 105.80 |
| 1 | 16S1 | 716 | A | N3-C4-N9 | 6.83 | 132.86 | 127.40 |
| 1 | 16S1 | 909 | A | C5-N7-C8 | 6.83 | 107.31 | 103.90 |
| 1 | 16S1 | 101 | A | C4-C5-C6 | 6.83 | 120.41 | 117.00 |
| 22 | 23S1 | 478 | A | N3-C4-N9 | 6.83 | 132.86 | 127.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 1572 | A | C4-C5-C6 | 6.83 | 120.41 | 117.00 |
| 22 | 23S1 | 1998 | A | N3-C4-N9 | 6.83 | 132.86 | 127.40 |
| 22 | 23S1 | 900 | A | N3-C4-N9 | 6.82 | 132.86 | 127.40 |
| 22 | 23S1 | 1342 | A | C8-N9-C4 | 6.82 | 108.53 | 105.80 |
| 22 | 23S1 | 2476 | A | N3-C4-N9 | 6.82 | 132.86 | 127.40 |
| 1 | 16S1 | 1252 | A | N3-C4-N9 | 6.82 | 132.86 | 127.40 |
| 22 | 23S1 | 1327 | A | C5-N7-C8 | 6.82 | 107.31 | 103.90 |
| 55 | PTR1 | 23 | A | C5-C6-N1 | 6.82 | 121.11 | 117.70 |
| 22 | 23S1 | 532 | A | C4-C5-C6 | 6.82 | 120.41 | 117.00 |
| 1 | 16S1 | 459 | A | N3-C4-N9 | 6.82 | 132.85 | 127.40 |
| 1 | 16S1 | 1005 | A | C8-N9-C4 | 6.82 | 108.53 | 105.80 |
| 22 | 23S1 | 544 | C | N3-C2-O2 | -6.82 | 117.13 | 121.90 |
| 22 | 23S1 | 1928 | A | C4-C5-C6 | 6.82 | 120.41 | 117.00 |
| 22 | 23S1 | 2449 | U | C5-C4-O4 | -6.82 | 121.81 | 125.90 |
| 23 | 05S1 | 46 | A | N9-C4-C5 | 6.82 | 108.53 | 105.80 |
| 1 | 16S1 | 1503 | A | N3-C4-N9 | 6.81 | 132.85 | 127.40 |
| 22 | 23S1 | 362 | A | C8-N9-C4 | 6.81 | 108.53 | 105.80 |
| 1 | 16S1 | 270 | A | N3-C4-N9 | 6.81 | 132.85 | 127.40 |
| 22 | 23S1 | 478 | A | C4-C5-C6 | 6.81 | 120.41 | 117.00 |
| 22 | 23S1 | 2225 | A | N3-C4-N9 | 6.81 | 132.85 | 127.40 |
| 22 | 23S1 | 190 | A | N3-C4-N9 | 6.81 | 132.85 | 127.40 |
| 22 | 23S1 | 1395 | A | C5-N7-C8 | 6.81 | 107.30 | 103.90 |
| 22 | 23S1 | 2082 | A | N3-C4-N9 | 6.81 | 132.84 | 127.40 |
| 22 | 23S1 | 2199 | A | C4-C5-C6 | 6.81 | 120.40 | 117.00 |
| 55 | PTR1 | 26 | A | C8-N9-C4 | 6.80 | 108.52 | 105.80 |
| 22 | 23S1 | 608 | A | C4-C5-C6 | 6.80 | 120.40 | 117.00 |
| 22 | 23S1 | 1314 | C | C5-C6-N1 | 6.80 | 124.40 | 121.00 |
| 1 | 16S1 | 441 | A | C8-N9-C4 | 6.80 | 108.52 | 105.80 |
| 1 | 16S1 | 1306 | A | C8-N9-C4 | 6.80 | 108.52 | 105.80 |
| 22 | 23S1 | 374 | A | C8-N9-C4 | 6.80 | 108.52 | 105.80 |
| 22 | 23S1 | 646 | U | C4-C5-C6 | 6.80 | 123.78 | 119.70 |
| 22 | 23S1 | 918 | A | C5-N7-C8 | 6.80 | 107.30 | 103.90 |
| 22 | 23S1 | 1877 | A | C4-C5-C6 | 6.80 | 120.40 | 117.00 |
| 1 | 16S1 | 172 | A | C5-N7-C8 | 6.80 | 107.30 | 103.90 |
| 22 | 23S1 | 181 | A | C4-C5-C6 | 6.80 | 120.40 | 117.00 |
| 22 | 23S1 | 529 | A | N9-C4-C5 | 6.80 | 108.52 | 105.80 |
| 22 | 23S1 | 1608 | A | C5-N7-C8 | 6.80 | 107.30 | 103.90 |
| 22 | 23S1 | 1735 | A | C4-C5-C6 | 6.79 | 120.40 | 117.00 |
| 55 | PTR1 | 69 | A | N3-C4-N9 | 6.79 | 132.84 | 127.40 |
| 1 | 16S1 | 1081 | A | C4-C5-C6 | 6.79 | 120.40 | 117.00 |
| 22 | 23S1 | 19 | A | N3-C4-N9 | 6.79 | 132.84 | 127.40 |
| 22 | 23S1 | 173 | A | C5-N7-C8 | 6.79 | 107.30 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 244 | A | N3-C4-N9 | 6.79 | 132.84 | 127.40 |
| 22 | 23S1 | 718 | A | C4-C5-C6 | 6.79 | 120.40 | 117.00 |
| 22 | 23S1 | 861 | A | N3-C4-N9 | 6.79 | 132.83 | 127.40 |
| 22 | 23S1 | 2679 | A | N3-C4-N9 | 6.79 | 132.83 | 127.40 |
| 1 | 16S1 | 80 | A | C5-N7-C8 | 6.79 | 107.30 | 103.90 |
| 22 | 23S1 | 256 | A | C4-C5-C6 | 6.79 | 120.39 | 117.00 |
| 22 | 23S1 | 1590 | A | C5-N7-C8 | 6.79 | 107.30 | 103.90 |
| 22 | 23S1 | 1040 | A | C8-N9-C4 | 6.79 | 108.52 | 105.80 |
| 22 | 23S1 | 181 | A | N3-C4-N9 | 6.79 | 132.83 | 127.40 |
| 22 | 23S1 | 1784 | A | C5-N7-C8 | 6.79 | 107.30 | 103.90 |
| 22 | 23S1 | 2033 | A | N9-C4-C5 | 6.79 | 108.52 | 105.80 |
| 22 | 23S1 | 2700 | A | N3-C4-N9 | 6.79 | 132.83 | 127.40 |
| 1 | 16S1 | 192 | A | C4-C5-C6 | 6.79 | 120.39 | 117.00 |
| 1 | 16S1 | 1507 | A | N3-C4-N9 | 6.79 | 132.83 | 127.40 |
| 22 | 23S1 | 750 | A | N3-C4-N9 | 6.78 | 132.83 | 127.40 |
| 22 | 23S1 | 1522 | A | C5-C6-N1 | 6.78 | 121.09 | 117.70 |
| 1 | 16S1 | 130 | A | N3-C4-N9 | 6.78 | 132.83 | 127.40 |
| 22 | 23S1 | 501 | A | C5-N7-C8 | 6.78 | 107.29 | 103.90 |
| 22 | 23S1 | 1591 | A | C4-C5-C6 | 6.78 | 120.39 | 117.00 |
| 22 | 23S1 | 2171 | A | C5-N7-C8 | 6.78 | 107.29 | 103.90 |
| 22 | 23S1 | 1969 | A | C4-C5-C6 | 6.78 | 120.39 | 117.00 |
| 22 | 23S1 | 2309 | A | C8-N9-C4 | 6.78 | 108.51 | 105.80 |
| 22 | 23S1 | 2425 | A | N3-C4-N9 | 6.78 | 132.82 | 127.40 |
| 1 | 16S1 | 435 | A | C8-N9-C4 | 6.78 | 108.51 | 105.80 |
| 1 | 16S1 | 635 | A | N3-C4-N9 | 6.78 | 132.82 | 127.40 |
| 1 | 16S1 | 1396 | A | C5-N7-C8 | 6.78 | 107.29 | 103.90 |
| 22 | 23S1 | 1689 | A | N3-C4-N9 | 6.78 | 132.82 | 127.40 |
| 23 | 05S1 | 24 | G | C6-N1-C2 | -6.78 | 121.03 | 125.10 |
| 1 | 16S1 | 1350 | A | C5-N7-C8 | 6.77 | 107.29 | 103.90 |
| 22 | 23S1 | 49 | A | N3-C4-N9 | 6.77 | 132.82 | 127.40 |
| 22 | 23S1 | 213 | A | N3-C4-N9 | 6.77 | 132.82 | 127.40 |
| 22 | 23S1 | 911 | A | C4-C5-C6 | 6.77 | 120.39 | 117.00 |
| 1 | 16S1 | 1157 | A | C4-C5-C6 | 6.77 | 120.39 | 117.00 |
| 1 | 16S1 | 2 | A | N9-C4-C5 | 6.77 | 108.51 | 105.80 |
| 22 | 23S1 | 190 | A | C4-C5-C6 | 6.77 | 120.38 | 117.00 |
| 1 | 16S1 | 452 | A | C4-C5-C6 | 6.76 | 120.38 | 117.00 |
| 22 | 23S1 | 734 | A | C4-C5-C6 | 6.76 | 120.38 | 117.00 |
| 22 | 23S1 | 1403 | A | C4-C5-C6 | 6.76 | 120.38 | 117.00 |
| 1 | 16S1 | 523 | A | C4-C5-C6 | 6.76 | 120.38 | 117.00 |
| 1 | 16S1 | 1110 | A | C5-N7-C8 | 6.76 | 107.28 | 103.90 |
| 22 | 23S1 | 1144 | A | N3-C4-N9 | 6.76 | 132.81 | 127.40 |
| 22 | 23S1 | 2781 | A | C5-N7-C8 | 6.76 | 107.28 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 16S1 | 174 | A | N3-C4-N9 | 6.76 | 132.81 | 127.40 |
| 1 | 16S1 | 465 | A | C5-C6-N1 | 6.76 | 121.08 | 117.70 |
| 1 | 16S1 | 1256 | A | C8-N9-C4 | 6.76 | 108.50 | 105.80 |
| 22 | 23S1 | 621 | A | C5-N7-C8 | 6.76 | 107.28 | 103.90 |
| 22 | 23S1 | 2634 | A | N3-C4-N9 | 6.76 | 132.81 | 127.40 |
| 22 | 23S1 | 1392 | A | N9-C4-C5 | 6.76 | 108.50 | 105.80 |
| 22 | 23S1 | 2281 | A | N3-C4-N9 | 6.75 | 132.80 | 127.40 |
| 55 | PTR1 | 59 | A | C8-N9-C4 | 6.75 | 108.50 | 105.80 |
| 22 | 23S1 | 270 | A | C8-N9-C4 | 6.75 | 108.50 | 105.80 |
| 22 | 23S1 | 324 | A | N3-C4-N9 | 6.75 | 132.80 | 127.40 |
| 22 | 23S1 | 477 | A | N3-C4-N9 | 6.75 | 132.80 | 127.40 |
| 22 | 23S1 | 173 | A | N3-C4-N9 | 6.75 | 132.80 | 127.40 |
| 22 | 23S1 | 1111 | A | N3-C4-N9 | 6.75 | 132.80 | 127.40 |
| 22 | 23S1 | 2459 | A | C8-N9-C4 | 6.75 | 108.50 | 105.80 |
| 1 | 16S1 | 353 | A | C8-N9-C4 | 6.75 | 108.50 | 105.80 |
| 22 | 23S1 | 71 | A | N3-C4-N9 | 6.75 | 132.80 | 127.40 |
| 22 | 23S1 | 91 | A | C8-N9-C4 | 6.75 | 108.50 | 105.80 |
| 22 | 23S1 | 1020 | A | C5-N7-C8 | 6.75 | 107.27 | 103.90 |
| 22 | 23S1 | 1593 | A | N3-C4-N9 | 6.74 | 132.79 | 127.40 |
| 22 | 23S1 | 1801 | A | C5-N7-C8 | 6.74 | 107.27 | 103.90 |
| 22 | 23S1 | 1858 | A | N3-C4-N9 | 6.74 | 132.79 | 127.40 |
| 22 | 23S1 | 2615 | U | N3-C2-O2 | -6.74 | 117.48 | 122.20 |
| 22 | 23S1 | 689 | A | C4-C5-C6 | 6.74 | 120.37 | 117.00 |
| 22 | 23S1 | 781 | A | C4-C5-C6 | 6.74 | 120.37 | 117.00 |
| 1 | 16S1 | 754 | C | C6-N1-C2 | -6.74 | 117.61 | 120.30 |
| 22 | 23S1 | 1549 | A | C5-N7-C8 | 6.74 | 107.27 | 103.90 |
| 22 | 23S1 | 2273 | A | C4-C5-C6 | 6.74 | 120.37 | 117.00 |
| 22 | 23S1 | 348 | A | C4-C5-C6 | 6.74 | 120.37 | 117.00 |
| 22 | 23S1 | 782 | A | N3-C4-N9 | 6.74 | 132.79 | 127.40 |
| 22 | 23S1 | 191 | A | N3-C4-N9 | 6.74 | 132.79 | 127.40 |
| 22 | 23S1 | 2893 | A | C8-N9-C4 | 6.74 | 108.49 | 105.80 |
| 1 | 16S1 | 1468 | A | C5-C6-N1 | 6.73 | 121.07 | 117.70 |
| 22 | 23S1 | 2273 | A | N3-C4-N9 | 6.73 | 132.79 | 127.40 |
| 1 | 16S1 | 338 | A | C5-N7-C8 | 6.73 | 107.27 | 103.90 |
| 22 | 23S1 | 6 | A | N3-C4-N9 | 6.73 | 132.78 | 127.40 |
| 22 | 23S1 | 127 | A | C5-N7-C8 | 6.73 | 107.27 | 103.90 |
| 22 | 23S1 | 863 | A | C4-C5-C6 | 6.73 | 120.36 | 117.00 |
| 55 | PTR1 | 73 | A | C8-N9-C4 | 6.73 | 108.49 | 105.80 |
| 22 | 23S1 | 928 | A | N3-C4-N9 | 6.73 | 132.78 | 127.40 |
| 22 | 23S1 | 1308 | A | C4-C5-N7 | -6.73 | 107.33 | 110.70 |
| 22 | 23S1 | 2014 | A | C8-N9-C4 | 6.73 | 108.49 | 105.80 |
| 1 | 16S1 | 270 | A | C4-C5-C6 | 6.73 | 120.36 | 117.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 782 | A | C4-C5-C6 | 6.73 | 120.36 | 117.00 |
| 22 | 23S1 | 821 | A | N9-C4-C5 | 6.73 | 108.49 | 105.80 |
| 22 | 23S1 | 1403 | A | N3-C4-N9 | 6.73 | 132.78 | 127.40 |
| 1 | 16S1 | 1093 | A | C4-C5-C6 | 6.73 | 120.36 | 117.00 |
| 1 | 16S1 | 743 | A | N3-C4-N9 | 6.72 | 132.78 | 127.40 |
| 22 | 23S1 | 928 | A | C4-C5-C6 | 6.72 | 120.36 | 117.00 |
| 22 | 23S1 | 933 | A | C4-C5-C6 | 6.72 | 120.36 | 117.00 |
| 22 | 23S1 | 2660 | A | C8-N9-C4 | 6.72 | 108.49 | 105.80 |
| 1 | 16S1 | 1324 | A | C5-N7-C8 | 6.72 | 107.26 | 103.90 |
| 1 | 16S1 | 1446 | A | N3-C4-N9 | 6.72 | 132.78 | 127.40 |
| 22 | 23S1 | 2453 | A | C4-C5-N7 | -6.72 | 107.34 | 110.70 |
| 1 | 16S1 | 382 | A | C4-C5-C6 | 6.72 | 120.36 | 117.00 |
| 22 | 23S1 | 1794 | A | N3-C4-N9 | 6.72 | 132.78 | 127.40 |
| 23 | 05S1 | 50 | A | N3-C4-N9 | 6.72 | 132.78 | 127.40 |
| 22 | 23S1 | 2031 | A | C8-N9-C4 | 6.72 | 108.49 | 105.80 |
| 22 | 23S1 | 142 | A | C5-C6-N6 | 6.71 | 129.07 | 123.70 |
| 22 | 23S1 | 1969 | A | N3-C4-N9 | 6.71 | 132.77 | 127.40 |
| 23 | 05S1 | 45 | A | C8-N9-C4 | 6.71 | 108.48 | 105.80 |
| 22 | 23S1 | 233 | A | N3-C4-N9 | 6.71 | 132.77 | 127.40 |
| 22 | 23S1 | 1927 | A | N9-C4-C5 | 6.71 | 108.48 | 105.80 |
| 22 | 23S1 | 2725 | A | N3-C4-N9 | 6.71 | 132.77 | 127.40 |
| 23 | 05S1 | 58 | A | C4-C5-C6 | 6.71 | 120.35 | 117.00 |
| 55 | PTR1 | 62 | C | N1-C2-O2 | 6.71 | 122.92 | 118.90 |
| 1 | 16S1 | 1117 | A | C8-N9-C4 | 6.70 | 108.48 | 105.80 |
| 22 | 23S1 | 739 | A | C4-C5-C6 | 6.70 | 120.35 | 117.00 |
| 22 | 23S1 | 758 | C | N3-C2-O2 | -6.70 | 117.21 | 121.90 |
| 22 | 23S1 | 1028 | A | N3-C4-N9 | 6.70 | 132.76 | 127.40 |
| 1 | 16S1 | 432 | A | N3-C4-N9 | 6.70 | 132.76 | 127.40 |
| 22 | 23S1 | 2366 | A | C4-C5-C6 | 6.70 | 120.35 | 117.00 |
| 22 | 23S1 | 2873 | A | C4-C5-C6 | 6.70 | 120.35 | 117.00 |
| 22 | 23S1 | 142 | A | N9-C4-C5 | 6.70 | 108.48 | 105.80 |
| 22 | 23S1 | 1080 | A | N3-C4-N9 | 6.70 | 132.76 | 127.40 |
| 22 | 23S1 | 2013 | A | N3-C4-N9 | 6.70 | 132.76 | 127.40 |
| 22 | 23S1 | 2088 | A | C4-C5-C6 | 6.69 | 120.35 | 117.00 |
| 1 | 16S1 | 66 | A | C5-N7-C8 | 6.69 | 107.25 | 103.90 |
| 1 | 16S1 | 430 | A | N3-C4-N9 | 6.69 | 132.75 | 127.40 |
| 22 | 23S1 | 144 | A | C4-C5-C6 | 6.69 | 120.35 | 117.00 |
| 22 | 23S1 | 788 | A | C8-N9-C4 | 6.69 | 108.48 | 105.80 |
| 22 | 23S1 | 1966 | A | N3-C4-N9 | 6.69 | 132.75 | 127.40 |
| 1 | 16S1 | 1324 | A | N3-C4-N9 | 6.69 | 132.75 | 127.40 |
| 22 | 23S1 | 789 | A | C8-N9-C4 | 6.69 | 108.48 | 105.80 |
| 22 | 23S1 | 2860 | A | C5-N7-C8 | 6.69 | 107.25 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 16S1 | 1042 | A | C8-N9-C4 | 6.69 | 108.47 | 105.80 |
| 22 | 23S1 | 2411 | A | C8-N9-C4 | 6.69 | 108.47 | 105.80 |
| 1 | 16S1 | 2 | A | C5-C6-N1 | 6.68 | 121.04 | 117.70 |
| 1 | 16S1 | 728 | A | N3-C4-N9 | 6.68 | 132.75 | 127.40 |
| 1 | 16S1 | 487 | A | N3-C4-N9 | 6.68 | 132.75 | 127.40 |
| 22 | 23S1 | 825 | A | N9-C4-C5 | 6.68 | 108.47 | 105.80 |
| 22 | 23S1 | 384 | A | N3-C4-N9 | 6.68 | 132.74 | 127.40 |
| 22 | 23S1 | 1641 | A | C4-C5-C6 | 6.68 | 120.34 | 117.00 |
| 22 | 23S1 | 73 | A | C5-N7-C8 | 6.68 | 107.24 | 103.90 |
| 22 | 23S1 | 155 | A | N3-C4-N9 | 6.68 | 132.74 | 127.40 |
| 22 | 23S1 | 1912 | A | C4-C5-C6 | 6.68 | 120.34 | 117.00 |
| 1 | 16S1 | 155 | A | N3-C4-N9 | 6.68 | 132.74 | 127.40 |
| 22 | 23S1 | 2023 | C | N3-C2-O2 | -6.68 | 117.23 | 121.90 |
| 22 | 23S1 | 2560 | A | C4-C5-C6 | 6.68 | 120.34 | 117.00 |
| 22 | 23S1 | 173 | A | C4-C5-C6 | 6.67 | 120.34 | 117.00 |
| 22 | 23S1 | 863 | A | C5-C6-N1 | 6.67 | 121.04 | 117.70 |
| 22 | 23S1 | 2675 | A | N3-C4-N9 | 6.67 | 132.74 | 127.40 |
| 22 | 23S1 | 2705 | A | C5-N7-C8 | 6.67 | 107.23 | 103.90 |
| 1 | 16S1 | 978 | A | C4-C5-N7 | -6.67 | 107.37 | 110.70 |
| 22 | 23S1 | 807 | U | N1-C2-N3 | 6.67 | 118.90 | 114.90 |
| 22 | 23S1 | 1913 | A | C8-N9-C4 | 6.67 | 108.47 | 105.80 |
| 23 | 05S1 | 73 | A | C4-C5-C6 | 6.67 | 120.33 | 117.00 |
| 1 | 16S1 | 199 | A | C4-C5-C6 | 6.67 | 120.33 | 117.00 |
| 1 | 16S1 | 1306 | A | N3-C4-N9 | 6.67 | 132.73 | 127.40 |
| 22 | 23S1 | 1147 | A | N9-C4-C5 | 6.67 | 108.47 | 105.80 |
| 1 | 16S1 | 1507 | A | C5-N7-C8 | 6.66 | 107.23 | 103.90 |
| 22 | 23S1 | 116 | C | N3-C2-O2 | -6.66 | 117.23 | 121.90 |
| 22 | 23S1 | 347 | A | C4-C5-C6 | 6.66 | 120.33 | 117.00 |
| 22 | 23S1 | 1515 | A | N9-C4-C5 | 6.66 | 108.47 | 105.80 |
| 1 | 16S1 | 383 | A | C5-N7-C8 | 6.66 | 107.23 | 103.90 |
| 1 | 16S1 | 435 | A | N3-C4-N9 | 6.66 | 132.73 | 127.40 |
| 1 | 16S1 | 983 | A | C4-C5-C6 | 6.66 | 120.33 | 117.00 |
| 22 | 23S1 | 1701 | A | C5-C6-N1 | 6.66 | 121.03 | 117.70 |
| 1 | 16S1 | 1503 | A | C4-C5-C6 | 6.66 | 120.33 | 117.00 |
| 1 | 16S1 | 675 | A | C8-N9-C4 | 6.66 | 108.46 | 105.80 |
| 22 | 23S1 | 362 | A | C5-N7-C8 | 6.66 | 107.23 | 103.90 |
| 22 | 23S1 | 272 | A | C4-C5-C6 | 6.65 | 120.33 | 117.00 |
| 22 | 23S1 | 716 | A | C4-C5-C6 | 6.65 | 120.33 | 117.00 |
| 22 | 23S1 | 2333 | A | C8-N9-C4 | 6.65 | 108.46 | 105.80 |
| 1 | 16S1 | 1531 | A | C5-N7-C8 | 6.65 | 107.22 | 103.90 |
| 22 | 23S1 | 1912 | A | C8-N9-C4 | 6.65 | 108.46 | 105.80 |
| 22 | 23S1 | 2764 | A | C8-N9-C4 | 6.65 | 108.46 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 22 | 23S1 | 1749 | A | N3-C4-N9 | 6.65 | 132.72 | 127.40 |
| 1 | 16S1 | 1229 | A | C4-C5-C6 | 6.64 | 120.32 | 117.00 |
| 22 | 23S1 | 1151 | A | N3-C4-N9 | 6.64 | 132.72 | 127.40 |
| 22 | 23S1 | 1801 | A | C4-C5-C6 | 6.64 | 120.32 | 117.00 |
| 22 | 23S1 | 1801 | A | N3-C4-N9 | 6.64 | 132.72 | 127.40 |
| 1 | 16S1 | 190 | A | C5-N7-C8 | 6.64 | 107.22 | 103.90 |
| 22 | 23S1 | 309 | A | N3-C4-N9 | 6.64 | 132.72 | 127.40 |
| 22 | 23S1 | 1143 | A | C4-C5-C6 | 6.64 | 120.32 | 117.00 |
| 22 | 23S1 | 788 | A | N3-C4-N9 | 6.64 | 132.71 | 127.40 |
| 23 | 05S1 | 58 | A | N3-C4-N9 | 6.64 | 132.71 | 127.40 |
| 1 | 16S1 | 309 | A | C8-N9-C4 | 6.64 | 108.45 | 105.80 |
| 1 | 16S1 | 408 | A | C4-C5-C6 | 6.64 | 120.32 | 117.00 |
| 22 | 23S1 | 1213 | A | N3-C4-N9 | 6.64 | 132.71 | 127.40 |
| 22 | 23S1 | 2097 | A | N3-C4-N9 | 6.64 | 132.71 | 127.40 |
| 22 | 23S1 | 2154 | A | C4-C5-C6 | 6.64 | 120.32 | 117.00 |
| 22 | 23S1 | 892 | A | C4-C5-C6 | 6.64 | 120.32 | 117.00 |
| 22 | 23S1 | 1987 | A | N3-C4-N9 | 6.64 | 132.71 | 127.40 |
| 22 | 23S1 | 2665 | A | N3-C4-N9 | 6.64 | 132.71 | 127.40 |
| 22 | 23S1 | 10 | A | C8-N9-C4 | 6.64 | 108.45 | 105.80 |
| 22 | 23S1 | 324 | A | C5-C6-N1 | 6.64 | 121.02 | 117.70 |
| 22 | 23S1 | 2135 | A | N3-C4-N9 | 6.64 | 132.71 | 127.40 |
| 22 | 23S1 | 2311 | A | N9-C4-C5 | 6.64 | 108.45 | 105.80 |
| 22 | 23S1 | 344 | A | C8-N9-C4 | 6.63 | 108.45 | 105.80 |
| 22 | 23S1 | 1205 | A | C8-N9-C4 | 6.63 | 108.45 | 105.80 |
| 1 | 16S1 | 635 | A | C8-N9-C4 | 6.63 | 108.45 | 105.80 |
| 22 | 23S1 | 2335 | A | C4-C5-C6 | 6.63 | 120.32 | 117.00 |
| 1 | 16S1 | 687 | A | C4-C5-C6 | 6.63 | 120.31 | 117.00 |
| 22 | 23S1 | 2757 | A | N3-C4-N9 | 6.63 | 132.70 | 127.40 |
| 1 | 16S1 | 448 | A | C4-C5-C6 | 6.63 | 120.31 | 117.00 |
| 22 | 23S1 | 753 | A | N3-C4-N9 | 6.63 | 132.70 | 127.40 |
| 1 | 16S1 | 1151 | A | N3-C4-N9 | 6.63 | 132.70 | 127.40 |
| 22 | 23S1 | 348 | A | N3-C4-N9 | 6.63 | 132.70 | 127.40 |
| 22 | 23S1 | 1668 | A | N9-C4-C5 | 6.63 | 108.45 | 105.80 |
| 22 | 23S1 | 2639 | A | C5-N7-C8 | 6.62 | 107.21 | 103.90 |
| 1 | 16S1 | 72 | A | C8-N9-C4 | 6.62 | 108.45 | 105.80 |
| 1 | 16S1 | 482 | A | N3-C4-N9 | 6.62 | 132.70 | 127.40 |
| 1 | 16S1 | 787 | A | C8-N9-C4 | 6.62 | 108.45 | 105.80 |
| 1 | 16S1 | 1288 | A | C5-N7-C8 | 6.62 | 107.21 | 103.90 |
| 22 | 23S1 | 980 | A | C5-N7-C8 | 6.62 | 107.21 | 103.90 |
| 22 | 23S1 | 2080 | A | C5-N7-C8 | 6.62 | 107.21 | 103.90 |
| 22 | 23S1 | 2679 | A | C4-C5-C6 | 6.62 | 120.31 | 117.00 |
| 22 | 23S1 | 722 | A | C4-C5-C6 | 6.62 | 120.31 | 117.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 959 | A | N3-C4-N9 | 6.62 | 132.69 | 127.40 |
| 22 | 23S1 | 1580 | A | N3-C4-N9 | 6.62 | 132.69 | 127.40 |
| 1 | 16S1 | 704 | A | N9-C4-C5 | 6.62 | 108.45 | 105.80 |
| 1 | 16S1 | 1363 | A | C4-C5-C6 | 6.62 | 120.31 | 117.00 |
| 22 | 23S1 | 943 | A | N3-C4-N9 | 6.62 | 132.69 | 127.40 |
| 22 | 23S1 | 626 | A | C5-N7-C8 | 6.62 | 107.21 | 103.90 |
| 22 | 23S1 | 1431 | A | N3-C4-N9 | 6.62 | 132.69 | 127.40 |
| 22 | 23S1 | 2725 | A | C5-N7-C8 | 6.62 | 107.21 | 103.90 |
| 22 | 23S1 | 2809 | A | C4-C5-C6 | 6.62 | 120.31 | 117.00 |
| 1 | 16S1 | 1324 | A | C4-C5-C6 | 6.61 | 120.31 | 117.00 |
| 22 | 23S1 | 2392 | A | N3-C4-N9 | 6.61 | 132.69 | 127.40 |
| 23 | 05S1 | 29 | A | C4-C5-N7 | -6.61 | 107.39 | 110.70 |
| 1 | 16S1 | 181 | A | C4-C5-C6 | 6.61 | 120.31 | 117.00 |
| 22 | 23S1 | 526 | A | C5-N7-C8 | 6.61 | 107.20 | 103.90 |
| 22 | 23S1 | 1439 | A | C8-N9-C4 | 6.61 | 108.44 | 105.80 |
| 22 | 23S1 | 1586 | A | N3-C4-N9 | 6.61 | 132.69 | 127.40 |
| 22 | 23S1 | 1598 | A | N3-C4-N9 | 6.61 | 132.69 | 127.40 |
| 22 | 23S1 | 2268 | A | C4-C5-C6 | 6.61 | 120.31 | 117.00 |
| 22 | 23S1 | 2510 | C | N3-C2-O2 | -6.61 | 117.27 | 121.90 |
| 22 | 23S1 | 1803 | A | C5-N7-C8 | 6.61 | 107.20 | 103.90 |
| 1 | 16S1 | 55 | A | C8-N9-C4 | 6.61 | 108.44 | 105.80 |
| 22 | 23S1 | 2482 | A | C4-C5-C6 | 6.61 | 120.30 | 117.00 |
| 1 | 16S1 | 1499 | A | N3-C4-N9 | 6.60 | 132.68 | 127.40 |
| 22 | 23S1 | 352 | A | C8-N9-C4 | 6.60 | 108.44 | 105.80 |
| 1 | 16S1 | 451 | A | C8-N9-C4 | 6.60 | 108.44 | 105.80 |
| 22 | 23S1 | 472 | A | C5-N7-C8 | 6.60 | 107.20 | 103.90 |
| 22 | 23S1 | 1900 | A | C5-N7-C8 | 6.60 | 107.20 | 103.90 |
| 1 | 16S1 | 579 | A | C4-C5-C6 | 6.60 | 120.30 | 117.00 |
| 1 | 16S1 | 1196 | A | C8-N9-C4 | 6.60 | 108.44 | 105.80 |
| 22 | 23S1 | 2757 | A | C4-C5-C6 | 6.60 | 120.30 | 117.00 |
| 1 | 16S1 | 640 | A | C4-C5-C6 | 6.60 | 120.30 | 117.00 |
| 22 | 23S1 | 439 | A | C4-C5-C6 | 6.60 | 120.30 | 117.00 |
| 22 | 23S1 | 1304 | A | N9-C4-C5 | 6.60 | 108.44 | 105.80 |
| 22 | 23S1 | 1373 | A | C4-C5-C6 | 6.60 | 120.30 | 117.00 |
| 22 | 23S1 | 1899 | A | C5-N7-C8 | 6.59 | 107.20 | 103.90 |
| 22 | 23S1 | 2154 | A | N3-C4-N9 | 6.59 | 132.67 | 127.40 |
| 22 | 23S1 | 2868 | A | C4-C5-C6 | 6.59 | 120.30 | 117.00 |
| 1 | 16S1 | 50 | A | N3-C4-N9 | 6.59 | 132.67 | 127.40 |
| 1 | 16S1 | 743 | A | C5-C6-N1 | 6.59 | 121.00 | 117.70 |
| 22 | 23S1 | 152 | A | N3-C4-N9 | 6.59 | 132.67 | 127.40 |
| 22 | 23S1 | 1580 | A | C8-N9-C4 | 6.59 | 108.44 | 105.80 |
| 22 | 23S1 | 2459 | A | C4-C5-C6 | 6.59 | 120.30 | 117.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 55 | PTR1 | 17 | U | C5-C4-O4 | -6.59 | 121.94 | 125.90 |
| 1 | 16S1 | 223 | A | N3-C4-N9 | 6.59 | 132.67 | 127.40 |
| 1 | 16S1 | 1275 | A | N3-C4-N9 | 6.59 | 132.67 | 127.40 |
| 1 | 16S1 | 1350 | A | C4-C5-C6 | 6.59 | 120.30 | 117.00 |
| 22 | 23S1 | 1746 | A | C4-C5-C6 | 6.59 | 120.30 | 117.00 |
| 22 | 23S1 | 742 | A | N3-C4-N9 | 6.59 | 132.67 | 127.40 |
| 1 | 16S1 | 336 | A | C5-N7-C8 | 6.59 | 107.19 | 103.90 |
| 1 | 16S1 | 1219 | A | C5-N7-C8 | 6.59 | 107.19 | 103.90 |
| 22 | 23S1 | 1650 | A | N3-C4-N9 | 6.59 | 132.67 | 127.40 |
| 22 | 23S1 | 1885 | A | C8-N9-C4 | 6.59 | 108.44 | 105.80 |
| 22 | 23S1 | 2682 | A | C8-N9-C4 | 6.58 | 108.43 | 105.80 |
| 1 | 16S1 | 815 | A | C8-N9-C4 | 6.58 | 108.43 | 105.80 |
| 1 | 16S1 | 1219 | A | C4-C5-C6 | 6.58 | 120.29 | 117.00 |
| 22 | 23S1 | 505 | A | C4-C5-C6 | 6.58 | 120.29 | 117.00 |
| 22 | 23S1 | 727 | A | N3-C4-N9 | 6.58 | 132.67 | 127.40 |
| 1 | 16S1 | 1044 | A | N3-C4-N9 | 6.58 | 132.66 | 127.40 |
| 22 | 23S1 | 233 | A | C8-N9-C4 | 6.58 | 108.43 | 105.80 |
| 22 | 23S1 | 1711 | A | C4-C5-C6 | 6.58 | 120.29 | 117.00 |
| 22 | 23S1 | 2094 | A | C5-C6-N1 | 6.58 | 120.99 | 117.70 |
| 22 | 23S1 | 2810 | A | C4-C5-C6 | 6.58 | 120.29 | 117.00 |
| 1 | 16S1 | 87 | C | N1-C2-O2 | 6.58 | 122.85 | 118.90 |
| 1 | 16S1 | 329 | A | N3-C4-N9 | 6.58 | 132.66 | 127.40 |
| 22 | 23S1 | 131 | A | C4-C5-C6 | 6.58 | 120.29 | 117.00 |
| 22 | 23S1 | 251 | A | N7-C8-N9 | -6.58 | 110.51 | 113.80 |
| 22 | 23S1 | 1246 | A | N3-C4-N9 | 6.58 | 132.66 | 127.40 |
| 22 | 23S1 | 1938 | A | C8-N9-C4 | 6.58 | 108.43 | 105.80 |
| 1 | 16S1 | 1092 | A | N9-C4-C5 | 6.58 | 108.43 | 105.80 |
| 22 | 23S1 | 633 | A | C5-N7-C8 | 6.58 | 107.19 | 103.90 |
| 22 | 23S1 | 52 | A | N3-C4-N9 | 6.57 | 132.66 | 127.40 |
| 22 | 23S1 | 477 | A | C5-N7-C8 | 6.57 | 107.19 | 103.90 |
| 22 | 23S1 | 2899 | A | C8-N9-C4 | 6.57 | 108.43 | 105.80 |
| 22 | 23S1 | 322 | A | C8-N9-C4 | 6.57 | 108.43 | 105.80 |
| 22 | 23S1 | 1307 | A | C4-C5-C6 | 6.57 | 120.28 | 117.00 |
| 22 | 23S1 | 1515 | A | C5-C6-N1 | 6.57 | 120.98 | 117.70 |
| 22 | 23S1 | 2241 | A | C4-C5-C6 | 6.57 | 120.28 | 117.00 |
| 22 | 23S1 | 2602 | A | C8-N9-C4 | 6.57 | 108.43 | 105.80 |
| 23 | 05S1 | 45 | A | C5-N7-C8 | 6.57 | 107.19 | 103.90 |
| 1 | 16S1 | 794 | A | N3-C4-N9 | 6.57 | 132.66 | 127.40 |
| 22 | 23S1 | 5 | A | C4-C5-C6 | 6.57 | 120.28 | 117.00 |
| 22 | 23S1 | 721 | A | N3-C4-N9 | 6.57 | 132.66 | 127.40 |
| 1 | 16S1 | 596 | A | C8-N9-C4 | 6.57 | 108.43 | 105.80 |
| 22 | 23S1 | 460 | A | N3-C4-N9 | 6.57 | 132.66 | 127.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 16S1 | 73 | C | C6-N1-C2 | -6.57 | 117.67 | 120.30 |
| 1 | 16S1 | 918 | A | N9-C4-C5 | 6.57 | 108.43 | 105.80 |
| 22 | 23S1 | 945 | A | C4-C5-C6 | 6.57 | 120.28 | 117.00 |
| 1 | 16S1 | 907 | A | C4-C5-C6 | 6.56 | 120.28 | 117.00 |
| 22 | 23S1 | 1143 | A | C5-N7-C8 | 6.56 | 107.18 | 103.90 |
| 22 | 23S1 | 2059 | A | C4-C5-C6 | 6.56 | 120.28 | 117.00 |
| 22 | 23S1 | 2071 | A | C4-C5-C6 | 6.56 | 120.28 | 117.00 |
| 22 | 23S1 | 582 | A | N3-C4-N9 | 6.56 | 132.65 | 127.40 |
| 1 | 16S1 | 1081 | A | N3-C4-N9 | 6.56 | 132.65 | 127.40 |
| 1 | 16S1 | 1357 | A | N3-C4-N9 | 6.56 | 132.65 | 127.40 |
| 1 | 16S1 | 946 | A | C4-C5-C6 | 6.56 | 120.28 | 117.00 |
| 22 | 23S1 | 925 | A | C8-N9-C4 | 6.56 | 108.42 | 105.80 |
| 22 | 23S1 | 1553 | A | C4-C5-C6 | 6.56 | 120.28 | 117.00 |
| 22 | 23S1 | 1650 | A | C8-N9-C4 | 6.56 | 108.42 | 105.80 |
| 22 | 23S1 | 2814 | A | C4-C5-C6 | 6.56 | 120.28 | 117.00 |
| 1 | 16S1 | 1360 | A | C4-C5-N7 | -6.56 | 107.42 | 110.70 |
| 1 | 16S1 | 414 | A | N9-C4-C5 | 6.55 | 108.42 | 105.80 |
| 22 | 23S1 | 1302 | A | C8-N9-C4 | 6.55 | 108.42 | 105.80 |
| 22 | 23S1 | 2406 | A | C8-N9-C4 | 6.55 | 108.42 | 105.80 |
| 22 | 23S1 | 2476 | A | C4-C5-C6 | 6.55 | 120.28 | 117.00 |
| 1 | 16S1 | 913 | A | C8-N9-C4 | 6.55 | 108.42 | 105.80 |
| 22 | 23S1 | 1419 | A | C8-N9-C4 | 6.55 | 108.42 | 105.80 |
| 22 | 23S1 | 1597 | A | N9-C4-C5 | 6.55 | 108.42 | 105.80 |
| 22 | 23S1 | 1810 | A | N7-C8-N9 | -6.55 | 110.52 | 113.80 |
| 1 | 16S1 | 78 | A | C4-C5-C6 | 6.55 | 120.27 | 117.00 |
| 1 | 16S1 | 460 | A | N3-C4-N9 | 6.55 | 132.64 | 127.40 |
| 1 | 16S1 | 1398 | A | N9-C4-C5 | 6.55 | 108.42 | 105.80 |
| 22 | 23S1 | 330 | A | C4-C5-C6 | 6.55 | 120.28 | 117.00 |
| 22 | 23S1 | 323 | C | N1-C2-O2 | 6.55 | 122.83 | 118.90 |
| 22 | 23S1 | 959 | A | C4-C5-C6 | 6.55 | 120.27 | 117.00 |
| 1 | 16S1 | 1274 | A | C4-C5-C6 | 6.55 | 120.27 | 117.00 |
| 22 | 23S1 | 56 | A | N3-C4-N9 | 6.55 | 132.64 | 127.40 |
| 22 | 23S1 | 661 | A | C5-C6-N1 | 6.55 | 120.97 | 117.70 |
| 22 | 23S1 | 900 | A | C4-C5-C6 | 6.55 | 120.27 | 117.00 |
| 22 | 23S1 | 1308 | A | N9-C4-C5 | 6.55 | 108.42 | 105.80 |
| 1 | 16S1 | 640 | A | N3-C4-N9 | 6.54 | 132.64 | 127.40 |
| 1 | 16S1 | 728 | A | C5-C6-N1 | 6.54 | 120.97 | 117.70 |
| 22 | 23S1 | 172 | A | N3-C4-N9 | 6.54 | 132.64 | 127.40 |
| 22 | 23S1 | 1395 | A | N9-C4-C5 | 6.54 | 108.42 | 105.80 |
| 1 | 16S1 | 622 | A | N9-C4-C5 | 6.54 | 108.42 | 105.80 |
| 1 | 16S1 | 1236 | A | N3-C4-N9 | 6.54 | 132.63 | 127.40 |
| 22 | 23S1 | 1579 | A | C8-N9-C4 | 6.54 | 108.42 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 2792 | A | N3-C4-N9 | 6.54 | 132.63 | 127.40 |
| 1 | 16S1 | 1332 | A | C4-C5-C6 | 6.54 | 120.27 | 117.00 |
| 1 | 16S1 | 197 | A | C8-N9-C4 | 6.54 | 108.42 | 105.80 |
| 1 | 16S1 | 1229 | A | N3-C4-N9 | 6.54 | 132.63 | 127.40 |
| 1 | 16S1 | 1275 | A | C8-N9-C4 | 6.54 | 108.42 | 105.80 |
| 16 | S161 | 14 | ARG | NE-CZ-NH1 | -6.54 | 117.03 | 120.30 |
| 22 | 23S1 | 2868 | A | N3-C4-N9 | 6.54 | 132.63 | 127.40 |
| 1 | 16S1 | 573 | A | N3-C4-N9 | 6.54 | 132.63 | 127.40 |
| 1 | 16S1 | 872 | A | N3-C4-N9 | 6.54 | 132.63 | 127.40 |
| 22 | 23S1 | 449 | A | C5-C6-N1 | 6.54 | 120.97 | 117.70 |
| 22 | 23S1 | 1746 | A | N3-C4-N9 | 6.54 | 132.63 | 127.40 |
| 1 | 16S1 | 461 | A | C8-N9-C4 | 6.53 | 108.41 | 105.80 |
| 1 | 16S1 | 768 | A | N9-C4-C5 | 6.53 | 108.41 | 105.80 |
| 1 | 16S1 | 938 | A | C5-C6-N1 | 6.53 | 120.97 | 117.70 |
| 22 | 23S1 | 1244 | A | N3-C4-N9 | 6.53 | 132.63 | 127.40 |
| 22 | 23S1 | 149 | A | N3-C4-N9 | 6.53 | 132.62 | 127.40 |
| 22 | 23S1 | 480 | A | N9-C4-C5 | 6.53 | 108.41 | 105.80 |
| 22 | 23S1 | 1039 | A | C4-C5-C6 | 6.53 | 120.27 | 117.00 |
| 22 | 23S1 | 1070 | A | C4-C5-C6 | 6.53 | 120.27 | 117.00 |
| 22 | 23S1 | 2014 | A | N3-C4-N9 | 6.53 | 132.62 | 127.40 |
| 1 | 16S1 | 1080 | A | C4-C5-C6 | 6.53 | 120.26 | 117.00 |
| 22 | 23S1 | 2386 | A | N3-C4-N9 | 6.53 | 132.62 | 127.40 |
| 22 | 23S1 | 1419 | A | C5-N7-C8 | 6.53 | 107.16 | 103.90 |
| 22 | 23S1 | 2189 | U | N3-C2-O2 | -6.53 | 117.63 | 122.20 |
| 22 | 23S1 | 340 | A | C4-C5-C6 | 6.52 | 120.26 | 117.00 |
| 22 | 23S1 | 1134 | A | C8-N9-C4 | 6.52 | 108.41 | 105.80 |
| 22 | 23S1 | 1998 | A | N9-C4-C5 | 6.52 | 108.41 | 105.80 |
| 1 | 16S1 | 81 | A | N9-C4-C5 | 6.52 | 108.41 | 105.80 |
| 22 | 23S1 | 1054 | A | N3-C4-N9 | 6.52 | 132.62 | 127.40 |
| 22 | 23S1 | 1590 | A | N3-C4-N9 | 6.52 | 132.62 | 127.40 |
| 22 | 23S1 | 1847 | A | N3-C4-N9 | 6.52 | 132.62 | 127.40 |
| 22 | 23S1 | 2173 | A | C5-C6-N1 | 6.52 | 120.96 | 117.70 |
| 1 | 16S1 | 621 | A | C4-C5-C6 | 6.52 | 120.26 | 117.00 |
| 22 | 23S1 | 13 | A | N3-C4-N9 | 6.52 | 132.61 | 127.40 |
| 1 | 16S1 | 509 | A | C4-C5-C6 | 6.51 | 120.26 | 117.00 |
| 2 | S021 | 57 | LEU | CB-CG-CD2 | -6.51 | 99.92 | 111.00 |
| 1 | 16S1 | 325 | A | C4-C5-C6 | 6.51 | 120.26 | 117.00 |
| 1 | 16S1 | 780 | A | C4-C5-C6 | 6.51 | 120.25 | 117.00 |
| 1 | 16S1 | 831 | A | C8-N9-C4 | 6.51 | 108.41 | 105.80 |
| 22 | 23S1 | 1073 | A | N3-C4-N9 | 6.51 | 132.61 | 127.40 |
| 22 | 23S1 | 1469 | A | C8-N9-C4 | 6.51 | 108.41 | 105.80 |
| 22 | 23S1 | 1966 | A | C8-N9-C4 | 6.51 | 108.40 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 1134 | A | C4-C5-C6 | 6.51 | 120.25 | 117.00 |
| 22 | 23S1 | 1665 | A | N3-C4-N9 | 6.51 | 132.61 | 127.40 |
| 22 | 23S1 | 125 | A | C8-N9-C4 | 6.51 | 108.40 | 105.80 |
| 22 | 23S1 | 1433 | A | C4-C5-C6 | 6.51 | 120.25 | 117.00 |
| 1 | 16S1 | 681 | A | C4-C5-C6 | 6.50 | 120.25 | 117.00 |
| 1 | 16S1 | 915 | A | C8-N9-C4 | 6.50 | 108.40 | 105.80 |
| 1 | 16S1 | 1036 | A | C4-C5-C6 | 6.50 | 120.25 | 117.00 |
| 22 | 23S1 | 374 | A | N3-C4-N9 | 6.50 | 132.60 | 127.40 |
| 22 | 23S1 | 633 | A | C4-C5-C6 | 6.50 | 120.25 | 117.00 |
| 22 | 23S1 | 2598 | A | C4-C5-C6 | 6.50 | 120.25 | 117.00 |
| 1 | 16S1 | 393 | A | C4-C5-C6 | 6.50 | 120.25 | 117.00 |
| 1 | 16S1 | 983 | A | C5-C6-N1 | 6.50 | 120.95 | 117.70 |
| 22 | 23S1 | 241 | A | C8-N9-C4 | 6.50 | 108.40 | 105.80 |
| 22 | 23S1 | 689 | A | N3-C4-N9 | 6.50 | 132.60 | 127.40 |
| 22 | 23S1 | 734 | A | N3-C4-N9 | 6.50 | 132.60 | 127.40 |
| 22 | 23S1 | 1084 | A | C4-C5-C6 | 6.50 | 120.25 | 117.00 |
| 22 | 23S1 | 1630 | A | N9-C4-C5 | 6.50 | 108.40 | 105.80 |
| 22 | 23S1 | 1744 | A | N3-C4-N9 | 6.50 | 132.60 | 127.40 |
| 1 | 16S1 | 162 | A | C5-C6-N6 | 6.50 | 128.90 | 123.70 |
| 1 | 16S1 | 913 | A | C6-N1-C2 | 6.50 | 122.50 | 118.60 |
| 22 | 23S1 | 1572 | A | C5-N7-C8 | 6.50 | 107.15 | 103.90 |
| 22 | 23S1 | 2176 | A | C4-C5-C6 | 6.50 | 120.25 | 117.00 |
| 22 | 23S1 | 422 | A | C5-N7-C8 | 6.50 | 107.15 | 103.90 |
| 22 | 23S1 | 1705 | A | N3-C4-N9 | 6.50 | 132.60 | 127.40 |
| 22 | 23S1 | 2366 | A | N3-C4-N9 | 6.50 | 132.60 | 127.40 |
| 22 | 23S1 | 428 | A | N3-C4-N9 | 6.50 | 132.60 | 127.40 |
| 22 | 23S1 | 1630 | A | C4-C5-N7 | -6.50 | 107.45 | 110.70 |
| 22 | 23S1 | 2191 | A | C5-N7-C8 | 6.50 | 107.15 | 103.90 |
| 55 | PTR1 | 21 | A | C5-N7-C8 | 6.50 | 107.15 | 103.90 |
| 1 | 16S1 | 130 | A | C8-N9-C4 | 6.50 | 108.40 | 105.80 |
| 1 | 16S1 | 535 | A | C8-N9-C4 | 6.49 | 108.40 | 105.80 |
| 1 | 16S1 | 1468 | A | C5-N7-C8 | 6.49 | 107.15 | 103.90 |
| 22 | 23S1 | 53 | A | N3-C4-N9 | 6.49 | 132.59 | 127.40 |
| 22 | 23S1 | 1755 | A | N9-C4-C5 | 6.49 | 108.40 | 105.80 |
| 22 | 23S1 | 2430 | A | N7-C8-N9 | -6.49 | 110.55 | 113.80 |
| 22 | 23S1 | 2266 | A | C5-N7-C8 | 6.49 | 107.15 | 103.90 |
| 22 | 23S1 | 2340 | A | N3-C4-N9 | 6.49 | 132.59 | 127.40 |
| 1 | 16S1 | 681 | A | N3-C4-N9 | 6.49 | 132.59 | 127.40 |
| 22 | 23S1 | 71 | A | C4-C5-C6 | 6.49 | 120.24 | 117.00 |
| 22 | 23S1 | 1050 | A | N3-C4-N9 | 6.49 | 132.59 | 127.40 |
| 22 | 23S1 | 917 | A | C4-C5-C6 | 6.49 | 120.24 | 117.00 |
| 1 | 16S1 | 161 | A | N3-C4-N9 | 6.49 | 132.59 | 127.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 16S1 | 1004 | A | C4-C5-C6 | 6.49 | 120.24 | 117.00 |
| 22 | 23S1 | 849 | A | N3-C4-N9 | 6.49 | 132.59 | 127.40 |
| 1 | 16S1 | 19 | A | N3-C4-N9 | 6.48 | 132.59 | 127.40 |
| 22 | 23S1 | 2003 | A | N3-C4-N9 | 6.48 | 132.59 | 127.40 |
| 1 | 16S1 | 325 | A | N3-C4-N9 | 6.48 | 132.59 | 127.40 |
| 22 | 23S1 | 1353 | A | C5-C6-N1 | 6.48 | 120.94 | 117.70 |
| 22 | 23S1 | 2386 | A | C5-C6-N1 | 6.48 | 120.94 | 117.70 |
| 1 | 16S1 | 509 | A | N3-C4-N9 | 6.48 | 132.58 | 127.40 |
| 1 | 16S1 | 648 | A | N3-C4-N9 | 6.48 | 132.59 | 127.40 |
| 1 | 16S1 | 807 | A | C4-C5-C6 | 6.48 | 120.24 | 117.00 |
| 1 | 16S1 | 1492 | A | C4-C5-C6 | 6.48 | 120.24 | 117.00 |
| 22 | 23S1 | 743 | A | C5-N7-C8 | 6.48 | 107.14 | 103.90 |
| 22 | 23S1 | 829 | A | C8-N9-C4 | 6.48 | 108.39 | 105.80 |
| 1 | 16S1 | 1204 | A | C4-C5-C6 | 6.48 | 120.24 | 117.00 |
| 1 | 16S1 | 1339 | A | C5-N7-C8 | 6.48 | 107.14 | 103.90 |
| 1 | 16S1 | 1163 | A | C5-C6-N1 | 6.48 | 120.94 | 117.70 |
| 22 | 23S1 | 2051 | A | C5-N7-C8 | 6.48 | 107.14 | 103.90 |
| 22 | 23S1 | 2328 | A | C5-N7-C8 | 6.48 | 107.14 | 103.90 |
| 22 | 23S1 | 2711 | A | C4-C5-C6 | 6.48 | 120.24 | 117.00 |
| 22 | 23S1 | 1711 | A | N3-C4-N9 | 6.48 | 132.58 | 127.40 |
| 22 | 23S1 | 1809 | A | C5-C6-N1 | 6.48 | 120.94 | 117.70 |
| 22 | 23S1 | 1262 | A | N3-C4-N9 | 6.47 | 132.58 | 127.40 |
| 22 | 23S1 | 1598 | A | C4-C5-C6 | 6.47 | 120.24 | 117.00 |
| 22 | 23S1 | 2340 | A | C4-C5-C6 | 6.47 | 120.24 | 117.00 |
| 1 | 16S1 | 1163 | A | C4-C5-C6 | 6.47 | 120.24 | 117.00 |
| 22 | 23S1 | 161 | A | N9-C4-C5 | 6.47 | 108.39 | 105.80 |
| 22 | 23S1 | 635 | C | C6-N1-C2 | -6.47 | 117.71 | 120.30 |
| 22 | 23S1 | 654 | A | C4-C5-C6 | 6.47 | 120.24 | 117.00 |
| 22 | 23S1 | 2534 | A | N3-C4-N9 | 6.47 | 132.58 | 127.40 |
| 1 | 16S1 | 600 | A | C4-C5-C6 | 6.47 | 120.23 | 117.00 |
| 22 | 23S1 | 1230 | A | N3-C4-N9 | 6.47 | 132.57 | 127.40 |
| 22 | 23S1 | 1819 | A | C4-C5-C6 | 6.47 | 120.23 | 117.00 |
| 22 | 23S1 | 2482 | A | N3-C4-N9 | 6.47 | 132.58 | 127.40 |
| 1 | 16S1 | 151 | A | C5-C6-N1 | 6.47 | 120.93 | 117.70 |
| 1 | 16S1 | 466 | A | N9-C4-C5 | 6.47 | 108.39 | 105.80 |
| 1 | 16S1 | 1225 | A | C5-C6-N1 | 6.47 | 120.93 | 117.70 |
| 22 | 23S1 | 1169 | A | N3-C4-N9 | 6.47 | 132.57 | 127.40 |
| 22 | 23S1 | 1785 | A | N9-C4-C5 | 6.47 | 108.39 | 105.80 |
| 13 | S131 | 79 | ARG | NE-CZ-NH1 | -6.46 | 117.07 | 120.30 |
| 22 | 23S1 | 344 | A | C4-C5-C6 | 6.46 | 120.23 | 117.00 |
| 22 | 23S1 | 1080 | A | C8-N9-C4 | 6.46 | 108.39 | 105.80 |
| 22 | 23S1 | 1287 | A | N3-C4-N9 | 6.46 | 132.57 | 127.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 22 | 23S1 | 2346 | A | C4-C5-C6 | 6.46 | 120.23 | 117.00 |
| 23 | 05S1 | 119 | A | N3-C4-N9 | 6.46 | 132.57 | 127.40 |
| 1 | 16S1 | 408 | A | N3-C4-N9 | 6.46 | 132.57 | 127.40 |
| 1 | 16S1 | 321 | A | C8-N9-C4 | 6.46 | 108.38 | 105.80 |
| 22 | 23S1 | 943 | A | C4-C5-C6 | 6.46 | 120.23 | 117.00 |
| 22 | 23S1 | 2530 | A | C4-C5-C6 | 6.46 | 120.23 | 117.00 |
| 22 | 23S1 | 131 | A | C5-C6-N1 | 6.46 | 120.93 | 117.70 |
| 22 | 23S1 | 1054 | A | C4-C5-C6 | 6.46 | 120.23 | 117.00 |
| 1 | 16S1 | 487 | A | C4-C5-C6 | 6.46 | 120.23 | 117.00 |
| 22 | 23S1 | 1610 | A | C5-N7-C8 | 6.46 | 107.13 | 103.90 |
| 1 | 16S1 | 78 | A | C5-N7-C8 | 6.46 | 107.13 | 103.90 |
| 22 | 23S1 | 1070 | A | N3-C4-N9 | 6.46 | 132.56 | 127.40 |
| 22 | 23S1 | 1900 | A | N3-C4-N9 | 6.46 | 132.57 | 127.40 |
| 22 | 23S1 | 2899 | A | N3-C4-N9 | 6.46 | 132.57 | 127.40 |
| 23 | 05S1 | 66 | A | C5-N7-C8 | 6.46 | 107.13 | 103.90 |
| 1 | 16S1 | 435 | A | C4-C5-C6 | 6.46 | 120.23 | 117.00 |
| 22 | 23S1 | 2821 | A | N3-C4-N9 | 6.46 | 132.56 | 127.40 |
| 22 | 23S1 | 1103 | A | C4-C5-C6 | 6.45 | 120.23 | 117.00 |
| 22 | 23S1 | 1328 | A | N9-C4-C5 | 6.45 | 108.38 | 105.80 |
| 22 | 23S1 | 53 | A | C8-N9-C4 | 6.45 | 108.38 | 105.80 |
| 22 | 23S1 | 735 | A | C8-N9-C4 | 6.45 | 108.38 | 105.80 |
| 22 | 23S1 | 1134 | A | N3-C4-N9 | 6.45 | 132.56 | 127.40 |
| 1 | 16S1 | 523 | A | N3-C4-N9 | 6.45 | 132.56 | 127.40 |
| 1 | 16S1 | 747 | A | N9-C4-C5 | 6.45 | 108.38 | 105.80 |
| 22 | 23S1 | 743 | A | N3-C4-N9 | 6.45 | 132.56 | 127.40 |
| 22 | 23S1 | 910 | A | N9-C4-C5 | 6.45 | 108.38 | 105.80 |
| 22 | 23S1 | 2005 | A | C8-N9-C4 | 6.45 | 108.38 | 105.80 |
| 22 | 23S1 | 1848 | A | C5-N7-C8 | 6.45 | 107.12 | 103.90 |
| 22 | 23S1 | 1901 | A | C5-N7-C8 | 6.45 | 107.12 | 103.90 |
| 22 | 23S1 | 2071 | A | N3-C4-N9 | 6.45 | 132.56 | 127.40 |
| 1 | 16S1 | 629 | A | C4-C5-C6 | 6.45 | 120.22 | 117.00 |
| 22 | 23S1 | 21 | A | N3-C4-N9 | 6.45 | 132.56 | 127.40 |
| 22 | 23S1 | 28 | A | C8-N9-C4 | 6.45 | 108.38 | 105.80 |
| 22 | 23S1 | 197 | A | C4-C5-C6 | 6.45 | 120.22 | 117.00 |
| 22 | 23S1 | 2734 | A | C8-N9-C4 | 6.45 | 108.38 | 105.80 |
| 22 | 23S1 | 1901 | A | N3-C4-N9 | 6.44 | 132.56 | 127.40 |
| 22 | 23S1 | 1970 | A | C4-C5-C6 | 6.44 | 120.22 | 117.00 |
| 1 | 16S1 | 26 | A | C5-C6-N1 | 6.44 | 120.92 | 117.70 |
| 1 | 16S1 | 196 | A | N9-C4-C5 | 6.44 | 108.38 | 105.80 |
| 1 | 16S1 | 389 | A | N9-C4-C5 | 6.44 | 108.38 | 105.80 |
| 1 | 16S1 | 559 | A | N3-C4-N9 | 6.44 | 132.55 | 127.40 |
| 1 | 16S1 | 1146 | A | C4-C5-C6 | 6.44 | 120.22 | 117.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 16S1 | 1306 | A | C4-C5-C6 | 6.44 | 120.22 | 117.00 |
| 22 | 23S1 | 299 | A | N9-C4-C5 | 6.44 | 108.38 | 105.80 |
| 22 | 23S1 | 483 | A | C8-N9-C4 | 6.44 | 108.38 | 105.80 |
| 22 | 23S1 | 1535 | A | N3-C4-N9 | 6.44 | 132.55 | 127.40 |
| 22 | 23S1 | 1773 | A | C4-C5-C6 | 6.44 | 120.22 | 117.00 |
| 22 | 23S1 | 2748 | A | C4-C5-C6 | 6.44 | 120.22 | 117.00 |
| 1 | 16S1 | 77 | A | C5-C6-N1 | 6.44 | 120.92 | 117.70 |
| 1 | 16S1 | 665 | A | N9-C4-C5 | 6.44 | 108.38 | 105.80 |
| 22 | 23S1 | 1508 | A | C5-N7-C8 | 6.44 | 107.12 | 103.90 |
| 22 | 23S1 | 1635 | A | N3-C4-N9 | 6.44 | 132.55 | 127.40 |
| 22 | 23S1 | 1717 | A | C8-N9-C4 | 6.44 | 108.38 | 105.80 |
| 1 | 16S1 | 767 | A | N3-C4-N9 | 6.44 | 132.55 | 127.40 |
| 10 | S101 | 27 | GLU | CB-CA-C | -6.43 | 97.53 | 110.40 |
| 22 | 23S1 | 661 | A | C8-N9-C4 | 6.43 | 108.37 | 105.80 |
| 22 | 23S1 | 2654 | A | N3-C4-N9 | 6.43 | 132.55 | 127.40 |
| 1 | 16S1 | 608 | A | N3-C4-N9 | 6.43 | 132.54 | 127.40 |
| 1 | 16S1 | 609 | A | N3-C4-N9 | 6.43 | 132.55 | 127.40 |
| 22 | 23S1 | 666 | A | N3-C4-N9 | 6.43 | 132.55 | 127.40 |
| 22 | 23S1 | 794 | A | C5-C6-N1 | 6.43 | 120.92 | 117.70 |
| 22 | 23S1 | 996 | A | C4-C5-C6 | 6.43 | 120.22 | 117.00 |
| 22 | 23S1 | 1373 | A | N3-C4-N9 | 6.43 | 132.55 | 127.40 |
| 22 | 23S1 | 2297 | A | C4-C5-N7 | -6.43 | 107.48 | 110.70 |
| 22 | 23S1 | 1393 | A | C5-N7-C8 | 6.43 | 107.12 | 103.90 |
| 22 | 23S1 | 1810 | A | C5-C6-N6 | 6.43 | 128.84 | 123.70 |
| 22 | 23S1 | 2378 | A | C4-C5-C6 | 6.43 | 120.22 | 117.00 |
| 1 | 16S1 | 696 | A | C5-N7-C8 | 6.43 | 107.11 | 103.90 |
| 1 | 16S1 | 1318 | A | C4-C5-C6 | 6.43 | 120.22 | 117.00 |
| 22 | 23S1 | 74 | A | N3-C4-N9 | 6.43 | 132.54 | 127.40 |
| 22 | 23S1 | 765 | C | N1-C2-O2 | 6.43 | 122.76 | 118.90 |
| 22 | 23S1 | 1027 | A | C4-C5-C6 | 6.43 | 120.21 | 117.00 |
| 22 | 23S1 | 1050 | A | C4-C5-C6 | 6.43 | 120.22 | 117.00 |
| 22 | 23S1 | 2023 | C | N1-C2-O2 | 6.43 | 122.76 | 118.90 |
| 1 | 16S1 | 19 | A | C4-C5-C6 | 6.43 | 120.21 | 117.00 |
| 22 | 23S1 | 347 | A | N3-C4-N9 | 6.43 | 132.54 | 127.40 |
| 22 | 23S1 | 996 | A | N3-C4-N9 | 6.43 | 132.54 | 127.40 |
| 22 | 23S1 | 1048 | A | C4-C5-C6 | 6.43 | 120.21 | 117.00 |
| 22 | 23S1 | 2516 | A | C8-N9-C4 | 6.43 | 108.37 | 105.80 |
| 22 | 23S1 | 2635 | A | N9-C4-C5 | 6.43 | 108.37 | 105.80 |
| 22 | 23S1 | 454 | A | N9-C4-C5 | 6.43 | 108.37 | 105.80 |
| 22 | 23S1 | 590 | A | C4-C5-C6 | 6.43 | 120.21 | 117.00 |
| 22 | 23S1 | 1085 | A | C4-C5-N7 | -6.43 | 107.49 | 110.70 |
| 22 | 23S1 | 2823 | A | N3-C4-N9 | 6.43 | 132.54 | 127.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 16S1 | 448 | A | C8-N9-C4 | 6.42 | 108.37 | 105.80 |
| 22 | 23S1 | 454 | A | C4-C5-N7 | -6.42 | 107.49 | 110.70 |
| 22 | 23S1 | 661 | A | N3-C4-N9 | 6.42 | 132.54 | 127.40 |
| 22 | 23S1 | 2097 | A | C4-C5-C6 | 6.42 | 120.21 | 117.00 |
| 22 | 23S1 | 743 | A | C4-C5-C6 | 6.42 | 120.21 | 117.00 |
| 22 | 23S1 | 2740 | A | N3-C4-N9 | 6.42 | 132.54 | 127.40 |
| 1 | 16S1 | 1102 | A | N3-C4-N9 | 6.42 | 132.54 | 127.40 |
| 1 | 16S1 | 1246 | A | N3-C4-N9 | 6.42 | 132.54 | 127.40 |
| 1 | 16S1 | 1339 | A | N3-C4-N9 | 6.42 | 132.54 | 127.40 |
| 1 | 16S1 | 1219 | A | C5-C6-N1 | 6.42 | 120.91 | 117.70 |
| 1 | 16S1 | 1349 | A | N3-C4-N9 | 6.42 | 132.53 | 127.40 |
| 22 | 23S1 | 1626 | A | N3-C4-N9 | 6.42 | 132.53 | 127.40 |
| 22 | 23S1 | 1730 | C | C5-C6-N1 | 6.42 | 124.21 | 121.00 |
| 1 | 16S1 | 1005 | A | N3-C4-N9 | 6.42 | 132.53 | 127.40 |
| 1 | 16S1 | 1044 | A | C5-C6-N1 | 6.42 | 120.91 | 117.70 |
| 1 | 16S1 | 1476 | A | N3-C4-N9 | 6.42 | 132.53 | 127.40 |
| 22 | 23S1 | 156 | A | N3-C4-N9 | 6.41 | 132.53 | 127.40 |
| 22 | 23S1 | 2634 | A | C4-C5-C6 | 6.41 | 120.21 | 117.00 |
| 22 | 23S1 | 2706 | A | C5-N7-C8 | 6.41 | 107.11 | 103.90 |
| 1 | 16S1 | 3 | A | N9-C4-C5 | 6.41 | 108.36 | 105.80 |
| 1 | 16S1 | 74 | A | N9-C4-C5 | 6.41 | 108.36 | 105.80 |
| 1 | 16S1 | 1285 | A | C8-N9-C4 | 6.41 | 108.36 | 105.80 |
| 1 | 16S1 | 1004 | A | C5-C6-N1 | 6.41 | 120.91 | 117.70 |
| 1 | 16S1 | 1176 | A | C4-C5-C6 | 6.41 | 120.20 | 117.00 |
| 22 | 23S1 | 1009 | A | N3-C4-N9 | 6.41 | 132.53 | 127.40 |
| 22 | 23S1 | 1810 | A | C6-C5-N7 | -6.41 | 127.81 | 132.30 |
| 22 | 23S1 | 2882 | A | C8-N9-C4 | 6.41 | 108.36 | 105.80 |
| 1 | 16S1 | 460 | A | C5-C6-N1 | 6.41 | 120.90 | 117.70 |
| 1 | 16S1 | 1204 | A | N9-C4-C5 | 6.41 | 108.36 | 105.80 |
| 22 | 23S1 | 1877 | A | N3-C4-N9 | 6.41 | 132.52 | 127.40 |
| 22 | 23S1 | 2052 | A | N3-C4-N9 | 6.41 | 132.53 | 127.40 |
| 22 | 23S1 | 2298 | A | C8-N9-C4 | 6.41 | 108.36 | 105.80 |
| 1 | 16S1 | 1363 | A | C5-C6-N1 | 6.40 | 120.90 | 117.70 |
| 22 | 23S1 | 693 | A | C4-C5-C6 | 6.40 | 120.20 | 117.00 |
| 22 | 23S1 | 2497 | A | C4-C5-C6 | 6.40 | 120.20 | 117.00 |
| 1 | 16S1 | 794 | A | C8-N9-C4 | 6.40 | 108.36 | 105.80 |
| 22 | 23S1 | 38 | A | N9-C4-C5 | 6.40 | 108.36 | 105.80 |
| 22 | 23S1 | 988 | A | C4-C5-C6 | 6.40 | 120.20 | 117.00 |
| 22 | 23S1 | 2031 | A | N3-C4-N9 | 6.40 | 132.52 | 127.40 |
| 22 | 23S1 | 13 | A | C4-C5-C6 | 6.40 | 120.20 | 117.00 |
| 22 | 23S1 | 1608 | A | N3-C4-N9 | 6.40 | 132.52 | 127.40 |
| 1 | 16S1 | 1227 | A | N9-C4-C5 | 6.40 | 108.36 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 616 | A | C8-N9-C4 | 6.40 | 108.36 | 105.80 |
| 1 | 16S1 | 687 | A | C8-N9-C4 | 6.40 | 108.36 | 105.80 |
| 22 | 23S1 | 947 | A | C8-N9-C4 | 6.40 | 108.36 | 105.80 |
| 22 | 23S1 | 1304 | A | C4-C5-N7 | -6.40 | 107.50 | 110.70 |
| 1 | 16S1 | 938 | A | N3-C4-N9 | 6.40 | 132.52 | 127.40 |
| 22 | 23S1 | 1490 | A | C5-C6-N1 | 6.40 | 120.90 | 117.70 |
| 22 | 23S1 | 1515 | A | C5-N7-C8 | 6.40 | 107.10 | 103.90 |
| 1 | 16S1 | 439 | U | C2-N3-C4 | -6.39 | 123.16 | 127.00 |
| 22 | 23S1 | 1919 | A | N3-C4-N9 | 6.39 | 132.52 | 127.40 |
| 22 | 23S1 | 2565 | A | C4-C5-C6 | 6.39 | 120.20 | 117.00 |
| 1 | 16S1 | 1176 | A | N3-C4-N9 | 6.39 | 132.51 | 127.40 |
| 22 | 23S1 | 272 | A | N3-C4-N9 | 6.39 | 132.51 | 127.40 |
| 22 | 23S1 | 514 | A | N3-C4-N9 | 6.39 | 132.51 | 127.40 |
| 1 | 16S1 | 53 | A | N3-C4-N9 | 6.39 | 132.51 | 127.40 |
| 1 | 16S1 | 459 | A | C5-N7-C8 | 6.39 | 107.09 | 103.90 |
| 1 | 16S1 | 546 | A | N3-C4-N9 | 6.39 | 132.51 | 127.40 |
| 1 | 16S1 | 1105 | A | C8-N9-C4 | 6.39 | 108.36 | 105.80 |
| 22 | 23S1 | 2900 | A | C4-C5-C6 | 6.39 | 120.19 | 117.00 |
| 1 | 16S1 | 1191 | A | C5-N7-C8 | 6.39 | 107.09 | 103.90 |
| 22 | 23S1 | 1359 | A | N9-C4-C5 | 6.39 | 108.36 | 105.80 |
| 22 | 23S1 | 1632 | A | N3-C4-N9 | 6.39 | 132.51 | 127.40 |
| 22 | 23S1 | 172 | A | C4-C5-C6 | 6.38 | 120.19 | 117.00 |
| 22 | 23S1 | 2108 | A | N9-C4-C5 | 6.38 | 108.35 | 105.80 |
| 22 | 23S1 | 2721 | A | N3-C4-N9 | 6.38 | 132.51 | 127.40 |
| 22 | 23S1 | 2738 | A | C5-N7-C8 | 6.38 | 107.09 | 103.90 |
| 1 | 16S1 | 1042 | A | N3-C4-N9 | 6.38 | 132.51 | 127.40 |
| 1 | 16S1 | 155 | A | C4-C5-C6 | 6.38 | 120.19 | 117.00 |
| 1 | 16S1 | 338 | A | C4-C5-C6 | 6.38 | 120.19 | 117.00 |
| 1 | 16S1 | 600 | A | N3-C4-N9 | 6.38 | 132.50 | 127.40 |
| 22 | 23S1 | 320 | A | N3-C4-N9 | 6.38 | 132.50 | 127.40 |
| 22 | 23S1 | 342 | A | C4-C5-C6 | 6.38 | 120.19 | 117.00 |
| 22 | 23S1 | 1829 | A | N3-C4-N9 | 6.38 | 132.51 | 127.40 |
| 23 | 05S1 | 78 | A | C8-N9-C4 | 6.38 | 108.35 | 105.80 |
| 1 | 16S1 | 1197 | A | N3-C4-N9 | 6.38 | 132.50 | 127.40 |
| 22 | 23S1 | 38 | A | C4-C5-C6 | 6.38 | 120.19 | 117.00 |
| 22 | 23S1 | 1144 | A | C4-C5-C6 | 6.38 | 120.19 | 117.00 |
| 1 | 16S1 | 161 | A | C5-N7-C8 | 6.38 | 107.09 | 103.90 |
| 1 | 16S1 | 179 | A | C4-C5-N7 | -6.38 | 107.51 | 110.70 |
| 1 | 16S1 | 223 | A | C4-C5-C6 | 6.38 | 120.19 | 117.00 |
| 22 | 23S1 | 538 | A | C4-C5-C6 | 6.38 | 120.19 | 117.00 |
| 22 | 23S1 | 1268 | A | N3-C4-N9 | 6.38 | 132.50 | 127.40 |
| 1 | 16S1 | 532 | A | C4-C5-C6 | 6.38 | 120.19 | 117.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 16S1 | 946 | A | N3-C4-N9 | 6.38 | 132.50 | 127.40 |
| 1 | 16S1 | 1394 | A | C4-C5-C6 | 6.37 | 120.19 | 117.00 |
| 22 | 23S1 | 505 | A | C8-N9-C4 | 6.37 | 108.35 | 105.80 |
| 22 | 23S1 | 602 | A | N3-C4-N9 | 6.37 | 132.50 | 127.40 |
| 22 | 23S1 | 1147 | A | C4-C5-N7 | -6.37 | 107.52 | 110.70 |
| 22 | 23S1 | 1762 | A | N9-C4-C5 | 6.37 | 108.35 | 105.80 |
| 22 | 23S1 | 1791 | A | C4-C5-C6 | 6.37 | 120.19 | 117.00 |
| 22 | 23S1 | 2392 | A | C5-N7-C8 | 6.37 | 107.09 | 103.90 |
| 55 | PTR1 | 9 | A | C4-C5-C6 | 6.37 | 120.19 | 117.00 |
| 22 | 23S1 | 1048 | A | N3-C4-N9 | 6.37 | 132.50 | 127.40 |
| 22 | 23S1 | 2566 | A | C4-C5-N7 | -6.37 | 107.52 | 110.70 |
| 1 | 16S1 | 373 | A | C8-N9-C4 | 6.37 | 108.35 | 105.80 |
| 1 | 16S1 | 1410 | A | C4-C5-C6 | 6.37 | 120.18 | 117.00 |
| 1 | 16S1 | 1531 | A | C4-C5-C6 | 6.37 | 120.18 | 117.00 |
| 22 | 23S1 | 1427 | A | C5-N7-C8 | 6.37 | 107.08 | 103.90 |
| 22 | 23S1 | 1829 | A | C4-C5-C6 | 6.37 | 120.18 | 117.00 |
| 22 | 23S1 | 2560 | A | C5-C6-N1 | 6.37 | 120.88 | 117.70 |
| 1 | 16S1 | 205 | A | C4-C5-C6 | 6.36 | 120.18 | 117.00 |
| 1 | 16S1 | 246 | A | C4-C5-C6 | 6.36 | 120.18 | 117.00 |
| 22 | 23S1 | 311 | A | N3-C4-N9 | 6.36 | 132.49 | 127.40 |
| 22 | 23S1 | 1735 | A | N3-C4-N9 | 6.36 | 132.49 | 127.40 |
| 1 | 16S1 | 1246 | A | C4-C5-C6 | 6.36 | 120.18 | 117.00 |
| 22 | 23S1 | 627 | A | C4-C5-C6 | 6.36 | 120.18 | 117.00 |
| 22 | 23S1 | 2346 | A | C8-N9-C4 | 6.36 | 108.34 | 105.80 |
| 22 | 23S1 | 116 | C | N1-C2-O2 | 6.36 | 122.72 | 118.90 |
| 22 | 23S1 | 282 | A | C4-C5-C6 | 6.36 | 120.18 | 117.00 |
| 22 | 23S1 | 910 | A | C4-C5-N7 | -6.36 | 107.52 | 110.70 |
| 22 | 23S1 | 936 | A | N3-C4-N9 | 6.36 | 132.49 | 127.40 |
| 1 | 16S1 | 211 | G | C5-C6-O6 | -6.36 | 124.79 | 128.60 |
| 1 | 16S1 | 648 | A | C4-C5-C6 | 6.36 | 120.18 | 117.00 |
| 1 | 16S1 | 964 | A | C5-N7-C8 | 6.36 | 107.08 | 103.90 |
| 22 | 23S1 | 1596 | A | C8-N9-C4 | 6.36 | 108.34 | 105.80 |
| 1 | 16S1 | 782 | A | C4-C5-C6 | 6.36 | 120.18 | 117.00 |
| 1 | 16S1 | 1155 | A | N3-C4-N9 | 6.36 | 132.49 | 127.40 |
| 22 | 23S1 | 219 | A | N9-C4-C5 | 6.36 | 108.34 | 105.80 |
| 22 | 23S1 | 1551 | A | N3-C4-N9 | 6.36 | 132.48 | 127.40 |
| 22 | 23S1 | 2614 | A | C4-C5-N7 | -6.36 | 107.52 | 110.70 |
| 1 | 16S1 | 78 | A | N3-C4-N9 | 6.35 | 132.48 | 127.40 |
| 1 | 16S1 | 1191 | A | N3-C4-N9 | 6.35 | 132.48 | 127.40 |
| 22 | 23S1 | 1127 | A | N3-C4-N9 | 6.35 | 132.48 | 127.40 |
| 22 | 23S1 | 1569 | A | C8-N9-C4 | 6.35 | 108.34 | 105.80 |
| 1 | 16S1 | 539 | A | N3-C4-N9 | 6.35 | 132.48 | 127.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 16S1 | 663 | A | C5-C6-N1 | 6.35 | 120.88 | 117.70 |
| 22 | 23S1 | 1103 | A | N3-C4-N9 | 6.35 | 132.48 | 127.40 |
| 22 | 23S1 | 2711 | A | C8-N9-C4 | 6.35 | 108.34 | 105.80 |
| 22 | 23S1 | 2893 | A | C4-C5-C6 | 6.35 | 120.18 | 117.00 |
| 55 | PTR1 | 20 | U | C5-C4-O4 | -6.35 | 122.09 | 125.90 |
| 1 | 16S1 | 510 | A | C4-C5-C6 | 6.35 | 120.17 | 117.00 |
| 22 | 23S1 | 1535 | A | C4-C5-C6 | 6.35 | 120.18 | 117.00 |
| 22 | 23S1 | 2205 | A | N9-C4-C5 | 6.35 | 108.34 | 105.80 |
| 22 | 23S1 | 2432 | A | C8-N9-C4 | 6.35 | 108.34 | 105.80 |
| 22 | 23S1 | 2469 | A | C5-C6-N1 | 6.35 | 120.88 | 117.70 |
| 1 | 16S1 | 199 | A | C5-C6-N1 | 6.35 | 120.88 | 117.70 |
| 1 | 16S1 | 1269 | A | N3-C4-N9 | 6.35 | 132.48 | 127.40 |
| 22 | 23S1 | 38 | A | N3-C4-N9 | 6.35 | 132.48 | 127.40 |
| 22 | 23S1 | 609 | A | C4-C5-C6 | 6.35 | 120.17 | 117.00 |
| 22 | 23S1 | 900 | A | C8-N9-C4 | 6.35 | 108.34 | 105.80 |
| 22 | 23S1 | 2054 | A | C5-C6-N1 | 6.35 | 120.88 | 117.70 |
| 22 | 23S1 | 2171 | A | C4-C5-C6 | 6.35 | 120.17 | 117.00 |
| 10 | S101 | 31 | ARG | NE-CZ-NH1 | 6.35 | 123.47 | 120.30 |
| 22 | 23S1 | 1143 | A | N3-C4-N9 | 6.35 | 132.48 | 127.40 |
| 22 | 23S1 | 1525 | A | N9-C4-C5 | 6.35 | 108.34 | 105.80 |
| 22 | 23S1 | 2726 | A | N9-C4-C5 | 6.35 | 108.34 | 105.80 |
| 23 | 05S1 | 39 | A | C8-N9-C4 | 6.35 | 108.34 | 105.80 |
| 1 | 16S1 | 151 | A | C4-C5-N7 | -6.35 | 107.53 | 110.70 |
| 1 | 16S1 | 95 | C | C2-N1-C1' | 6.34 | 125.78 | 118.80 |
| 22 | 23S1 | 2352 | A | N3-C4-N9 | 6.34 | 132.47 | 127.40 |
| 22 | 23S1 | 1265 | A | N3-C4-N9 | 6.34 | 132.47 | 127.40 |
| 22 | 23S1 | 2799 | A | C8-N9-C4 | 6.34 | 108.34 | 105.80 |
| 22 | 23S1 | 2900 | A | N3-C4-N9 | 6.34 | 132.47 | 127.40 |
| 22 | 23S1 | 282 | A | N3-C4-N9 | 6.34 | 132.47 | 127.40 |
| 22 | 23S1 | 1977 | A | C8-N9-C4 | 6.34 | 108.34 | 105.80 |
| 22 | 23S1 | 2278 | A | N3-C4-N9 | 6.34 | 132.47 | 127.40 |
| 1 | 16S1 | 59 | A | C4-C5-C6 | 6.34 | 120.17 | 117.00 |
| 23 | 05S1 | 94 | A | C4-C5-C6 | 6.34 | 120.17 | 117.00 |
| 10 | S101 | 85 | ASP | CB-CG-OD1 | 6.33 | 124.00 | 118.30 |
| 22 | 23S1 | 149 | A | C4-C5-C6 | 6.33 | 120.17 | 117.00 |
| 55 | PTR1 | 38 | A | C4-C5-C6 | 6.33 | 120.17 | 117.00 |
| 1 | 16S1 | 1000 | A | C4-C5-C6 | 6.33 | 120.17 | 117.00 |
| 22 | 23S1 | 1321 | A | C4-C5-C6 | 6.33 | 120.17 | 117.00 |
| 1 | 16S1 | 712 | A | C4-C5-C6 | 6.33 | 120.17 | 117.00 |
| 22 | 23S1 | 844 | A | N3-C4-N9 | 6.33 | 132.47 | 127.40 |
| 22 | 23S1 | 1821 | A | N9-C4-C5 | 6.33 | 108.33 | 105.80 |
| 22 | 23S1 | 430 | A | N9-C4-C5 | 6.33 | 108.33 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 2727 | A | C4-C5-C6 | 6.33 | 120.17 | 117.00 |
| 22 | 23S1 | 1789 | A | N3-C4-N9 | 6.33 | 132.46 | 127.40 |
| 22 | 23S1 | 670 | A | N3-C4-N9 | 6.33 | 132.46 | 127.40 |
| 22 | 23S1 | 1655 | A | C5-C6-N1 | 6.33 | 120.86 | 117.70 |
| 1 | 16S1 | 563 | A | C5-C6-N1 | 6.33 | 120.86 | 117.70 |
| 1 | 16S1 | 878 | A | C4-C5-C6 | 6.33 | 120.16 | 117.00 |
| 1 | 16S1 | 1032 | G | N3-C4-C5 | -6.32 | 125.44 | 128.60 |
| 22 | 23S1 | 632 | A | C4-C5-C6 | 6.32 | 120.16 | 117.00 |
| 22 | 23S1 | 764 | A | C5-N7-C8 | 6.32 | 107.06 | 103.90 |
| 22 | 23S1 | 1027 | A | N3-C4-N9 | 6.32 | 132.46 | 127.40 |
| 22 | 23S1 | 1275 | A | C8-N9-C4 | 6.32 | 108.33 | 105.80 |
| 1 | 16S1 | 792 | A | N3-C4-N9 | 6.32 | 132.46 | 127.40 |
| 22 | 23S1 | 941 | A | N3-C4-N9 | 6.32 | 132.46 | 127.40 |
| 22 | 23S1 | 1000 | A | N9-C4-C5 | 6.32 | 108.33 | 105.80 |
| 22 | 23S1 | 1918 | A | N3-C4-N9 | 6.32 | 132.46 | 127.40 |
| 22 | 23S1 | 2670 | A | N3-C4-N9 | 6.32 | 132.46 | 127.40 |
| 23 | 05S1 | 101 | A | C6-N1-C2 | -6.32 | 114.81 | 118.60 |
| 22 | 23S1 | 94 | A | N3-C4-N9 | 6.32 | 132.46 | 127.40 |
| 22 | 23S1 | 1655 | A | N3-C4-N9 | 6.32 | 132.46 | 127.40 |
| 22 | 23S1 | 1755 | A | C4-C5-N7 | -6.32 | 107.54 | 110.70 |
| 22 | 23S1 | 2531 | A | N3-C4-N9 | 6.32 | 132.46 | 127.40 |
| 1 | 16S1 | 602 | A | C5-C6-N1 | 6.32 | 120.86 | 117.70 |
| 1 | 16S1 | 815 | A | N3-C4-N9 | 6.32 | 132.45 | 127.40 |
| 22 | 23S1 | 2872 | A | C6-N1-C2 | 6.32 | 122.39 | 118.60 |
| 1 | 16S1 | 1465 | A | C5-C6-N1 | 6.32 | 120.86 | 117.70 |
| 23 | 05S1 | 15 | A | C8-N9-C4 | 6.31 | 108.33 | 105.80 |
| 1 | 16S1 | 53 | A | C4-C5-C6 | 6.31 | 120.16 | 117.00 |
| 22 | 23S1 | 471 | A | N3-C4-N9 | 6.31 | 132.45 | 127.40 |
| 22 | 23S1 | 1354 | A | N3-C4-N9 | 6.31 | 132.45 | 127.40 |
| 22 | 23S1 | 2781 | A | C4-C5-C6 | 6.31 | 120.16 | 117.00 |
| 22 | 23S1 | 1635 | A | C8-N9-C4 | 6.31 | 108.32 | 105.80 |
| 22 | 23S1 | 2037 | A | N3-C4-N9 | 6.31 | 132.45 | 127.40 |
| 1 | 16S1 | 574 | A | N9-C4-C5 | 6.31 | 108.32 | 105.80 |
| 22 | 23S1 | 160 | A | C4-C5-N7 | -6.31 | 107.55 | 110.70 |
| 22 | 23S1 | 2577 | A | N3-C4-N9 | 6.31 | 132.44 | 127.40 |
| 55 | PTR1 | 51 | A | C4-C5-N7 | -6.31 | 107.55 | 110.70 |
| 22 | 23S1 | 693 | A | C5-C6-N1 | 6.31 | 120.85 | 117.70 |
| 1 | 16S1 | 864 | A | N3-C4-N9 | 6.30 | 132.44 | 127.40 |
| 1 | 16S1 | 1350 | A | N3-C4-N9 | 6.30 | 132.44 | 127.40 |
| 22 | 23S1 | 176 | A | C5-C6-N1 | 6.30 | 120.85 | 117.70 |
| 22 | 23S1 | 256 | A | N3-C4-N9 | 6.30 | 132.44 | 127.40 |
| 22 | 23S1 | 1020 | A | C6-N1-C2 | 6.30 | 122.38 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 1791 | A | C5-N7-C8 | 6.30 | 107.05 | 103.90 |
| 1 | 16S1 | 959 | A | N3-C4-N9 | 6.30 | 132.44 | 127.40 |
| 22 | 23S1 | 1978 | A | C4-C5-C6 | 6.30 | 120.15 | 117.00 |
| 22 | 23S1 | 2142 | A | C4-C5-C6 | 6.30 | 120.15 | 117.00 |
| 22 | 23S1 | 2531 | A | C4-C5-C6 | 6.30 | 120.15 | 117.00 |
| 22 | 23S1 | 548 | G | C4-N9-C1' | 6.30 | 134.69 | 126.50 |
| 22 | 23S1 | 1470 | A | C4-C5-C6 | 6.30 | 120.15 | 117.00 |
| 22 | 23S1 | 1551 | A | C5-C6-N1 | 6.30 | 120.85 | 117.70 |
| 22 | 23S1 | 1931 | U | N1-C2-O2 | 6.30 | 127.21 | 122.80 |
| 22 | 23S1 | 2281 | A | C4-C5-C6 | 6.30 | 120.15 | 117.00 |
| 1 | 16S1 | 26 | A | N3-C4-N9 | 6.30 | 132.44 | 127.40 |
| 1 | 16S1 | 583 | A | C5-C6-N1 | 6.30 | 120.85 | 117.70 |
| 22 | 23S1 | 2126 | A | N3-C4-N9 | 6.30 | 132.44 | 127.40 |
| 22 | 23S1 | 449 | A | C4-C5-C6 | 6.30 | 120.15 | 117.00 |
| 22 | 23S1 | 1057 | A | C8-N9-C4 | 6.30 | 108.32 | 105.80 |
| 22 | 23S1 | 2158 | A | C8-N9-C4 | 6.30 | 108.32 | 105.80 |
| 22 | 23S1 | 2577 | A | C4-C5-N7 | -6.30 | 107.55 | 110.70 |
| 22 | 23S1 | 12 | U | C6-N1-C2 | -6.30 | 117.22 | 121.00 |
| 22 | 23S1 | 233 | A | C4-C5-C6 | 6.30 | 120.15 | 117.00 |
| 22 | 23S1 | 2267 | A | C4-C5-C6 | 6.30 | 120.15 | 117.00 |
| 1 | 16S1 | 236 | A | C4-C5-C6 | 6.29 | 120.15 | 117.00 |
| 22 | 23S1 | 2014 | A | C4-C5-C6 | 6.29 | 120.15 | 117.00 |
| 1 | 16S1 | 1271 | A | N3-C4-N9 | 6.29 | 132.44 | 127.40 |
| 22 | 23S1 | 503 | A | C5-C6-N1 | 6.29 | 120.85 | 117.70 |
| 22 | 23S1 | 915 | C | C6-N1-C2 | -6.29 | 117.78 | 120.30 |
| 1 | 16S1 | 1236 | A | C8-N9-C4 | 6.29 | 108.32 | 105.80 |
| 22 | 23S1 | 2042 | A | C8-N9-C4 | 6.29 | 108.32 | 105.80 |
| 22 | 23S1 | 2170 | A | C4-C5-C6 | 6.29 | 120.15 | 117.00 |
| 1 | 16S1 | 747 | A | C4-C5-C6 | 6.29 | 120.14 | 117.00 |
| 1 | 16S1 | 1256 | A | C4-C5-C6 | 6.29 | 120.14 | 117.00 |
| 22 | 23S1 | 207 | A | C8-N9-C4 | 6.29 | 108.32 | 105.80 |
| 22 | 23S1 | 1889 | A | N3-C4-N9 | 6.29 | 132.43 | 127.40 |
| 23 | 05S1 | 52 | A | C8-N9-C4 | 6.29 | 108.32 | 105.80 |
| 22 | 23S1 | 670 | A | C4-C5-C6 | 6.29 | 120.14 | 117.00 |
| 22 | 23S1 | 1953 | A | N3-C4-N9 | 6.29 | 132.43 | 127.40 |
| 22 | 23S1 | 2572 | A | C4-C5-N7 | -6.29 | 107.56 | 110.70 |
| 22 | 23S1 | 2095 | A | N9-C4-C5 | 6.29 | 108.31 | 105.80 |
| 22 | 23S1 | 2468 | A | C8-N9-C4 | 6.29 | 108.31 | 105.80 |
| 22 | 23S1 | 2513 | A | N9-C4-C5 | 6.29 | 108.31 | 105.80 |
| 22 | 23S1 | 94 | A | C8-N9-C4 | 6.28 | 108.31 | 105.80 |
| 22 | 23S1 | 471 | A | C8-N9-C4 | 6.28 | 108.31 | 105.80 |
| 22 | 23S1 | 1032 | A | C5-C6-N1 | 6.28 | 120.84 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|------|-------------|----------|
| 22 | 23S1 | 1365 | A | C4-C5-C6 | 6.28 | 120.14 | 117.00 |
| 1 | 16S1 | 211 | G | N3-C4-N9 | 6.28 | 129.77 | 126.00 |
| 22 | 23S1 | 1876 | A | C4-C5-C6 | 6.28 | 120.14 | 117.00 |
| 1 | 16S1 | 673 | A | C5-C6-N1 | 6.28 | 120.84 | 117.70 |
| 1 | 16S1 | 923 | A | C5-N7-C8 | 6.28 | 107.04 | 103.90 |
| 22 | 23S1 | 64 | A | N3-C4-N9 | 6.28 | 132.42 | 127.40 |
| 22 | 23S1 | 793 | A | N3-C4-N9 | 6.28 | 132.43 | 127.40 |
| 22 | 23S1 | 833 | A | C5-N7-C8 | 6.28 | 107.04 | 103.90 |
| 22 | 23S1 | 2062 | A | C4-C5-C6 | 6.28 | 120.14 | 117.00 |
| 1 | 16S1 | 1239 | A | N9-C4-C5 | 6.28 | 108.31 | 105.80 |
| 22 | 23S1 | 1057 | A | N3-C4-N9 | 6.28 | 132.42 | 127.40 |
| 1 | 16S1 | 815 | A | C4-C5-C6 | 6.28 | 120.14 | 117.00 |
| 22 | 23S1 | 155 | A | C4-C5-C6 | 6.28 | 120.14 | 117.00 |
| 22 | 23S1 | 480 | A | N3-C4-N9 | 6.28 | 132.42 | 127.40 |
| 22 | 23S1 | 1014 | A | C8-N9-C4 | 6.28 | 108.31 | 105.80 |
| 22 | 23S1 | 2189 | U | P-O3'-C3' | 6.28 | 127.23 | 119.70 |
| 22 | 23S1 | 2278 | A | C4-C5-C6 | 6.28 | 120.14 | 117.00 |
| 22 | 23S1 | 2335 | A | N3-C4-N9 | 6.28 | 132.42 | 127.40 |
| 22 | 23S1 | 2886 | A | N3-C4-N9 | 6.28 | 132.42 | 127.40 |
| 22 | 23S1 | 111 | A | C8-N9-C4 | 6.28 | 108.31 | 105.80 |
| 22 | 23S1 | 218 | A | N3-C4-N9 | 6.28 | 132.42 | 127.40 |
| 22 | 23S1 | 244 | A | C4-C5-C6 | 6.28 | 120.14 | 117.00 |
| 22 | 23S1 | 279 | A | C4-C5-C6 | 6.28 | 120.14 | 117.00 |
| 22 | 23S1 | 1762 | A | C4-C5-C6 | 6.28 | 120.14 | 117.00 |
| 22 | 23S1 | 1977 | A | N3-C4-N9 | 6.28 | 132.42 | 127.40 |
| 22 | 23S1 | 2298 | A | C4-C5-C6 | 6.28 | 120.14 | 117.00 |
| 23 | 05S1 | 119 | A | C4-C5-C6 | 6.28 | 120.14 | 117.00 |
| 22 | 23S1 | 2114 | A | C5-C6-N1 | 6.27 | 120.84 | 117.70 |
| 1 | 16S1 | 10 | A | N3-C4-N9 | 6.27 | 132.42 | 127.40 |
| 22 | 23S1 | 56 | A | C4-C5-C6 | 6.27 | 120.14 | 117.00 |
| 22 | 23S1 | 231 | A | C4-C5-C6 | 6.27 | 120.14 | 117.00 |
| 22 | 23S1 | 753 | A | C4-C5-C6 | 6.27 | 120.14 | 117.00 |
| 22 | 23S1 | 1552 | A | N3-C4-N9 | 6.27 | 132.42 | 127.40 |
| 22 | 23S1 | 2471 | A | N9-C4-C5 | 6.27 | 108.31 | 105.80 |
| 23 | 05S1 | 34 | A | C4-C5-C6 | 6.27 | 120.14 | 117.00 |
| 1 | 16S1 | 1396 | A | C4-C5-C6 | 6.27 | 120.14 | 117.00 |
| 22 | 23S1 | 988 | A | N3-C4-N9 | 6.27 | 132.42 | 127.40 |
| 1 | 16S1 | 729 | A | N3-C4-N9 | 6.27 | 132.42 | 127.40 |
| 22 | 23S1 | 152 | A | C8-N9-C4 | 6.27 | 108.31 | 105.80 |
| 22 | 23S1 | 299 | A | N3-C4-N9 | 6.27 | 132.41 | 127.40 |
| 22 | 23S1 | 909 | A | C5-C6-N1 | 6.27 | 120.83 | 117.70 |
| 22 | 23S1 | 1096 | A | C4-C5-C6 | 6.27 | 120.13 | 117.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 2311 | A | C4-C5-N7 | -6.27 | 107.57 | 110.70 |
| 22 | 23S1 | 2711 | A | N3-C4-N9 | 6.27 | 132.41 | 127.40 |
| 1 | 16S1 | 1394 | A | C8-N9-C4 | 6.27 | 108.31 | 105.80 |
| 22 | 23S1 | 19 | A | C4-C5-C6 | 6.26 | 120.13 | 117.00 |
| 22 | 23S1 | 38 | A | C4-C5-N7 | -6.26 | 107.57 | 110.70 |
| 22 | 23S1 | 207 | A | N3-C4-N9 | 6.26 | 132.41 | 127.40 |
| 22 | 23S1 | 1089 | A | N3-C4-N9 | 6.26 | 132.41 | 127.40 |
| 22 | 23S1 | 1532 | A | C8-N9-C4 | 6.26 | 108.31 | 105.80 |
| 22 | 23S1 | 1998 | A | C4-C5-N7 | -6.26 | 107.57 | 110.70 |
| 22 | 23S1 | 344 | A | N3-C4-N9 | 6.26 | 132.41 | 127.40 |
| 22 | 23S1 | 1014 | A | N3-C4-N9 | 6.26 | 132.41 | 127.40 |
| 22 | 23S1 | 1495 | A | N9-C4-C5 | 6.26 | 108.31 | 105.80 |
| 22 | 23S1 | 1655 | A | C8-N9-C4 | 6.26 | 108.31 | 105.80 |
| 23 | 05S1 | 66 | A | C4-C5-C6 | 6.26 | 120.13 | 117.00 |
| 22 | 23S1 | 64 | A | C4-C5-C6 | 6.26 | 120.13 | 117.00 |
| 22 | 23S1 | 2297 | A | N9-C4-C5 | 6.26 | 108.30 | 105.80 |
| 1 | 16S1 | 1437 | A | C8-N9-C4 | 6.26 | 108.30 | 105.80 |
| 22 | 23S1 | 1028 | A | C8-N9-C4 | 6.26 | 108.30 | 105.80 |
| 22 | 23S1 | 1762 | A | N3-C4-N9 | 6.26 | 132.41 | 127.40 |
| 22 | 23S1 | 2660 | A | N3-C4-N9 | 6.26 | 132.41 | 127.40 |
| 1 | 16S1 | 819 | A | C4-C5-C6 | 6.25 | 120.13 | 117.00 |
| 1 | 16S1 | 1225 | A | C4-C5-C6 | 6.25 | 120.13 | 117.00 |
| 22 | 23S1 | 2134 | A | N3-C4-N9 | 6.25 | 132.40 | 127.40 |
| 22 | 23S1 | 2298 | A | N3-C4-N9 | 6.25 | 132.40 | 127.40 |
| 1 | 16S1 | 179 | A | N9-C4-C5 | 6.25 | 108.30 | 105.80 |
| 22 | 23S1 | 979 | A | C8-N9-C4 | 6.25 | 108.30 | 105.80 |
| 22 | 23S1 | 1322 | A | C8-N9-C4 | 6.25 | 108.30 | 105.80 |
| 22 | 23S1 | 2516 | A | N3-C4-N9 | 6.25 | 132.40 | 127.40 |
| 55 | PTR1 | 58 | A | N9-C4-C5 | 6.25 | 108.30 | 105.80 |
| 1 | 16S1 | 974 | A | N3-C4-N9 | 6.25 | 132.40 | 127.40 |
| 22 | 23S1 | 1829 | A | C4-C5-N7 | -6.25 | 107.57 | 110.70 |
| 22 | 23S1 | 2274 | A | C5-N7-C8 | 6.25 | 107.03 | 103.90 |
| 55 | PTR1 | 42 | A | N3-C4-N9 | 6.25 | 132.40 | 127.40 |
| 1 | 16S1 | 1012 | A | C4-C5-C6 | 6.25 | 120.12 | 117.00 |
| 22 | 23S1 | 586 | A | C4-C5-C6 | 6.25 | 120.12 | 117.00 |
| 22 | 23S1 | 1745 | A | C5-N7-C8 | 6.25 | 107.03 | 103.90 |
| 22 | 23S1 | 1226 | A | C5-N7-C8 | 6.25 | 107.02 | 103.90 |
| 22 | 23S1 | 1713 | A | N3-C4-N9 | 6.25 | 132.40 | 127.40 |
| 22 | 23S1 | 2433 | A | N3-C4-N9 | 6.25 | 132.40 | 127.40 |
| 22 | 23S1 | 2530 | A | C8-N9-C4 | 6.25 | 108.30 | 105.80 |
| 1 | 16S1 | 493 | A | C5-N7-C8 | 6.25 | 107.02 | 103.90 |
| 1 | 16S1 | 1105 | A | C4-C5-C6 | 6.25 | 120.12 | 117.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 16S1 | 1513 | A | N3-C4-N9 | 6.25 | 132.40 | 127.40 |
| 22 | 23S1 | 472 | A | C4-C5-C6 | 6.25 | 120.12 | 117.00 |
| 23 | 05S1 | 30 | C | C6-N1-C2 | -6.25 | 117.80 | 120.30 |
| 22 | 23S1 | 2778 | A | C4-C5-C6 | 6.24 | 120.12 | 117.00 |
| 1 | 16S1 | 935 | A | N3-C4-N9 | 6.24 | 132.39 | 127.40 |
| 22 | 23S1 | 513 | A | C5-N7-C8 | 6.24 | 107.02 | 103.90 |
| 22 | 23S1 | 324 | A | C4-C5-C6 | 6.24 | 120.12 | 117.00 |
| 22 | 23S1 | 2750 | A | C8-N9-C4 | 6.24 | 108.30 | 105.80 |
| 1 | 16S1 | 1012 | A | N3-C4-N9 | 6.24 | 132.39 | 127.40 |
| 22 | 23S1 | 340 | A | N3-C4-N9 | 6.24 | 132.39 | 127.40 |
| 22 | 23S1 | 422 | A | C5-C6-N1 | 6.24 | 120.82 | 117.70 |
| 22 | 23S1 | 2426 | A | C4-C5-C6 | 6.24 | 120.12 | 117.00 |
| 1 | 16S1 | 609 | A | C4-C5-C6 | 6.24 | 120.12 | 117.00 |
| 22 | 23S1 | 911 | A | N3-C4-N9 | 6.24 | 132.39 | 127.40 |
| 22 | 23S1 | 2015 | A | N3-C4-N9 | 6.24 | 132.39 | 127.40 |
| 1 | 16S1 | 718 | A | C4-C5-C6 | 6.24 | 120.12 | 117.00 |
| 1 | 16S1 | 1374 | A | C4-C5-C6 | 6.24 | 120.12 | 117.00 |
| 22 | 23S1 | 382 | A | N9-C4-C5 | 6.24 | 108.29 | 105.80 |
| 22 | 23S1 | 1269 | A | N3-C4-N9 | 6.24 | 132.39 | 127.40 |
| 22 | 23S1 | 354 | A | C8-N9-C4 | 6.23 | 108.29 | 105.80 |
| 22 | 23S1 | 861 | A | C4-C5-C6 | 6.23 | 120.12 | 117.00 |
| 22 | 23S1 | 1244 | A | C8-N9-C4 | 6.23 | 108.29 | 105.80 |
| 1 | 16S1 | 440 | C | N1-C2-O2 | 6.23 | 122.64 | 118.90 |
| 1 | 16S1 | 533 | A | C4-C5-N7 | -6.23 | 107.58 | 110.70 |
| 1 | 16S1 | 621 | A | C5-C6-N1 | 6.23 | 120.82 | 117.70 |
| 22 | 23S1 | 802 | A | N3-C4-N9 | 6.23 | 132.39 | 127.40 |
| 22 | 23S1 | 1133 | A | C4-C5-C6 | 6.23 | 120.12 | 117.00 |
| 22 | 23S1 | 1314 | C | N3-C2-O2 | -6.23 | 117.54 | 121.90 |
| 22 | 23S1 | 1665 | A | C5-C6-N1 | 6.23 | 120.82 | 117.70 |
| 22 | 23S1 | 2346 | A | N3-C4-N9 | 6.23 | 132.39 | 127.40 |
| 22 | 23S1 | 689 | A | N9-C4-C5 | 6.23 | 108.29 | 105.80 |
| 22 | 23S1 | 804 | A | C4-C5-N7 | -6.23 | 107.58 | 110.70 |
| 22 | 23S1 | 2376 | A | N3-C4-N9 | 6.23 | 132.38 | 127.40 |
| 22 | 23S1 | 2513 | A | N3-C4-N9 | 6.23 | 132.38 | 127.40 |
| 1 | 16S1 | 573 | A | C4-C5-C6 | 6.23 | 120.11 | 117.00 |
| 22 | 23S1 | 382 | A | C5-C6-N1 | 6.23 | 120.81 | 117.70 |
| 1 | 16S1 | 749 | A | C8-N9-C4 | 6.23 | 108.29 | 105.80 |
| 1 | 16S1 | 900 | A | C5-C6-N1 | 6.23 | 120.81 | 117.70 |
| 22 | 23S1 | 1244 | A | C4-C5-C6 | 6.23 | 120.11 | 117.00 |
| 22 | 23S1 | 1936 | A | C5-N7-C8 | 6.23 | 107.01 | 103.90 |
| 1 | 16S1 | 1507 | A | C4-C5-C6 | 6.23 | 120.11 | 117.00 |
| 22 | 23S1 | 844 | A | C4-C5-C6 | 6.23 | 120.11 | 117.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 1378 | A | N9-C4-C5 | 6.23 | 108.29 | 105.80 |
| 1 | 16S1 | 753 | A | N3-C4-N9 | 6.22 | 132.38 | 127.40 |
| 1 | 16S1 | 1000 | A | C5-C6-N1 | 6.22 | 120.81 | 117.70 |
| 22 | 23S1 | 644 | A | C4-C5-N7 | -6.22 | 107.59 | 110.70 |
| 22 | 23S1 | 920 | A | C8-N9-C4 | 6.22 | 108.29 | 105.80 |
| 22 | 23S1 | 1169 | A | C4-C5-C6 | 6.22 | 120.11 | 117.00 |
| 22 | 23S1 | 1630 | A | C8-N9-C4 | 6.22 | 108.29 | 105.80 |
| 22 | 23S1 | 1652 | A | N9-C4-C5 | 6.22 | 108.29 | 105.80 |
| 22 | 23S1 | 2288 | A | C8-N9-C4 | 6.22 | 108.29 | 105.80 |
| 22 | 23S1 | 2600 | A | N3-C4-N9 | 6.22 | 132.38 | 127.40 |
| 1 | 16S1 | 439 | U | C2-N1-C1' | 6.22 | 125.17 | 117.70 |
| 22 | 23S1 | 693 | A | C8-N9-C4 | 6.22 | 108.29 | 105.80 |
| 22 | 23S1 | 2327 | A | C4-C5-C6 | 6.22 | 120.11 | 117.00 |
| 22 | 23S1 | 2354 | C | N1-C2-O2 | 6.22 | 122.63 | 118.90 |
| 22 | 23S1 | 2447 | G | C5-C6-N1 | 6.22 | 114.61 | 111.50 |
| 1 | 16S1 | 1172 | C | C2-N1-C1' | 6.22 | 125.64 | 118.80 |
| 22 | 23S1 | 582 | A | C5-C6-N1 | 6.22 | 120.81 | 117.70 |
| 1 | 16S1 | 152 | A | C5-C6-N1 | 6.22 | 120.81 | 117.70 |
| 1 | 16S1 | 794 | A | C4-C5-C6 | 6.22 | 120.11 | 117.00 |
| 1 | 16S1 | 974 | A | C4-C5-C6 | 6.22 | 120.11 | 117.00 |
| 22 | 23S1 | 89 | A | C8-N9-C4 | 6.22 | 108.29 | 105.80 |
| 22 | 23S1 | 2163 | A | N3-C4-N9 | 6.22 | 132.38 | 127.40 |
| 22 | 23S1 | 2753 | A | N9-C4-C5 | 6.22 | 108.29 | 105.80 |
| 1 | 16S1 | 32 | A | C8-N9-C4 | 6.22 | 108.29 | 105.80 |
| 1 | 16S1 | 489 | C | C6-N1-C1' | -6.22 | 113.34 | 120.80 |
| 22 | 23S1 | 44 | A | N3-C4-N9 | 6.22 | 132.37 | 127.40 |
| 22 | 23S1 | 602 | A | C8-N9-C4 | 6.22 | 108.29 | 105.80 |
| 22 | 23S1 | 761 | A | C5-C6-N1 | 6.22 | 120.81 | 117.70 |
| 22 | 23S1 | 866 | A | C8-N9-C4 | 6.22 | 108.29 | 105.80 |
| 22 | 23S1 | 1247 | A | N3-C4-N9 | 6.22 | 132.37 | 127.40 |
| 22 | 23S1 | 1603 | A | C4-C5-C6 | 6.22 | 120.11 | 117.00 |
| 22 | 23S1 | 1745 | A | N3-C4-N9 | 6.22 | 132.37 | 127.40 |
| 23 | 05S1 | 75 | G | C5-C6-N1 | 6.22 | 114.61 | 111.50 |
| 1 | 16S1 | 196 | A | C5-N7-C8 | 6.21 | 107.01 | 103.90 |
| 22 | 23S1 | 311 | A | C4-C5-C6 | 6.21 | 120.11 | 117.00 |
| 22 | 23S1 | 1084 | A | N3-C4-N9 | 6.21 | 132.37 | 127.40 |
| 22 | 23S1 | 1392 | A | C4-C5-C6 | 6.21 | 120.11 | 117.00 |
| 23 | 05S1 | 119 | A | C8-N9-C4 | 6.21 | 108.28 | 105.80 |
| 1 | 16S1 | 33 | A | C8-N9-C4 | 6.21 | 108.28 | 105.80 |
| 1 | 16S1 | 298 | A | C8-N9-C4 | 6.21 | 108.28 | 105.80 |
| 1 | 16S1 | 1332 | A | N3-C4-N9 | 6.21 | 132.37 | 127.40 |
| 22 | 23S1 | 309 | A | C4-C5-C6 | 6.21 | 120.11 | 117.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 346 | A | N3-C4-N9 | 6.21 | 132.37 | 127.40 |
| 1 | 16S1 | 1410 | A | N3-C4-N9 | 6.21 | 132.37 | 127.40 |
| 22 | 23S1 | 83 | A | N3-C4-N9 | 6.21 | 132.37 | 127.40 |
| 22 | 23S1 | 332 | A | C8-N9-C4 | 6.21 | 108.28 | 105.80 |
| 22 | 23S1 | 2111 | U | N3-C2-O2 | -6.21 | 117.85 | 122.20 |
| 22 | 23S1 | 2850 | A | C4-C5-C6 | 6.21 | 120.11 | 117.00 |
| 22 | 23S1 | 21 | A | C5-C6-N1 | 6.21 | 120.80 | 117.70 |
| 22 | 23S1 | 1230 | A | C4-C5-C6 | 6.21 | 120.11 | 117.00 |
| 22 | 23S1 | 2095 | A | C8-N9-C4 | 6.21 | 108.28 | 105.80 |
| 1 | 16S1 | 1275 | A | C4-C5-C6 | 6.21 | 120.10 | 117.00 |
| 1 | 16S1 | 1350 | A | N9-C4-C5 | 6.21 | 108.28 | 105.80 |
| 1 | 16S1 | 155 | A | C5-C6-N1 | 6.21 | 120.80 | 117.70 |
| 22 | 23S1 | 1147 | A | C5-C6-N1 | 6.21 | 120.80 | 117.70 |
| 22 | 23S1 | 2100 | G | N3-C4-N9 | 6.21 | 129.72 | 126.00 |
| 22 | 23S1 | 2705 | A | C4-C5-C6 | 6.21 | 120.10 | 117.00 |
| 1 | 16S1 | 189 | A | N3-C4-N9 | 6.20 | 132.36 | 127.40 |
| 1 | 16S1 | 465 | A | C4-C5-C6 | 6.20 | 120.10 | 117.00 |
| 22 | 23S1 | 975 | A | C8-N9-C4 | 6.20 | 108.28 | 105.80 |
| 22 | 23S1 | 1204 | A | C5-C6-N1 | 6.20 | 120.80 | 117.70 |
| 55 | PTR1 | 3 | A | C4-C5-C6 | 6.20 | 120.10 | 117.00 |
| 1 | 16S1 | 694 | A | C8-N9-C4 | 6.20 | 108.28 | 105.80 |
| 22 | 23S1 | 1085 | A | N9-C4-C5 | 6.20 | 108.28 | 105.80 |
| 22 | 23S1 | 2327 | A | N3-C4-N9 | 6.20 | 132.36 | 127.40 |
| 1 | 16S1 | 482 | A | C4-C5-C6 | 6.20 | 120.10 | 117.00 |
| 1 | 16S1 | 914 | A | C6-N1-C2 | 6.20 | 122.32 | 118.60 |
| 1 | 16S1 | 975 | A | C5-N7-C8 | 6.20 | 107.00 | 103.90 |
| 22 | 23S1 | 362 | A | C5-C6-N1 | 6.20 | 120.80 | 117.70 |
| 22 | 23S1 | 599 | A | N3-C4-N9 | 6.20 | 132.36 | 127.40 |
| 22 | 23S1 | 1268 | A | C4-C5-C6 | 6.20 | 120.10 | 117.00 |
| 22 | 23S1 | 1854 | A | C5-N7-C8 | 6.20 | 107.00 | 103.90 |
| 22 | 23S1 | 2042 | A | N3-C4-N9 | 6.20 | 132.36 | 127.40 |
| 1 | 16S1 | 71 | A | N3-C4-N9 | 6.20 | 132.36 | 127.40 |
| 1 | 16S1 | 784 | A | C5-C6-N1 | 6.20 | 120.80 | 117.70 |
| 22 | 23S1 | 53 | A | C5-C6-N1 | 6.20 | 120.80 | 117.70 |
| 22 | 23S1 | 574 | A | N3-C4-N9 | 6.20 | 132.36 | 127.40 |
| 22 | 23S1 | 1626 | A | C8-N9-C4 | 6.20 | 108.28 | 105.80 |
| 1 | 16S1 | 192 | A | N3-C4-N9 | 6.20 | 132.36 | 127.40 |
| 1 | 16S1 | 665 | A | C5-N7-C8 | 6.20 | 107.00 | 103.90 |
| 22 | 23S1 | 63 | A | C8-N9-C4 | 6.20 | 108.28 | 105.80 |
| 22 | 23S1 | 899 | A | C4-C5-C6 | 6.20 | 120.10 | 117.00 |
| 22 | 23S1 | 2646 | C | C5-C6-N1 | 6.20 | 124.10 | 121.00 |
| 22 | 23S1 | 685 | A | N3-C4-N9 | 6.20 | 132.36 | 127.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 2725 | A | C5-C6-N1 | 6.20 | 120.80 | 117.70 |
| 22 | 23S1 | 756 | A | N3-C4-N9 | 6.19 | 132.35 | 127.40 |
| 22 | 23S1 | 2534 | A | C4-C5-C6 | 6.19 | 120.10 | 117.00 |
| 22 | 23S1 | 2721 | A | C8-N9-C4 | 6.19 | 108.28 | 105.80 |
| 1 | 16S1 | 169 | C | C5-C4-N4 | 6.19 | 124.53 | 120.20 |
| 1 | 16S1 | 784 | A | N3-C4-N9 | 6.19 | 132.35 | 127.40 |
| 1 | 16S1 | 1016 | A | C8-N9-C4 | 6.19 | 108.28 | 105.80 |
| 22 | 23S1 | 1020 | A | N3-C4-C5 | -6.19 | 122.47 | 126.80 |
| 22 | 23S1 | 1090 | A | N9-C4-C5 | 6.19 | 108.28 | 105.80 |
| 22 | 23S1 | 1745 | A | C4-C5-C6 | 6.19 | 120.10 | 117.00 |
| 22 | 23S1 | 1757 | A | N3-C4-N9 | 6.19 | 132.35 | 127.40 |
| 22 | 23S1 | 1889 | A | C4-C5-C6 | 6.19 | 120.10 | 117.00 |
| 1 | 16S1 | 1229 | A | C5-C6-N1 | 6.19 | 120.80 | 117.70 |
| 22 | 23S1 | 980 | A | C5-C6-N1 | 6.19 | 120.80 | 117.70 |
| 22 | 23S1 | 1274 | A | N9-C4-C5 | 6.19 | 108.28 | 105.80 |
| 22 | 23S1 | 1809 | A | N9-C4-C5 | 6.19 | 108.28 | 105.80 |
| 22 | 23S1 | 2333 | A | N3-C4-N9 | 6.19 | 132.35 | 127.40 |
| 22 | 23S1 | 2654 | A | C4-C5-C6 | 6.19 | 120.09 | 117.00 |
| 1 | 16S1 | 1238 | A | N9-C4-C5 | 6.19 | 108.28 | 105.80 |
| 22 | 23S1 | 505 | A | N3-C4-N9 | 6.19 | 132.35 | 127.40 |
| 22 | 23S1 | 1327 | A | N3-C4-N9 | 6.19 | 132.35 | 127.40 |
| 22 | 23S1 | 1566 | A | C8-N9-C4 | 6.19 | 108.28 | 105.80 |
| 1 | 16S1 | 935 | A | C5-C6-N1 | 6.19 | 120.79 | 117.70 |
| 22 | 23S1 | 213 | A | C4-C5-C6 | 6.19 | 120.09 | 117.00 |
| 22 | 23S1 | 1847 | A | C5-N7-C8 | 6.19 | 106.99 | 103.90 |
| 22 | 23S1 | 222 | A | N3-C4-N9 | 6.19 | 132.35 | 127.40 |
| 1 | 16S1 | 781 | A | N3-C4-N9 | 6.18 | 132.35 | 127.40 |
| 1 | 16S1 | 1446 | A | C4-C5-C6 | 6.18 | 120.09 | 117.00 |
| 22 | 23S1 | 1899 | A | N3-C4-N9 | 6.18 | 132.35 | 127.40 |
| 22 | 23S1 | 2267 | A | C5-C6-N1 | 6.18 | 120.79 | 117.70 |
| 23 | 05S1 | 29 | A | N3-C4-N9 | 6.18 | 132.35 | 127.40 |
| 1 | 16S1 | 1396 | A | C5-C6-N1 | 6.18 | 120.79 | 117.70 |
| 22 | 23S1 | 449 | A | C4-C5-N7 | -6.18 | 107.61 | 110.70 |
| 22 | 23S1 | 1634 | A | N9-C4-C5 | 6.18 | 108.27 | 105.80 |
| 22 | 23S1 | 1885 | A | N3-C4-N9 | 6.18 | 132.35 | 127.40 |
| 22 | 23S1 | 2412 | A | N3-C4-N9 | 6.18 | 132.35 | 127.40 |
| 22 | 23S1 | 2721 | A | C4-C5-C6 | 6.18 | 120.09 | 117.00 |
| 54 | MRN1 | 1 | G | N3-C2-N2 | -6.18 | 115.57 | 119.90 |
| 1 | 16S1 | 1492 | A | N3-C4-N9 | 6.18 | 132.34 | 127.40 |
| 22 | 23S1 | 877 | A | N9-C4-C5 | 6.18 | 108.27 | 105.80 |
| 23 | 05S1 | 52 | A | C4-C5-C6 | 6.18 | 120.09 | 117.00 |
| 22 | 23S1 | 2134 | A | C4-C5-C6 | 6.18 | 120.09 | 117.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 2530 | A | N3-C4-N9 | 6.18 | 132.34 | 127.40 |
| 1 | 16S1 | 1394 | A | N3-C4-N9 | 6.18 | 132.34 | 127.40 |
| 22 | 23S1 | 2726 | A | C4-C5-N7 | -6.18 | 107.61 | 110.70 |
| 22 | 23S1 | 203 | A | C4-C5-C6 | 6.17 | 120.09 | 117.00 |
| 22 | 23S1 | 460 | A | C4-C5-C6 | 6.17 | 120.09 | 117.00 |
| 22 | 23S1 | 2225 | A | C4-C5-C6 | 6.17 | 120.09 | 117.00 |
| 22 | 23S1 | 2407 | A | C5-C6-N1 | 6.17 | 120.79 | 117.70 |
| 22 | 23S1 | 382 | A | N3-C4-N9 | 6.17 | 132.34 | 127.40 |
| 22 | 23S1 | 1641 | A | N3-C4-N9 | 6.17 | 132.34 | 127.40 |
| 22 | 23S1 | 2654 | A | C8-N9-C4 | 6.17 | 108.27 | 105.80 |
| 1 | 16S1 | 819 | A | N3-C4-N9 | 6.17 | 132.34 | 127.40 |
| 1 | 16S1 | 1158 | C | C6-N1-C1' | -6.17 | 113.39 | 120.80 |
| 22 | 23S1 | 721 | A | C8-N9-C4 | 6.17 | 108.27 | 105.80 |
| 22 | 23S1 | 2468 | A | N3-C4-N9 | 6.17 | 132.34 | 127.40 |
| 22 | 23S1 | 2541 | A | N3-C4-N9 | 6.17 | 132.34 | 127.40 |
| 22 | 23S1 | 2665 | A | C4-C5-C6 | 6.17 | 120.09 | 117.00 |
| 55 | PTR1 | 38 | A | C5-C6-N1 | 6.17 | 120.78 | 117.70 |
| 1 | 16S1 | 1014 | A | N3-C4-N9 | 6.17 | 132.34 | 127.40 |
| 22 | 23S1 | 144 | A | C5-C6-N1 | 6.17 | 120.78 | 117.70 |
| 22 | 23S1 | 300 | A | C4-C5-C6 | 6.17 | 120.08 | 117.00 |
| 1 | 16S1 | 139 | A | C8-N9-C4 | 6.17 | 108.27 | 105.80 |
| 1 | 16S1 | 454 | G | N3-C2-N2 | 6.17 | 124.22 | 119.90 |
| 1 | 16S1 | 676 | A | C4-C5-C6 | 6.17 | 120.08 | 117.00 |
| 1 | 16S1 | 1055 | A | N3-C4-N9 | 6.17 | 132.33 | 127.40 |
| 22 | 23S1 | 1046 | A | C8-N9-C4 | 6.17 | 108.27 | 105.80 |
| 22 | 23S1 | 2090 | A | C5-C6-N1 | 6.17 | 120.78 | 117.70 |
| 22 | 23S1 | 2097 | A | C5-C6-N1 | 6.17 | 120.78 | 117.70 |
| 22 | 23S1 | 2471 | A | C4-C5-C6 | 6.17 | 120.08 | 117.00 |
| 22 | 23S1 | 2821 | A | C4-C5-C6 | 6.17 | 120.08 | 117.00 |
| 23 | 05S1 | 29 | A | C5-C6-N1 | 6.17 | 120.78 | 117.70 |
| 1 | 16S1 | 923 | A | C5-C6-N1 | 6.17 | 120.78 | 117.70 |
| 55 | PTR1 | 9 | A | C8-N9-C4 | 6.17 | 108.27 | 105.80 |
| 55 | PTR1 | 14 | A | C8-N9-C4 | 6.17 | 108.27 | 105.80 |
| 22 | 23S1 | 221 | A | C6-N1-C2 | 6.17 | 122.30 | 118.60 |
| 22 | 23S1 | 1785 | A | C5-N7-C8 | 6.17 | 106.98 | 103.90 |
| 22 | 23S1 | 2635 | A | C4-C5-N7 | -6.17 | 107.62 | 110.70 |
| 22 | 23S1 | 1616 | A | N3-C4-N9 | 6.16 | 132.33 | 127.40 |
| 22 | 23S1 | 1749 | A | C5-C6-N1 | 6.16 | 120.78 | 117.70 |
| 22 | 23S1 | 1858 | A | C5-C6-N1 | 6.16 | 120.78 | 117.70 |
| 22 | 23S1 | 1916 | A | N3-C4-N9 | 6.16 | 132.33 | 127.40 |
| 22 | 23S1 | 2837 | A | C4-C5-C6 | 6.16 | 120.08 | 117.00 |
| 1 | 16S1 | 1155 | A | C4-C5-C6 | 6.16 | 120.08 | 117.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 1142 | A | C4-C5-C6 | 6.16 | 120.08 | 117.00 |
| 22 | 23S1 | 1672 | A | N3-C4-N9 | 6.16 | 132.33 | 127.40 |
| 22 | 23S1 | 2632 | A | C4-C5-N7 | -6.16 | 107.62 | 110.70 |
| 1 | 16S1 | 728 | A | C4-C5-C6 | 6.16 | 120.08 | 117.00 |
| 1 | 16S1 | 1236 | A | C5-C6-N1 | 6.16 | 120.78 | 117.70 |
| 22 | 23S1 | 84 | A | N9-C4-C5 | 6.16 | 108.26 | 105.80 |
| 22 | 23S1 | 592 | A | N3-C4-N9 | 6.16 | 132.33 | 127.40 |
| 22 | 23S1 | 1916 | A | C4-C5-C6 | 6.16 | 120.08 | 117.00 |
| 23 | 05S1 | 15 | A | N3-C4-N9 | 6.16 | 132.33 | 127.40 |
| 1 | 16S1 | 44 | A | C4-C5-N7 | -6.16 | 107.62 | 110.70 |
| 1 | 16S1 | 60 | A | N9-C4-C5 | 6.16 | 108.26 | 105.80 |
| 1 | 16S1 | 1362 | A | N3-C4-N9 | 6.16 | 132.33 | 127.40 |
| 22 | 23S1 | 761 | A | N9-C4-C5 | 6.16 | 108.26 | 105.80 |
| 22 | 23S1 | 2100 | G | C5-C6-O6 | -6.16 | 124.91 | 128.60 |
| 22 | 23S1 | 2411 | A | N3-C4-N9 | 6.16 | 132.33 | 127.40 |
| 1 | 16S1 | 456 | A | N9-C4-C5 | 6.16 | 108.26 | 105.80 |
| 22 | 23S1 | 2288 | A | N3-C4-N9 | 6.16 | 132.33 | 127.40 |
| 1 | 16S1 | 356 | A | C8-N9-C4 | 6.16 | 108.26 | 105.80 |
| 22 | 23S1 | 449 | A | N9-C4-C5 | 6.16 | 108.26 | 105.80 |
| 22 | 23S1 | 1413 | A | N3-C4-N9 | 6.16 | 132.32 | 127.40 |
| 22 | 23S1 | 2461 | A | C4-C5-C6 | 6.16 | 120.08 | 117.00 |
| 22 | 23S1 | 2880 | C | N1-C2-O2 | 6.16 | 122.59 | 118.90 |
| 55 | PTR1 | 21 | A | C4-C5-C6 | 6.16 | 120.08 | 117.00 |
| 22 | 23S1 | 941 | A | C4-C5-C6 | 6.15 | 120.08 | 117.00 |
| 22 | 23S1 | 1626 | A | C4-C5-C6 | 6.15 | 120.08 | 117.00 |
| 1 | 16S1 | 77 | A | C5-N7-C8 | 6.15 | 106.98 | 103.90 |
| 1 | 16S1 | 459 | A | C4-C5-C6 | 6.15 | 120.08 | 117.00 |
| 1 | 16S1 | 814 | A | C5-C6-N1 | 6.15 | 120.78 | 117.70 |
| 22 | 23S1 | 1057 | A | C4-C5-C6 | 6.15 | 120.08 | 117.00 |
| 22 | 23S1 | 1654 | A | N3-C4-N9 | 6.15 | 132.32 | 127.40 |
| 22 | 23S1 | 1700 | A | N3-C4-N9 | 6.15 | 132.32 | 127.40 |
| 22 | 23S1 | 1774 | C | C6-N1-C2 | -6.15 | 117.84 | 120.30 |
| 1 | 16S1 | 807 | A | C5-C6-N1 | 6.15 | 120.78 | 117.70 |
| 22 | 23S1 | 1151 | A | C4-C5-C6 | 6.15 | 120.08 | 117.00 |
| 23 | 05S1 | 34 | A | N3-C4-N9 | 6.15 | 132.32 | 127.40 |
| 1 | 16S1 | 1105 | A | N3-C4-N9 | 6.15 | 132.32 | 127.40 |
| 22 | 23S1 | 563 | A | N3-C4-N9 | 6.15 | 132.32 | 127.40 |
| 1 | 16S1 | 50 | A | C4-C5-C6 | 6.15 | 120.07 | 117.00 |
| 1 | 16S1 | 1044 | A | C4-C5-C6 | 6.15 | 120.07 | 117.00 |
| 22 | 23S1 | 633 | A | N3-C4-N9 | 6.15 | 132.32 | 127.40 |
| 22 | 23S1 | 2013 | A | C8-N9-C4 | 6.15 | 108.26 | 105.80 |
| 1 | 16S1 | 441 | A | C4-C5-C6 | 6.15 | 120.07 | 117.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 16S1 | 621 | A | N9-C4-C5 | 6.15 | 108.26 | 105.80 |
| 1 | 16S1 | 767 | A | C4-C5-C6 | 6.15 | 120.07 | 117.00 |
| 1 | 16S1 | 1311 | A | N3-C4-N9 | 6.14 | 132.31 | 127.40 |
| 22 | 23S1 | 104 | A | C4-C5-C6 | 6.14 | 120.07 | 117.00 |
| 22 | 23S1 | 1254 | A | C8-N9-C4 | 6.14 | 108.26 | 105.80 |
| 22 | 23S1 | 1287 | A | C8-N9-C4 | 6.14 | 108.26 | 105.80 |
| 22 | 23S1 | 2753 | A | C4-C5-N7 | -6.14 | 107.63 | 110.70 |
| 1 | 16S1 | 321 | A | C4-C5-C6 | 6.14 | 120.07 | 117.00 |
| 22 | 23S1 | 256 | A | C8-N9-C4 | 6.14 | 108.26 | 105.80 |
| 22 | 23S1 | 2425 | A | C8-N9-C4 | 6.14 | 108.26 | 105.80 |
| 22 | 23S1 | 2736 | A | C8-N9-C4 | 6.14 | 108.26 | 105.80 |
| 22 | 23S1 | 2810 | A | N3-C4-N9 | 6.14 | 132.31 | 127.40 |
| 1 | 16S1 | 33 | A | C4-C5-C6 | 6.14 | 120.07 | 117.00 |
| 1 | 16S1 | 630 | A | N3-C4-N9 | 6.14 | 132.31 | 127.40 |
| 22 | 23S1 | 1313 | U | C6-N1-C1' | -6.14 | 112.61 | 121.20 |
| 22 | 23S1 | 1871 | A | N3-C4-N9 | 6.14 | 132.31 | 127.40 |
| 1 | 16S1 | 1288 | A | N3-C4-N9 | 6.14 | 132.31 | 127.40 |
| 1 | 16S1 | 1456 | A | C4-C5-C6 | 6.14 | 120.07 | 117.00 |
| 1 | 16S1 | 1171 | A | C5-C6-N1 | 6.14 | 120.77 | 117.70 |
| 22 | 23S1 | 423 | A | N9-C4-C5 | 6.14 | 108.25 | 105.80 |
| 22 | 23S1 | 715 | A | C4-C5-C6 | 6.14 | 120.07 | 117.00 |
| 22 | 23S1 | 1046 | A | N3-C4-N9 | 6.14 | 132.31 | 127.40 |
| 22 | 23S1 | 2340 | A | C8-N9-C4 | 6.14 | 108.25 | 105.80 |
| 1 | 16S1 | 583 | A | N9-C4-C5 | 6.13 | 108.25 | 105.80 |
| 1 | 16S1 | 790 | A | N3-C4-N9 | 6.13 | 132.31 | 127.40 |
| 22 | 23S1 | 429 | A | C4-C5-C6 | 6.13 | 120.07 | 117.00 |
| 22 | 23S1 | 1650 | A | C4-C5-C6 | 6.13 | 120.07 | 117.00 |
| 22 | 23S1 | 2471 | A | C4-C5-N7 | -6.13 | 107.63 | 110.70 |
| 22 | 23S1 | 2792 | A | C4-C5-C6 | 6.13 | 120.07 | 117.00 |
| 1 | 16S1 | 179 | A | C4-C5-C6 | 6.13 | 120.07 | 117.00 |
| 1 | 16S1 | 1251 | A | C4-C5-C6 | 6.13 | 120.07 | 117.00 |
| 22 | 23S1 | 590 | A | N9-C4-C5 | 6.13 | 108.25 | 105.80 |
| 22 | 23S1 | 632 | A | N3-C4-N9 | 6.13 | 132.31 | 127.40 |
| 22 | 23S1 | 825 | A | N3-C4-N9 | 6.13 | 132.31 | 127.40 |
| 22 | 23S1 | 833 | A | N3-C4-N9 | 6.13 | 132.31 | 127.40 |
| 22 | 23S1 | 1522 | A | N3-C4-N9 | 6.13 | 132.31 | 127.40 |
| 1 | 16S1 | 1102 | A | C4-C5-C6 | 6.13 | 120.06 | 117.00 |
| 22 | 23S1 | 1284 | A | C8-N9-C4 | 6.13 | 108.25 | 105.80 |
| 23 | 05S1 | 109 | A | N3-C4-N9 | 6.13 | 132.30 | 127.40 |
| 22 | 23S1 | 849 | A | C4-C5-C6 | 6.13 | 120.06 | 117.00 |
| 1 | 16S1 | 389 | A | C4-C5-C6 | 6.13 | 120.06 | 117.00 |
| 1 | 16S1 | 520 | A | C4-C5-C6 | 6.13 | 120.06 | 117.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 2003 | A | C5-C6-N1 | 6.13 | 120.76 | 117.70 |
| 22 | 23S1 | 2088 | A | C8-N9-C4 | 6.13 | 108.25 | 105.80 |
| 22 | 23S1 | 2418 | A | N3-C4-N9 | 6.13 | 132.30 | 127.40 |
| 22 | 23S1 | 599 | A | C8-N9-C4 | 6.12 | 108.25 | 105.80 |
| 22 | 23S1 | 1067 | A | N3-C4-N9 | 6.12 | 132.30 | 127.40 |
| 22 | 23S1 | 1089 | A | C4-C5-C6 | 6.12 | 120.06 | 117.00 |
| 1 | 16S1 | 1 | A | C8-N9-C4 | 6.12 | 108.25 | 105.80 |
| 1 | 16S1 | 371 | A | N3-C4-N9 | 6.12 | 132.30 | 127.40 |
| 22 | 23S1 | 556 | A | N3-C4-N9 | 6.12 | 132.30 | 127.40 |
| 22 | 23S1 | 899 | A | N3-C4-N9 | 6.12 | 132.30 | 127.40 |
| 22 | 23S1 | 1420 | A | N3-C4-N9 | 6.12 | 132.30 | 127.40 |
| 22 | 23S1 | 1847 | A | N9-C4-C5 | 6.12 | 108.25 | 105.80 |
| 1 | 16S1 | 489 | C | C6-N1-C2 | -6.12 | 117.85 | 120.30 |
| 1 | 16S1 | 753 | A | C4-C5-C6 | 6.12 | 120.06 | 117.00 |
| 1 | 16S1 | 759 | A | C4-C5-C6 | 6.12 | 120.06 | 117.00 |
| 1 | 16S1 | 1042 | A | C4-C5-C6 | 6.12 | 120.06 | 117.00 |
| 1 | 16S1 | 1110 | A | N9-C4-C5 | 6.12 | 108.25 | 105.80 |
| 1 | 16S1 | 1180 | A | C4-C5-C6 | 6.12 | 120.06 | 117.00 |
| 22 | 23S1 | 1918 | A | C4-C5-C6 | 6.12 | 120.06 | 117.00 |
| 22 | 23S1 | 2547 | A | N3-C4-N9 | 6.12 | 132.30 | 127.40 |
| 1 | 16S1 | 1360 | A | C4-C5-C6 | 6.12 | 120.06 | 117.00 |
| 22 | 23S1 | 1246 | A | C4-C5-C6 | 6.12 | 120.06 | 117.00 |
| 22 | 23S1 | 1652 | A | C4-C5-N7 | -6.12 | 107.64 | 110.70 |
| 22 | 23S1 | 1705 | A | C4-C5-C6 | 6.12 | 120.06 | 117.00 |
| 22 | 23S1 | 2158 | A | N3-C4-N9 | 6.12 | 132.29 | 127.40 |
| 22 | 23S1 | 44 | A | C4-C5-C6 | 6.12 | 120.06 | 117.00 |
| 22 | 23S1 | 222 | A | C4-C5-C6 | 6.12 | 120.06 | 117.00 |
| 22 | 23S1 | 910 | A | N3-C4-N9 | 6.12 | 132.29 | 127.40 |
| 22 | 23S1 | 1328 | A | C4-C5-N7 | -6.12 | 107.64 | 110.70 |
| 22 | 23S1 | 2792 | A | C5-C6-N1 | 6.12 | 120.76 | 117.70 |
| 22 | 23S1 | 1254 | A | N3-C4-N9 | 6.12 | 132.29 | 127.40 |
| 22 | 23S1 | 1502 | A | N3-C4-N9 | 6.12 | 132.29 | 127.40 |
| 22 | 23S1 | 1549 | A | N3-C4-N9 | 6.12 | 132.29 | 127.40 |
| 1 | 16S1 | 306 | A | N3-C4-N9 | 6.11 | 132.29 | 127.40 |
| 1 | 16S1 | 1288 | A | C4-C5-C6 | 6.11 | 120.06 | 117.00 |
| 1 | 16S1 | 1465 | A | N3-C4-N9 | 6.11 | 132.29 | 127.40 |
| 22 | 23S1 | 980 | A | N3-C4-N9 | 6.11 | 132.29 | 127.40 |
| 22 | 23S1 | 1773 | A | N3-C4-N9 | 6.11 | 132.29 | 127.40 |
| 22 | 23S1 | 2497 | A | N9-C4-C5 | 6.11 | 108.25 | 105.80 |
| 55 | PTR1 | 69 | A | C4-C5-C6 | 6.11 | 120.06 | 117.00 |
| 22 | 23S1 | 1780 | A | N3-C4-N9 | 6.11 | 132.29 | 127.40 |
| 23 | 05S1 | 34 | A | C8-N9-C4 | 6.11 | 108.25 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 16S1 | 1333 | A | C4-C5-N7 | -6.11 | 107.64 | 110.70 |
| 1 | 16S1 | 1413 | A | N9-C4-C5 | 6.11 | 108.24 | 105.80 |
| 1 | 16S1 | 338 | A | N3-C4-N9 | 6.11 | 132.29 | 127.40 |
| 1 | 16S1 | 1261 | A | N3-C4-N9 | 6.11 | 132.29 | 127.40 |
| 22 | 23S1 | 1079 | C | N1-C2-O2 | 6.11 | 122.57 | 118.90 |
| 1 | 16S1 | 411 | A | N3-C4-N9 | 6.11 | 132.29 | 127.40 |
| 1 | 16S1 | 1145 | A | C5-C6-N1 | 6.11 | 120.75 | 117.70 |
| 22 | 23S1 | 466 | A | N3-C4-N9 | 6.11 | 132.28 | 127.40 |
| 1 | 16S1 | 364 | A | C8-N9-C4 | 6.11 | 108.24 | 105.80 |
| 1 | 16S1 | 958 | A | N3-C4-N9 | 6.11 | 132.28 | 127.40 |
| 1 | 16S1 | 1311 | A | C5-C6-N1 | 6.11 | 120.75 | 117.70 |
| 22 | 23S1 | 262 | A | N9-C4-C5 | 6.11 | 108.24 | 105.80 |
| 22 | 23S1 | 735 | A | N3-C4-N9 | 6.11 | 132.28 | 127.40 |
| 22 | 23S1 | 947 | A | C4-C5-C6 | 6.11 | 120.05 | 117.00 |
| 22 | 23S1 | 2589 | A | N3-C4-N9 | 6.11 | 132.28 | 127.40 |
| 22 | 23S1 | 2734 | A | N3-C4-N9 | 6.11 | 132.28 | 127.40 |
| 22 | 23S1 | 83 | A | C8-N9-C4 | 6.10 | 108.24 | 105.80 |
| 22 | 23S1 | 453 | A | C4-C5-C6 | 6.10 | 120.05 | 117.00 |
| 1 | 16S1 | 1157 | A | C8-N9-C4 | 6.10 | 108.24 | 105.80 |
| 1 | 16S1 | 1256 | A | N3-C4-N9 | 6.10 | 132.28 | 127.40 |
| 22 | 23S1 | 1301 | A | C5-C6-N1 | 6.10 | 120.75 | 117.70 |
| 1 | 16S1 | 630 | A | C4-C5-C6 | 6.10 | 120.05 | 117.00 |
| 1 | 16S1 | 767 | A | C8-N9-C4 | 6.10 | 108.24 | 105.80 |
| 1 | 16S1 | 313 | A | N3-C4-N9 | 6.10 | 132.28 | 127.40 |
| 1 | 16S1 | 1191 | A | C4-C5-C6 | 6.10 | 120.05 | 117.00 |
| 1 | 16S1 | 1413 | A | C4-C5-N7 | -6.10 | 107.65 | 110.70 |
| 22 | 23S1 | 1858 | A | C4-C5-C6 | 6.10 | 120.05 | 117.00 |
| 22 | 23S1 | 2432 | A | N3-C4-N9 | 6.10 | 132.28 | 127.40 |
| 22 | 23S1 | 702 | U | N3-C2-O2 | -6.10 | 117.93 | 122.20 |
| 1 | 16S1 | 1476 | A | C4-C5-C6 | 6.09 | 120.05 | 117.00 |
| 22 | 23S1 | 1579 | A | N3-C4-N9 | 6.09 | 132.28 | 127.40 |
| 22 | 23S1 | 460 | A | C8-N9-C4 | 6.09 | 108.24 | 105.80 |
| 55 | PTR1 | 58 | A | C4-C5-N7 | -6.09 | 107.65 | 110.70 |
| 1 | 16S1 | 243 | A | C8-N9-C4 | 6.09 | 108.24 | 105.80 |
| 1 | 16S1 | 802 | A | C8-N9-C4 | 6.09 | 108.24 | 105.80 |
| 22 | 23S1 | 515 | A | N9-C4-C5 | 6.09 | 108.24 | 105.80 |
| 22 | 23S1 | 975 | A | N3-C4-N9 | 6.09 | 132.27 | 127.40 |
| 22 | 23S1 | 1040 | A | N3-C4-N9 | 6.09 | 132.27 | 127.40 |
| 22 | 23S1 | 1156 | A | N3-C4-N9 | 6.09 | 132.27 | 127.40 |
| 22 | 23S1 | 2090 | A | C4-C5-C6 | 6.09 | 120.05 | 117.00 |
| 22 | 23S1 | 538 | A | C8-N9-C4 | 6.09 | 108.24 | 105.80 |
| 22 | 23S1 | 1609 | A | C4-C5-C6 | 6.09 | 120.05 | 117.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 16S1 | 1152 | A | C5-N7-C8 | 6.09 | 106.94 | 103.90 |
| 1 | 16S1 | 1216 | A | N9-C4-C5 | 6.09 | 108.23 | 105.80 |
| 22 | 23S1 | 2670 | A | C5-C6-N1 | 6.09 | 120.74 | 117.70 |
| 1 | 16S1 | 1377 | A | C4-C5-C6 | 6.09 | 120.04 | 117.00 |
| 22 | 23S1 | 103 | A | C4-C5-C6 | 6.09 | 120.04 | 117.00 |
| 22 | 23S1 | 354 | A | N9-C4-C5 | 6.09 | 108.23 | 105.80 |
| 22 | 23S1 | 428 | A | C4-C5-C6 | 6.09 | 120.04 | 117.00 |
| 22 | 23S1 | 1746 | A | C5-C6-N1 | 6.09 | 120.74 | 117.70 |
| 22 | 23S1 | 2297 | A | C4-C5-C6 | 6.09 | 120.04 | 117.00 |
| 22 | 23S1 | 2799 | A | C5-C6-N1 | 6.09 | 120.74 | 117.70 |
| 1 | 16S1 | 26 | A | C5-N7-C8 | 6.08 | 106.94 | 103.90 |
| 1 | 16S1 | 694 | A | C4-C5-N7 | -6.08 | 107.66 | 110.70 |
| 22 | 23S1 | 182 | A | N3-C4-N9 | 6.08 | 132.27 | 127.40 |
| 1 | 16S1 | 279 | A | C4-C5-C6 | 6.08 | 120.04 | 117.00 |
| 22 | 23S1 | 631 | A | N3-C4-N9 | 6.08 | 132.27 | 127.40 |
| 22 | 23S1 | 715 | A | N3-C4-N9 | 6.08 | 132.27 | 127.40 |
| 22 | 23S1 | 1000 | A | N3-C4-N9 | 6.08 | 132.27 | 127.40 |
| 1 | 16S1 | 221 | C | N1-C2-O2 | 6.08 | 122.55 | 118.90 |
| 22 | 23S1 | 702 | U | N1-C2-O2 | 6.08 | 127.06 | 122.80 |
| 22 | 23S1 | 1039 | A | N3-C4-N9 | 6.08 | 132.26 | 127.40 |
| 22 | 23S1 | 1544 | A | N3-C4-N9 | 6.08 | 132.27 | 127.40 |
| 1 | 16S1 | 44 | A | N9-C4-C5 | 6.08 | 108.23 | 105.80 |
| 22 | 23S1 | 1676 | A | N3-C4-N9 | 6.08 | 132.26 | 127.40 |
| 1 | 16S1 | 872 | A | C5-C6-N1 | 6.08 | 120.74 | 117.70 |
| 1 | 16S1 | 1021 | A | N3-C4-N9 | 6.08 | 132.26 | 127.40 |
| 1 | 16S1 | 1169 | A | C8-N9-C4 | 6.08 | 108.23 | 105.80 |
| 1 | 16S1 | 1357 | A | C5-C6-N1 | 6.08 | 120.74 | 117.70 |
| 1 | 16S1 | 816 | A | N3-C4-N9 | 6.08 | 132.26 | 127.40 |
| 22 | 23S1 | 103 | A | N3-C4-N9 | 6.08 | 132.26 | 127.40 |
| 1 | 16S1 | 374 | A | N3-C4-N9 | 6.08 | 132.26 | 127.40 |
| 1 | 16S1 | 560 | A | N3-C4-N9 | 6.08 | 132.26 | 127.40 |
| 1 | 16S1 | 1531 | A | N3-C4-N9 | 6.08 | 132.26 | 127.40 |
| 22 | 23S1 | 447 | A | N3-C4-N9 | 6.08 | 132.26 | 127.40 |
| 22 | 23S1 | 56 | A | C8-N9-C4 | 6.07 | 108.23 | 105.80 |
| 22 | 23S1 | 538 | A | N3-C4-N9 | 6.07 | 132.26 | 127.40 |
| 22 | 23S1 | 933 | A | C5-C6-N1 | 6.07 | 120.74 | 117.70 |
| 22 | 23S1 | 1285 | A | C4-C5-C6 | 6.07 | 120.04 | 117.00 |
| 1 | 16S1 | 676 | A | N3-C4-N9 | 6.07 | 132.26 | 127.40 |
| 1 | 16S1 | 1101 | A | N9-C4-C5 | 6.07 | 108.23 | 105.80 |
| 1 | 16S1 | 1483 | A | N3-C4-N9 | 6.07 | 132.26 | 127.40 |
| 22 | 23S1 | 176 | A | N3-C4-N9 | 6.07 | 132.26 | 127.40 |
| 22 | 23S1 | 2080 | A | C4-C5-C6 | 6.07 | 120.04 | 117.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 156 | A | C4-C5-C6 | 6.07 | 120.03 | 117.00 |
| 22 | 23S1 | 483 | A | N3-C4-N9 | 6.07 | 132.26 | 127.40 |
| 22 | 23S1 | 1433 | A | N3-C4-N9 | 6.07 | 132.26 | 127.40 |
| 22 | 23S1 | 1676 | A | C4-C5-C6 | 6.07 | 120.03 | 117.00 |
| 22 | 23S1 | 2799 | A | C5-N7-C8 | 6.07 | 106.94 | 103.90 |
| 1 | 16S1 | 1227 | A | N7-C8-N9 | -6.07 | 110.77 | 113.80 |
| 22 | 23S1 | 371 | A | C8-N9-C4 | 6.07 | 108.23 | 105.80 |
| 22 | 23S1 | 1786 | A | N9-C4-C5 | 6.07 | 108.23 | 105.80 |
| 22 | 23S1 | 1876 | A | N3-C4-N9 | 6.07 | 132.25 | 127.40 |
| 1 | 16S1 | 236 | A | N3-C4-N9 | 6.07 | 132.25 | 127.40 |
| 22 | 23S1 | 1126 | A | C4-C5-C6 | 6.07 | 120.03 | 117.00 |
| 22 | 23S1 | 1919 | A | C5-N7-C8 | 6.07 | 106.93 | 103.90 |
| 22 | 23S1 | 2070 | A | N3-C4-N9 | 6.07 | 132.25 | 127.40 |
| 23 | 05S1 | 59 | A | C4-C5-N7 | -6.07 | 107.67 | 110.70 |
| 1 | 16S1 | 1101 | A | C8-N9-C4 | 6.07 | 108.23 | 105.80 |
| 10 | S101 | 27 | GLU | CA-CB-CG | 6.07 | 126.75 | 113.40 |
| 22 | 23S1 | 2247 | A | N3-C4-N9 | 6.07 | 132.25 | 127.40 |
| 22 | 23S1 | 2459 | A | C5-C6-N1 | 6.07 | 120.73 | 117.70 |
| 1 | 16S1 | 130 | A | C4-C5-C6 | 6.06 | 120.03 | 117.00 |
| 1 | 16S1 | 1036 | A | N9-C4-C5 | 6.06 | 108.23 | 105.80 |
| 1 | 16S1 | 1204 | A | C4-C5-N7 | -6.06 | 107.67 | 110.70 |
| 22 | 23S1 | 782 | A | N9-C4-C5 | 6.06 | 108.23 | 105.80 |
| 22 | 23S1 | 1365 | A | N9-C4-C5 | 6.06 | 108.23 | 105.80 |
| 22 | 23S1 | 2270 | A | N9-C4-C5 | 6.06 | 108.23 | 105.80 |
| 22 | 23S1 | 2758 | A | N9-C4-C5 | 6.06 | 108.23 | 105.80 |
| 1 | 16S1 | 74 | A | C8-N9-C4 | 6.06 | 108.22 | 105.80 |
| 1 | 16S1 | 120 | A | C8-N9-C4 | 6.06 | 108.22 | 105.80 |
| 1 | 16S1 | 553 | A | C8-N9-C4 | 6.06 | 108.22 | 105.80 |
| 1 | 16S1 | 1257 | A | N3-C4-N9 | 6.06 | 132.25 | 127.40 |
| 22 | 23S1 | 758 | C | C6-N1-C2 | -6.06 | 117.88 | 120.30 |
| 22 | 23S1 | 1126 | A | N9-C4-C5 | 6.06 | 108.22 | 105.80 |
| 22 | 23S1 | 1632 | A | C4-C5-C6 | 6.06 | 120.03 | 117.00 |
| 22 | 23S1 | 2182 | U | N3-C2-O2 | -6.06 | 117.96 | 122.20 |
| 22 | 23S1 | 231 | A | N3-C4-N9 | 6.06 | 132.25 | 127.40 |
| 22 | 23S1 | 1866 | A | N3-C4-N9 | 6.06 | 132.25 | 127.40 |
| 22 | 23S1 | 821 | A | C8-N9-C4 | 6.06 | 108.22 | 105.80 |
| 22 | 23S1 | 1302 | A | N3-C4-N9 | 6.06 | 132.25 | 127.40 |
| 22 | 23S1 | 2761 | A | N3-C4-N9 | 6.06 | 132.25 | 127.40 |
| 1 | 16S1 | 743 | A | C8-N9-C4 | 6.06 | 108.22 | 105.80 |
| 22 | 23S1 | 447 | A | C4-C5-C6 | 6.06 | 120.03 | 117.00 |
| 22 | 23S1 | 675 | A | N9-C4-C5 | 6.06 | 108.22 | 105.80 |
| 1 | 16S1 | 781 | A | C8-N9-C4 | 6.05 | 108.22 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 16S1 | 918 | A | C4-C5-C6 | 6.05 | 120.03 | 117.00 |
| 22 | 23S1 | 734 | A | C8-N9-C4 | 6.05 | 108.22 | 105.80 |
| 22 | 23S1 | 2188 | U | P-O3'-C3' | 6.05 | 126.97 | 119.70 |
| 1 | 16S1 | 1169 | A | C4-C5-C6 | 6.05 | 120.03 | 117.00 |
| 22 | 23S1 | 1585 | C | C6-N1-C2 | -6.05 | 117.88 | 120.30 |
| 22 | 23S1 | 1757 | A | C8-N9-C4 | 6.05 | 108.22 | 105.80 |
| 22 | 23S1 | 1952 | A | N3-C4-N9 | 6.05 | 132.24 | 127.40 |
| 22 | 23S1 | 2513 | A | C4-C5-C6 | 6.05 | 120.03 | 117.00 |
| 1 | 16S1 | 408 | A | N9-C4-C5 | 6.05 | 108.22 | 105.80 |
| 22 | 23S1 | 21 | A | C4-C5-C6 | 6.05 | 120.03 | 117.00 |
| 22 | 23S1 | 2766 | A | C5-C6-N1 | 6.05 | 120.73 | 117.70 |
| 1 | 16S1 | 190 | A | C6-C5-N7 | -6.05 | 128.06 | 132.30 |
| 22 | 23S1 | 788 | A | C4-C5-C6 | 6.05 | 120.03 | 117.00 |
| 22 | 23S1 | 1717 | A | N3-C4-N9 | 6.05 | 132.24 | 127.40 |
| 22 | 23S1 | 2108 | A | N3-C4-N9 | 6.05 | 132.24 | 127.40 |
| 22 | 23S1 | 2176 | A | N3-C4-N9 | 6.05 | 132.24 | 127.40 |
| 22 | 23S1 | 2388 | A | C8-N9-C4 | 6.05 | 108.22 | 105.80 |
| 22 | 23S1 | 2778 | A | N3-C4-N9 | 6.05 | 132.24 | 127.40 |
| 1 | 16S1 | 19 | A | C4-C5-N7 | -6.05 | 107.68 | 110.70 |
| 1 | 16S1 | 1299 | A | C5-C6-N1 | 6.05 | 120.72 | 117.70 |
| 22 | 23S1 | 2761 | A | C4-C5-C6 | 6.05 | 120.02 | 117.00 |
| 1 | 16S1 | 596 | A | N3-C4-N9 | 6.05 | 132.24 | 127.40 |
| 1 | 16S1 | 1374 | A | C8-N9-C4 | 6.05 | 108.22 | 105.80 |
| 1 | 16S1 | 1429 | A | N3-C4-N9 | 6.05 | 132.24 | 127.40 |
| 22 | 23S1 | 1032 | A | N9-C4-C5 | 6.05 | 108.22 | 105.80 |
| 22 | 23S1 | 1165 | A | C8-N9-C4 | 6.05 | 108.22 | 105.80 |
| 1 | 16S1 | 694 | A | N3-C4-N9 | 6.04 | 132.24 | 127.40 |
| 23 | 05S1 | 50 | A | C5-C6-N1 | 6.04 | 120.72 | 117.70 |
| 1 | 16S1 | 288 | A | N3-C4-N9 | 6.04 | 132.24 | 127.40 |
| 1 | 16S1 | 1476 | A | C5-C6-N1 | 6.04 | 120.72 | 117.70 |
| 22 | 23S1 | 2054 | A | C4-C5-C6 | 6.04 | 120.02 | 117.00 |
| 55 | PTR1 | 56 | C | C5-C6-N1 | 6.04 | 124.02 | 121.00 |
| 1 | 16S1 | 461 | A | C5-C6-N1 | 6.04 | 120.72 | 117.70 |
| 22 | 23S1 | 582 | A | C4-C5-C6 | 6.04 | 120.02 | 117.00 |
| 22 | 23S1 | 1470 | A | N3-C4-N9 | 6.04 | 132.23 | 127.40 |
| 1 | 16S1 | 228 | A | N3-C4-N9 | 6.04 | 132.23 | 127.40 |
| 22 | 23S1 | 1354 | A | C4-C5-C6 | 6.04 | 120.02 | 117.00 |
| 1 | 16S1 | 120 | A | N3-C4-N9 | 6.04 | 132.23 | 127.40 |
| 1 | 16S1 | 831 | A | N3-C4-N9 | 6.04 | 132.23 | 127.40 |
| 1 | 16S1 | 878 | A | N3-C4-N9 | 6.04 | 132.23 | 127.40 |
| 22 | 23S1 | 300 | A | N3-C4-N9 | 6.04 | 132.23 | 127.40 |
| 22 | 23S1 | 345 | A | N3-C4-N9 | 6.04 | 132.23 | 127.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22 | 23S1 | 508 | A | C4-C5-C6 | 6.04 | 120.02 | 117.00 |
| 22 | 23S1 | 532 | A | C5-C6-N1 | 6.04 | 120.72 | 117.70 |
| 22 | 23S1 | 1419 | A | C5-C6-N1 | 6.04 | 120.72 | 117.70 |
| 22 | 23S1 | 1609 | A | N3-C4-N9 | 6.04 | 132.23 | 127.40 |
| 22 | 23S1 | 1978 | A | N3-C4-N9 | 6.04 | 132.23 | 127.40 |
| 23 | 05S1 | 104 | A | C4-C5-C6 | 6.04 | 120.02 | 117.00 |
| 1 | 16S1 | 282 | A | N3-C4-N9 | 6.04 | 132.23 | 127.40 |
| 1 | 16S1 | 374 | A | C4-C5-C6 | 6.04 | 120.02 | 117.00 |
| 1 | 16S1 | 969 | A | C4-C5-C6 | 6.04 | 120.02 | 117.00 |
| 1 | 16S1 | 1261 | A | C8-N9-C4 | 6.04 | 108.22 | 105.80 |
| 22 | 23S1 | 382 | A | C4-C5-C6 | 6.04 | 120.02 | 117.00 |
| 22 | 23S1 | 1505 | A | C4-C5-C6 | 6.04 | 120.02 | 117.00 |
| 22 | 23S1 | 2719 | G | N9-C4-C5 | -6.04 | 102.99 | 105.40 |
| 22 | 23S1 | 2211 | A | N9-C4-C5 | 6.03 | 108.21 | 105.80 |
| 22 | 23S1 | 2835 | A | N9-C4-C5 | 6.03 | 108.21 | 105.80 |
| 1 | 16S1 | 502 | A | C5-C6-N1 | 6.03 | 120.72 | 117.70 |
| 1 | 16S1 | 1254 | A | N3-C4-N9 | 6.03 | 132.23 | 127.40 |
| 13 | S131 | 4 | ILE | CG1-CB-CG2 | -6.03 | 98.13 | 111.40 |
| 22 | 23S1 | 1165 | A | N3-C4-N9 | 6.03 | 132.23 | 127.40 |
| 22 | 23S1 | 1821 | A | C4-C5-C6 | 6.03 | 120.02 | 117.00 |
| 55 | PTR1 | 58 | A | C4-C5-C6 | 6.03 | 120.02 | 117.00 |
| 1 | 16S1 | 28 | A | N3-C4-N9 | 6.03 | 132.22 | 127.40 |
| 1 | 16S1 | 1197 | A | C4-C5-C6 | 6.03 | 120.02 | 117.00 |
| 1 | 16S1 | 174 | A | C8-N9-C4 | 6.03 | 108.21 | 105.80 |
| 22 | 23S1 | 1214 | A | N9-C4-C5 | 6.03 | 108.21 | 105.80 |
| 22 | 23S1 | 1431 | A | C4-C5-C6 | 6.03 | 120.02 | 117.00 |
| 22 | 23S1 | 1713 | A | C4-C5-C6 | 6.03 | 120.01 | 117.00 |
| 22 | 23S1 | 2183 | A | C4-C5-N7 | -6.03 | 107.69 | 110.70 |
| 1 | 16S1 | 167 | A | N3-C4-N9 | 6.03 | 132.22 | 127.40 |
| 1 | 16S1 | 412 | A | N9-C4-C5 | 6.03 | 108.21 | 105.80 |
| 22 | 23S1 | 165 | A | C4-C5-N7 | -6.03 | 107.69 | 110.70 |
| 22 | 23S1 | 1353 | A | N3-C4-N9 | 6.03 | 132.22 | 127.40 |
| 22 | 23S1 | 2094 | A | C4-C5-C6 | 6.03 | 120.01 | 117.00 |
| 1 | 16S1 | 815 | A | C4-C5-N7 | -6.03 | 107.69 | 110.70 |
| 1 | 16S1 | 1180 | A | N3-C4-N9 | 6.03 | 132.22 | 127.40 |
| 22 | 23S1 | 203 | A | N3-C4-N9 | 6.03 | 132.22 | 127.40 |
| 22 | 23S1 | 541 | A | C4-C5-C6 | 6.03 | 120.01 | 117.00 |
| 23 | 05S1 | 115 | A | C8-N9-C4 | 6.03 | 108.21 | 105.80 |
| 1 | 16S1 | 640 | A | C5-C6-N1 | 6.02 | 120.71 | 117.70 |
| 22 | 23S1 | 233 | A | C5-C6-N1 | 6.02 | 120.71 | 117.70 |
| 22 | 23S1 | 1347 | A | N3-C4-N9 | 6.02 | 132.22 | 127.40 |
| 22 | 23S1 | 1829 | A | N9-C4-C5 | 6.02 | 108.21 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 16S1 | 768 | A | C4-C5-N7 | -6.02 | 107.69 | 110.70 |
| 22 | 23S1 | 56 | A | C5-C6-N1 | 6.02 | 120.71 | 117.70 |
| 22 | 23S1 | 2497 | A | N3-C4-N9 | 6.02 | 132.22 | 127.40 |
| 22 | 23S1 | 1151 | A | C5-C6-N1 | 6.02 | 120.71 | 117.70 |
| 1 | 16S1 | 366 | A | C4-C5-C6 | 6.02 | 120.01 | 117.00 |
| 1 | 16S1 | 702 | A | C8-N9-C4 | 6.02 | 108.21 | 105.80 |
| 22 | 23S1 | 374 | A | C4-C5-C6 | 6.02 | 120.01 | 117.00 |
| 22 | 23S1 | 821 | A | C4-C5-N7 | -6.02 | 107.69 | 110.70 |
| 22 | 23S1 | 2600 | A | C4-C5-C6 | 6.02 | 120.01 | 117.00 |
| 55 | PTR1 | 3 | A | N3-C4-N9 | 6.02 | 132.22 | 127.40 |
| 55 | PTR1 | 62 | C | C2-N1-C1' | 6.02 | 125.42 | 118.80 |
| 22 | 23S1 | 789 | A | N3-C4-N9 | 6.02 | 132.21 | 127.40 |
| 22 | 23S1 | 2352 | A | N9-C4-C5 | 6.02 | 108.21 | 105.80 |
| 1 | 16S1 | 55 | A | C4-C5-N7 | -6.02 | 107.69 | 110.70 |
| 1 | 16S1 | 461 | A | N3-C4-N9 | 6.01 | 132.21 | 127.40 |
| 22 | 23S1 | 217 | A | N3-C4-N9 | 6.01 | 132.21 | 127.40 |
| 22 | 23S1 | 1672 | A | C4-C5-C6 | 6.01 | 120.01 | 117.00 |
| 22 | 23S1 | 2063 | C | C6-N1-C2 | -6.01 | 117.89 | 120.30 |
| 22 | 23S1 | 2198 | A | C8-N9-C4 | 6.01 | 108.21 | 105.80 |
| 23 | 05S1 | 59 | A | C6-N1-C2 | -6.01 | 114.99 | 118.60 |
| 1 | 16S1 | 1271 | A | C4-C5-C6 | 6.01 | 120.01 | 117.00 |
| 1 | 16S1 | 1480 | A | N9-C4-C5 | 6.01 | 108.20 | 105.80 |
| 22 | 23S1 | 2095 | A | C4-C5-N7 | -6.01 | 107.69 | 110.70 |
| 22 | 23S1 | 2726 | A | C8-N9-C4 | 6.01 | 108.20 | 105.80 |
| 1 | 16S1 | 414 | A | C5-C6-N1 | 6.01 | 120.70 | 117.70 |
| 1 | 16S1 | 958 | A | N9-C4-C5 | 6.01 | 108.20 | 105.80 |
| 22 | 23S1 | 182 | A | C4-C5-C6 | 6.01 | 120.00 | 117.00 |
| 22 | 23S1 | 216 | A | N3-C4-N9 | 6.01 | 132.21 | 127.40 |
| 22 | 23S1 | 1246 | A | N9-C4-C5 | 6.01 | 108.20 | 105.80 |
| 22 | 23S1 | 2019 | A | N3-C4-N9 | 6.01 | 132.21 | 127.40 |
| 22 | 23S1 | 2873 | A | N9-C4-C5 | 6.01 | 108.20 | 105.80 |
| 1 | 16S1 | 1329 | A | C5-C6-N1 | 6.01 | 120.70 | 117.70 |
| 22 | 23S1 | 1169 | A | C8-N9-C4 | 6.01 | 108.20 | 105.80 |
| 22 | 23S1 | 1393 | A | C4-C5-C6 | 6.01 | 120.00 | 117.00 |
| 22 | 23S1 | 2354 | C | C6-N1-C2 | -6.01 | 117.90 | 120.30 |
| 23 | 05S1 | 119 | A | C5-C6-N1 | 6.01 | 120.70 | 117.70 |
| 1 | 16S1 | 792 | A | C8-N9-C4 | 6.00 | 108.20 | 105.80 |
| 1 | 16S1 | 1410 | A | C5-C6-N1 | 6.00 | 120.70 | 117.70 |
| 1 | 16S1 | 1434 | A | N3-C4-N9 | 6.00 | 132.20 | 127.40 |
| 22 | 23S1 | 199 | A | C4-C5-C6 | 6.00 | 120.00 | 117.00 |
| 22 | 23S1 | 1142 | A | C5-C6-N1 | 6.00 | 120.70 | 117.70 |
| 22 | 23S1 | 1586 | A | C5-N7-C8 | 6.00 | 106.90 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 2107 | G | N1-C6-O6 | -6.00 | 116.30 | 119.90 |
| 22 | 23S1 | 2268 | A | N3-C4-N9 | 6.00 | 132.20 | 127.40 |
| 1 | 16S1 | 10 | A | C4-C5-C6 | 6.00 | 120.00 | 117.00 |
| 1 | 16S1 | 892 | A | N3-C4-N9 | 6.00 | 132.20 | 127.40 |
| 22 | 23S1 | 1679 | A | C4-C5-C6 | 6.00 | 120.00 | 117.00 |
| 22 | 23S1 | 2826 | A | N3-C4-N9 | 6.00 | 132.20 | 127.40 |
| 1 | 16S1 | 190 | A | C5-C6-N6 | 6.00 | 128.50 | 123.70 |
| 1 | 16S1 | 814 | A | C8-N9-C4 | 6.00 | 108.20 | 105.80 |
| 1 | 16S1 | 1167 | A | N3-C4-N9 | 6.00 | 132.20 | 127.40 |
| 22 | 23S1 | 404 | A | C5-N7-C8 | 6.00 | 106.90 | 103.90 |
| 22 | 23S1 | 621 | A | N9-C4-C5 | 6.00 | 108.20 | 105.80 |
| 22 | 23S1 | 2478 | A | N3-C4-N9 | 6.00 | 132.20 | 127.40 |
| 1 | 16S1 | 919 | A | N9-C4-C5 | 6.00 | 108.20 | 105.80 |
| 1 | 16S1 | 958 | A | C5-C6-N1 | 6.00 | 120.70 | 117.70 |
| 22 | 23S1 | 945 | A | N9-C4-C5 | 6.00 | 108.20 | 105.80 |
| 1 | 16S1 | 1000 | A | C8-N9-C4 | 6.00 | 108.20 | 105.80 |
| 22 | 23S1 | 1783 | A | N9-C4-C5 | 6.00 | 108.20 | 105.80 |
| 22 | 23S1 | 1987 | A | C8-N9-C4 | 6.00 | 108.20 | 105.80 |
| 22 | 23S1 | 2314 | A | N3-C4-N9 | 6.00 | 132.20 | 127.40 |
| 22 | 23S1 | 2453 | A | N3-C4-N9 | 6.00 | 132.20 | 127.40 |
| 1 | 16S1 | 595 | A | N3-C4-N9 | 6.00 | 132.20 | 127.40 |
| 1 | 16S1 | 608 | A | C4-C5-C6 | 6.00 | 120.00 | 117.00 |
| 22 | 23S1 | 428 | A | C8-N9-C4 | 6.00 | 108.20 | 105.80 |
| 22 | 23S1 | 721 | A | C4-C5-C6 | 6.00 | 120.00 | 117.00 |
| 22 | 23S1 | 2734 | A | C5-C6-N1 | 6.00 | 120.70 | 117.70 |
| 55 | PTR1 | 9 | A | N3-C4-N9 | 6.00 | 132.20 | 127.40 |
| 1 | 16S1 | 1151 | A | C8-N9-C4 | 5.99 | 108.20 | 105.80 |
| 1 | 16S1 | 1250 | A | N9-C4-C5 | 5.99 | 108.20 | 105.80 |
| 22 | 23S1 | 689 | A | C5-C6-N1 | 5.99 | 120.70 | 117.70 |
| 22 | 23S1 | 1433 | A | N9-C4-C5 | 5.99 | 108.20 | 105.80 |
| 22 | 23S1 | 2270 | A | N3-C4-N9 | 5.99 | 132.19 | 127.40 |
| 1 | 16S1 | 960 | U | C2-N1-C1' | 5.99 | 124.89 | 117.70 |
| 1 | 16S1 | 969 | A | N9-C4-C5 | 5.99 | 108.20 | 105.80 |
| 1 | 16S1 | 205 | A | N3-C4-N9 | 5.99 | 132.19 | 127.40 |
| 1 | 16S1 | 968 | A | N3-C4-N9 | 5.99 | 132.19 | 127.40 |
| 22 | 23S1 | 793 | A | C4-C5-C6 | 5.99 | 120.00 | 117.00 |
| 22 | 23S1 | 925 | A | C5-C6-N1 | 5.99 | 120.69 | 117.70 |
| 22 | 23S1 | 1570 | A | C4-C5-N7 | -5.99 | 107.70 | 110.70 |
| 1 | 16S1 | 919 | A | C4-C5-C6 | 5.99 | 119.99 | 117.00 |
| 22 | 23S1 | 1805 | A | N3-C4-N9 | 5.99 | 132.19 | 127.40 |
| 22 | 23S1 | 2547 | A | C4-C5-C6 | 5.99 | 119.99 | 117.00 |
| 1 | 16S1 | 996 | A | N3-C4-N9 | 5.99 | 132.19 | 127.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 44 | A | C8-N9-C4 | 5.99 | 108.19 | 105.80 |
| 22 | 23S1 | 544 | C | C6-N1-C1' | -5.99 | 113.62 | 120.80 |
| 22 | 23S1 | 614 | A | C8-N9-C4 | 5.99 | 108.19 | 105.80 |
| 22 | 23S1 | 2792 | A | C8-N9-C4 | 5.99 | 108.19 | 105.80 |
| 23 | 05S1 | 15 | A | C4-C5-C6 | 5.99 | 119.99 | 117.00 |
| 1 | 16S1 | 728 | A | C4-C5-N7 | -5.98 | 107.71 | 110.70 |
| 22 | 23S1 | 2088 | A | C5-C6-N1 | 5.98 | 120.69 | 117.70 |
| 1 | 16S1 | 1274 | A | C8-N9-C4 | 5.98 | 108.19 | 105.80 |
| 22 | 23S1 | 756 | A | C5-C6-N1 | 5.98 | 120.69 | 117.70 |
| 22 | 23S1 | 829 | A | N3-C4-N9 | 5.98 | 132.19 | 127.40 |
| 22 | 23S1 | 1477 | A | C4-C5-C6 | 5.98 | 119.99 | 117.00 |
| 22 | 23S1 | 1665 | A | C4-C5-C6 | 5.98 | 119.99 | 117.00 |
| 22 | 23S1 | 2058 | A | N3-C4-N9 | 5.98 | 132.19 | 127.40 |
| 22 | 23S1 | 2725 | A | C4-C5-C6 | 5.98 | 119.99 | 117.00 |
| 1 | 16S1 | 595 | A | C4-C5-C6 | 5.98 | 119.99 | 117.00 |
| 1 | 16S1 | 1163 | A | C8-N9-C4 | 5.98 | 108.19 | 105.80 |
| 22 | 23S1 | 42 | A | N3-C4-N9 | 5.98 | 132.19 | 127.40 |
| 22 | 23S1 | 1260 | A | N9-C4-C5 | 5.98 | 108.19 | 105.80 |
| 22 | 23S1 | 1759 | A | C5-C6-N1 | 5.98 | 120.69 | 117.70 |
| 1 | 16S1 | 327 | A | C8-N9-C4 | 5.98 | 108.19 | 105.80 |
| 22 | 23S1 | 146 | A | C5-C6-N1 | 5.98 | 120.69 | 117.70 |
| 22 | 23S1 | 541 | A | N3-C4-N9 | 5.98 | 132.18 | 127.40 |
| 22 | 23S1 | 2434 | A | C4-C5-C6 | 5.98 | 119.99 | 117.00 |
| 22 | 23S1 | 2761 | A | N9-C4-C5 | 5.98 | 108.19 | 105.80 |
| 1 | 16S1 | 28 | A | C4-C5-C6 | 5.98 | 119.99 | 117.00 |
| 1 | 16S1 | 560 | A | C5-C6-N1 | 5.98 | 120.69 | 117.70 |
| 1 | 16S1 | 563 | A | C8-N9-C4 | 5.98 | 108.19 | 105.80 |
| 1 | 16S1 | 994 | A | C8-N9-C4 | 5.98 | 108.19 | 105.80 |
| 1 | 16S1 | 1168 | U | N1-C2-O2 | 5.98 | 126.98 | 122.80 |
| 1 | 16S1 | 1437 | A | N3-C4-N9 | 5.98 | 132.18 | 127.40 |
| 22 | 23S1 | 5 | A | C5-C6-N1 | 5.98 | 120.69 | 117.70 |
| 22 | 23S1 | 1053 | C | N1-C2-O2 | 5.98 | 122.49 | 118.90 |
| 22 | 23S1 | 1387 | A | C5-C6-N1 | 5.98 | 120.69 | 117.70 |
| 22 | 23S1 | 1427 | A | C5-C6-N1 | 5.98 | 120.69 | 117.70 |
| 22 | 23S1 | 1593 | A | C5-C6-N1 | 5.98 | 120.69 | 117.70 |
| 22 | 23S1 | 1773 | A | N9-C4-C5 | 5.98 | 108.19 | 105.80 |
| 1 | 16S1 | 349 | A | N3-C4-N9 | 5.98 | 132.18 | 127.40 |
| 22 | 23S1 | 42 | A | C4-C5-C6 | 5.98 | 119.99 | 117.00 |
| 22 | 23S1 | 825 | A | C4-C5-N7 | -5.98 | 107.71 | 110.70 |
| 22 | 23S1 | 1644 | C | N1-C2-O2 | 5.98 | 122.49 | 118.90 |
| 1 | 16S1 | 468 | A | N3-C4-N9 | 5.97 | 132.18 | 127.40 |
| 22 | 23S1 | 616 | A | N3-C4-N9 | 5.97 | 132.18 | 127.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 927 | A | N3-C4-N9 | 5.97 | 132.18 | 127.40 |
| 22 | 23S1 | 2317 | A | N3-C4-N9 | 5.97 | 132.18 | 127.40 |
| 1 | 16S1 | 535 | A | C4-C5-C6 | 5.97 | 119.99 | 117.00 |
| 1 | 16S1 | 900 | A | N9-C4-C5 | 5.97 | 108.19 | 105.80 |
| 22 | 23S1 | 342 | A | C8-N9-C4 | 5.97 | 108.19 | 105.80 |
| 22 | 23S1 | 750 | A | C5-C6-N1 | 5.97 | 120.69 | 117.70 |
| 22 | 23S1 | 2439 | A | C4-C5-C6 | 5.97 | 119.99 | 117.00 |
| 1 | 16S1 | 51 | A | N3-C4-N9 | 5.97 | 132.18 | 127.40 |
| 1 | 16S1 | 1157 | A | C5-C6-N1 | 5.97 | 120.68 | 117.70 |
| 22 | 23S1 | 368 | A | C4-C5-C6 | 5.97 | 119.98 | 117.00 |
| 22 | 23S1 | 384 | A | C4-C5-C6 | 5.97 | 119.98 | 117.00 |
| 22 | 23S1 | 453 | A | N3-C4-N9 | 5.97 | 132.18 | 127.40 |
| 22 | 23S1 | 739 | A | N9-C4-C5 | 5.97 | 108.19 | 105.80 |
| 22 | 23S1 | 1353 | A | C4-C5-N7 | -5.97 | 107.72 | 110.70 |
| 22 | 23S1 | 1365 | A | N3-C4-N9 | 5.97 | 132.18 | 127.40 |
| 22 | 23S1 | 2147 | A | N9-C4-C5 | 5.97 | 108.19 | 105.80 |
| 22 | 23S1 | 2572 | A | N9-C4-C5 | 5.97 | 108.19 | 105.80 |
| 23 | 05S1 | 35 | C | N1-C2-O2 | 5.97 | 122.48 | 118.90 |
| 22 | 23S1 | 199 | A | N3-C4-N9 | 5.97 | 132.17 | 127.40 |
| 22 | 23S1 | 631 | A | N9-C4-C5 | 5.97 | 108.19 | 105.80 |
| 22 | 23S1 | 1912 | A | C4-C5-N7 | -5.97 | 107.72 | 110.70 |
| 22 | 23S1 | 2108 | A | C4-C5-N7 | -5.97 | 107.72 | 110.70 |
| 1 | 16S1 | 715 | A | C8-N9-C4 | 5.97 | 108.19 | 105.80 |
| 22 | 23S1 | 706 | A | C8-N9-C4 | 5.97 | 108.19 | 105.80 |
| 22 | 23S1 | 1744 | A | C5-C6-N1 | 5.97 | 120.68 | 117.70 |
| 22 | 23S1 | 2020 | A | C8-N9-C4 | 5.97 | 108.19 | 105.80 |
| 22 | 23S1 | 2070 | A | C4-C5-C6 | 5.97 | 119.98 | 117.00 |
| 22 | 23S1 | 2273 | A | N9-C4-C5 | 5.97 | 108.19 | 105.80 |
| 22 | 23S1 | 2665 | A | C8-N9-C4 | 5.97 | 108.19 | 105.80 |
| 22 | 23S1 | 2761 | A | C5-C6-N1 | 5.97 | 120.68 | 117.70 |
| 22 | 23S1 | 2850 | A | N3-C4-N9 | 5.97 | 132.17 | 127.40 |
| 1 | 16S1 | 968 | A | C8-N9-C4 | 5.96 | 108.19 | 105.80 |
| 22 | 23S1 | 1552 | A | C4-C5-C6 | 5.96 | 119.98 | 117.00 |
| 1 | 16S1 | 825 | A | C8-N9-C4 | 5.96 | 108.19 | 105.80 |
| 1 | 16S1 | 1428 | A | N3-C4-N9 | 5.96 | 132.17 | 127.40 |
| 22 | 23S1 | 480 | A | C4-C5-N7 | -5.96 | 107.72 | 110.70 |
| 22 | 23S1 | 1230 | A | C5-C6-N1 | 5.96 | 120.68 | 117.70 |
| 22 | 23S1 | 1635 | A | C4-C5-C6 | 5.96 | 119.98 | 117.00 |
| 22 | 23S1 | 2516 | A | C5-C6-N1 | 5.96 | 120.68 | 117.70 |
| 22 | 23S1 | 2542 | A | C4-C5-N7 | -5.96 | 107.72 | 110.70 |
| 22 | 23S1 | 2632 | A | N3-C4-N9 | 5.96 | 132.17 | 127.40 |
| 1 | 16S1 | 1433 | A | N9-C4-C5 | 5.96 | 108.18 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 16S1 | 174 | A | C4-C5-C6 | 5.96 | 119.98 | 117.00 |
| 22 | 23S1 | 152 | A | C5-C6-N1 | 5.96 | 120.68 | 117.70 |
| 22 | 23S1 | 616 | A | C4-C5-C6 | 5.96 | 119.98 | 117.00 |
| 22 | 23S1 | 1126 | A | N3-C4-N9 | 5.96 | 132.17 | 127.40 |
| 22 | 23S1 | 1836 | C | C6-N1-C2 | -5.96 | 117.92 | 120.30 |
| 22 | 23S1 | 2080 | A | C5-C6-N1 | 5.96 | 120.68 | 117.70 |
| 22 | 23S1 | 2183 | A | N9-C4-C5 | 5.96 | 108.18 | 105.80 |
| 22 | 23S1 | 2266 | A | C5-C6-N1 | 5.96 | 120.68 | 117.70 |
| 22 | 23S1 | 2733 | A | C4-C5-C6 | 5.96 | 119.98 | 117.00 |
| 1 | 16S1 | 160 | A | C4-C5-C6 | 5.96 | 119.98 | 117.00 |
| 1 | 16S1 | 759 | A | N3-C4-N9 | 5.96 | 132.17 | 127.40 |
| 1 | 16S1 | 1349 | A | C4-C5-C6 | 5.96 | 119.98 | 117.00 |
| 22 | 23S1 | 2411 | A | C4-C5-C6 | 5.96 | 119.98 | 117.00 |
| 23 | 05S1 | 115 | A | N3-C4-N9 | 5.96 | 132.16 | 127.40 |
| 22 | 23S1 | 706 | A | C5-C6-N1 | 5.96 | 120.68 | 117.70 |
| 22 | 23S1 | 2003 | A | C4-C5-C6 | 5.96 | 119.98 | 117.00 |
| 1 | 16S1 | 1377 | A | N3-C4-N9 | 5.95 | 132.16 | 127.40 |
| 22 | 23S1 | 575 | A | C4-C5-C6 | 5.95 | 119.98 | 117.00 |
| 22 | 23S1 | 1977 | A | C4-C5-C6 | 5.95 | 119.98 | 117.00 |
| 22 | 23S1 | 371 | A | C4-C5-N7 | -5.95 | 107.72 | 110.70 |
| 1 | 16S1 | 274 | A | C5-C6-N1 | 5.95 | 120.68 | 117.70 |
| 22 | 23S1 | 1794 | A | C5-C6-N1 | 5.95 | 120.67 | 117.70 |
| 55 | PTR1 | 42 | A | C4-C5-C6 | 5.95 | 119.98 | 117.00 |
| 1 | 16S1 | 149 | A | C4-C5-C6 | 5.95 | 119.97 | 117.00 |
| 1 | 16S1 | 181 | A | C5-C6-N1 | 5.95 | 120.67 | 117.70 |
| 1 | 16S1 | 238 | A | C8-N9-C4 | 5.95 | 108.18 | 105.80 |
| 1 | 16S1 | 320 | A | N3-C4-N9 | 5.95 | 132.16 | 127.40 |
| 1 | 16S1 | 510 | A | N3-C4-N9 | 5.95 | 132.16 | 127.40 |
| 22 | 23S1 | 866 | A | C4-C5-C6 | 5.95 | 119.97 | 117.00 |
| 22 | 23S1 | 1156 | A | C8-N9-C4 | 5.95 | 108.18 | 105.80 |
| 22 | 23S1 | 1269 | A | N9-C4-C5 | 5.95 | 108.18 | 105.80 |
| 22 | 23S1 | 1998 | A | C5-C6-N1 | 5.95 | 120.67 | 117.70 |
| 23 | 05S1 | 119 | A | C4-C5-N7 | -5.95 | 107.73 | 110.70 |
| 22 | 23S1 | 219 | A | N3-C4-N9 | 5.95 | 132.16 | 127.40 |
| 22 | 23S1 | 1431 | A | C8-N9-C4 | 5.95 | 108.18 | 105.80 |
| 22 | 23S1 | 1593 | A | C4-C5-C6 | 5.95 | 119.97 | 117.00 |
| 22 | 23S1 | 2184 | A | N9-C4-C5 | 5.94 | 108.18 | 105.80 |
| 22 | 23S1 | 2634 | A | C5-C6-N1 | 5.94 | 120.67 | 117.70 |
| 1 | 16S1 | 2 | A | C4-C5-C6 | 5.94 | 119.97 | 117.00 |
| 1 | 16S1 | 432 | A | C8-N9-C4 | 5.94 | 108.18 | 105.80 |
| 1 | 16S1 | 935 | A | C4-C5-C6 | 5.94 | 119.97 | 117.00 |
| 22 | 23S1 | 119 | A | C5-C6-N1 | 5.94 | 120.67 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 412 | A | N3-C4-N9 | 5.94 | 132.15 | 127.40 |
| 55 | PTR1 | 62 | C | C6-N1-C2 | -5.94 | 117.92 | 120.30 |
| 1 | 16S1 | 906 | A | N3-C4-N9 | 5.94 | 132.15 | 127.40 |
| 1 | 16S1 | 1329 | A | N3-C4-N9 | 5.94 | 132.15 | 127.40 |
| 22 | 23S1 | 1327 | A | C8-N9-C4 | 5.94 | 108.18 | 105.80 |
| 22 | 23S1 | 1794 | A | C4-C5-C6 | 5.94 | 119.97 | 117.00 |
| 22 | 23S1 | 1960 | A | N3-C4-N9 | 5.94 | 132.15 | 127.40 |
| 22 | 23S1 | 2205 | A | C4-C5-N7 | -5.94 | 107.73 | 110.70 |
| 22 | 23S1 | 2705 | A | N9-C4-C5 | 5.94 | 108.18 | 105.80 |
| 22 | 23S1 | 2826 | A | C8-N9-C4 | 5.94 | 108.18 | 105.80 |
| 22 | 23S1 | 718 | A | N3-C4-N9 | 5.94 | 132.15 | 127.40 |
| 22 | 23S1 | 756 | A | C4-C5-C6 | 5.94 | 119.97 | 117.00 |
| 22 | 23S1 | 1614 | A | C4-C5-C6 | 5.94 | 119.97 | 117.00 |
| 55 | PTR1 | 23 | A | N3-C4-N9 | 5.94 | 132.15 | 127.40 |
| 1 | 16S1 | 1229 | A | N9-C4-C5 | 5.94 | 108.17 | 105.80 |
| 22 | 23S1 | 2281 | A | C5-C6-N1 | 5.94 | 120.67 | 117.70 |
| 1 | 16S1 | 306 | A | C5-C6-N1 | 5.94 | 120.67 | 117.70 |
| 1 | 16S1 | 1274 | A | N3-C4-N9 | 5.94 | 132.15 | 127.40 |
| 1 | 16S1 | 1495 | U | C2-N1-C1' | 5.94 | 124.82 | 117.70 |
| 22 | 23S1 | 1155 | A | N9-C4-C5 | 5.94 | 108.17 | 105.80 |
| 22 | 23S1 | 2587 | A | C4-C5-C6 | 5.94 | 119.97 | 117.00 |
| 22 | 23S1 | 432 | A | N3-C4-N9 | 5.93 | 132.15 | 127.40 |
| 22 | 23S1 | 1427 | A | N9-C4-C5 | 5.93 | 108.17 | 105.80 |
| 22 | 23S1 | 2119 | A | C4-C5-C6 | 5.93 | 119.97 | 117.00 |
| 22 | 23S1 | 2274 | A | C4-C5-C6 | 5.93 | 119.97 | 117.00 |
| 22 | 23S1 | 2327 | A | N9-C4-C5 | 5.93 | 108.17 | 105.80 |
| 1 | 16S1 | 303 | A | C8-N9-C4 | 5.93 | 108.17 | 105.80 |
| 22 | 23S1 | 1784 | A | N3-C4-N9 | 5.93 | 132.15 | 127.40 |
| 22 | 23S1 | 2381 | A | N3-C4-N9 | 5.93 | 132.15 | 127.40 |
| 1 | 16S1 | 1082 | A | N3-C4-N9 | 5.93 | 132.15 | 127.40 |
| 1 | 16S1 | 1534 | A | N9-C4-C5 | 5.93 | 108.17 | 105.80 |
| 22 | 23S1 | 1260 | A | N3-C4-N9 | 5.93 | 132.15 | 127.40 |
| 22 | 23S1 | 1336 | A | C5-C6-N1 | 5.93 | 120.67 | 117.70 |
| 1 | 16S1 | 503 | C | C6-N1-C2 | -5.93 | 117.93 | 120.30 |
| 1 | 16S1 | 532 | A | N3-C4-N9 | 5.93 | 132.14 | 127.40 |
| 22 | 23S1 | 430 | A | C4-C5-C6 | 5.93 | 119.97 | 117.00 |
| 22 | 23S1 | 439 | A | C5-C6-N1 | 5.93 | 120.67 | 117.70 |
| 22 | 23S1 | 2435 | A | C4-C5-N7 | -5.93 | 107.73 | 110.70 |
| 1 | 16S1 | 918 | A | N3-C4-N9 | 5.93 | 132.14 | 127.40 |
| 1 | 16S1 | 1447 | A | C8-N9-C4 | 5.93 | 108.17 | 105.80 |
| 22 | 23S1 | 94 | A | C4-C5-C6 | 5.93 | 119.96 | 117.00 |
| 22 | 23S1 | 155 | A | C8-N9-C4 | 5.93 | 108.17 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 849 | A | N9-C4-C5 | 5.93 | 108.17 | 105.80 |
| 22 | 23S1 | 1502 | A | C4-C5-C6 | 5.93 | 119.96 | 117.00 |
| 1 | 16S1 | 938 | A | C4-C5-C6 | 5.92 | 119.96 | 117.00 |
| 1 | 16S1 | 1408 | A | N9-C4-C5 | 5.92 | 108.17 | 105.80 |
| 22 | 23S1 | 28 | A | N3-C4-N9 | 5.92 | 132.14 | 127.40 |
| 22 | 23S1 | 156 | A | C5-C6-N1 | 5.92 | 120.66 | 117.70 |
| 22 | 23S1 | 265 | A | C8-N9-C4 | 5.92 | 108.17 | 105.80 |
| 22 | 23S1 | 1090 | A | C4-C5-N7 | -5.92 | 107.74 | 110.70 |
| 22 | 23S1 | 1274 | A | C4-C5-C6 | 5.92 | 119.96 | 117.00 |
| 22 | 23S1 | 1677 | A | C4-C5-C6 | 5.92 | 119.96 | 117.00 |
| 23 | 05S1 | 94 | A | C5-C6-N1 | 5.92 | 120.66 | 117.70 |
| 1 | 16S1 | 32 | A | C5-C6-N1 | 5.92 | 120.66 | 117.70 |
| 22 | 23S1 | 1809 | A | C4-C5-C6 | 5.92 | 119.96 | 117.00 |
| 22 | 23S1 | 2058 | A | C4-C5-C6 | 5.92 | 119.96 | 117.00 |
| 22 | 23S1 | 2322 | A | C8-N9-C4 | 5.92 | 108.17 | 105.80 |
| 1 | 16S1 | 1046 | A | C4-C5-N7 | -5.92 | 107.74 | 110.70 |
| 1 | 16S1 | 1362 | A | C4-C5-C6 | 5.92 | 119.96 | 117.00 |
| 22 | 23S1 | 1791 | A | N3-C4-N9 | 5.92 | 132.14 | 127.40 |
| 1 | 16S1 | 182 | A | N3-C4-N9 | 5.92 | 132.14 | 127.40 |
| 1 | 16S1 | 1035 | A | C4-C5-C6 | 5.92 | 119.96 | 117.00 |
| 22 | 23S1 | 401 | A | N3-C4-N9 | 5.92 | 132.14 | 127.40 |
| 22 | 23S1 | 483 | A | C4-C5-C6 | 5.92 | 119.96 | 117.00 |
| 22 | 23S1 | 2322 | A | C4-C5-C6 | 5.92 | 119.96 | 117.00 |
| 1 | 16S1 | 315 | A | N3-C4-N9 | 5.92 | 132.13 | 127.40 |
| 1 | 16S1 | 749 | A | N3-C4-N9 | 5.92 | 132.13 | 127.40 |
| 22 | 23S1 | 1637 | A | N3-C4-N9 | 5.92 | 132.13 | 127.40 |
| 22 | 23S1 | 2031 | A | C4-C5-N7 | -5.92 | 107.74 | 110.70 |
| 1 | 16S1 | 330 | C | N1-C2-O2 | 5.92 | 122.45 | 118.90 |
| 1 | 16S1 | 468 | A | C5-C6-N1 | 5.92 | 120.66 | 117.70 |
| 1 | 16S1 | 845 | A | N3-C4-N9 | 5.92 | 132.13 | 127.40 |
| 1 | 16S1 | 1368 | A | N3-C4-N9 | 5.92 | 132.13 | 127.40 |
| 22 | 23S1 | 909 | A | N9-C4-C5 | 5.92 | 108.17 | 105.80 |
| 22 | 23S1 | 1009 | A | N9-C4-C5 | 5.92 | 108.17 | 105.80 |
| 22 | 23S1 | 1027 | A | C8-N9-C4 | 5.92 | 108.17 | 105.80 |
| 22 | 23S1 | 1590 | A | C4-C5-C6 | 5.92 | 119.96 | 117.00 |
| 22 | 23S1 | 1932 | A | C8-N9-C4 | 5.92 | 108.17 | 105.80 |
| 22 | 23S1 | 2247 | A | C8-N9-C4 | 5.92 | 108.17 | 105.80 |
| 22 | 23S1 | 2577 | A | C8-N9-C4 | 5.92 | 108.17 | 105.80 |
| 55 | PTR1 | 21 | A | N9-C4-C5 | 5.92 | 108.17 | 105.80 |
| 1 | 16S1 | 608 | A | C5-C6-N1 | 5.92 | 120.66 | 117.70 |
| 22 | 23S1 | 1367 | A | C4-C5-C6 | 5.92 | 119.96 | 117.00 |
| 22 | 23S1 | 1508 | A | C8-N9-C4 | 5.92 | 108.17 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 16S1 | 969 | A | C4-C5-N7 | -5.91 | 107.74 | 110.70 |
| 22 | 23S1 | 556 | A | C4-C5-C6 | 5.91 | 119.96 | 117.00 |
| 22 | 23S1 | 699 | A | C4-C5-C6 | 5.91 | 119.96 | 117.00 |
| 22 | 23S1 | 1205 | A | N9-C4-C5 | 5.91 | 108.17 | 105.80 |
| 22 | 23S1 | 1918 | A | N9-C4-C5 | 5.91 | 108.17 | 105.80 |
| 1 | 16S1 | 460 | A | C4-C5-C6 | 5.91 | 119.96 | 117.00 |
| 1 | 16S1 | 602 | A | N3-C4-N9 | 5.91 | 132.13 | 127.40 |
| 22 | 23S1 | 2700 | A | C4-C5-C6 | 5.91 | 119.96 | 117.00 |
| 1 | 16S1 | 236 | A | N9-C4-C5 | 5.91 | 108.16 | 105.80 |
| 1 | 16S1 | 488 | C | N1-C2-O2 | 5.91 | 122.45 | 118.90 |
| 1 | 16S1 | 968 | A | C4-C5-C6 | 5.91 | 119.95 | 117.00 |
| 22 | 23S1 | 401 | A | C4-C5-C6 | 5.91 | 119.95 | 117.00 |
| 22 | 23S1 | 1090 | A | C8-N9-C4 | 5.91 | 108.17 | 105.80 |
| 1 | 16S1 | 1169 | A | N3-C4-N9 | 5.91 | 132.13 | 127.40 |
| 1 | 16S1 | 1349 | A | C8-N9-C4 | 5.91 | 108.16 | 105.80 |
| 22 | 23S1 | 936 | A | C5-C6-N1 | 5.91 | 120.65 | 117.70 |
| 22 | 23S1 | 1900 | A | C8-N9-C4 | 5.91 | 108.16 | 105.80 |
| 22 | 23S1 | 2377 | A | N3-C4-N9 | 5.91 | 132.13 | 127.40 |
| 22 | 23S1 | 2736 | A | C4-C5-N7 | -5.91 | 107.75 | 110.70 |
| 1 | 16S1 | 909 | A | N9-C4-C5 | 5.91 | 108.16 | 105.80 |
| 22 | 23S1 | 829 | A | C4-C5-C6 | 5.91 | 119.95 | 117.00 |
| 22 | 23S1 | 800 | A | N9-C4-C5 | 5.91 | 108.16 | 105.80 |
| 22 | 23S1 | 979 | A | N3-C4-N9 | 5.91 | 132.12 | 127.40 |
| 22 | 23S1 | 1014 | A | C4-C5-C6 | 5.91 | 119.95 | 117.00 |
| 22 | 23S1 | 1144 | A | C5-C6-N1 | 5.91 | 120.65 | 117.70 |
| 1 | 16S1 | 59 | A | C8-N9-C4 | 5.90 | 108.16 | 105.80 |
| 1 | 16S1 | 171 | A | N9-C4-C5 | 5.90 | 108.16 | 105.80 |
| 1 | 16S1 | 722 | G | N3-C4-N9 | 5.90 | 129.54 | 126.00 |
| 22 | 23S1 | 877 | A | C4-C5-C6 | 5.90 | 119.95 | 117.00 |
| 1 | 16S1 | 66 | A | N3-C4-N9 | 5.90 | 132.12 | 127.40 |
| 1 | 16S1 | 116 | A | C8-N9-C4 | 5.90 | 108.16 | 105.80 |
| 1 | 16S1 | 1019 | A | C8-N9-C4 | 5.90 | 108.16 | 105.80 |
| 22 | 23S1 | 299 | A | C4-C5-C6 | 5.90 | 119.95 | 117.00 |
| 22 | 23S1 | 1046 | A | C4-C5-C6 | 5.90 | 119.95 | 117.00 |
| 22 | 23S1 | 2205 | A | C4-C5-C6 | 5.90 | 119.95 | 117.00 |
| 22 | 23S1 | 2469 | A | N3-C4-N9 | 5.90 | 132.12 | 127.40 |
| 1 | 16S1 | 687 | A | N3-C4-N9 | 5.90 | 132.12 | 127.40 |
| 1 | 16S1 | 1248 | A | C8-N9-C4 | 5.90 | 108.16 | 105.80 |
| 5 | S051 | 112 | ARG | NE-CZ-NH1 | -5.90 | 117.35 | 120.30 |
| 22 | 23S1 | 111 | A | N3-C4-N9 | 5.90 | 132.12 | 127.40 |
| 22 | 23S1 | 1586 | A | N9-C4-C5 | 5.90 | 108.16 | 105.80 |
| 22 | 23S1 | 1700 | A | C4-C5-C6 | 5.90 | 119.95 | 117.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 2227 | A | C4-C5-N7 | -5.90 | 107.75 | 110.70 |
| 23 | 05S1 | 31 | C | N1-C2-O2 | 5.90 | 122.44 | 118.90 |
| 1 | 16S1 | 60 | A | C4-C5-C6 | 5.90 | 119.95 | 117.00 |
| 1 | 16S1 | 7 | A | C8-N9-C4 | 5.90 | 108.16 | 105.80 |
| 1 | 16S1 | 780 | A | N3-C4-N9 | 5.90 | 132.12 | 127.40 |
| 1 | 16S1 | 782 | A | C8-N9-C4 | 5.90 | 108.16 | 105.80 |
| 1 | 16S1 | 1430 | A | C4-C5-C6 | 5.90 | 119.95 | 117.00 |
| 22 | 23S1 | 227 | A | N3-C4-N9 | 5.90 | 132.12 | 127.40 |
| 22 | 23S1 | 275 | C | C6-N1-C2 | -5.90 | 117.94 | 120.30 |
| 22 | 23S1 | 685 | A | C8-N9-C4 | 5.90 | 108.16 | 105.80 |
| 22 | 23S1 | 1194 | A | N9-C4-C5 | 5.90 | 108.16 | 105.80 |
| 1 | 16S1 | 1428 | A | C4-C5-C6 | 5.89 | 119.95 | 117.00 |
| 22 | 23S1 | 1080 | A | C4-C5-C6 | 5.89 | 119.95 | 117.00 |
| 22 | 23S1 | 1247 | A | C5-C6-N1 | 5.89 | 120.65 | 117.70 |
| 22 | 23S1 | 1265 | A | C4-C5-C6 | 5.89 | 119.95 | 117.00 |
| 22 | 23S1 | 1285 | A | N9-C4-C5 | 5.89 | 108.16 | 105.80 |
| 22 | 23S1 | 1301 | A | C4-C5-C6 | 5.89 | 119.95 | 117.00 |
| 22 | 23S1 | 1403 | A | C5-C6-N1 | 5.89 | 120.65 | 117.70 |
| 22 | 23S1 | 1614 | A | C8-N9-C4 | 5.89 | 108.16 | 105.80 |
| 22 | 23S1 | 1819 | A | C8-N9-C4 | 5.89 | 108.16 | 105.80 |
| 22 | 23S1 | 2212 | A | N3-C4-N9 | 5.89 | 132.12 | 127.40 |
| 23 | 05S1 | 31 | C | C6-N1-C2 | -5.89 | 117.94 | 120.30 |
| 23 | 05S1 | 50 | A | C4-C5-C6 | 5.89 | 119.95 | 117.00 |
| 55 | PTR1 | 76 | A | N3-C4-N9 | 5.89 | 132.12 | 127.40 |
| 1 | 16S1 | 116 | A | C5-C6-N1 | 5.89 | 120.65 | 117.70 |
| 1 | 16S1 | 1171 | A | C8-N9-C4 | 5.89 | 108.16 | 105.80 |
| 22 | 23S1 | 1532 | A | N3-C4-N9 | 5.89 | 132.12 | 127.40 |
| 22 | 23S1 | 2810 | A | N9-C4-C5 | 5.89 | 108.16 | 105.80 |
| 23 | 05S1 | 50 | A | C8-N9-C4 | 5.89 | 108.16 | 105.80 |
| 1 | 16S1 | 211 | G | N3-C4-C5 | -5.89 | 125.65 | 128.60 |
| 22 | 23S1 | 89 | A | N3-C4-N9 | 5.89 | 132.11 | 127.40 |
| 22 | 23S1 | 1610 | A | C8-N9-C4 | 5.89 | 108.16 | 105.80 |
| 22 | 23S1 | 2162 | G | OP1-P-O3' | 5.89 | 118.16 | 105.20 |
| 22 | 23S1 | 2602 | A | C4-C5-N7 | -5.89 | 107.75 | 110.70 |
| 1 | 16S1 | 98 | A | C5-C6-N1 | 5.89 | 120.64 | 117.70 |
| 1 | 16S1 | 583 | A | C5-N7-C8 | 5.89 | 106.84 | 103.90 |
| 1 | 16S1 | 1111 | A | C4-C5-C6 | 5.89 | 119.94 | 117.00 |
| 1 | 16S1 | 1167 | A | C4-C5-C6 | 5.89 | 119.94 | 117.00 |
| 22 | 23S1 | 155 | A | C5-C6-N1 | 5.89 | 120.64 | 117.70 |
| 22 | 23S1 | 626 | A | C4-C5-C6 | 5.89 | 119.94 | 117.00 |
| 22 | 23S1 | 905 | A | C8-N9-C4 | 5.89 | 108.16 | 105.80 |
| 22 | 23S1 | 2212 | A | N9-C4-C5 | 5.89 | 108.16 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 1 | 16S1 | 262 | A | N3-C4-N9 | 5.89 | 132.11 | 127.40 |
| 1 | 16S1 | 336 | A | N3-C4-N9 | 5.89 | 132.11 | 127.40 |
| 1 | 16S1 | 629 | A | N3-C4-N9 | 5.89 | 132.11 | 127.40 |
| 1 | 16S1 | 716 | A | C5-C6-N1 | 5.89 | 120.64 | 117.70 |
| 1 | 16S1 | 946 | A | C5-C6-N1 | 5.89 | 120.64 | 117.70 |
| 22 | 23S1 | 666 | A | C8-N9-C4 | 5.89 | 108.16 | 105.80 |
| 22 | 23S1 | 945 | A | N3-C4-N9 | 5.89 | 132.11 | 127.40 |
| 22 | 23S1 | 1260 | A | C4-C5-C6 | 5.89 | 119.94 | 117.00 |
| 22 | 23S1 | 1632 | A | N9-C4-C5 | 5.89 | 108.16 | 105.80 |
| 22 | 23S1 | 1932 | A | N3-C4-N9 | 5.89 | 132.11 | 127.40 |
| 22 | 23S1 | 2856 | A | N3-C4-N9 | 5.89 | 132.11 | 127.40 |
| 1 | 16S1 | 33 | A | C5-C6-N1 | 5.88 | 120.64 | 117.70 |
| 1 | 16S1 | 119 | A | N9-C4-C5 | 5.88 | 108.15 | 105.80 |
| 1 | 16S1 | 181 | A | C8-N9-C4 | 5.88 | 108.15 | 105.80 |
| 1 | 16S1 | 228 | A | C4-C5-C6 | 5.88 | 119.94 | 117.00 |
| 22 | 23S1 | 655 | A | N3-C4-N9 | 5.88 | 132.11 | 127.40 |
| 22 | 23S1 | 753 | A | C5-C6-N1 | 5.88 | 120.64 | 117.70 |
| 22 | 23S1 | 1711 | A | C5-C6-N1 | 5.88 | 120.64 | 117.70 |
| 22 | 23S1 | 2376 | A | C4-C5-C6 | 5.88 | 119.94 | 117.00 |
| 23 | 05S1 | 52 | A | N3-C4-N9 | 5.88 | 132.11 | 127.40 |
| 1 | 16S1 | 787 | A | N3-C4-N9 | 5.88 | 132.11 | 127.40 |
| 1 | 16S1 | 1350 | A | C5-C6-N1 | 5.88 | 120.64 | 117.70 |
| 22 | 23S1 | 2478 | A | C5-C6-N1 | 5.88 | 120.64 | 117.70 |
| 23 | 05S1 | 53 | A | C8-N9-C4 | 5.88 | 108.15 | 105.80 |
| 1 | 16S1 | 51 | A | C8-N9-C4 | 5.88 | 108.15 | 105.80 |
| 22 | 23S1 | 1383 | A | C4-C5-C6 | 5.88 | 119.94 | 117.00 |
| 22 | 23S1 | 2899 | A | C4-C5-C6 | 5.88 | 119.94 | 117.00 |
| 1 | 16S1 | 872 | A | N9-C4-C5 | 5.88 | 108.15 | 105.80 |
| 22 | 23S1 | 63 | A | N3-C4-N9 | 5.88 | 132.10 | 127.40 |
| 1 | 16S1 | 321 | A | N3-C4-N9 | 5.88 | 132.10 | 127.40 |
| 22 | 23S1 | 739 | A | C5-C6-N1 | 5.88 | 120.64 | 117.70 |
| 22 | 23S1 | 2765 | A | C5-C6-N1 | 5.88 | 120.64 | 117.70 |
| 22 | 23S1 | 2886 | A | C8-N9-C4 | 5.88 | 108.15 | 105.80 |
| 1 | 16S1 | 298 | A | N3-C4-N9 | 5.88 | 132.10 | 127.40 |
| 1 | 16S1 | 1130 | A | N9-C4-C5 | 5.88 | 108.15 | 105.80 |
| 23 | 05S1 | 104 | A | N3-C4-N9 | 5.88 | 132.10 | 127.40 |
| 1 | 16S1 | 313 | A | C4-C5-C6 | 5.87 | 119.94 | 117.00 |
| 22 | 23S1 | 1739 | A | C5-N7-C8 | 5.87 | 106.84 | 103.90 |
| 22 | 23S1 | 74 | A | C4-C5-C6 | 5.87 | 119.94 | 117.00 |
| 22 | 23S1 | 320 | A | C4-C5-C6 | 5.87 | 119.94 | 117.00 |
| 22 | 23S1 | 404 | A | C8-N9-C4 | 5.87 | 108.15 | 105.80 |
| 22 | 23S1 | 1264 | A | N9-C4-C5 | 5.87 | 108.15 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 1596 | A | C5-C6-N1 | 5.87 | 120.64 | 117.70 |
| 22 | 23S1 | 2189 | U | O5'-P-OP1 | -5.87 | 100.42 | 105.70 |
| 23 | 05S1 | 108 | A | C5-C6-N1 | 5.87 | 120.64 | 117.70 |
| 22 | 23S1 | 1805 | A | C4-C5-C6 | 5.87 | 119.94 | 117.00 |
| 1 | 16S1 | 1101 | A | C4-C5-N7 | -5.87 | 107.77 | 110.70 |
| 1 | 16S1 | 1261 | A | C5-C6-N1 | 5.87 | 120.63 | 117.70 |
| 22 | 23S1 | 1246 | A | C4-C5-N7 | -5.87 | 107.77 | 110.70 |
| 22 | 23S1 | 1672 | A | C8-N9-C4 | 5.87 | 108.15 | 105.80 |
| 22 | 23S1 | 1711 | A | C8-N9-C4 | 5.87 | 108.15 | 105.80 |
| 22 | 23S1 | 2449 | U | C6-N1-C2 | 5.87 | 124.52 | 121.00 |
| 22 | 23S1 | 676 | A | N9-C4-C5 | 5.87 | 108.15 | 105.80 |
| 22 | 23S1 | 2748 | A | N3-C4-N9 | 5.87 | 132.09 | 127.40 |
| 1 | 16S1 | 937 | A | N9-C4-C5 | 5.87 | 108.15 | 105.80 |
| 1 | 16S1 | 1238 | A | N3-C4-N9 | 5.87 | 132.09 | 127.40 |
| 22 | 23S1 | 1549 | A | C4-C5-C6 | 5.87 | 119.93 | 117.00 |
| 22 | 23S1 | 1853 | A | C8-N9-C4 | 5.87 | 108.15 | 105.80 |
| 23 | 05S1 | 39 | A | N3-C4-N9 | 5.87 | 132.09 | 127.40 |
| 22 | 23S1 | 412 | A | C8-N9-C4 | 5.86 | 108.14 | 105.80 |
| 22 | 23S1 | 510 | C | N3-C2-O2 | -5.86 | 117.80 | 121.90 |
| 22 | 23S1 | 920 | A | N3-C4-N9 | 5.86 | 132.09 | 127.40 |
| 22 | 23S1 | 1069 | A | N3-C4-N9 | 5.86 | 132.09 | 127.40 |
| 22 | 23S1 | 1637 | A | N9-C4-C5 | 5.86 | 108.14 | 105.80 |
| 22 | 23S1 | 2354 | C | N3-C2-O2 | -5.86 | 117.80 | 121.90 |
| 22 | 23S1 | 2471 | A | N3-C4-N9 | 5.86 | 132.09 | 127.40 |
| 22 | 23S1 | 1652 | A | C8-N9-C4 | 5.86 | 108.14 | 105.80 |
| 1 | 16S1 | 149 | A | N3-C4-N9 | 5.86 | 132.09 | 127.40 |
| 1 | 16S1 | 327 | A | N3-C4-N9 | 5.86 | 132.09 | 127.40 |
| 1 | 16S1 | 1534 | A | N3-C4-N9 | 5.86 | 132.09 | 127.40 |
| 22 | 23S1 | 936 | A | C8-N9-C4 | 5.86 | 108.14 | 105.80 |
| 1 | 16S1 | 845 | A | C4-C5-C6 | 5.86 | 119.93 | 117.00 |
| 22 | 23S1 | 279 | A | N3-C4-N9 | 5.86 | 132.09 | 127.40 |
| 22 | 23S1 | 590 | A | N3-C4-N9 | 5.86 | 132.09 | 127.40 |
| 22 | 23S1 | 1927 | A | N3-C4-N9 | 5.86 | 132.09 | 127.40 |
| 22 | 23S1 | 2418 | A | N9-C4-C5 | 5.86 | 108.14 | 105.80 |
| 22 | 23S1 | 2826 | A | C5-C6-N1 | 5.86 | 120.63 | 117.70 |
| 1 | 16S1 | 366 | A | N3-C4-N9 | 5.86 | 132.08 | 127.40 |
| 1 | 16S1 | 1441 | A | N3-C4-N9 | 5.86 | 132.09 | 127.40 |
| 22 | 23S1 | 165 | A | N9-C4-C5 | 5.86 | 108.14 | 105.80 |
| 22 | 23S1 | 199 | A | N9-C4-C5 | 5.86 | 108.14 | 105.80 |
| 22 | 23S1 | 354 | A | C4-C5-N7 | -5.86 | 107.77 | 110.70 |
| 22 | 23S1 | 668 | A | C8-N9-C4 | 5.86 | 108.14 | 105.80 |
| 22 | 23S1 | 2565 | A | C8-N9-C4 | 5.86 | 108.14 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 55 | PTR1 | 69 | A | C8-N9-C4 | 5.86 | 108.14 | 105.80 |
| 1 | 16S1 | 546 | A | C4-C5-C6 | 5.85 | 119.93 | 117.00 |
| 1 | 16S1 | 655 | A | C5-C6-N1 | 5.85 | 120.63 | 117.70 |
| 22 | 23S1 | 2225 | A | C8-N9-C4 | 5.85 | 108.14 | 105.80 |
| 22 | 23S1 | 2598 | A | N3-C4-N9 | 5.85 | 132.08 | 127.40 |
| 1 | 16S1 | 1251 | A | N3-C4-N9 | 5.85 | 132.08 | 127.40 |
| 22 | 23S1 | 2634 | A | C8-N9-C4 | 5.85 | 108.14 | 105.80 |
| 23 | 05S1 | 75 | G | N3-C4-N9 | 5.85 | 129.51 | 126.00 |
| 1 | 16S1 | 1271 | A | C8-N9-C4 | 5.85 | 108.14 | 105.80 |
| 1 | 16S1 | 58 | C | C6-N1-C2 | -5.85 | 117.96 | 120.30 |
| 1 | 16S1 | 675 | A | N3-C4-N9 | 5.85 | 132.08 | 127.40 |
| 1 | 16S1 | 1289 | A | N9-C4-C5 | 5.85 | 108.14 | 105.80 |
| 1 | 16S1 | 1360 | A | N3-C4-N9 | 5.85 | 132.08 | 127.40 |
| 1 | 16S1 | 1513 | A | C4-C5-C6 | 5.85 | 119.92 | 117.00 |
| 22 | 23S1 | 125 | A | N3-C4-N9 | 5.85 | 132.08 | 127.40 |
| 22 | 23S1 | 217 | A | C4-C5-C6 | 5.85 | 119.92 | 117.00 |
| 22 | 23S1 | 262 | A | C4-C5-N7 | -5.85 | 107.78 | 110.70 |
| 22 | 23S1 | 550 | C | C6-N1-C2 | -5.85 | 117.96 | 120.30 |
| 22 | 23S1 | 609 | A | N9-C4-C5 | 5.85 | 108.14 | 105.80 |
| 22 | 23S1 | 742 | A | C5-C6-N1 | 5.85 | 120.62 | 117.70 |
| 22 | 23S1 | 1914 | C | C6-N1-C2 | -5.85 | 117.96 | 120.30 |
| 1 | 16S1 | 1 | A | N3-C4-N9 | 5.85 | 132.08 | 127.40 |
| 1 | 16S1 | 747 | A | N3-C4-N9 | 5.85 | 132.08 | 127.40 |
| 1 | 16S1 | 1493 | A | C8-N9-C4 | 5.85 | 108.14 | 105.80 |
| 22 | 23S1 | 401 | A | C8-N9-C4 | 5.85 | 108.14 | 105.80 |
| 22 | 23S1 | 643 | A | N3-C4-N9 | 5.85 | 132.08 | 127.40 |
| 22 | 23S1 | 905 | A | N3-C4-N9 | 5.85 | 132.08 | 127.40 |
| 22 | 23S1 | 1359 | A | C5-C6-N1 | 5.85 | 120.62 | 117.70 |
| 1 | 16S1 | 16 | A | C4-C5-N7 | -5.85 | 107.78 | 110.70 |
| 1 | 16S1 | 1239 | A | C8-N9-C4 | 5.85 | 108.14 | 105.80 |
| 22 | 23S1 | 1420 | A | C4-C5-C6 | 5.85 | 119.92 | 117.00 |
| 22 | 23S1 | 1668 | A | C4-C5-N7 | -5.85 | 107.78 | 110.70 |
| 22 | 23S1 | 207 | A | C5-C6-N1 | 5.84 | 120.62 | 117.70 |
| 22 | 23S1 | 1596 | A | N3-C4-N9 | 5.84 | 132.07 | 127.40 |
| 22 | 23S1 | 1952 | A | N9-C4-C5 | 5.84 | 108.14 | 105.80 |
| 22 | 23S1 | 2199 | A | C8-N9-C4 | 5.84 | 108.14 | 105.80 |
| 22 | 23S1 | 2270 | A | C4-C5-N7 | -5.84 | 107.78 | 110.70 |
| 1 | 16S1 | 1168 | U | N3-C2-O2 | -5.84 | 118.11 | 122.20 |
| 22 | 23S1 | 2184 | A | C4-C5-C6 | 5.84 | 119.92 | 117.00 |
| 1 | 16S1 | 50 | A | C8-N9-C4 | 5.84 | 108.14 | 105.80 |
| 22 | 23S1 | 1050 | A | C4-C5-N7 | -5.84 | 107.78 | 110.70 |
| 22 | 23S1 | 2119 | A | N3-C4-N9 | 5.84 | 132.07 | 127.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 23 | 05S1 | 29 | A | C4-C5-C6 | 5.84 | 119.92 | 117.00 |
| 22 | 23S1 | 167 | A | N3-C4-N9 | 5.84 | 132.07 | 127.40 |
| 22 | 23S1 | 429 | A | N9-C4-C5 | 5.84 | 108.14 | 105.80 |
| 22 | 23S1 | 2042 | A | C4-C5-C6 | 5.84 | 119.92 | 117.00 |
| 22 | 23S1 | 792 | A | C8-N9-C4 | 5.84 | 108.14 | 105.80 |
| 22 | 23S1 | 1551 | A | N9-C4-C5 | 5.84 | 108.14 | 105.80 |
| 22 | 23S1 | 1678 | A | C8-N9-C4 | 5.84 | 108.14 | 105.80 |
| 22 | 23S1 | 1866 | A | N9-C4-C5 | 5.84 | 108.14 | 105.80 |
| 1 | 16S1 | 1046 | A | N9-C4-C5 | 5.84 | 108.13 | 105.80 |
| 22 | 23S1 | 346 | A | C4-C5-C6 | 5.84 | 119.92 | 117.00 |
| 22 | 23S1 | 609 | A | N3-C4-N9 | 5.84 | 132.07 | 127.40 |
| 22 | 23S1 | 716 | A | C8-N9-C4 | 5.84 | 108.13 | 105.80 |
| 22 | 23S1 | 1096 | A | N3-C4-N9 | 5.84 | 132.07 | 127.40 |
| 22 | 23S1 | 2278 | A | C8-N9-C4 | 5.84 | 108.13 | 105.80 |
| 1 | 16S1 | 246 | A | N3-C4-N9 | 5.83 | 132.07 | 127.40 |
| 1 | 16S1 | 907 | A | C8-N9-C4 | 5.83 | 108.13 | 105.80 |
| 22 | 23S1 | 165 | A | C8-N9-C4 | 5.83 | 108.13 | 105.80 |
| 22 | 23S1 | 1021 | A | C5-C6-N1 | 5.83 | 120.62 | 117.70 |
| 22 | 23S1 | 1786 | A | C4-C5-N7 | -5.83 | 107.78 | 110.70 |
| 22 | 23S1 | 1848 | A | N3-C4-N9 | 5.83 | 132.07 | 127.40 |
| 1 | 16S1 | 371 | A | C5-C6-N1 | 5.83 | 120.62 | 117.70 |
| 1 | 16S1 | 1196 | A | N3-C4-N9 | 5.83 | 132.07 | 127.40 |
| 22 | 23S1 | 716 | A | N3-C4-N9 | 5.83 | 132.07 | 127.40 |
| 22 | 23S1 | 2184 | A | N3-C4-N9 | 5.83 | 132.07 | 127.40 |
| 22 | 23S1 | 915 | C | N1-C2-O2 | 5.83 | 122.40 | 118.90 |
| 22 | 23S1 | 1503 | A | N9-C4-C5 | 5.83 | 108.13 | 105.80 |
| 22 | 23S1 | 2033 | A | C4-C5-N7 | -5.83 | 107.78 | 110.70 |
| 22 | 23S1 | 2450 | A | C5-N7-C8 | 5.83 | 106.81 | 103.90 |
| 22 | 23S1 | 643 | A | C8-N9-C4 | 5.83 | 108.13 | 105.80 |
| 23 | 05S1 | 78 | A | N3-C4-N9 | 5.83 | 132.06 | 127.40 |
| 1 | 16S1 | 279 | A | C5-N7-C8 | 5.83 | 106.81 | 103.90 |
| 1 | 16S1 | 908 | A | N3-C4-N9 | 5.83 | 132.06 | 127.40 |
| 22 | 23S1 | 348 | A | C8-N9-C4 | 5.83 | 108.13 | 105.80 |
| 22 | 23S1 | 586 | A | N9-C4-C5 | 5.83 | 108.13 | 105.80 |
| 22 | 23S1 | 743 | A | N9-C4-C5 | 5.83 | 108.13 | 105.80 |
| 22 | 23S1 | 1395 | A | C5-C6-N1 | 5.83 | 120.61 | 117.70 |
| 22 | 23S1 | 2198 | A | C4-C5-C6 | 5.83 | 119.91 | 117.00 |
| 22 | 23S1 | 2381 | A | C5-C6-N1 | 5.83 | 120.61 | 117.70 |
| 1 | 16S1 | 205 | A | N9-C4-C5 | 5.83 | 108.13 | 105.80 |
| 1 | 16S1 | 935 | A | C8-N9-C4 | 5.83 | 108.13 | 105.80 |
| 22 | 23S1 | 2311 | A | C5-C6-N1 | 5.83 | 120.61 | 117.70 |
| 1 | 16S1 | 320 | A | C5-C6-N1 | 5.83 | 120.61 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 528 | A | C4-C5-C6 | 5.83 | 119.91 | 117.00 |
| 22 | 23S1 | 1095 | A | C4-C5-C6 | 5.83 | 119.91 | 117.00 |
| 22 | 23S1 | 1095 | A | N9-C4-C5 | 5.83 | 108.13 | 105.80 |
| 22 | 23S1 | 1759 | A | C4-C5-C6 | 5.83 | 119.91 | 117.00 |
| 22 | 23S1 | 2227 | A | N9-C4-C5 | 5.83 | 108.13 | 105.80 |
| 1 | 16S1 | 743 | A | C4-C5-C6 | 5.82 | 119.91 | 117.00 |
| 22 | 23S1 | 2873 | A | N3-C4-N9 | 5.82 | 132.06 | 127.40 |
| 22 | 23S1 | 1286 | A | C5-C6-N1 | 5.82 | 120.61 | 117.70 |
| 1 | 16S1 | 1410 | A | N9-C4-C5 | 5.82 | 108.13 | 105.80 |
| 1 | 16S1 | 1499 | A | C8-N9-C4 | 5.82 | 108.13 | 105.80 |
| 22 | 23S1 | 362 | A | C5-C6-N6 | 5.82 | 128.36 | 123.70 |
| 22 | 23S1 | 1780 | A | C4-C5-C6 | 5.82 | 119.91 | 117.00 |
| 22 | 23S1 | 2378 | A | N3-C4-N9 | 5.82 | 132.06 | 127.40 |
| 22 | 23S1 | 1679 | A | N3-C4-N9 | 5.82 | 132.06 | 127.40 |
| 1 | 16S1 | 199 | A | C8-N9-C4 | 5.82 | 108.13 | 105.80 |
| 1 | 16S1 | 454 | G | N3-C4-N9 | 5.82 | 129.49 | 126.00 |
| 22 | 23S1 | 1156 | A | C4-C5-C6 | 5.82 | 119.91 | 117.00 |
| 1 | 16S1 | 622 | A | C5-N7-C8 | 5.82 | 106.81 | 103.90 |
| 22 | 23S1 | 1230 | A | C4-C5-N7 | -5.82 | 107.79 | 110.70 |
| 22 | 23S1 | 382 | A | C4-C5-N7 | -5.81 | 107.79 | 110.70 |
| 22 | 23S1 | 878 | A | C4-C5-N7 | -5.81 | 107.79 | 110.70 |
| 22 | 23S1 | 2314 | A | C4-C5-C6 | 5.81 | 119.91 | 117.00 |
| 1 | 16S1 | 523 | A | C8-N9-C4 | 5.81 | 108.12 | 105.80 |
| 1 | 16S1 | 777 | A | N3-C4-N9 | 5.81 | 132.05 | 127.40 |
| 1 | 16S1 | 782 | A | C4-C5-N7 | -5.81 | 107.79 | 110.70 |
| 1 | 16S1 | 1179 | A | N9-C4-C5 | 5.81 | 108.12 | 105.80 |
| 1 | 16S1 | 1329 | A | C4-C5-N7 | -5.81 | 107.79 | 110.70 |
| 1 | 16S1 | 1408 | A | C8-N9-C4 | 5.81 | 108.12 | 105.80 |
| 22 | 23S1 | 1532 | A | C4-C5-C6 | 5.81 | 119.91 | 117.00 |
| 22 | 23S1 | 2700 | A | C5-C6-N1 | 5.81 | 120.61 | 117.70 |
| 1 | 16S1 | 139 | A | N3-C4-N9 | 5.81 | 132.05 | 127.40 |
| 1 | 16S1 | 553 | A | C4-C5-N7 | -5.81 | 107.79 | 110.70 |
| 1 | 16S1 | 1035 | A | N3-C4-N9 | 5.81 | 132.05 | 127.40 |
| 22 | 23S1 | 371 | A | N9-C4-C5 | 5.81 | 108.12 | 105.80 |
| 22 | 23S1 | 1505 | A | N9-C4-C5 | 5.81 | 108.12 | 105.80 |
| 22 | 23S1 | 1522 | A | C8-N9-C4 | 5.81 | 108.12 | 105.80 |
| 22 | 23S1 | 2170 | A | N3-C4-N9 | 5.81 | 132.05 | 127.40 |
| 1 | 16S1 | 477 | C | N3-C2-O2 | -5.81 | 117.83 | 121.90 |
| 22 | 23S1 | 508 | A | N3-C4-N9 | 5.81 | 132.05 | 127.40 |
| 22 | 23S1 | 644 | A | C5-C6-N1 | 5.81 | 120.61 | 117.70 |
| 22 | 23S1 | 825 | A | C5-C6-N1 | 5.81 | 120.60 | 117.70 |
| 22 | 23S1 | 1509 | A | C4-C5-C6 | 5.81 | 119.90 | 117.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 16S1 | 503 | C | N3-C2-O2 | -5.81 | 117.83 | 121.90 |
| 1 | 16S1 | 535 | A | N3-C4-N9 | 5.81 | 132.05 | 127.40 |
| 1 | 16S1 | 573 | A | N9-C4-C5 | 5.81 | 108.12 | 105.80 |
| 1 | 16S1 | 649 | A | N9-C4-C5 | 5.81 | 108.12 | 105.80 |
| 22 | 23S1 | 384 | A | C8-N9-C4 | 5.81 | 108.12 | 105.80 |
| 22 | 23S1 | 838 | C | N3-C2-O2 | -5.81 | 117.83 | 121.90 |
| 22 | 23S1 | 975 | A | C4-C5-C6 | 5.81 | 119.90 | 117.00 |
| 22 | 23S1 | 1927 | A | C4-C5-C6 | 5.81 | 119.90 | 117.00 |
| 22 | 23S1 | 1080 | A | C5-C6-N1 | 5.81 | 120.60 | 117.70 |
| 22 | 23S1 | 2052 | A | C4-C5-C6 | 5.81 | 119.90 | 117.00 |
| 22 | 23S1 | 637 | A | C8-N9-C4 | 5.80 | 108.12 | 105.80 |
| 22 | 23S1 | 866 | A | N3-C4-N9 | 5.80 | 132.04 | 127.40 |
| 22 | 23S1 | 947 | A | C5-C6-N1 | 5.80 | 120.60 | 117.70 |
| 22 | 23S1 | 1347 | A | C4-C5-N7 | -5.80 | 107.80 | 110.70 |
| 22 | 23S1 | 1637 | A | C4-C5-C6 | 5.80 | 119.90 | 117.00 |
| 22 | 23S1 | 1916 | A | N9-C4-C5 | 5.80 | 108.12 | 105.80 |
| 1 | 16S1 | 1110 | A | C4-C5-C6 | 5.80 | 119.90 | 117.00 |
| 22 | 23S1 | 1698 | A | N3-C4-N9 | 5.80 | 132.04 | 127.40 |
| 22 | 23S1 | 2170 | A | N9-C4-C5 | 5.80 | 108.12 | 105.80 |
| 22 | 23S1 | 2675 | A | C8-N9-C4 | 5.80 | 108.12 | 105.80 |
| 55 | PTR1 | 73 | A | N3-C4-N9 | 5.80 | 132.04 | 127.40 |
| 1 | 16S1 | 1080 | A | N3-C4-N9 | 5.80 | 132.04 | 127.40 |
| 22 | 23S1 | 1494 | A | N9-C4-C5 | 5.80 | 108.12 | 105.80 |
| 22 | 23S1 | 1789 | A | C4-C5-C6 | 5.80 | 119.90 | 117.00 |
| 22 | 23S1 | 1938 | A | N3-C4-N9 | 5.80 | 132.04 | 127.40 |
| 22 | 23S1 | 2333 | A | C4-C5-C6 | 5.80 | 119.90 | 117.00 |
| 1 | 16S1 | 380 | G | C2-N3-C4 | -5.80 | 109.00 | 111.90 |
| 22 | 23S1 | 1287 | A | C4-C5-C6 | 5.80 | 119.90 | 117.00 |
| 23 | 05S1 | 104 | A | C8-N9-C4 | 5.80 | 108.12 | 105.80 |
| 1 | 16S1 | 192 | A | N9-C4-C5 | 5.79 | 108.12 | 105.80 |
| 1 | 16S1 | 262 | A | C4-C5-C6 | 5.79 | 119.90 | 117.00 |
| 1 | 16S1 | 722 | G | N3-C4-C5 | -5.79 | 125.70 | 128.60 |
| 1 | 16S1 | 1238 | A | C4-C5-C6 | 5.79 | 119.90 | 117.00 |
| 22 | 23S1 | 592 | A | C8-N9-C4 | 5.79 | 108.12 | 105.80 |
| 22 | 23S1 | 742 | A | C4-C5-C6 | 5.79 | 119.90 | 117.00 |
| 22 | 23S1 | 1803 | A | C4-C5-C6 | 5.79 | 119.90 | 117.00 |
| 22 | 23S1 | 2740 | A | C5-C6-N1 | 5.79 | 120.60 | 117.70 |
| 1 | 16S1 | 250 | A | N3-C4-N9 | 5.79 | 132.03 | 127.40 |
| 1 | 16S1 | 336 | A | C4-C5-C6 | 5.79 | 119.89 | 117.00 |
| 1 | 16S1 | 364 | A | C4-C5-N7 | -5.79 | 107.81 | 110.70 |
| 1 | 16S1 | 932 | C | N1-C2-O2 | 5.79 | 122.37 | 118.90 |
| 22 | 23S1 | 1502 | A | C5-C6-N1 | 5.79 | 120.59 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 16S1 | 60 | A | C4-C5-N7 | -5.79 | 107.81 | 110.70 |
| 1 | 16S1 | 547 | A | C4-C5-C6 | 5.79 | 119.89 | 117.00 |
| 1 | 16S1 | 1500 | A | C8-N9-C4 | 5.79 | 108.12 | 105.80 |
| 22 | 23S1 | 990 | A | N3-C4-N9 | 5.79 | 132.03 | 127.40 |
| 22 | 23S1 | 1413 | A | C4-C5-C6 | 5.79 | 119.89 | 117.00 |
| 22 | 23S1 | 1437 | C | N1-C2-O2 | 5.79 | 122.37 | 118.90 |
| 22 | 23S1 | 1590 | A | C5-C6-N1 | 5.79 | 120.59 | 117.70 |
| 22 | 23S1 | 2015 | A | C4-C5-C6 | 5.79 | 119.89 | 117.00 |
| 23 | 05S1 | 108 | A | N3-C4-N9 | 5.79 | 132.03 | 127.40 |
| 1 | 16S1 | 80 | A | N9-C4-C5 | 5.79 | 108.11 | 105.80 |
| 22 | 23S1 | 800 | A | C4-C5-N7 | -5.79 | 107.81 | 110.70 |
| 1 | 16S1 | 1428 | A | C4-C5-N7 | -5.79 | 107.81 | 110.70 |
| 22 | 23S1 | 340 | A | C8-N9-C4 | 5.79 | 108.11 | 105.80 |
| 22 | 23S1 | 541 | A | N9-C4-C5 | 5.79 | 108.11 | 105.80 |
| 22 | 23S1 | 1077 | A | C8-N9-C4 | 5.79 | 108.11 | 105.80 |
| 22 | 23S1 | 1913 | A | N3-C4-N9 | 5.79 | 132.03 | 127.40 |
| 22 | 23S1 | 1960 | A | C5-C6-N1 | 5.79 | 120.59 | 117.70 |
| 22 | 23S1 | 2297 | A | N3-C4-N9 | 5.79 | 132.03 | 127.40 |
| 1 | 16S1 | 94 | G | O5'-P-OP2 | -5.78 | 100.50 | 105.70 |
| 1 | 16S1 | 602 | A | C4-C5-C6 | 5.78 | 119.89 | 117.00 |
| 1 | 16S1 | 1433 | A | C4-C5-C6 | 5.78 | 119.89 | 117.00 |
| 22 | 23S1 | 668 | A | C4-C5-C6 | 5.78 | 119.89 | 117.00 |
| 22 | 23S1 | 1347 | A | N9-C4-C5 | 5.78 | 108.11 | 105.80 |
| 22 | 23S1 | 2439 | A | C8-N9-C4 | 5.78 | 108.11 | 105.80 |
| 1 | 16S1 | 1430 | A | N3-C4-N9 | 5.78 | 132.03 | 127.40 |
| 22 | 23S1 | 49 | A | C4-C5-N7 | -5.78 | 107.81 | 110.70 |
| 22 | 23S1 | 472 | A | N3-C4-N9 | 5.78 | 132.03 | 127.40 |
| 22 | 23S1 | 2013 | A | C4-C5-C6 | 5.78 | 119.89 | 117.00 |
| 22 | 23S1 | 2247 | A | C4-C5-C6 | 5.78 | 119.89 | 117.00 |
| 22 | 23S1 | 2590 | A | C4-C5-N7 | -5.78 | 107.81 | 110.70 |
| 23 | 05S1 | 99 | A | C4-C5-C6 | 5.78 | 119.89 | 117.00 |
| 1 | 16S1 | 649 | A | C4-C5-C6 | 5.78 | 119.89 | 117.00 |
| 22 | 23S1 | 501 | A | N3-C4-N9 | 5.78 | 132.02 | 127.40 |
| 22 | 23S1 | 1664 | A | C5-C6-N1 | 5.78 | 120.59 | 117.70 |
| 22 | 23S1 | 1670 | C | C6-N1-C2 | -5.78 | 117.99 | 120.30 |
| 22 | 23S1 | 1997 | C | C6-N1-C2 | -5.78 | 117.99 | 120.30 |
| 22 | 23S1 | 2388 | A | C4-C5-C6 | 5.78 | 119.89 | 117.00 |
| 1 | 16S1 | 1082 | A | C4-C5-C6 | 5.78 | 119.89 | 117.00 |
| 1 | 16S1 | 28 | A | C5-C6-N1 | 5.77 | 120.59 | 117.70 |
| 1 | 16S1 | 313 | A | N9-C4-C5 | 5.77 | 108.11 | 105.80 |
| 22 | 23S1 | 1304 | A | C8-N9-C4 | 5.77 | 108.11 | 105.80 |
| 1 | 16S1 | 1239 | A | C4-C5-N7 | -5.77 | 107.81 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 324 | A | C8-N9-C4 | 5.77 | 108.11 | 105.80 |
| 1 | 16S1 | 1319 | A | C8-N9-C4 | 5.77 | 108.11 | 105.80 |
| 22 | 23S1 | 142 | A | N3-C4-N9 | 5.77 | 132.02 | 127.40 |
| 22 | 23S1 | 300 | A | N9-C4-C5 | 5.77 | 108.11 | 105.80 |
| 1 | 16S1 | 274 | A | N3-C4-N9 | 5.77 | 132.02 | 127.40 |
| 1 | 16S1 | 315 | A | C5-C6-N1 | 5.77 | 120.58 | 117.70 |
| 1 | 16S1 | 1250 | A | C8-N9-C4 | 5.77 | 108.11 | 105.80 |
| 22 | 23S1 | 626 | A | N3-C4-N9 | 5.77 | 132.02 | 127.40 |
| 22 | 23S1 | 2513 | A | C4-C5-N7 | -5.77 | 107.81 | 110.70 |
| 1 | 16S1 | 315 | A | C8-N9-C4 | 5.77 | 108.11 | 105.80 |
| 1 | 16S1 | 1082 | A | N9-C4-C5 | 5.77 | 108.11 | 105.80 |
| 22 | 23S1 | 219 | A | C5-C6-N1 | 5.77 | 120.58 | 117.70 |
| 22 | 23S1 | 1286 | A | N9-C4-C5 | 5.77 | 108.11 | 105.80 |
| 22 | 23S1 | 1927 | A | C4-C5-N7 | -5.77 | 107.82 | 110.70 |
| 1 | 16S1 | 1269 | A | N9-C4-C5 | 5.77 | 108.11 | 105.80 |
| 22 | 23S1 | 428 | A | C5-C6-N1 | 5.77 | 120.58 | 117.70 |
| 22 | 23S1 | 2856 | A | C4-C5-C6 | 5.77 | 119.88 | 117.00 |
| 1 | 16S1 | 1287 | A | C8-N9-C4 | 5.76 | 108.11 | 105.80 |
| 22 | 23S1 | 752 | A | C4-C5-C6 | 5.76 | 119.88 | 117.00 |
| 22 | 23S1 | 1204 | A | N9-C4-C5 | 5.76 | 108.11 | 105.80 |
| 22 | 23S1 | 1690 | A | C8-N9-C4 | 5.76 | 108.11 | 105.80 |
| 22 | 23S1 | 1701 | A | N9-C4-C5 | 5.76 | 108.11 | 105.80 |
| 22 | 23S1 | 2059 | A | C5-C6-N1 | 5.76 | 120.58 | 117.70 |
| 22 | 23S1 | 973 | A | N9-C4-C5 | 5.76 | 108.11 | 105.80 |
| 22 | 23S1 | 1566 | A | N3-C4-N9 | 5.76 | 132.01 | 127.40 |
| 1 | 16S1 | 349 | A | C5-C6-N1 | 5.76 | 120.58 | 117.70 |
| 1 | 16S1 | 790 | A | C4-C5-C6 | 5.76 | 119.88 | 117.00 |
| 22 | 23S1 | 751 | A | C8-N9-C4 | 5.76 | 108.11 | 105.80 |
| 22 | 23S1 | 1496 | A | N3-C4-N9 | 5.76 | 132.01 | 127.40 |
| 22 | 23S1 | 2662 | A | C5-N7-C8 | 5.76 | 106.78 | 103.90 |
| 1 | 16S1 | 1012 | A | C8-N9-C4 | 5.76 | 108.10 | 105.80 |
| 1 | 16S1 | 1311 | A | N9-C4-C5 | 5.76 | 108.10 | 105.80 |
| 22 | 23S1 | 429 | A | N3-C4-N9 | 5.76 | 132.01 | 127.40 |
| 22 | 23S1 | 1762 | A | C5-C6-N1 | 5.76 | 120.58 | 117.70 |
| 22 | 23S1 | 2376 | A | C5-C6-N1 | 5.76 | 120.58 | 117.70 |
| 22 | 23S1 | 2541 | A | C5-C6-N1 | 5.76 | 120.58 | 117.70 |
| 1 | 16S1 | 4 | U | C2-N1-C1' | -5.76 | 110.79 | 117.70 |
| 1 | 16S1 | 116 | A | C4-C5-C6 | 5.76 | 119.88 | 117.00 |
| 1 | 16S1 | 918 | A | C4-C5-N7 | -5.76 | 107.82 | 110.70 |
| 1 | 16S1 | 1434 | A | C4-C5-C6 | 5.76 | 119.88 | 117.00 |
| 1 | 16S1 | 1456 | A | N9-C4-C5 | 5.76 | 108.10 | 105.80 |
| 22 | 23S1 | 1640 | A | N9-C4-C5 | 5.76 | 108.10 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 2037 | A | C8-N9-C4 | 5.76 | 108.10 | 105.80 |
| 1 | 16S1 | 792 | A | C4-C5-C6 | 5.75 | 119.88 | 117.00 |
| 22 | 23S1 | 176 | A | C8-N9-C4 | 5.75 | 108.10 | 105.80 |
| 22 | 23S1 | 541 | A | C5-C6-N1 | 5.75 | 120.58 | 117.70 |
| 22 | 23S1 | 1885 | A | C5-C6-N1 | 5.75 | 120.58 | 117.70 |
| 22 | 23S1 | 2052 | A | C5-C6-N1 | 5.75 | 120.58 | 117.70 |
| 22 | 23S1 | 2406 | A | C4-C5-C6 | 5.75 | 119.88 | 117.00 |
| 1 | 16S1 | 87 | C | N3-C2-O2 | -5.75 | 117.87 | 121.90 |
| 1 | 16S1 | 1357 | A | C4-C5-C6 | 5.75 | 119.88 | 117.00 |
| 22 | 23S1 | 1376 | C | N1-C2-O2 | 5.75 | 122.35 | 118.90 |
| 22 | 23S1 | 1783 | A | C4-C5-N7 | -5.75 | 107.82 | 110.70 |
| 22 | 23S1 | 1890 | A | N9-C4-C5 | 5.75 | 108.10 | 105.80 |
| 22 | 23S1 | 2227 | A | C4-C5-C6 | 5.75 | 119.88 | 117.00 |
| 1 | 16S1 | 845 | A | N9-C4-C5 | 5.75 | 108.10 | 105.80 |
| 22 | 23S1 | 402 | A | C8-N9-C4 | 5.75 | 108.10 | 105.80 |
| 22 | 23S1 | 792 | A | N3-C4-N9 | 5.75 | 132.00 | 127.40 |
| 22 | 23S1 | 1597 | A | C8-N9-C4 | 5.75 | 108.10 | 105.80 |
| 22 | 23S1 | 1938 | A | C4-C5-C6 | 5.75 | 119.88 | 117.00 |
| 22 | 23S1 | 2736 | A | C4-C5-C6 | 5.75 | 119.88 | 117.00 |
| 1 | 16S1 | 1377 | A | N9-C4-C5 | 5.75 | 108.10 | 105.80 |
| 22 | 23S1 | 2388 | A | N3-C4-N9 | 5.75 | 132.00 | 127.40 |
| 1 | 16S1 | 1329 | A | N9-C4-C5 | 5.75 | 108.10 | 105.80 |
| 1 | 16S1 | 1428 | A | N9-C4-C5 | 5.75 | 108.10 | 105.80 |
| 22 | 23S1 | 825 | A | C4-C5-C6 | 5.75 | 119.88 | 117.00 |
| 22 | 23S1 | 1204 | A | C8-N9-C4 | 5.75 | 108.10 | 105.80 |
| 22 | 23S1 | 2733 | A | N3-C4-N9 | 5.75 | 132.00 | 127.40 |
| 1 | 16S1 | 452 | A | C8-N9-C4 | 5.75 | 108.10 | 105.80 |
| 1 | 16S1 | 1252 | A | C5-C6-N1 | 5.75 | 120.57 | 117.70 |
| 1 | 16S1 | 468 | A | C4-C5-N7 | -5.75 | 107.83 | 110.70 |
| 1 | 16S1 | 873 | A | C8-N9-C4 | 5.75 | 108.10 | 105.80 |
| 22 | 23S1 | 800 | A | C8-N9-C4 | 5.74 | 108.10 | 105.80 |
| 22 | 23S1 | 1496 | A | C4-C5-C6 | 5.74 | 119.87 | 117.00 |
| 1 | 16S1 | 1111 | A | N3-C4-N9 | 5.74 | 131.99 | 127.40 |
| 1 | 16S1 | 1349 | A | C5-C6-N1 | 5.74 | 120.57 | 117.70 |
| 1 | 16S1 | 131 | A | C8-N9-C4 | 5.74 | 108.10 | 105.80 |
| 1 | 16S1 | 1431 | A | N3-C4-N9 | 5.74 | 131.99 | 127.40 |
| 22 | 23S1 | 1509 | A | N9-C4-C5 | 5.74 | 108.10 | 105.80 |
| 22 | 23S1 | 2388 | A | C4-C5-N7 | -5.74 | 107.83 | 110.70 |
| 22 | 23S1 | 2749 | A | N3-C4-N9 | 5.74 | 131.99 | 127.40 |
| 1 | 16S1 | 553 | A | N9-C4-C5 | 5.74 | 108.09 | 105.80 |
| 1 | 16S1 | 596 | A | C4-C5-C6 | 5.74 | 119.87 | 117.00 |
| 1 | 16S1 | 1254 | A | C4-C5-C6 | 5.74 | 119.87 | 117.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 1095 | A | C4-C5-N7 | -5.74 | 107.83 | 110.70 |
| 1 | 16S1 | 629 | A | N9-C4-C5 | 5.74 | 108.09 | 105.80 |
| 22 | 23S1 | 1439 | A | N3-C4-N9 | 5.74 | 131.99 | 127.40 |
| 22 | 23S1 | 2317 | A | C5-C6-N1 | 5.74 | 120.57 | 117.70 |
| 22 | 23S1 | 2829 | A | N9-C4-C5 | 5.74 | 108.09 | 105.80 |
| 1 | 16S1 | 309 | A | C5-C6-N1 | 5.74 | 120.57 | 117.70 |
| 1 | 16S1 | 536 | C | N1-C2-O2 | 5.74 | 122.34 | 118.90 |
| 1 | 16S1 | 595 | A | C8-N9-C4 | 5.74 | 108.09 | 105.80 |
| 1 | 16S1 | 1188 | A | N3-C4-N9 | 5.74 | 131.99 | 127.40 |
| 1 | 16S1 | 1429 | A | C4-C5-C6 | 5.74 | 119.87 | 117.00 |
| 1 | 16S1 | 160 | A | C8-N9-C4 | 5.73 | 108.09 | 105.80 |
| 1 | 16S1 | 640 | A | C8-N9-C4 | 5.73 | 108.09 | 105.80 |
| 1 | 16S1 | 782 | A | N3-C4-N9 | 5.73 | 131.99 | 127.40 |
| 1 | 16S1 | 1251 | A | N9-C4-C5 | 5.73 | 108.09 | 105.80 |
| 22 | 23S1 | 1308 | A | C4-C5-C6 | 5.73 | 119.87 | 117.00 |
| 22 | 23S1 | 1591 | A | C5-C6-N1 | 5.73 | 120.57 | 117.70 |
| 22 | 23S1 | 1952 | A | C5-C6-N1 | 5.73 | 120.57 | 117.70 |
| 1 | 16S1 | 270 | A | C5-C6-N1 | 5.73 | 120.57 | 117.70 |
| 1 | 16S1 | 649 | A | N3-C4-N9 | 5.73 | 131.99 | 127.40 |
| 22 | 23S1 | 529 | A | C5-C6-N1 | 5.73 | 120.57 | 117.70 |
| 22 | 23S1 | 1583 | A | C4-C5-N7 | -5.73 | 107.83 | 110.70 |
| 22 | 23S1 | 1746 | A | N9-C4-C5 | 5.73 | 108.09 | 105.80 |
| 22 | 23S1 | 2418 | A | C4-C5-C6 | 5.73 | 119.87 | 117.00 |
| 22 | 23S1 | 2670 | A | N9-C4-C5 | 5.73 | 108.09 | 105.80 |
| 1 | 16S1 | 374 | A | C8-N9-C4 | 5.73 | 108.09 | 105.80 |
| 22 | 23S1 | 812 | C | C6-N1-C2 | -5.73 | 118.01 | 120.30 |
| 22 | 23S1 | 1786 | A | N3-C4-N9 | 5.73 | 131.99 | 127.40 |
| 22 | 23S1 | 2468 | A | C4-C5-C6 | 5.73 | 119.87 | 117.00 |
| 1 | 16S1 | 536 | C | C6-N1-C2 | -5.73 | 118.01 | 120.30 |
| 1 | 16S1 | 1329 | A | C8-N9-C4 | 5.73 | 108.09 | 105.80 |
| 1 | 16S1 | 26 | A | C4-C5-C6 | 5.73 | 119.86 | 117.00 |
| 1 | 16S1 | 1151 | A | C4-C5-C6 | 5.73 | 119.86 | 117.00 |
| 22 | 23S1 | 348 | A | C5-C6-N1 | 5.73 | 120.56 | 117.70 |
| 22 | 23S1 | 1544 | A | C4-C5-N7 | -5.73 | 107.84 | 110.70 |
| 1 | 16S1 | 1036 | A | N3-C4-N9 | 5.72 | 131.98 | 127.40 |
| 22 | 23S1 | 251 | A | C5-N7-C8 | 5.72 | 106.76 | 103.90 |
| 22 | 23S1 | 1966 | A | C5-C6-N1 | 5.72 | 120.56 | 117.70 |
| 1 | 16S1 | 253 | A | C8-N9-C4 | 5.72 | 108.09 | 105.80 |
| 1 | 16S1 | 553 | A | N3-C4-N9 | 5.72 | 131.98 | 127.40 |
| 1 | 16S1 | 946 | A | C8-N9-C4 | 5.72 | 108.09 | 105.80 |
| 1 | 16S1 | 1150 | A | C8-N9-C4 | 5.72 | 108.09 | 105.80 |
| 22 | 23S1 | 371 | A | N3-C4-N9 | 5.72 | 131.98 | 127.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 676 | A | C5-C6-N1 | 5.72 | 120.56 | 117.70 |
| 22 | 23S1 | 909 | A | N3-C4-N9 | 5.72 | 131.98 | 127.40 |
| 22 | 23S1 | 2635 | A | C5-C6-N1 | 5.72 | 120.56 | 117.70 |
| 1 | 16S1 | 8 | A | N3-C4-N9 | 5.72 | 131.98 | 127.40 |
| 1 | 16S1 | 1093 | A | C8-N9-C4 | 5.72 | 108.09 | 105.80 |
| 22 | 23S1 | 603 | A | C8-N9-C4 | 5.72 | 108.09 | 105.80 |
| 22 | 23S1 | 2675 | A | C4-C5-C6 | 5.72 | 119.86 | 117.00 |
| 22 | 23S1 | 2736 | A | N9-C4-C5 | 5.72 | 108.09 | 105.80 |
| 55 | PTR1 | 17 | U | C4-C5-C6 | -5.72 | 116.27 | 119.70 |
| 1 | 16S1 | 109 | A | C4-C5-C6 | 5.72 | 119.86 | 117.00 |
| 1 | 16S1 | 171 | A | C5-C6-N1 | 5.72 | 120.56 | 117.70 |
| 1 | 16S1 | 794 | A | C4-C5-N7 | -5.72 | 107.84 | 110.70 |
| 1 | 16S1 | 1311 | A | C4-C5-C6 | 5.72 | 119.86 | 117.00 |
| 22 | 23S1 | 430 | A | N3-C4-N9 | 5.72 | 131.97 | 127.40 |
| 22 | 23S1 | 706 | A | N3-C4-N9 | 5.72 | 131.98 | 127.40 |
| 22 | 23S1 | 1247 | A | C4-C5-C6 | 5.72 | 119.86 | 117.00 |
| 22 | 23S1 | 1644 | C | N3-C2-O2 | -5.72 | 117.90 | 121.90 |
| 22 | 23S1 | 1772 | A | C4-C5-C6 | 5.72 | 119.86 | 117.00 |
| 22 | 23S1 | 2173 | A | C4-C5-C6 | 5.72 | 119.86 | 117.00 |
| 22 | 23S1 | 2851 | A | C8-N9-C4 | 5.72 | 108.09 | 105.80 |
| 22 | 23S1 | 2856 | A | C5-C6-N1 | 5.72 | 120.56 | 117.70 |
| 1 | 16S1 | 782 | A | N9-C4-C5 | 5.72 | 108.09 | 105.80 |
| 1 | 16S1 | 825 | A | N3-C4-N9 | 5.72 | 131.97 | 127.40 |
| 22 | 23S1 | 804 | A | C4-C5-C6 | 5.72 | 119.86 | 117.00 |
| 22 | 23S1 | 1505 | A | N3-C4-N9 | 5.72 | 131.97 | 127.40 |
| 1 | 16S1 | 162 | A | C6-C5-N7 | -5.72 | 128.30 | 132.30 |
| 1 | 16S1 | 313 | A | C4-C5-N7 | -5.72 | 107.84 | 110.70 |
| 1 | 16S1 | 949 | A | C4-C5-N7 | -5.72 | 107.84 | 110.70 |
| 1 | 16S1 | 1150 | A | N9-C4-C5 | 5.72 | 108.09 | 105.80 |
| 22 | 23S1 | 227 | A | C4-C5-C6 | 5.72 | 119.86 | 117.00 |
| 22 | 23S1 | 1385 | A | N9-C4-C5 | 5.72 | 108.09 | 105.80 |
| 22 | 23S1 | 1772 | A | N3-C4-N9 | 5.72 | 131.97 | 127.40 |
| 22 | 23S1 | 1815 | A | C5-N7-C8 | 5.72 | 106.76 | 103.90 |
| 22 | 23S1 | 2716 | C | N1-C2-O2 | 5.72 | 122.33 | 118.90 |
| 55 | PTR1 | 42 | A | C5-C6-N1 | 5.72 | 120.56 | 117.70 |
| 1 | 16S1 | 288 | A | C4-C5-C6 | 5.71 | 119.86 | 117.00 |
| 1 | 16S1 | 327 | A | C4-C5-C6 | 5.71 | 119.86 | 117.00 |
| 1 | 16S1 | 498 | A | C6-N1-C2 | -5.71 | 115.17 | 118.60 |
| 1 | 16S1 | 553 | A | C5-C6-N1 | 5.71 | 120.56 | 117.70 |
| 1 | 16S1 | 766 | A | N9-C4-C5 | 5.71 | 108.09 | 105.80 |
| 1 | 16S1 | 1374 | A | C5-C6-N1 | 5.71 | 120.56 | 117.70 |
| 22 | 23S1 | 347 | A | C4-C5-N7 | -5.71 | 107.84 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 510 | C | N1-C2-O2 | 5.71 | 122.33 | 118.90 |
| 22 | 23S1 | 548 | G | N3-C4-N9 | 5.71 | 129.43 | 126.00 |
| 22 | 23S1 | 563 | A | N9-C4-C5 | 5.71 | 108.09 | 105.80 |
| 22 | 23S1 | 699 | A | N9-C4-C5 | 5.71 | 108.09 | 105.80 |
| 22 | 23S1 | 1169 | A | C5-C6-N1 | 5.71 | 120.56 | 117.70 |
| 22 | 23S1 | 1302 | A | C4-C5-C6 | 5.71 | 119.86 | 117.00 |
| 22 | 23S1 | 1383 | A | N3-C4-N9 | 5.71 | 131.97 | 127.40 |
| 1 | 16S1 | 1 | A | C4-C5-C6 | 5.71 | 119.86 | 117.00 |
| 22 | 23S1 | 1503 | A | N3-C4-N9 | 5.71 | 131.97 | 127.40 |
| 22 | 23S1 | 1890 | A | C8-N9-C4 | 5.71 | 108.08 | 105.80 |
| 22 | 23S1 | 2733 | A | N9-C4-C5 | 5.71 | 108.08 | 105.80 |
| 1 | 16S1 | 1480 | A | C4-C5-C6 | 5.71 | 119.86 | 117.00 |
| 22 | 23S1 | 432 | A | C4-C5-C6 | 5.71 | 119.86 | 117.00 |
| 22 | 23S1 | 802 | A | C4-C5-C6 | 5.71 | 119.86 | 117.00 |
| 22 | 23S1 | 1525 | A | C4-C5-N7 | -5.71 | 107.84 | 110.70 |
| 1 | 16S1 | 777 | A | N9-C4-C5 | 5.71 | 108.08 | 105.80 |
| 1 | 16S1 | 906 | A | C4-C5-C6 | 5.71 | 119.85 | 117.00 |
| 1 | 16S1 | 1434 | A | C5-C6-N1 | 5.71 | 120.55 | 117.70 |
| 22 | 23S1 | 508 | A | N9-C4-C5 | 5.71 | 108.08 | 105.80 |
| 22 | 23S1 | 1214 | A | C5-C6-N1 | 5.71 | 120.56 | 117.70 |
| 22 | 23S1 | 1900 | A | C4-C5-C6 | 5.71 | 119.85 | 117.00 |
| 22 | 23S1 | 2670 | A | C4-C5-C6 | 5.71 | 119.85 | 117.00 |
| 1 | 16S1 | 892 | A | C4-C5-C6 | 5.71 | 119.85 | 117.00 |
| 22 | 23S1 | 340 | A | C4-C5-N7 | -5.71 | 107.85 | 110.70 |
| 22 | 23S1 | 756 | A | N9-C4-C5 | 5.71 | 108.08 | 105.80 |
| 22 | 23S1 | 2602 | A | N3-C4-N9 | 5.71 | 131.97 | 127.40 |
| 55 | PTR1 | 6 | C | N1-C2-O2 | 5.71 | 122.32 | 118.90 |
| 22 | 23S1 | 1347 | A | C5-C6-N1 | 5.71 | 120.55 | 117.70 |
| 1 | 16S1 | 131 | A | C4-C5-C6 | 5.70 | 119.85 | 117.00 |
| 1 | 16S1 | 363 | A | C8-N9-C4 | 5.70 | 108.08 | 105.80 |
| 22 | 23S1 | 152 | A | C4-C5-C6 | 5.70 | 119.85 | 117.00 |
| 22 | 23S1 | 172 | A | C5-C6-N1 | 5.70 | 120.55 | 117.70 |
| 22 | 23S1 | 1143 | A | C8-N9-C4 | 5.70 | 108.08 | 105.80 |
| 22 | 23S1 | 1247 | A | C8-N9-C4 | 5.70 | 108.08 | 105.80 |
| 22 | 23S1 | 1701 | A | N3-C4-N9 | 5.70 | 131.96 | 127.40 |
| 22 | 23S1 | 2003 | A | C8-N9-C4 | 5.70 | 108.08 | 105.80 |
| 22 | 23S1 | 2350 | C | N3-C2-O2 | -5.70 | 117.91 | 121.90 |
| 1 | 16S1 | 282 | A | C4-C5-C6 | 5.70 | 119.85 | 117.00 |
| 1 | 16S1 | 321 | A | C4-C5-N7 | -5.70 | 107.85 | 110.70 |
| 1 | 16S1 | 958 | A | C4-C5-C6 | 5.70 | 119.85 | 117.00 |
| 22 | 23S1 | 1871 | A | C4-C5-N7 | -5.70 | 107.85 | 110.70 |
| 22 | 23S1 | 2706 | A | C5-C6-N1 | 5.70 | 120.55 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 167 | A | C5-C6-N1 | 5.70 | 120.55 | 117.70 |
| 22 | 23S1 | 196 | A | N9-C4-C5 | 5.70 | 108.08 | 105.80 |
| 22 | 23S1 | 1253 | A | C5-C6-N1 | 5.70 | 120.55 | 117.70 |
| 22 | 23S1 | 1366 | A | C4-C5-C6 | 5.70 | 119.85 | 117.00 |
| 22 | 23S1 | 2358 | A | N3-C4-N9 | 5.70 | 131.96 | 127.40 |
| 22 | 23S1 | 1306 | C | N1-C2-O2 | 5.70 | 122.32 | 118.90 |
| 1 | 16S1 | 171 | A | N3-C4-N9 | 5.70 | 131.96 | 127.40 |
| 22 | 23S1 | 2471 | A | C5-C6-N1 | 5.70 | 120.55 | 117.70 |
| 22 | 23S1 | 2587 | A | C4-C5-N7 | -5.70 | 107.85 | 110.70 |
| 22 | 23S1 | 2711 | A | C4-C5-N7 | -5.70 | 107.85 | 110.70 |
| 1 | 16S1 | 98 | A | N9-C4-C5 | 5.69 | 108.08 | 105.80 |
| 22 | 23S1 | 83 | A | C5-C6-N1 | 5.69 | 120.55 | 117.70 |
| 1 | 16S1 | 975 | A | C8-N9-C4 | 5.69 | 108.08 | 105.80 |
| 1 | 16S1 | 1019 | A | N3-C4-N9 | 5.69 | 131.95 | 127.40 |
| 22 | 23S1 | 226 | A | N3-C4-N9 | 5.69 | 131.95 | 127.40 |
| 22 | 23S1 | 497 | A | N9-C4-C5 | 5.69 | 108.08 | 105.80 |
| 22 | 23S1 | 685 | A | C5-C6-N1 | 5.69 | 120.55 | 117.70 |
| 22 | 23S1 | 1095 | A | N3-C4-N9 | 5.69 | 131.95 | 127.40 |
| 1 | 16S1 | 1429 | A | C5-C6-N1 | 5.69 | 120.55 | 117.70 |
| 1 | 16S1 | 1431 | A | C8-N9-C4 | 5.69 | 108.08 | 105.80 |
| 1 | 16S1 | 1499 | A | C5-C6-N1 | 5.69 | 120.55 | 117.70 |
| 22 | 23S1 | 345 | A | C4-C5-C6 | 5.69 | 119.84 | 117.00 |
| 22 | 23S1 | 1535 | A | C4-C5-N7 | -5.69 | 107.86 | 110.70 |
| 22 | 23S1 | 2126 | A | C4-C5-N7 | -5.69 | 107.86 | 110.70 |
| 22 | 23S1 | 2835 | A | N3-C4-N9 | 5.69 | 131.95 | 127.40 |
| 1 | 16S1 | 356 | A | C5-C6-N1 | 5.69 | 120.54 | 117.70 |
| 1 | 16S1 | 1005 | A | C4-C5-C6 | 5.69 | 119.84 | 117.00 |
| 22 | 23S1 | 497 | A | C8-N9-C4 | 5.69 | 108.08 | 105.80 |
| 22 | 23S1 | 1366 | A | N3-C4-N9 | 5.69 | 131.95 | 127.40 |
| 22 | 23S1 | 2850 | A | C8-N9-C4 | 5.69 | 108.08 | 105.80 |
| 1 | 16S1 | 81 | A | N3-C4-N9 | 5.69 | 131.95 | 127.40 |
| 22 | 23S1 | 172 | A | C8-N9-C4 | 5.69 | 108.08 | 105.80 |
| 22 | 23S1 | 614 | A | C4-C5-N7 | -5.69 | 107.86 | 110.70 |
| 22 | 23S1 | 1247 | A | C4-C5-N7 | -5.69 | 107.86 | 110.70 |
| 22 | 23S1 | 2176 | A | C5-N7-C8 | 5.69 | 106.74 | 103.90 |
| 22 | 23S1 | 2227 | A | N3-C4-N9 | 5.69 | 131.95 | 127.40 |
| 1 | 16S1 | 300 | A | C5-C6-N6 | 5.69 | 128.25 | 123.70 |
| 1 | 16S1 | 364 | A | N9-C4-C5 | 5.69 | 108.08 | 105.80 |
| 1 | 16S1 | 415 | A | C4-C5-N7 | -5.69 | 107.86 | 110.70 |
| 1 | 16S1 | 1021 | A | C8-N9-C4 | 5.69 | 108.07 | 105.80 |
| 22 | 23S1 | 927 | A | C5-C6-N1 | 5.69 | 120.54 | 117.70 |
| 22 | 23S1 | 1070 | A | C4-C5-N7 | -5.69 | 107.86 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 2378 | A | C8-N9-C4 | 5.69 | 108.07 | 105.80 |
| 22 | 23S1 | 2435 | A | N9-C4-C5 | 5.69 | 108.08 | 105.80 |
| 1 | 16S1 | 109 | A | N3-C4-N9 | 5.68 | 131.95 | 127.40 |
| 1 | 16S1 | 1248 | A | N3-C4-N9 | 5.68 | 131.95 | 127.40 |
| 22 | 23S1 | 118 | A | C8-N9-C4 | 5.68 | 108.07 | 105.80 |
| 22 | 23S1 | 727 | A | C4-C5-C6 | 5.68 | 119.84 | 117.00 |
| 22 | 23S1 | 1014 | A | C5-C6-N1 | 5.68 | 120.54 | 117.70 |
| 22 | 23S1 | 1276 | A | C8-N9-C4 | 5.68 | 108.07 | 105.80 |
| 22 | 23S1 | 2009 | A | N3-C4-N9 | 5.68 | 131.95 | 127.40 |
| 22 | 23S1 | 2333 | A | C5-C6-N1 | 5.68 | 120.54 | 117.70 |
| 22 | 23S1 | 2753 | A | C4-C5-C6 | 5.68 | 119.84 | 117.00 |
| 23 | 05S1 | 46 | A | C4-C5-N7 | -5.68 | 107.86 | 110.70 |
| 1 | 16S1 | 814 | A | C4-C5-C6 | 5.68 | 119.84 | 117.00 |
| 1 | 16S1 | 1362 | A | C5-C6-N1 | 5.68 | 120.54 | 117.70 |
| 1 | 16S1 | 1446 | A | N9-C4-C5 | 5.68 | 108.07 | 105.80 |
| 22 | 23S1 | 1253 | A | N9-C4-C5 | 5.68 | 108.07 | 105.80 |
| 22 | 23S1 | 2284 | A | C5-C6-N1 | 5.68 | 120.54 | 117.70 |
| 22 | 23S1 | 2317 | A | C4-C5-C6 | 5.68 | 119.84 | 117.00 |
| 23 | 05S1 | 57 | A | N3-C4-N9 | 5.68 | 131.95 | 127.40 |
| 22 | 23S1 | 126 | A | N3-C4-N9 | 5.68 | 131.94 | 127.40 |
| 22 | 23S1 | 279 | A | N9-C4-C5 | 5.68 | 108.07 | 105.80 |
| 22 | 23S1 | 309 | A | C5-C6-N1 | 5.68 | 120.54 | 117.70 |
| 22 | 23S1 | 1966 | A | C4-C5-C6 | 5.68 | 119.84 | 117.00 |
| 22 | 23S1 | 2114 | A | C5-N7-C8 | 5.68 | 106.74 | 103.90 |
| 1 | 16S1 | 900 | A | N3-C4-N9 | 5.68 | 131.94 | 127.40 |
| 22 | 23S1 | 63 | A | C4-C5-C6 | 5.68 | 119.84 | 117.00 |
| 22 | 23S1 | 262 | A | C8-N9-C4 | 5.68 | 108.07 | 105.80 |
| 22 | 23S1 | 270 | A | C4-C5-N7 | -5.68 | 107.86 | 110.70 |
| 22 | 23S1 | 1874 | C | N3-C2-O2 | -5.68 | 117.92 | 121.90 |
| 22 | 23S1 | 2432 | A | C4-C5-C6 | 5.68 | 119.84 | 117.00 |
| 22 | 23S1 | 2587 | A | N9-C4-C5 | 5.68 | 108.07 | 105.80 |
| 23 | 05S1 | 109 | A | C4-C5-C6 | 5.68 | 119.84 | 117.00 |
| 1 | 16S1 | 1492 | A | N9-C4-C5 | 5.68 | 108.07 | 105.80 |
| 1 | 16S1 | 1429 | A | C8-N9-C4 | 5.68 | 108.07 | 105.80 |
| 22 | 23S1 | 910 | A | C4-C5-C6 | 5.68 | 119.84 | 117.00 |
| 22 | 23S1 | 1230 | A | N9-C4-C5 | 5.68 | 108.07 | 105.80 |
| 1 | 16S1 | 129 | A | C8-N9-C4 | 5.67 | 108.07 | 105.80 |
| 1 | 16S1 | 167 | A | C5-C6-N1 | 5.67 | 120.54 | 117.70 |
| 1 | 16S1 | 1332 | A | C5-N7-C8 | 5.67 | 106.74 | 103.90 |
| 22 | 23S1 | 6 | A | C5-C6-N1 | 5.67 | 120.54 | 117.70 |
| 22 | 23S1 | 479 | A | N3-C4-N9 | 5.67 | 131.94 | 127.40 |
| 22 | 23S1 | 602 | A | C5-C6-N1 | 5.67 | 120.54 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 1383 | A | N9-C4-C5 | 5.67 | 108.07 | 105.80 |
| 22 | 23S1 | 1874 | C | N1-C2-O2 | 5.67 | 122.30 | 118.90 |
| 22 | 23S1 | 2052 | A | C8-N9-C4 | 5.67 | 108.07 | 105.80 |
| 22 | 23S1 | 2589 | A | C8-N9-C4 | 5.67 | 108.07 | 105.80 |
| 22 | 23S1 | 1477 | A | N3-C4-N9 | 5.67 | 131.94 | 127.40 |
| 1 | 16S1 | 66 | A | N9-C4-C5 | 5.67 | 108.07 | 105.80 |
| 1 | 16S1 | 816 | A | C4-C5-C6 | 5.67 | 119.84 | 117.00 |
| 1 | 16S1 | 1105 | A | C4-C5-N7 | -5.67 | 107.86 | 110.70 |
| 1 | 16S1 | 1483 | A | N9-C4-C5 | 5.67 | 108.07 | 105.80 |
| 22 | 23S1 | 575 | A | N3-C4-N9 | 5.67 | 131.94 | 127.40 |
| 22 | 23S1 | 1265 | A | N9-C4-C5 | 5.67 | 108.07 | 105.80 |
| 22 | 23S1 | 2813 | A | N9-C4-C5 | 5.67 | 108.07 | 105.80 |
| 22 | 23S1 | 2814 | A | N3-C4-N9 | 5.67 | 131.94 | 127.40 |
| 22 | 23S1 | 722 | A | C8-N9-C4 | 5.67 | 108.07 | 105.80 |
| 22 | 23S1 | 750 | A | C8-N9-C4 | 5.67 | 108.07 | 105.80 |
| 23 | 05S1 | 115 | A | C4-C5-C6 | 5.67 | 119.83 | 117.00 |
| 1 | 16S1 | 509 | A | C4-C5-N7 | -5.67 | 107.87 | 110.70 |
| 1 | 16S1 | 1055 | A | C8-N9-C4 | 5.67 | 108.07 | 105.80 |
| 1 | 16S1 | 1216 | A | C4-C5-C6 | 5.67 | 119.83 | 117.00 |
| 22 | 23S1 | 143 | C | N1-C2-O2 | 5.67 | 122.30 | 118.90 |
| 22 | 23S1 | 368 | A | N3-C4-N9 | 5.67 | 131.94 | 127.40 |
| 22 | 23S1 | 718 | A | C4-C5-N7 | -5.67 | 107.87 | 110.70 |
| 22 | 23S1 | 1545 | A | C4-C5-C6 | 5.67 | 119.83 | 117.00 |
| 22 | 23S1 | 1931 | U | N3-C2-O2 | -5.67 | 118.23 | 122.20 |
| 1 | 16S1 | 498 | A | N9-C4-C5 | 5.67 | 108.07 | 105.80 |
| 22 | 23S1 | 2887 | A | N3-C4-N9 | 5.67 | 131.93 | 127.40 |
| 55 | PTR1 | 3 | A | C8-N9-C4 | 5.67 | 108.07 | 105.80 |
| 1 | 16S1 | 468 | A | C8-N9-C4 | 5.67 | 108.07 | 105.80 |
| 22 | 23S1 | 74 | A | N9-C4-C5 | 5.67 | 108.07 | 105.80 |
| 22 | 23S1 | 1853 | A | N9-C4-C5 | 5.67 | 108.07 | 105.80 |
| 22 | 23S1 | 761 | A | N3-C4-N9 | 5.66 | 131.93 | 127.40 |
| 22 | 23S1 | 1453 | A | N9-C4-C5 | 5.66 | 108.06 | 105.80 |
| 22 | 23S1 | 1544 | A | C4-C5-C6 | 5.66 | 119.83 | 117.00 |
| 22 | 23S1 | 1579 | A | C4-C5-C6 | 5.66 | 119.83 | 117.00 |
| 22 | 23S1 | 1676 | A | C5-N7-C8 | 5.66 | 106.73 | 103.90 |
| 22 | 23S1 | 1084 | A | C4-C5-N7 | -5.66 | 107.87 | 110.70 |
| 1 | 16S1 | 320 | A | C4-C5-N7 | -5.66 | 107.87 | 110.70 |
| 1 | 16S1 | 440 | C | N3-C2-O2 | -5.66 | 117.94 | 121.90 |
| 1 | 16S1 | 1311 | A | C4-C5-N7 | -5.66 | 107.87 | 110.70 |
| 22 | 23S1 | 21 | A | N9-C4-C5 | 5.66 | 108.06 | 105.80 |
| 22 | 23S1 | 548 | G | C8-N9-C1' | -5.66 | 119.64 | 127.00 |
| 22 | 23S1 | 563 | A | C4-C5-C6 | 5.66 | 119.83 | 117.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 668 | A | N3-C4-N9 | 5.66 | 131.93 | 127.40 |
| 22 | 23S1 | 721 | A | C5-C6-N1 | 5.66 | 120.53 | 117.70 |
| 22 | 23S1 | 1668 | A | C5-C6-N1 | 5.66 | 120.53 | 117.70 |
| 22 | 23S1 | 2900 | A | C8-N9-C4 | 5.66 | 108.06 | 105.80 |
| 1 | 16S1 | 238 | A | C4-C5-C6 | 5.66 | 119.83 | 117.00 |
| 1 | 16S1 | 607 | A | C6-N1-C2 | 5.66 | 122.00 | 118.60 |
| 22 | 23S1 | 666 | A | C4-C5-C6 | 5.66 | 119.83 | 117.00 |
| 22 | 23S1 | 983 | A | N3-C4-N9 | 5.66 | 131.93 | 127.40 |
| 22 | 23S1 | 1274 | A | C4-C5-N7 | -5.66 | 107.87 | 110.70 |
| 22 | 23S1 | 1821 | A | C4-C5-N7 | -5.66 | 107.87 | 110.70 |
| 22 | 23S1 | 1901 | A | C5-C6-N1 | 5.66 | 120.53 | 117.70 |
| 22 | 23S1 | 2358 | A | C4-C5-C6 | 5.66 | 119.83 | 117.00 |
| 22 | 23S1 | 2750 | A | C4-C5-C6 | 5.66 | 119.83 | 117.00 |
| 29 | L091 | 70 | GLU | C-N-CA | 5.66 | 135.85 | 121.70 |
| 1 | 16S1 | 1324 | A | C5-C6-N1 | 5.66 | 120.53 | 117.70 |
| 22 | 23S1 | 1040 | A | C5-C6-N1 | 5.66 | 120.53 | 117.70 |
| 22 | 23S1 | 2037 | A | C5-C6-N1 | 5.66 | 120.53 | 117.70 |
| 22 | 23S1 | 2450 | A | N9-C4-C5 | 5.66 | 108.06 | 105.80 |
| 1 | 16S1 | 238 | A | N3-C4-N9 | 5.66 | 131.93 | 127.40 |
| 1 | 16S1 | 977 | A | C5-C6-N1 | 5.66 | 120.53 | 117.70 |
| 22 | 23S1 | 195 | A | C5-C6-N1 | 5.66 | 120.53 | 117.70 |
| 22 | 23S1 | 699 | A | N3-C4-N9 | 5.66 | 131.93 | 127.40 |
| 22 | 23S1 | 1147 | A | N3-C4-N9 | 5.66 | 131.92 | 127.40 |
| 22 | 23S1 | 2019 | A | C4-C5-C6 | 5.66 | 119.83 | 117.00 |
| 22 | 23S1 | 2764 | A | C5-C6-N1 | 5.66 | 120.53 | 117.70 |
| 22 | 23S1 | 103 | A | C8-N9-C4 | 5.65 | 108.06 | 105.80 |
| 22 | 23S1 | 347 | A | N9-C4-C5 | 5.65 | 108.06 | 105.80 |
| 22 | 23S1 | 2439 | A | N3-C4-N9 | 5.65 | 131.92 | 127.40 |
| 1 | 16S1 | 344 | A | N3-C4-N9 | 5.65 | 131.92 | 127.40 |
| 1 | 16S1 | 371 | A | C4-C5-N7 | -5.65 | 107.87 | 110.70 |
| 1 | 16S1 | 1246 | A | C5-C6-N1 | 5.65 | 120.53 | 117.70 |
| 1 | 16S1 | 1476 | A | N9-C4-C5 | 5.65 | 108.06 | 105.80 |
| 22 | 23S1 | 10 | A | N9-C4-C5 | 5.65 | 108.06 | 105.80 |
| 22 | 23S1 | 1050 | A | C5-C6-N1 | 5.65 | 120.53 | 117.70 |
| 22 | 23S1 | 1987 | A | C4-C5-C6 | 5.65 | 119.83 | 117.00 |
| 22 | 23S1 | 2835 | A | C4-C5-N7 | -5.65 | 107.87 | 110.70 |
| 1 | 16S1 | 648 | A | C5-C6-N1 | 5.65 | 120.53 | 117.70 |
| 1 | 16S1 | 1216 | A | C8-N9-C4 | 5.65 | 108.06 | 105.80 |
| 22 | 23S1 | 2095 | A | C4-C5-C6 | 5.65 | 119.83 | 117.00 |
| 22 | 23S1 | 2418 | A | C5-C6-N1 | 5.65 | 120.53 | 117.70 |
| 1 | 16S1 | 1502 | A | C8-N9-C4 | 5.65 | 108.06 | 105.80 |
| 22 | 23S1 | 2283 | C | N3-C2-O2 | -5.65 | 117.95 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 2564 | A | N9-C4-C5 | 5.65 | 108.06 | 105.80 |
| 1 | 16S1 | 766 | A | C8-N9-C4 | 5.65 | 108.06 | 105.80 |
| 22 | 23S1 | 844 | A | C8-N9-C4 | 5.65 | 108.06 | 105.80 |
| 22 | 23S1 | 2070 | A | N9-C4-C5 | 5.65 | 108.06 | 105.80 |
| 1 | 16S1 | 344 | A | C4-C5-C6 | 5.65 | 119.82 | 117.00 |
| 1 | 16S1 | 1368 | A | N9-C4-C5 | 5.65 | 108.06 | 105.80 |
| 22 | 23S1 | 849 | A | C4-C5-N7 | -5.65 | 107.88 | 110.70 |
| 22 | 23S1 | 2851 | A | N3-C4-N9 | 5.65 | 131.92 | 127.40 |
| 29 | L091 | 58 | LEU | CA-CB-CG | 5.65 | 128.29 | 115.30 |
| 1 | 16S1 | 665 | A | C5-C6-N1 | 5.64 | 120.52 | 117.70 |
| 1 | 16S1 | 937 | A | N3-C4-N9 | 5.64 | 131.92 | 127.40 |
| 1 | 16S1 | 1213 | A | C4-C5-C6 | 5.64 | 119.82 | 117.00 |
| 22 | 23S1 | 412 | A | C4-C5-C6 | 5.64 | 119.82 | 117.00 |
| 22 | 23S1 | 979 | A | C4-C5-C6 | 5.64 | 119.82 | 117.00 |
| 22 | 23S1 | 1717 | A | C4-C5-C6 | 5.64 | 119.82 | 117.00 |
| 1 | 16S1 | 10 | A | C5-C6-N1 | 5.64 | 120.52 | 117.70 |
| 1 | 16S1 | 160 | A | N3-C4-N9 | 5.64 | 131.91 | 127.40 |
| 1 | 16S1 | 167 | A | C4-C5-C6 | 5.64 | 119.82 | 117.00 |
| 1 | 16S1 | 547 | A | C8-N9-C4 | 5.64 | 108.06 | 105.80 |
| 1 | 16S1 | 602 | A | N9-C4-C5 | 5.64 | 108.06 | 105.80 |
| 1 | 16S1 | 889 | A | N9-C4-C5 | 5.64 | 108.06 | 105.80 |
| 1 | 16S1 | 974 | A | C5-C6-N1 | 5.64 | 120.52 | 117.70 |
| 1 | 16S1 | 1476 | A | C4-C5-N7 | -5.64 | 107.88 | 110.70 |
| 1 | 16S1 | 250 | A | C4-C5-C6 | 5.64 | 119.82 | 117.00 |
| 1 | 16S1 | 1346 | A | C4-C5-N7 | -5.64 | 107.88 | 110.70 |
| 22 | 23S1 | 294 | A | N3-C4-N9 | 5.64 | 131.91 | 127.40 |
| 22 | 23S1 | 371 | A | C4-C5-C6 | 5.64 | 119.82 | 117.00 |
| 22 | 23S1 | 1665 | A | C8-N9-C4 | 5.64 | 108.06 | 105.80 |
| 22 | 23S1 | 1877 | A | N9-C4-C5 | 5.64 | 108.06 | 105.80 |
| 22 | 23S1 | 2054 | A | C8-N9-C4 | 5.64 | 108.06 | 105.80 |
| 1 | 16S1 | 1014 | A | N9-C4-C5 | 5.64 | 108.06 | 105.80 |
| 22 | 23S1 | 1393 | A | N3-C4-N9 | 5.64 | 131.91 | 127.40 |
| 22 | 23S1 | 2070 | A | C5-C6-N1 | 5.64 | 120.52 | 117.70 |
| 23 | 05S1 | 31 | C | N3-C2-O2 | -5.64 | 117.95 | 121.90 |
| 1 | 16S1 | 1225 | A | N9-C4-C5 | 5.64 | 108.05 | 105.80 |
| 22 | 23S1 | 310 | A | N9-C4-C5 | 5.64 | 108.06 | 105.80 |
| 22 | 23S1 | 1502 | A | N9-C4-C5 | 5.64 | 108.06 | 105.80 |
| 22 | 23S1 | 2327 | A | C4-C5-N7 | -5.64 | 107.88 | 110.70 |
| 22 | 23S1 | 2377 | A | C8-N9-C4 | 5.64 | 108.06 | 105.80 |
| 22 | 23S1 | 2635 | A | N3-C4-N9 | 5.64 | 131.91 | 127.40 |
| 22 | 23S1 | 346 | A | C5-C6-N1 | 5.63 | 120.52 | 117.70 |
| 22 | 23S1 | 920 | A | C4-C5-C6 | 5.63 | 119.82 | 117.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 1133 | A | N9-C4-C5 | 5.63 | 108.05 | 105.80 |
| 22 | 23S1 | 1762 | A | C4-C5-N7 | -5.63 | 107.88 | 110.70 |
| 22 | 23S1 | 1801 | A | C8-N9-C4 | 5.63 | 108.05 | 105.80 |
| 1 | 16S1 | 1216 | A | C4-C5-N7 | -5.63 | 107.88 | 110.70 |
| 22 | 23S1 | 13 | A | N9-C4-C5 | 5.63 | 108.05 | 105.80 |
| 22 | 23S1 | 454 | A | C4-C5-C6 | 5.63 | 119.82 | 117.00 |
| 1 | 16S1 | 432 | A | C4-C5-N7 | -5.63 | 107.88 | 110.70 |
| 1 | 16S1 | 1465 | A | N9-C4-C5 | 5.63 | 108.05 | 105.80 |
| 22 | 23S1 | 743 | A | C5-C6-N1 | 5.63 | 120.52 | 117.70 |
| 22 | 23S1 | 990 | A | C4-C5-C6 | 5.63 | 119.81 | 117.00 |
| 22 | 23S1 | 1705 | A | C8-N9-C4 | 5.63 | 108.05 | 105.80 |
| 1 | 16S1 | 539 | A | C4-C5-C6 | 5.63 | 119.81 | 117.00 |
| 1 | 16S1 | 1032 | G | N3-C4-N9 | 5.63 | 129.38 | 126.00 |
| 22 | 23S1 | 2336 | A | N3-C4-N9 | 5.63 | 131.90 | 127.40 |
| 22 | 23S1 | 2675 | A | C5-C6-N1 | 5.63 | 120.52 | 117.70 |
| 1 | 16S1 | 1437 | A | C5-C6-N1 | 5.63 | 120.51 | 117.70 |
| 22 | 23S1 | 1378 | A | C5-C6-N1 | 5.63 | 120.51 | 117.70 |
| 22 | 23S1 | 1384 | A | N9-C4-C5 | 5.63 | 108.05 | 105.80 |
| 22 | 23S1 | 2682 | A | N3-C4-N9 | 5.63 | 131.90 | 127.40 |
| 22 | 23S1 | 345 | A | C8-N9-C4 | 5.63 | 108.05 | 105.80 |
| 22 | 23S1 | 1000 | A | C5-C6-N1 | 5.63 | 120.51 | 117.70 |
| 22 | 23S1 | 1086 | A | C4-C5-N7 | -5.63 | 107.89 | 110.70 |
| 22 | 23S1 | 2190 | G | N7-C8-N9 | 5.62 | 115.91 | 113.10 |
| 1 | 16S1 | 371 | A | N9-C4-C5 | 5.62 | 108.05 | 105.80 |
| 22 | 23S1 | 501 | A | C4-C5-C6 | 5.62 | 119.81 | 117.00 |
| 22 | 23S1 | 614 | A | N3-C4-N9 | 5.62 | 131.90 | 127.40 |
| 22 | 23S1 | 2748 | A | N9-C4-C5 | 5.62 | 108.05 | 105.80 |
| 1 | 16S1 | 452 | A | C5-C6-N1 | 5.62 | 120.51 | 117.70 |
| 1 | 16S1 | 938 | A | N9-C4-C5 | 5.62 | 108.05 | 105.80 |
| 22 | 23S1 | 83 | A | C4-C5-C6 | 5.62 | 119.81 | 117.00 |
| 22 | 23S1 | 165 | A | C4-C5-C6 | 5.62 | 119.81 | 117.00 |
| 22 | 23S1 | 1453 | A | N3-C4-N9 | 5.62 | 131.90 | 127.40 |
| 22 | 23S1 | 1608 | A | N9-C4-C5 | 5.62 | 108.05 | 105.80 |
| 1 | 16S1 | 65 | A | N3-C4-N9 | 5.62 | 131.90 | 127.40 |
| 1 | 16S1 | 959 | A | C5-N7-C8 | 5.62 | 106.71 | 103.90 |
| 22 | 23S1 | 899 | A | N9-C4-C5 | 5.62 | 108.05 | 105.80 |
| 22 | 23S1 | 1260 | A | C5-C6-N1 | 5.62 | 120.51 | 117.70 |
| 1 | 16S1 | 44 | A | N3-C4-N9 | 5.62 | 131.90 | 127.40 |
| 22 | 23S1 | 526 | A | C8-N9-C4 | 5.62 | 108.05 | 105.80 |
| 22 | 23S1 | 1544 | A | C5-C6-N1 | 5.62 | 120.51 | 117.70 |
| 1 | 16S1 | 681 | A | C5-C6-N1 | 5.62 | 120.51 | 117.70 |
| 1 | 16S1 | 1433 | A | N3-C4-N9 | 5.62 | 131.89 | 127.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 1009 | A | C4-C5-C6 | 5.62 | 119.81 | 117.00 |
| 22 | 23S1 | 1129 | A | C8-N9-C4 | 5.62 | 108.05 | 105.80 |
| 22 | 23S1 | 1367 | A | C8-N9-C4 | 5.62 | 108.05 | 105.80 |
| 22 | 23S1 | 1583 | A | N9-C4-C5 | 5.62 | 108.05 | 105.80 |
| 1 | 16S1 | 44 | A | C4-C5-C6 | 5.62 | 119.81 | 117.00 |
| 1 | 16S1 | 790 | A | C8-N9-C4 | 5.62 | 108.05 | 105.80 |
| 22 | 23S1 | 792 | A | N9-C4-C5 | 5.62 | 108.05 | 105.80 |
| 22 | 23S1 | 1090 | A | C4-C5-C6 | 5.62 | 119.81 | 117.00 |
| 22 | 23S1 | 1321 | A | C8-N9-C4 | 5.62 | 108.05 | 105.80 |
| 22 | 23S1 | 2307 | G | N9-C4-C5 | -5.62 | 103.15 | 105.40 |
| 22 | 23S1 | 2336 | A | C4-C5-C6 | 5.62 | 119.81 | 117.00 |
| 22 | 23S1 | 2381 | A | C8-N9-C4 | 5.62 | 108.05 | 105.80 |
| 22 | 23S1 | 2516 | A | C4-C5-C6 | 5.62 | 119.81 | 117.00 |
| 1 | 16S1 | 315 | A | C4-C5-C6 | 5.61 | 119.81 | 117.00 |
| 1 | 16S1 | 596 | A | C4-C5-N7 | -5.61 | 107.89 | 110.70 |
| 1 | 16S1 | 1507 | A | C8-N9-C4 | 5.61 | 108.05 | 105.80 |
| 22 | 23S1 | 792 | A | C4-C5-C6 | 5.61 | 119.81 | 117.00 |
| 22 | 23S1 | 1126 | A | C5-C6-N1 | 5.61 | 120.51 | 117.70 |
| 22 | 23S1 | 2510 | C | N1-C2-O2 | 5.61 | 122.27 | 118.90 |
| 22 | 23S1 | 2823 | A | C8-N9-C4 | 5.61 | 108.05 | 105.80 |
| 1 | 16S1 | 1204 | A | N3-C4-N9 | 5.61 | 131.89 | 127.40 |
| 22 | 23S1 | 2635 | A | C4-C5-C6 | 5.61 | 119.81 | 117.00 |
| 22 | 23S1 | 161 | A | C8-N9-C4 | 5.61 | 108.05 | 105.80 |
| 22 | 23S1 | 198 | C | C5-C6-N1 | 5.61 | 123.81 | 121.00 |
| 22 | 23S1 | 502 | A | N9-C4-C5 | 5.61 | 108.04 | 105.80 |
| 22 | 23S1 | 751 | A | N3-C4-N9 | 5.61 | 131.89 | 127.40 |
| 22 | 23S1 | 1010 | A | N3-C4-N9 | 5.61 | 131.89 | 127.40 |
| 22 | 23S1 | 1698 | A | C8-N9-C4 | 5.61 | 108.04 | 105.80 |
| 22 | 23S1 | 1918 | A | C5-C6-N1 | 5.61 | 120.50 | 117.70 |
| 22 | 23S1 | 2322 | A | N3-C4-N9 | 5.61 | 131.89 | 127.40 |
| 55 | PTR1 | 58 | A | N3-C4-N9 | 5.61 | 131.89 | 127.40 |
| 22 | 23S1 | 262 | A | C5-C6-N1 | 5.61 | 120.50 | 117.70 |
| 22 | 23S1 | 423 | A | C4-C5-C6 | 5.61 | 119.80 | 117.00 |
| 22 | 23S1 | 1504 | A | N3-C4-N9 | 5.61 | 131.89 | 127.40 |
| 22 | 23S1 | 1597 | A | C4-C5-C6 | 5.61 | 119.80 | 117.00 |
| 22 | 23S1 | 1928 | A | N9-C4-C5 | 5.61 | 108.04 | 105.80 |
| 22 | 23S1 | 2198 | A | N3-C4-N9 | 5.61 | 131.89 | 127.40 |
| 22 | 23S1 | 2829 | A | C4-C5-N7 | -5.61 | 107.90 | 110.70 |
| 1 | 16S1 | 441 | A | C5-C6-N1 | 5.61 | 120.50 | 117.70 |
| 1 | 16S1 | 1285 | A | N3-C4-N9 | 5.61 | 131.88 | 127.40 |
| 1 | 16S1 | 1447 | A | N3-C4-N9 | 5.61 | 131.89 | 127.40 |
| 22 | 23S1 | 342 | A | C5-C6-N1 | 5.61 | 120.50 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 2182 | U | C2-N1-C1' | 5.61 | 124.43 | 117.70 |
| 22 | 23S1 | 2317 | A | C8-N9-C4 | 5.61 | 108.04 | 105.80 |
| 1 | 16S1 | 182 | A | C4-C5-C6 | 5.61 | 119.80 | 117.00 |
| 1 | 16S1 | 1250 | A | C4-C5-N7 | -5.61 | 107.90 | 110.70 |
| 22 | 23S1 | 71 | A | C8-N9-C4 | 5.61 | 108.04 | 105.80 |
| 22 | 23S1 | 675 | A | N3-C4-N9 | 5.61 | 131.88 | 127.40 |
| 22 | 23S1 | 1194 | A | N3-C4-N9 | 5.61 | 131.88 | 127.40 |
| 22 | 23S1 | 1746 | A | C4-C5-N7 | -5.61 | 107.90 | 110.70 |
| 1 | 16S1 | 363 | A | N3-C4-N9 | 5.60 | 131.88 | 127.40 |
| 22 | 23S1 | 2165 | C | C6-N1-C2 | -5.60 | 118.06 | 120.30 |
| 1 | 16S1 | 600 | A | C5-C6-N1 | 5.60 | 120.50 | 117.70 |
| 1 | 16S1 | 1172 | C | N3-C2-O2 | -5.60 | 117.98 | 121.90 |
| 22 | 23S1 | 781 | A | C5-C6-N1 | 5.60 | 120.50 | 117.70 |
| 22 | 23S1 | 1545 | A | C8-N9-C4 | 5.60 | 108.04 | 105.80 |
| 22 | 23S1 | 2740 | A | C4-C5-C6 | 5.60 | 119.80 | 117.00 |
| 22 | 23S1 | 2541 | A | C4-C5-C6 | 5.60 | 119.80 | 117.00 |
| 1 | 16S1 | 172 | A | N9-C4-C5 | 5.60 | 108.04 | 105.80 |
| 1 | 16S1 | 546 | A | C8-N9-C4 | 5.60 | 108.04 | 105.80 |
| 1 | 16S1 | 621 | A | C4-C5-N7 | -5.60 | 107.90 | 110.70 |
| 1 | 16S1 | 1446 | A | C5-C6-N1 | 5.60 | 120.50 | 117.70 |
| 22 | 23S1 | 219 | A | C4-C5-N7 | -5.60 | 107.90 | 110.70 |
| 22 | 23S1 | 586 | A | C5-N7-C8 | 5.60 | 106.70 | 103.90 |
| 22 | 23S1 | 1067 | A | C4-C5-C6 | 5.60 | 119.80 | 117.00 |
| 22 | 23S1 | 1794 | A | C4-C5-N7 | -5.60 | 107.90 | 110.70 |
| 22 | 23S1 | 2518 | A | C5-C6-N1 | 5.60 | 120.50 | 117.70 |
| 1 | 16S1 | 44 | A | C8-N9-C4 | 5.60 | 108.04 | 105.80 |
| 1 | 16S1 | 309 | A | N3-C4-N9 | 5.60 | 131.88 | 127.40 |
| 1 | 16S1 | 553 | A | C4-C5-C6 | 5.60 | 119.80 | 117.00 |
| 1 | 16S1 | 1257 | A | C4-C5-C6 | 5.60 | 119.80 | 117.00 |
| 22 | 23S1 | 912 | C | N1-C2-O2 | 5.60 | 122.26 | 118.90 |
| 22 | 23S1 | 1545 | A | N9-C4-C5 | 5.60 | 108.04 | 105.80 |
| 22 | 23S1 | 2350 | C | N1-C2-O2 | 5.60 | 122.26 | 118.90 |
| 1 | 16S1 | 149 | A | N9-C4-C5 | 5.60 | 108.04 | 105.80 |
| 22 | 23S1 | 718 | A | N9-C4-C5 | 5.60 | 108.04 | 105.80 |
| 1 | 16S1 | 579 | A | C8-N9-C4 | 5.59 | 108.04 | 105.80 |
| 1 | 16S1 | 1437 | A | C4-C5-C6 | 5.59 | 119.80 | 117.00 |
| 1 | 16S1 | 1447 | A | N9-C4-C5 | 5.59 | 108.04 | 105.80 |
| 22 | 23S1 | 1597 | A | C5-C6-N1 | 5.59 | 120.50 | 117.70 |
| 22 | 23S1 | 2126 | A | N9-C4-C5 | 5.59 | 108.04 | 105.80 |
| 1 | 16S1 | 1431 | A | C5-C6-N1 | 5.59 | 120.50 | 117.70 |
| 22 | 23S1 | 1328 | A | C4-C5-C6 | 5.59 | 119.80 | 117.00 |
| 22 | 23S1 | 1757 | A | C5-C6-N1 | 5.59 | 120.50 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 2288 | A | C4-C5-C6 | 5.59 | 119.80 | 117.00 |
| 22 | 23S1 | 2882 | A | N3-C4-N9 | 5.59 | 131.87 | 127.40 |
| 1 | 16S1 | 74 | A | C4-C5-N7 | -5.59 | 107.91 | 110.70 |
| 1 | 16S1 | 344 | A | C8-N9-C4 | 5.59 | 108.04 | 105.80 |
| 1 | 16S1 | 753 | A | N9-C4-C5 | 5.59 | 108.03 | 105.80 |
| 1 | 16S1 | 909 | A | N3-C4-N9 | 5.59 | 131.87 | 127.40 |
| 22 | 23S1 | 160 | A | C5-C6-N1 | 5.59 | 120.49 | 117.70 |
| 22 | 23S1 | 272 | A | C8-N9-C4 | 5.59 | 108.04 | 105.80 |
| 22 | 23S1 | 1254 | A | C5-C6-N1 | 5.59 | 120.50 | 117.70 |
| 55 | PTR1 | 23 | A | N9-C4-C5 | 5.59 | 108.04 | 105.80 |
| 55 | PTR1 | 59 | A | C5-C6-N1 | 5.59 | 120.50 | 117.70 |
| 1 | 16S1 | 139 | A | C4-C5-C6 | 5.59 | 119.79 | 117.00 |
| 19 | S191 | 28 | LYS | CA-CB-CG | 5.59 | 125.69 | 113.40 |
| 22 | 23S1 | 599 | A | C4-C5-C6 | 5.59 | 119.79 | 117.00 |
| 1 | 16S1 | 309 | A | C4-C5-N7 | -5.59 | 107.91 | 110.70 |
| 1 | 16S1 | 363 | A | C4-C5-C6 | 5.59 | 119.79 | 117.00 |
| 1 | 16S1 | 749 | A | C5-C6-N1 | 5.59 | 120.49 | 117.70 |
| 22 | 23S1 | 751 | A | C4-C5-C6 | 5.59 | 119.79 | 117.00 |
| 22 | 23S1 | 1237 | A | C5-C6-N1 | 5.59 | 120.49 | 117.70 |
| 22 | 23S1 | 1614 | A | N3-C4-N9 | 5.59 | 131.87 | 127.40 |
| 1 | 16S1 | 1021 | A | C4-C5-C6 | 5.58 | 119.79 | 117.00 |
| 22 | 23S1 | 764 | A | N9-C4-C5 | 5.58 | 108.03 | 105.80 |
| 1 | 16S1 | 28 | A | C8-N9-C4 | 5.58 | 108.03 | 105.80 |
| 1 | 16S1 | 1340 | A | N3-C4-N9 | 5.58 | 131.87 | 127.40 |
| 1 | 16S1 | 1363 | A | C4-C5-N7 | -5.58 | 107.91 | 110.70 |
| 22 | 23S1 | 42 | A | C8-N9-C4 | 5.58 | 108.03 | 105.80 |
| 22 | 23S1 | 447 | A | C8-N9-C4 | 5.58 | 108.03 | 105.80 |
| 22 | 23S1 | 878 | A | N3-C4-N9 | 5.58 | 131.87 | 127.40 |
| 23 | 05S1 | 70 | C | N1-C2-O2 | 5.58 | 122.25 | 118.90 |
| 1 | 16S1 | 223 | A | C4-C5-N7 | -5.58 | 107.91 | 110.70 |
| 1 | 16S1 | 243 | A | C4-C5-C6 | 5.58 | 119.79 | 117.00 |
| 1 | 16S1 | 1229 | A | C4-C5-N7 | -5.58 | 107.91 | 110.70 |
| 22 | 23S1 | 722 | A | C5-C6-N1 | 5.58 | 120.49 | 117.70 |
| 22 | 23S1 | 1385 | A | C8-N9-C4 | 5.58 | 108.03 | 105.80 |
| 22 | 23S1 | 2616 | C | N3-C2-O2 | -5.58 | 117.99 | 121.90 |
| 22 | 23S1 | 73 | A | C4-C5-C6 | 5.58 | 119.79 | 117.00 |
| 22 | 23S1 | 833 | A | C5-C6-N1 | 5.58 | 120.49 | 117.70 |
| 22 | 23S1 | 1913 | A | C4-C5-C6 | 5.58 | 119.79 | 117.00 |
| 22 | 23S1 | 2212 | A | C8-N9-C4 | 5.58 | 108.03 | 105.80 |
| 22 | 23S1 | 735 | A | C4-C5-C6 | 5.58 | 119.79 | 117.00 |
| 55 | PTR1 | 51 | A | C8-N9-C4 | 5.58 | 108.03 | 105.80 |
| 1 | 16S1 | 1035 | A | N9-C4-C5 | 5.58 | 108.03 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 631 | A | C4-C5-C6 | 5.58 | 119.79 | 117.00 |
| 1 | 16S1 | 559 | A | C4-C5-C6 | 5.58 | 119.79 | 117.00 |
| 1 | 16S1 | 777 | A | C4-C5-C6 | 5.58 | 119.79 | 117.00 |
| 1 | 16S1 | 1130 | A | C4-C5-C6 | 5.58 | 119.79 | 117.00 |
| 1 | 16S1 | 1287 | A | N3-C4-N9 | 5.58 | 131.86 | 127.40 |
| 1 | 16S1 | 1395 | C | C6-N1-C2 | -5.58 | 118.07 | 120.30 |
| 1 | 16S1 | 1398 | A | C4-C5-C6 | 5.58 | 119.79 | 117.00 |
| 22 | 23S1 | 196 | A | C4-C5-N7 | -5.58 | 107.91 | 110.70 |
| 22 | 23S1 | 453 | A | N9-C4-C5 | 5.58 | 108.03 | 105.80 |
| 22 | 23S1 | 1226 | A | C4-C5-C6 | 5.58 | 119.79 | 117.00 |
| 1 | 16S1 | 253 | A | N3-C4-N9 | 5.57 | 131.86 | 127.40 |
| 1 | 16S1 | 1465 | A | C4-C5-C6 | 5.57 | 119.79 | 117.00 |
| 22 | 23S1 | 1504 | A | C4-C5-C6 | 5.57 | 119.79 | 117.00 |
| 22 | 23S1 | 1901 | A | N9-C4-C5 | 5.57 | 108.03 | 105.80 |
| 22 | 23S1 | 2321 | U | N1-C2-O2 | 5.57 | 126.70 | 122.80 |
| 1 | 16S1 | 414 | A | N3-C4-N9 | 5.57 | 131.86 | 127.40 |
| 1 | 16S1 | 602 | A | C8-N9-C4 | 5.57 | 108.03 | 105.80 |
| 1 | 16S1 | 1238 | A | C4-C5-N7 | -5.57 | 107.91 | 110.70 |
| 1 | 16S1 | 560 | A | C4-C5-C6 | 5.57 | 119.79 | 117.00 |
| 22 | 23S1 | 765 | C | N3-C2-O2 | -5.57 | 118.00 | 121.90 |
| 22 | 23S1 | 1096 | A | N9-C4-C5 | 5.57 | 108.03 | 105.80 |
| 22 | 23S1 | 1535 | A | N9-C4-C5 | 5.57 | 108.03 | 105.80 |
| 22 | 23S1 | 1551 | A | C4-C5-N7 | -5.57 | 107.92 | 110.70 |
| 55 | PTR1 | 20 | U | C6-N1-C2 | 5.57 | 124.34 | 121.00 |
| 22 | 23S1 | 792 | A | C4-C5-N7 | -5.57 | 107.92 | 110.70 |
| 22 | 23S1 | 1960 | A | N9-C4-C5 | 5.57 | 108.03 | 105.80 |
| 22 | 23S1 | 2163 | A | C8-N9-C4 | 5.57 | 108.03 | 105.80 |
| 22 | 23S1 | 1262 | A | C4-C5-C6 | 5.57 | 119.78 | 117.00 |
| 22 | 23S1 | 1549 | A | C5-C6-N1 | 5.57 | 120.48 | 117.70 |
| 22 | 23S1 | 2212 | A | C4-C5-C6 | 5.57 | 119.78 | 117.00 |
| 1 | 16S1 | 78 | A | C5-C6-N1 | 5.57 | 120.48 | 117.70 |
| 1 | 16S1 | 298 | A | C5-C6-N1 | 5.57 | 120.48 | 117.70 |
| 1 | 16S1 | 329 | A | C8-N9-C4 | 5.57 | 108.03 | 105.80 |
| 1 | 16S1 | 1158 | C | C5-C6-N1 | 5.57 | 123.78 | 121.00 |
| 1 | 16S1 | 1447 | A | C4-C5-C6 | 5.57 | 119.78 | 117.00 |
| 22 | 23S1 | 1495 | A | C4-C5-C6 | 5.57 | 119.78 | 117.00 |
| 22 | 23S1 | 1665 | A | C4-C5-N7 | -5.57 | 107.92 | 110.70 |
| 22 | 23S1 | 1749 | A | C4-C5-C6 | 5.56 | 119.78 | 117.00 |
| 22 | 23S1 | 2051 | A | C5-C6-N1 | 5.56 | 120.48 | 117.70 |
| 1 | 16S1 | 143 | A | N3-C4-N9 | 5.56 | 131.85 | 127.40 |
| 1 | 16S1 | 303 | A | N3-C4-N9 | 5.56 | 131.85 | 127.40 |
| 1 | 16S1 | 845 | A | C4-C5-N7 | -5.56 | 107.92 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 16S1 | 949 | A | C8-N9-C4 | 5.56 | 108.03 | 105.80 |
| 1 | 16S1 | 1261 | A | C4-C5-C6 | 5.56 | 119.78 | 117.00 |
| 1 | 16S1 | 1430 | A | N9-C4-C5 | 5.56 | 108.03 | 105.80 |
| 22 | 23S1 | 1340 | U | C2-N3-C4 | -5.56 | 123.66 | 127.00 |
| 22 | 23S1 | 1477 | A | C8-N9-C4 | 5.56 | 108.03 | 105.80 |
| 22 | 23S1 | 1677 | A | N3-C4-N9 | 5.56 | 131.85 | 127.40 |
| 22 | 23S1 | 310 | A | C8-N9-C4 | 5.56 | 108.02 | 105.80 |
| 22 | 23S1 | 670 | A | C8-N9-C4 | 5.56 | 108.02 | 105.80 |
| 22 | 23S1 | 1551 | A | C4-C5-C6 | 5.56 | 119.78 | 117.00 |
| 22 | 23S1 | 1901 | A | C4-C5-C6 | 5.56 | 119.78 | 117.00 |
| 1 | 16S1 | 288 | A | N9-C4-C5 | 5.56 | 108.02 | 105.80 |
| 1 | 16S1 | 528 | C | C6-N1-C2 | -5.56 | 118.08 | 120.30 |
| 1 | 16S1 | 1493 | A | N9-C4-C5 | 5.56 | 108.02 | 105.80 |
| 22 | 23S1 | 1175 | A | C5-C6-N1 | 5.56 | 120.48 | 117.70 |
| 22 | 23S1 | 1548 | A | C5-C6-N1 | 5.56 | 120.48 | 117.70 |
| 1 | 16S1 | 831 | A | C5-C6-N1 | 5.56 | 120.48 | 117.70 |
| 1 | 16S1 | 1271 | A | C5-C6-N1 | 5.56 | 120.48 | 117.70 |
| 9 | S091 | 61 | LEU | CA-CB-CG | 5.56 | 128.08 | 115.30 |
| 22 | 23S1 | 213 | A | C5-C6-N1 | 5.56 | 120.48 | 117.70 |
| 22 | 23S1 | 412 | A | C5-C6-N1 | 5.56 | 120.48 | 117.70 |
| 22 | 23S1 | 2150 | C | N3-C2-O2 | -5.56 | 118.01 | 121.90 |
| 22 | 23S1 | 2660 | A | C4-C5-C6 | 5.56 | 119.78 | 117.00 |
| 1 | 16S1 | 681 | A | C8-N9-C4 | 5.56 | 108.02 | 105.80 |
| 22 | 23S1 | 574 | A | C4-C5-C6 | 5.56 | 119.78 | 117.00 |
| 22 | 23S1 | 1040 | A | C4-C5-C6 | 5.56 | 119.78 | 117.00 |
| 55 | PTR1 | 59 | A | N3-C4-N9 | 5.55 | 131.84 | 127.40 |
| 1 | 16S1 | 131 | A | N9-C4-C5 | 5.55 | 108.02 | 105.80 |
| 22 | 23S1 | 1932 | A | C5-C6-N1 | 5.55 | 120.48 | 117.70 |
| 1 | 16S1 | 437 | U | N3-C2-O2 | -5.55 | 118.31 | 122.20 |
| 1 | 16S1 | 466 | A | N3-C4-N9 | 5.55 | 131.84 | 127.40 |
| 1 | 16S1 | 495 | A | N3-C4-N9 | 5.55 | 131.84 | 127.40 |
| 1 | 16S1 | 996 | A | C4-C5-C6 | 5.55 | 119.78 | 117.00 |
| 22 | 23S1 | 231 | A | C5-C6-N1 | 5.55 | 120.48 | 117.70 |
| 22 | 23S1 | 1783 | A | C4-C5-C6 | 5.55 | 119.78 | 117.00 |
| 22 | 23S1 | 1872 | A | C5-N7-C8 | 5.55 | 106.68 | 103.90 |
| 1 | 16S1 | 129 | A | N9-C4-C5 | 5.55 | 108.02 | 105.80 |
| 1 | 16S1 | 195 | A | C5-C6-N1 | 5.55 | 120.47 | 117.70 |
| 1 | 16S1 | 1413 | A | C8-N9-C4 | 5.55 | 108.02 | 105.80 |
| 22 | 23S1 | 95 | A | C5-C6-N1 | 5.55 | 120.47 | 117.70 |
| 22 | 23S1 | 127 | A | C6-N1-C2 | 5.55 | 121.93 | 118.60 |
| 22 | 23S1 | 1744 | A | C4-C5-C6 | 5.55 | 119.78 | 117.00 |
| 22 | 23S1 | 2587 | A | N3-C4-N9 | 5.55 | 131.84 | 127.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 16S1 | 509 | A | C8-N9-C4 | 5.55 | 108.02 | 105.80 |
| 1 | 16S1 | 1236 | A | C4-C5-C6 | 5.55 | 119.77 | 117.00 |
| 22 | 23S1 | 111 | A | C4-C5-C6 | 5.55 | 119.77 | 117.00 |
| 22 | 23S1 | 1205 | A | C4-C5-N7 | -5.55 | 107.93 | 110.70 |
| 22 | 23S1 | 2660 | A | C5-C6-N1 | 5.55 | 120.47 | 117.70 |
| 22 | 23S1 | 173 | A | C5-C6-N1 | 5.54 | 120.47 | 117.70 |
| 1 | 16S1 | 1500 | A | N3-C4-N9 | 5.54 | 131.83 | 127.40 |
| 22 | 23S1 | 1214 | A | N3-C4-N9 | 5.54 | 131.84 | 127.40 |
| 22 | 23S1 | 1509 | A | C8-N9-C4 | 5.54 | 108.02 | 105.80 |
| 22 | 23S1 | 1640 | A | N3-C4-N9 | 5.54 | 131.84 | 127.40 |
| 22 | 23S1 | 2736 | A | N3-C4-N9 | 5.54 | 131.84 | 127.40 |
| 22 | 23S1 | 2835 | A | C4-C5-C6 | 5.54 | 119.77 | 117.00 |
| 1 | 16S1 | 171 | A | C8-N9-C4 | 5.54 | 108.02 | 105.80 |
| 1 | 16S1 | 288 | A | C5-C6-N1 | 5.54 | 120.47 | 117.70 |
| 1 | 16S1 | 353 | A | C4-C5-C6 | 5.54 | 119.77 | 117.00 |
| 1 | 16S1 | 704 | A | C5-C6-N1 | 5.54 | 120.47 | 117.70 |
| 1 | 16S1 | 1441 | A | C4-C5-N7 | -5.54 | 107.93 | 110.70 |
| 22 | 23S1 | 370 | G | O4'-C1'-N9 | -5.54 | 103.77 | 108.20 |
| 22 | 23S1 | 526 | A | C5-C6-N1 | 5.54 | 120.47 | 117.70 |
| 22 | 23S1 | 705 | A | C8-N9-C4 | 5.54 | 108.02 | 105.80 |
| 22 | 23S1 | 804 | A | N3-C4-N9 | 5.54 | 131.83 | 127.40 |
| 22 | 23S1 | 1509 | A | N3-C4-N9 | 5.54 | 131.83 | 127.40 |
| 22 | 23S1 | 1805 | A | N9-C4-C5 | 5.54 | 108.02 | 105.80 |
| 22 | 23S1 | 2020 | A | C5-C6-N1 | 5.54 | 120.47 | 117.70 |
| 22 | 23S1 | 2309 | A | N3-C4-N9 | 5.54 | 131.83 | 127.40 |
| 22 | 23S1 | 2565 | A | N3-C4-N9 | 5.54 | 131.83 | 127.40 |
| 22 | 23S1 | 2821 | A | C8-N9-C4 | 5.54 | 108.02 | 105.80 |
| 1 | 16S1 | 253 | A | C5-C6-N1 | 5.54 | 120.47 | 117.70 |
| 1 | 16S1 | 753 | A | C5-C6-N1 | 5.54 | 120.47 | 117.70 |
| 1 | 16S1 | 1428 | A | C5-C6-N1 | 5.54 | 120.47 | 117.70 |
| 22 | 23S1 | 715 | A | C8-N9-C4 | 5.54 | 108.02 | 105.80 |
| 22 | 23S1 | 1000 | A | C4-C5-N7 | -5.54 | 107.93 | 110.70 |
| 22 | 23S1 | 1730 | C | C6-N1-C1' | -5.54 | 114.15 | 120.80 |
| 22 | 23S1 | 2311 | A | N3-C4-N9 | 5.54 | 131.83 | 127.40 |
| 22 | 23S1 | 2589 | A | C4-C5-C6 | 5.54 | 119.77 | 117.00 |
| 23 | 05S1 | 109 | A | C5-C6-N1 | 5.54 | 120.47 | 117.70 |
| 1 | 16S1 | 223 | A | N9-C4-C5 | 5.54 | 108.02 | 105.80 |
| 1 | 16S1 | 320 | A | N9-C4-C5 | 5.54 | 108.02 | 105.80 |
| 22 | 23S1 | 443 | A | N3-C4-N9 | 5.54 | 131.83 | 127.40 |
| 22 | 23S1 | 479 | A | C5-C6-N1 | 5.54 | 120.47 | 117.70 |
| 22 | 23S1 | 111 | A | C4-C5-N7 | -5.53 | 107.93 | 110.70 |
| 22 | 23S1 | 402 | A | C4-C5-C6 | 5.53 | 119.77 | 117.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 900 | A | C5-C6-N1 | 5.53 | 120.47 | 117.70 |
| 22 | 23S1 | 1000 | A | C4-C5-C6 | 5.53 | 119.77 | 117.00 |
| 1 | 16S1 | 408 | A | C4-C5-N7 | -5.53 | 107.93 | 110.70 |
| 22 | 23S1 | 2287 | A | C8-N9-C4 | 5.53 | 108.01 | 105.80 |
| 1 | 16S1 | 509 | A | N9-C4-C5 | 5.53 | 108.01 | 105.80 |
| 22 | 23S1 | 119 | A | C4-C5-N7 | -5.53 | 107.94 | 110.70 |
| 22 | 23S1 | 602 | A | C4-C5-C6 | 5.53 | 119.77 | 117.00 |
| 22 | 23S1 | 1103 | A | C8-N9-C4 | 5.53 | 108.01 | 105.80 |
| 22 | 23S1 | 1967 | C | N1-C2-O2 | 5.53 | 122.22 | 118.90 |
| 22 | 23S1 | 1981 | A | C8-N9-C4 | 5.53 | 108.01 | 105.80 |
| 22 | 23S1 | 2352 | A | C4-C5-N7 | -5.53 | 107.93 | 110.70 |
| 1 | 16S1 | 860 | A | N3-C4-N9 | 5.53 | 131.82 | 127.40 |
| 22 | 23S1 | 1508 | A | C5-C6-N1 | 5.53 | 120.46 | 117.70 |
| 1 | 16S1 | 371 | A | C4-C5-C6 | 5.53 | 119.76 | 117.00 |
| 1 | 16S1 | 842 | U | N3-C2-O2 | -5.53 | 118.33 | 122.20 |
| 1 | 16S1 | 909 | A | C4-C5-C6 | 5.53 | 119.76 | 117.00 |
| 22 | 23S1 | 64 | A | C8-N9-C4 | 5.53 | 108.01 | 105.80 |
| 22 | 23S1 | 146 | A | N9-C4-C5 | 5.53 | 108.01 | 105.80 |
| 22 | 23S1 | 749 | A | C8-N9-C4 | 5.53 | 108.01 | 105.80 |
| 22 | 23S1 | 965 | C | C6-N1-C2 | -5.53 | 118.09 | 120.30 |
| 22 | 23S1 | 1008 | A | C4-C5-C6 | 5.53 | 119.76 | 117.00 |
| 1 | 16S1 | 784 | A | C8-N9-C4 | 5.53 | 108.01 | 105.80 |
| 1 | 16S1 | 1456 | A | N3-C4-N9 | 5.53 | 131.82 | 127.40 |
| 22 | 23S1 | 1779 | U | C2-N1-C1' | 5.53 | 124.33 | 117.70 |
| 22 | 23S1 | 2154 | A | C8-N9-C4 | 5.53 | 108.01 | 105.80 |
| 1 | 16S1 | 649 | A | C4-C5-N7 | -5.52 | 107.94 | 110.70 |
| 22 | 23S1 | 1496 | A | N9-C4-C5 | 5.52 | 108.01 | 105.80 |
| 22 | 23S1 | 2019 | A | C8-N9-C4 | 5.52 | 108.01 | 105.80 |
| 22 | 23S1 | 2212 | A | C5-C6-N1 | 5.52 | 120.46 | 117.70 |
| 22 | 23S1 | 2705 | A | N3-C4-N9 | 5.52 | 131.82 | 127.40 |
| 1 | 16S1 | 918 | A | C5-C6-N1 | 5.52 | 120.46 | 117.70 |
| 22 | 23S1 | 95 | A | N9-C4-C5 | 5.52 | 108.01 | 105.80 |
| 22 | 23S1 | 631 | A | C5-C6-N1 | 5.52 | 120.46 | 117.70 |
| 22 | 23S1 | 892 | A | C4-C5-N7 | -5.52 | 107.94 | 110.70 |
| 22 | 23S1 | 2750 | A | N3-C4-N9 | 5.52 | 131.82 | 127.40 |
| 22 | 23S1 | 2776 | A | C4-C5-N7 | -5.52 | 107.94 | 110.70 |
| 1 | 16S1 | 409 | U | N1-C2-O2 | 5.52 | 126.67 | 122.80 |
| 22 | 23S1 | 272 | A | C5-C6-N1 | 5.52 | 120.46 | 117.70 |
| 22 | 23S1 | 1133 | A | N3-C4-N9 | 5.52 | 131.82 | 127.40 |
| 22 | 23S1 | 2031 | A | C4-C5-C6 | 5.52 | 119.76 | 117.00 |
| 22 | 23S1 | 2322 | A | N9-C4-C5 | 5.52 | 108.01 | 105.80 |
| 1 | 16S1 | 1332 | A | N9-C4-C5 | 5.52 | 108.01 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 73 | A | N9-C4-C5 | 5.52 | 108.01 | 105.80 |
| 22 | 23S1 | 353 | C | N1-C2-O2 | 5.52 | 122.21 | 118.90 |
| 1 | 16S1 | 648 | A | N9-C4-C5 | 5.52 | 108.01 | 105.80 |
| 22 | 23S1 | 514 | A | N9-C4-C5 | 5.52 | 108.01 | 105.80 |
| 22 | 23S1 | 2518 | A | C8-N9-C4 | 5.52 | 108.01 | 105.80 |
| 23 | 05S1 | 39 | A | C4-C5-C6 | 5.52 | 119.76 | 117.00 |
| 1 | 16S1 | 486 | U | N1-C2-O2 | 5.52 | 126.66 | 122.80 |
| 1 | 16S1 | 784 | A | C4-C5-C6 | 5.51 | 119.76 | 117.00 |
| 1 | 16S1 | 882 | C | N1-C2-O2 | 5.51 | 122.21 | 118.90 |
| 1 | 16S1 | 1146 | A | C5-C6-N1 | 5.51 | 120.46 | 117.70 |
| 22 | 23S1 | 265 | A | N3-C4-N9 | 5.51 | 131.81 | 127.40 |
| 22 | 23S1 | 1147 | A | C4-C5-C6 | 5.51 | 119.76 | 117.00 |
| 22 | 23S1 | 125 | A | C4-C5-C6 | 5.51 | 119.76 | 117.00 |
| 22 | 23S1 | 849 | A | C5-C6-N1 | 5.51 | 120.46 | 117.70 |
| 22 | 23S1 | 2727 | A | C5-C6-N1 | 5.51 | 120.46 | 117.70 |
| 22 | 23S1 | 2868 | A | N9-C4-C5 | 5.51 | 108.00 | 105.80 |
| 22 | 23S1 | 2880 | C | N3-C2-O2 | -5.51 | 118.04 | 121.90 |
| 1 | 16S1 | 81 | A | C4-C5-N7 | -5.51 | 107.94 | 110.70 |
| 1 | 16S1 | 655 | A | N9-C4-C5 | 5.51 | 108.00 | 105.80 |
| 1 | 16S1 | 842 | U | N1-C2-O2 | 5.51 | 126.66 | 122.80 |
| 1 | 16S1 | 1493 | A | C4-C5-N7 | -5.51 | 107.94 | 110.70 |
| 22 | 23S1 | 231 | A | N9-C4-C5 | 5.51 | 108.00 | 105.80 |
| 22 | 23S1 | 918 | A | N3-C4-N9 | 5.51 | 131.81 | 127.40 |
| 22 | 23S1 | 1264 | A | N3-C4-N9 | 5.51 | 131.81 | 127.40 |
| 22 | 23S1 | 1392 | A | C4-C5-N7 | -5.51 | 107.94 | 110.70 |
| 22 | 23S1 | 1772 | A | N9-C4-C5 | 5.51 | 108.00 | 105.80 |
| 22 | 23S1 | 1987 | A | C5-C6-N1 | 5.51 | 120.45 | 117.70 |
| 22 | 23S1 | 2169 | A | C4-C5-N7 | -5.51 | 107.94 | 110.70 |
| 55 | PTR1 | 14 | A | C4-C5-N7 | -5.51 | 107.94 | 110.70 |
| 1 | 16S1 | 1447 | A | C4-C5-N7 | -5.51 | 107.95 | 110.70 |
| 23 | 05S1 | 99 | A | C5-C6-N1 | 5.51 | 120.45 | 117.70 |
| 1 | 16S1 | 1441 | A | C4-C5-C6 | 5.51 | 119.75 | 117.00 |
| 22 | 23S1 | 761 | A | C5-N7-C8 | 5.51 | 106.65 | 103.90 |
| 22 | 23S1 | 1668 | A | N3-C4-N9 | 5.51 | 131.81 | 127.40 |
| 22 | 23S1 | 2386 | A | C4-C5-C6 | 5.51 | 119.75 | 117.00 |
| 22 | 23S1 | 2797 | U | N1-C2-O2 | 5.51 | 126.66 | 122.80 |
| 22 | 23S1 | 1786 | A | C4-C5-C6 | 5.50 | 119.75 | 117.00 |
| 1 | 16S1 | 468 | A | N9-C4-C5 | 5.50 | 108.00 | 105.80 |
| 1 | 16S1 | 768 | A | N3-C4-N9 | 5.50 | 131.80 | 127.40 |
| 22 | 23S1 | 6 | A | N9-C4-C5 | 5.50 | 108.00 | 105.80 |
| 22 | 23S1 | 927 | A | C4-C5-C6 | 5.50 | 119.75 | 117.00 |
| 22 | 23S1 | 1366 | A | C8-N9-C4 | 5.50 | 108.00 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 1508 | A | N3-C4-N9 | 5.50 | 131.80 | 127.40 |
| 22 | 23S1 | 1637 | A | C5-C6-N1 | 5.50 | 120.45 | 117.70 |
| 22 | 23S1 | 1805 | A | C4-C5-N7 | -5.50 | 107.95 | 110.70 |
| 22 | 23S1 | 2183 | A | C8-N9-C4 | 5.50 | 108.00 | 105.80 |
| 22 | 23S1 | 2266 | A | C4-C5-C6 | 5.50 | 119.75 | 117.00 |
| 1 | 16S1 | 1180 | A | N9-C4-C5 | 5.50 | 108.00 | 105.80 |
| 22 | 23S1 | 614 | A | C4-C5-C6 | 5.50 | 119.75 | 117.00 |
| 22 | 23S1 | 1008 | A | C8-N9-C4 | 5.50 | 108.00 | 105.80 |
| 22 | 23S1 | 1872 | A | N9-C4-C5 | 5.50 | 108.00 | 105.80 |
| 22 | 23S1 | 2212 | A | C4-C5-N7 | -5.50 | 107.95 | 110.70 |
| 22 | 23S1 | 2418 | A | C4-C5-N7 | -5.50 | 107.95 | 110.70 |
| 22 | 23S1 | 2851 | A | C4-C5-C6 | 5.50 | 119.75 | 117.00 |
| 23 | 05S1 | 66 | A | N3-C4-N9 | 5.50 | 131.80 | 127.40 |
| 1 | 16S1 | 547 | A | N3-C4-N9 | 5.50 | 131.80 | 127.40 |
| 22 | 23S1 | 14 | A | N9-C4-C5 | 5.50 | 108.00 | 105.80 |
| 22 | 23S1 | 782 | A | C4-C5-N7 | -5.50 | 107.95 | 110.70 |
| 22 | 23S1 | 1189 | A | C8-N9-C4 | 5.50 | 108.00 | 105.80 |
| 1 | 16S1 | 1502 | A | N3-C4-N9 | 5.50 | 131.80 | 127.40 |
| 22 | 23S1 | 637 | A | N9-C4-C5 | 5.50 | 108.00 | 105.80 |
| 22 | 23S1 | 1008 | A | N3-C4-N9 | 5.50 | 131.80 | 127.40 |
| 22 | 23S1 | 1032 | A | C8-N9-C4 | 5.50 | 108.00 | 105.80 |
| 22 | 23S1 | 1129 | A | N3-C4-N9 | 5.50 | 131.80 | 127.40 |
| 22 | 23S1 | 1376 | C | N3-C2-O2 | -5.50 | 118.05 | 121.90 |
| 22 | 23S1 | 1640 | A | C5-C6-N1 | 5.50 | 120.45 | 117.70 |
| 22 | 23S1 | 2562 | U | N3-C2-O2 | -5.50 | 118.35 | 122.20 |
| 22 | 23S1 | 2820 | A | C8-N9-C4 | 5.50 | 108.00 | 105.80 |
| 22 | 23S1 | 2900 | A | C5-C6-N1 | 5.50 | 120.45 | 117.70 |
| 1 | 16S1 | 88 | U | N1-C2-O2 | 5.50 | 126.65 | 122.80 |
| 1 | 16S1 | 179 | A | N3-C4-N9 | 5.50 | 131.80 | 127.40 |
| 22 | 23S1 | 541 | A | C4-C5-N7 | -5.50 | 107.95 | 110.70 |
| 22 | 23S1 | 1053 | C | N3-C2-O2 | -5.50 | 118.05 | 121.90 |
| 22 | 23S1 | 1077 | A | C4-C5-C6 | 5.50 | 119.75 | 117.00 |
| 22 | 23S1 | 2009 | A | C8-N9-C4 | 5.50 | 108.00 | 105.80 |
| 22 | 23S1 | 2247 | A | C4-C5-N7 | -5.50 | 107.95 | 110.70 |
| 55 | PTR1 | 26 | A | N3-C4-N9 | 5.50 | 131.80 | 127.40 |
| 1 | 16S1 | 675 | A | C4-C5-C6 | 5.50 | 119.75 | 117.00 |
| 1 | 16S1 | 969 | A | N3-C4-N9 | 5.49 | 131.79 | 127.40 |
| 1 | 16S1 | 1480 | A | C4-C5-N7 | -5.49 | 107.95 | 110.70 |
| 22 | 23S1 | 144 | A | N9-C4-C5 | 5.49 | 108.00 | 105.80 |
| 22 | 23S1 | 802 | A | N9-C4-C5 | 5.49 | 108.00 | 105.80 |
| 22 | 23S1 | 1010 | A | C4-C5-C6 | 5.49 | 119.75 | 117.00 |
| 22 | 23S1 | 1690 | A | N3-C4-N9 | 5.49 | 131.79 | 127.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 2281 | A | C8-N9-C4 | 5.49 | 108.00 | 105.80 |
| 1 | 16S1 | 1363 | A | N9-C4-C5 | 5.49 | 108.00 | 105.80 |
| 1 | 16S1 | 716 | A | C4-C5-C6 | 5.49 | 119.75 | 117.00 |
| 1 | 16S1 | 1396 | A | C8-N9-C4 | 5.49 | 108.00 | 105.80 |
| 22 | 23S1 | 432 | A | N9-C4-C5 | 5.49 | 108.00 | 105.80 |
| 22 | 23S1 | 838 | C | N1-C2-O2 | 5.49 | 122.19 | 118.90 |
| 22 | 23S1 | 1525 | A | C4-C5-C6 | 5.49 | 119.75 | 117.00 |
| 22 | 23S1 | 1803 | A | N3-C4-N9 | 5.49 | 131.79 | 127.40 |
| 23 | 05S1 | 57 | A | C4-C5-C6 | 5.49 | 119.75 | 117.00 |
| 1 | 16S1 | 253 | A | C4-C5-C6 | 5.49 | 119.75 | 117.00 |
| 1 | 16S1 | 1375 | A | C8-N9-C4 | 5.49 | 108.00 | 105.80 |
| 22 | 23S1 | 225 | C | N3-C2-O2 | -5.49 | 118.06 | 121.90 |
| 22 | 23S1 | 239 | C | N3-C2-O2 | -5.49 | 118.06 | 121.90 |
| 22 | 23S1 | 1005 | C | C6-N1-C2 | -5.49 | 118.11 | 120.30 |
| 22 | 23S1 | 1095 | A | C8-N9-C4 | 5.49 | 108.00 | 105.80 |
| 22 | 23S1 | 1616 | A | C5-C6-N1 | 5.49 | 120.44 | 117.70 |
| 22 | 23S1 | 1889 | A | C8-N9-C4 | 5.49 | 108.00 | 105.80 |
| 1 | 16S1 | 878 | A | N9-C4-C5 | 5.49 | 108.00 | 105.80 |
| 22 | 23S1 | 181 | A | C8-N9-C4 | 5.49 | 108.00 | 105.80 |
| 22 | 23S1 | 2639 | A | N3-C4-N9 | 5.49 | 131.79 | 127.40 |
| 1 | 16S1 | 7 | A | N3-C4-N9 | 5.49 | 131.79 | 127.40 |
| 1 | 16S1 | 364 | A | N3-C4-N9 | 5.49 | 131.79 | 127.40 |
| 1 | 16S1 | 716 | A | N9-C4-C5 | 5.49 | 107.99 | 105.80 |
| 22 | 23S1 | 515 | A | C5-C6-N1 | 5.49 | 120.44 | 117.70 |
| 22 | 23S1 | 1654 | A | C4-C5-C6 | 5.49 | 119.74 | 117.00 |
| 22 | 23S1 | 1794 | A | N9-C4-C5 | 5.49 | 107.99 | 105.80 |
| 22 | 23S1 | 2386 | A | C8-N9-C4 | 5.49 | 108.00 | 105.80 |
| 22 | 23S1 | 2740 | A | N9-C4-C5 | 5.49 | 108.00 | 105.80 |
| 22 | 23S1 | 2860 | A | C4-C5-C6 | 5.49 | 119.74 | 117.00 |
| 1 | 16S1 | 1333 | A | C5-C6-N1 | 5.48 | 120.44 | 117.70 |
| 22 | 23S1 | 19 | A | C8-N9-C4 | 5.48 | 107.99 | 105.80 |
| 22 | 23S1 | 111 | A | C5-C6-N1 | 5.48 | 120.44 | 117.70 |
| 22 | 23S1 | 1670 | C | N1-C2-O2 | 5.48 | 122.19 | 118.90 |
| 22 | 23S1 | 2531 | A | C5-C6-N1 | 5.48 | 120.44 | 117.70 |
| 22 | 23S1 | 2602 | A | C4-C5-C6 | 5.48 | 119.74 | 117.00 |
| 22 | 23S1 | 346 | A | C8-N9-C4 | 5.48 | 107.99 | 105.80 |
| 22 | 23S1 | 877 | A | N3-C4-N9 | 5.48 | 131.78 | 127.40 |
| 22 | 23S1 | 1367 | A | N3-C4-N9 | 5.48 | 131.79 | 127.40 |
| 22 | 23S1 | 1503 | A | C5-C6-N1 | 5.48 | 120.44 | 117.70 |
| 22 | 23S1 | 1634 | A | C4-C5-N7 | -5.48 | 107.96 | 110.70 |
| 22 | 23S1 | 1803 | A | N9-C4-C5 | 5.48 | 107.99 | 105.80 |
| 22 | 23S1 | 2243 | U | N3-C2-O2 | -5.48 | 118.36 | 122.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 2856 | A | C8-N9-C4 | 5.48 | 107.99 | 105.80 |
| 1 | 16S1 | 320 | A | C8-N9-C4 | 5.48 | 107.99 | 105.80 |
| 1 | 16S1 | 681 | A | C4-C5-N7 | -5.48 | 107.96 | 110.70 |
| 22 | 23S1 | 84 | A | C4-C5-N7 | -5.48 | 107.96 | 110.70 |
| 22 | 23S1 | 764 | A | N3-C4-N9 | 5.48 | 131.78 | 127.40 |
| 22 | 23S1 | 1327 | A | C4-C5-C6 | 5.48 | 119.74 | 117.00 |
| 22 | 23S1 | 599 | A | C5-C6-N1 | 5.48 | 120.44 | 117.70 |
| 22 | 23S1 | 905 | A | C5-C6-N1 | 5.48 | 120.44 | 117.70 |
| 22 | 23S1 | 1009 | A | C4-C5-N7 | -5.48 | 107.96 | 110.70 |
| 22 | 23S1 | 1194 | A | C4-C5-N7 | -5.48 | 107.96 | 110.70 |
| 22 | 23S1 | 1698 | A | C4-C5-C6 | 5.48 | 119.74 | 117.00 |
| 22 | 23S1 | 2183 | A | N3-C4-N9 | 5.48 | 131.78 | 127.40 |
| 1 | 16S1 | 1016 | A | N3-C4-N9 | 5.48 | 131.78 | 127.40 |
| 22 | 23S1 | 1111 | A | C8-N9-C4 | 5.48 | 107.99 | 105.80 |
| 22 | 23S1 | 1269 | A | C4-C5-N7 | -5.48 | 107.96 | 110.70 |
| 22 | 23S1 | 1678 | A | C4-C5-C6 | 5.48 | 119.74 | 117.00 |
| 1 | 16S1 | 1081 | A | C5-C6-N1 | 5.47 | 120.44 | 117.70 |
| 1 | 16S1 | 1176 | A | C5-C6-N1 | 5.47 | 120.44 | 117.70 |
| 22 | 23S1 | 1009 | A | C5-C6-N1 | 5.47 | 120.44 | 117.70 |
| 22 | 23S1 | 1822 | C | C6-N1-C2 | -5.47 | 118.11 | 120.30 |
| 22 | 23S1 | 2778 | A | N9-C4-C5 | 5.47 | 107.99 | 105.80 |
| 22 | 23S1 | 2829 | A | N3-C4-N9 | 5.47 | 131.78 | 127.40 |
| 1 | 16S1 | 495 | A | C8-N9-C4 | 5.47 | 107.99 | 105.80 |
| 1 | 16S1 | 892 | A | N9-C4-C5 | 5.47 | 107.99 | 105.80 |
| 22 | 23S1 | 176 | A | C4-C5-C6 | 5.47 | 119.74 | 117.00 |
| 22 | 23S1 | 239 | C | N1-C2-O2 | 5.47 | 122.18 | 118.90 |
| 1 | 16S1 | 969 | A | C8-N9-C4 | 5.47 | 107.99 | 105.80 |
| 22 | 23S1 | 19 | A | C5-C6-N1 | 5.47 | 120.44 | 117.70 |
| 22 | 23S1 | 502 | A | C5-C6-N1 | 5.47 | 120.44 | 117.70 |
| 22 | 23S1 | 2158 | A | C4-C5-C6 | 5.47 | 119.73 | 117.00 |
| 1 | 16S1 | 1311 | A | C8-N9-C4 | 5.47 | 107.99 | 105.80 |
| 22 | 23S1 | 749 | A | N9-C4-C5 | 5.47 | 107.99 | 105.80 |
| 22 | 23S1 | 2205 | A | N3-C4-N9 | 5.47 | 131.77 | 127.40 |
| 22 | 23S1 | 2887 | A | C5-C6-N1 | 5.47 | 120.43 | 117.70 |
| 1 | 16S1 | 2 | A | C4-C5-N7 | -5.47 | 107.97 | 110.70 |
| 1 | 16S1 | 411 | A | C5-C6-N1 | 5.47 | 120.43 | 117.70 |
| 1 | 16S1 | 792 | A | C5-C6-N1 | 5.47 | 120.43 | 117.70 |
| 1 | 16S1 | 1513 | A | C8-N9-C4 | 5.47 | 107.99 | 105.80 |
| 22 | 23S1 | 1328 | A | N3-C4-N9 | 5.47 | 131.77 | 127.40 |
| 22 | 23S1 | 2163 | A | C4-C5-C6 | 5.47 | 119.73 | 117.00 |
| 23 | 05S1 | 34 | A | C4-C5-N7 | -5.47 | 107.97 | 110.70 |
| 1 | 16S1 | 802 | A | N3-C4-N9 | 5.46 | 131.77 | 127.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 16S1 | 819 | A | N9-C4-C5 | 5.46 | 107.99 | 105.80 |
| 1 | 16S1 | 1180 | A | C8-N9-C4 | 5.46 | 107.99 | 105.80 |
| 22 | 23S1 | 443 | A | C8-N9-C4 | 5.46 | 107.99 | 105.80 |
| 22 | 23S1 | 471 | A | C4-C5-C6 | 5.46 | 119.73 | 117.00 |
| 22 | 23S1 | 1048 | A | C8-N9-C4 | 5.46 | 107.99 | 105.80 |
| 1 | 16S1 | 946 | A | C4-C5-N7 | -5.46 | 107.97 | 110.70 |
| 22 | 23S1 | 689 | A | C4-C5-N7 | -5.46 | 107.97 | 110.70 |
| 22 | 23S1 | 1285 | A | N3-C4-N9 | 5.46 | 131.77 | 127.40 |
| 22 | 23S1 | 1502 | A | C4-C5-N7 | -5.46 | 107.97 | 110.70 |
| 23 | 05S1 | 119 | A | N9-C4-C5 | 5.46 | 107.98 | 105.80 |
| 22 | 23S1 | 126 | A | N9-C4-C5 | 5.46 | 107.98 | 105.80 |
| 1 | 16S1 | 825 | A | C5-C6-N1 | 5.46 | 120.43 | 117.70 |
| 22 | 23S1 | 44 | A | C5-C6-N1 | 5.46 | 120.43 | 117.70 |
| 22 | 23S1 | 1735 | A | C8-N9-C4 | 5.46 | 107.98 | 105.80 |
| 22 | 23S1 | 2273 | A | C4-C5-N7 | -5.46 | 107.97 | 110.70 |
| 22 | 23S1 | 2750 | A | N9-C4-C5 | 5.46 | 107.98 | 105.80 |
| 55 | PTR1 | 21 | A | N3-C4-N9 | 5.46 | 131.77 | 127.40 |
| 1 | 16S1 | 640 | A | C4-C5-N7 | -5.46 | 107.97 | 110.70 |
| 22 | 23S1 | 730 | A | C5-C6-N1 | 5.46 | 120.43 | 117.70 |
| 22 | 23S1 | 1226 | A | N3-C4-N9 | 5.46 | 131.77 | 127.40 |
| 22 | 23S1 | 1669 | A | C5-C6-N1 | 5.46 | 120.43 | 117.70 |
| 22 | 23S1 | 2322 | A | C4-C5-N7 | -5.46 | 107.97 | 110.70 |
| 1 | 16S1 | 130 | A | C4-C5-N7 | -5.46 | 107.97 | 110.70 |
| 1 | 16S1 | 315 | A | N9-C4-C5 | 5.46 | 107.98 | 105.80 |
| 1 | 16S1 | 1012 | A | C5-C6-N1 | 5.46 | 120.43 | 117.70 |
| 1 | 16S1 | 1022 | A | N9-C4-C5 | 5.46 | 107.98 | 105.80 |
| 1 | 16S1 | 1468 | A | C8-N9-C4 | 5.46 | 107.98 | 105.80 |
| 22 | 23S1 | 14 | A | N3-C4-N9 | 5.46 | 131.76 | 127.40 |
| 22 | 23S1 | 529 | A | C4-C5-N7 | -5.46 | 107.97 | 110.70 |
| 22 | 23S1 | 1069 | A | C4-C5-N7 | -5.46 | 107.97 | 110.70 |
| 23 | 05S1 | 70 | C | N3-C2-O2 | -5.46 | 118.08 | 121.90 |
| 22 | 23S1 | 528 | A | C8-N9-C4 | 5.46 | 107.98 | 105.80 |
| 22 | 23S1 | 2764 | A | N3-C4-N9 | 5.46 | 131.76 | 127.40 |
| 1 | 16S1 | 53 | A | C5-C6-N1 | 5.45 | 120.43 | 117.70 |
| 1 | 16S1 | 120 | A | C4-C5-C6 | 5.45 | 119.73 | 117.00 |
| 1 | 16S1 | 393 | A | C5-C6-N1 | 5.45 | 120.43 | 117.70 |
| 1 | 16S1 | 437 | U | N1-C2-O2 | 5.45 | 126.62 | 122.80 |
| 1 | 16S1 | 810 | C | N3-C2-O2 | -5.45 | 118.08 | 121.90 |
| 1 | 16S1 | 975 | A | C4-C5-C6 | 5.45 | 119.73 | 117.00 |
| 22 | 23S1 | 1194 | A | C5-C6-N1 | 5.45 | 120.43 | 117.70 |
| 1 | 16S1 | 889 | A | C8-N9-C4 | 5.45 | 107.98 | 105.80 |
| 1 | 16S1 | 1067 | A | C8-N9-C4 | 5.45 | 107.98 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 2813 | A | N3-C4-N9 | 5.45 | 131.76 | 127.40 |
| 1 | 16S1 | 831 | A | C4-C5-C6 | 5.45 | 119.72 | 117.00 |
| 22 | 23S1 | 526 | A | N3-C4-N9 | 5.45 | 131.76 | 127.40 |
| 22 | 23S1 | 1096 | A | C4-C5-N7 | -5.45 | 107.97 | 110.70 |
| 22 | 23S1 | 1359 | A | C8-N9-C4 | 5.45 | 107.98 | 105.80 |
| 22 | 23S1 | 1553 | A | C8-N9-C4 | 5.45 | 107.98 | 105.80 |
| 22 | 23S1 | 1978 | A | N9-C4-C5 | 5.45 | 107.98 | 105.80 |
| 22 | 23S1 | 2170 | A | C4-C5-N7 | -5.45 | 107.97 | 110.70 |
| 22 | 23S1 | 2727 | A | C8-N9-C4 | 5.45 | 107.98 | 105.80 |
| 22 | 23S1 | 2870 | C | C6-N1-C2 | -5.45 | 118.12 | 120.30 |
| 1 | 16S1 | 306 | A | C4-C5-C6 | 5.45 | 119.72 | 117.00 |
| 22 | 23S1 | 104 | A | C8-N9-C4 | 5.45 | 107.98 | 105.80 |
| 22 | 23S1 | 346 | A | C4-C5-N7 | -5.45 | 107.98 | 110.70 |
| 22 | 23S1 | 2376 | A | N9-C4-C5 | 5.45 | 107.98 | 105.80 |
| 1 | 16S1 | 414 | A | C4-C5-N7 | -5.45 | 107.98 | 110.70 |
| 1 | 16S1 | 1448 | C | N1-C2-O2 | 5.45 | 122.17 | 118.90 |
| 22 | 23S1 | 204 | A | C5-C6-N1 | 5.45 | 120.42 | 117.70 |
| 22 | 23S1 | 753 | A | C8-N9-C4 | 5.45 | 107.98 | 105.80 |
| 22 | 23S1 | 1569 | A | C5-C6-N1 | 5.45 | 120.42 | 117.70 |
| 22 | 23S1 | 1641 | A | N9-C4-C5 | 5.45 | 107.98 | 105.80 |
| 22 | 23S1 | 2476 | A | C8-N9-C4 | 5.45 | 107.98 | 105.80 |
| 1 | 16S1 | 59 | A | C5-C6-N1 | 5.45 | 120.42 | 117.70 |
| 1 | 16S1 | 547 | A | C4-C5-N7 | -5.45 | 107.98 | 110.70 |
| 1 | 16S1 | 1480 | A | N3-C4-N9 | 5.45 | 131.76 | 127.40 |
| 22 | 23S1 | 391 | A | C8-N9-C4 | 5.45 | 107.98 | 105.80 |
| 22 | 23S1 | 2741 | A | N9-C4-C5 | 5.44 | 107.98 | 105.80 |
| 23 | 05S1 | 101 | A | C4-C5-N7 | -5.44 | 107.98 | 110.70 |
| 1 | 16S1 | 792 | A | C4-C5-N7 | -5.44 | 107.98 | 110.70 |
| 22 | 23S1 | 715 | A | N9-C4-C5 | 5.44 | 107.98 | 105.80 |
| 22 | 23S1 | 927 | A | C4-C5-N7 | -5.44 | 107.98 | 110.70 |
| 22 | 23S1 | 1383 | A | C8-N9-C4 | 5.44 | 107.98 | 105.80 |
| 22 | 23S1 | 1502 | A | C8-N9-C4 | 5.44 | 107.98 | 105.80 |
| 22 | 23S1 | 2013 | A | C5-C6-N1 | 5.44 | 120.42 | 117.70 |
| 1 | 16S1 | 780 | A | N9-C4-C5 | 5.44 | 107.98 | 105.80 |
| 1 | 16S1 | 1067 | A | C4-C5-C6 | 5.44 | 119.72 | 117.00 |
| 22 | 23S1 | 912 | C | N3-C2-O2 | -5.44 | 118.09 | 121.90 |
| 22 | 23S1 | 927 | A | N9-C4-C5 | 5.44 | 107.98 | 105.80 |
| 22 | 23S1 | 1284 | A | N3-C4-N9 | 5.44 | 131.75 | 127.40 |
| 22 | 23S1 | 1593 | A | C8-N9-C4 | 5.44 | 107.98 | 105.80 |
| 22 | 23S1 | 1705 | A | C5-C6-N1 | 5.44 | 120.42 | 117.70 |
| 1 | 16S1 | 746 | A | N9-C4-C5 | 5.44 | 107.98 | 105.80 |
| 22 | 23S1 | 2284 | A | C4-C5-N7 | -5.44 | 107.98 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 16S1 | 924 | C | C6-N1-C2 | -5.44 | 118.12 | 120.30 |
| 22 | 23S1 | 1144 | A | C8-N9-C4 | 5.44 | 107.97 | 105.80 |
| 22 | 23S1 | 1328 | A | C5-C6-N1 | 5.44 | 120.42 | 117.70 |
| 23 | 05S1 | 115 | A | C5-C6-N1 | 5.44 | 120.42 | 117.70 |
| 1 | 16S1 | 129 | A | N3-C4-N9 | 5.44 | 131.75 | 127.40 |
| 1 | 16S1 | 179 | A | C8-N9-C4 | 5.44 | 107.97 | 105.80 |
| 1 | 16S1 | 279 | A | N9-C4-C5 | 5.44 | 107.97 | 105.80 |
| 22 | 23S1 | 432 | A | C4-C5-N7 | -5.44 | 107.98 | 110.70 |
| 22 | 23S1 | 833 | A | N9-C4-C5 | 5.44 | 107.97 | 105.80 |
| 22 | 23S1 | 897 | C | C6-N1-C2 | -5.44 | 118.13 | 120.30 |
| 22 | 23S1 | 2478 | A | C4-C5-C6 | 5.44 | 119.72 | 117.00 |
| 22 | 23S1 | 443 | A | N9-C4-C5 | 5.43 | 107.97 | 105.80 |
| 22 | 23S1 | 1347 | A | C4-C5-C6 | 5.43 | 119.72 | 117.00 |
| 22 | 23S1 | 2134 | A | N9-C4-C5 | 5.43 | 107.97 | 105.80 |
| 1 | 16S1 | 363 | A | N9-C4-C5 | 5.43 | 107.97 | 105.80 |
| 22 | 23S1 | 1155 | A | N3-C4-N9 | 5.43 | 131.75 | 127.40 |
| 1 | 16S1 | 306 | A | C8-N9-C4 | 5.43 | 107.97 | 105.80 |
| 22 | 23S1 | 197 | A | C8-N9-C4 | 5.43 | 107.97 | 105.80 |
| 22 | 23S1 | 603 | A | N3-C4-N9 | 5.43 | 131.75 | 127.40 |
| 22 | 23S1 | 2740 | A | C8-N9-C4 | 5.43 | 107.97 | 105.80 |
| 1 | 16S1 | 303 | A | C4-C5-C6 | 5.43 | 119.72 | 117.00 |
| 1 | 16S1 | 560 | A | N9-C4-C5 | 5.43 | 107.97 | 105.80 |
| 1 | 16S1 | 1434 | A | C8-N9-C4 | 5.43 | 107.97 | 105.80 |
| 22 | 23S1 | 332 | A | N9-C4-C5 | 5.43 | 107.97 | 105.80 |
| 22 | 23S1 | 502 | A | N3-C4-N9 | 5.43 | 131.74 | 127.40 |
| 22 | 23S1 | 592 | A | C4-C5-C6 | 5.43 | 119.71 | 117.00 |
| 22 | 23S1 | 2809 | A | C5-C6-N1 | 5.43 | 120.42 | 117.70 |
| 23 | 05S1 | 57 | A | C8-N9-C4 | 5.43 | 107.97 | 105.80 |
| 1 | 16S1 | 282 | A | N9-C4-C5 | 5.43 | 107.97 | 105.80 |
| 1 | 16S1 | 325 | A | N9-C4-C5 | 5.43 | 107.97 | 105.80 |
| 1 | 16S1 | 496 | A | C5-N7-C8 | 5.43 | 106.61 | 103.90 |
| 1 | 16S1 | 906 | A | C8-N9-C4 | 5.43 | 107.97 | 105.80 |
| 22 | 23S1 | 892 | A | C5-C6-N1 | 5.43 | 120.41 | 117.70 |
| 22 | 23S1 | 1453 | A | C4-C5-C6 | 5.43 | 119.71 | 117.00 |
| 22 | 23S1 | 1772 | A | C4-C5-N7 | -5.43 | 107.99 | 110.70 |
| 22 | 23S1 | 2461 | A | C8-N9-C4 | 5.43 | 107.97 | 105.80 |
| 55 | PTR1 | 58 | A | C8-N9-C4 | 5.43 | 107.97 | 105.80 |
| 1 | 16S1 | 221 | C | N3-C2-O2 | -5.42 | 118.10 | 121.90 |
| 1 | 16S1 | 1303 | C | N1-C2-O2 | 5.42 | 122.16 | 118.90 |
| 1 | 16S1 | 1429 | A | N9-C4-C5 | 5.42 | 107.97 | 105.80 |
| 22 | 23S1 | 1877 | A | C5-C6-N1 | 5.42 | 120.41 | 117.70 |
| 22 | 23S1 | 2314 | A | C5-C6-N1 | 5.42 | 120.41 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 2829 | A | C8-N9-C4 | 5.42 | 107.97 | 105.80 |
| 1 | 16S1 | 729 | A | N9-C4-C5 | 5.42 | 107.97 | 105.80 |
| 1 | 16S1 | 1406 | U | C2-N3-C4 | -5.42 | 123.75 | 127.00 |
| 22 | 23S1 | 218 | A | N9-C4-C5 | 5.42 | 107.97 | 105.80 |
| 22 | 23S1 | 912 | C | C6-N1-C2 | -5.42 | 118.13 | 120.30 |
| 22 | 23S1 | 983 | A | C6-N1-C2 | 5.42 | 121.85 | 118.60 |
| 22 | 23S1 | 1439 | A | C4-C5-N7 | -5.42 | 107.99 | 110.70 |
| 22 | 23S1 | 2566 | A | C5-C6-N1 | 5.42 | 120.41 | 117.70 |
| 22 | 23S1 | 637 | A | C4-C5-N7 | -5.42 | 107.99 | 110.70 |
| 22 | 23S1 | 1494 | A | C4-C5-C6 | 5.42 | 119.71 | 117.00 |
| 1 | 16S1 | 1495 | U | C5-C6-N1 | 5.42 | 125.41 | 122.70 |
| 22 | 23S1 | 1378 | A | C4-C5-N7 | -5.42 | 107.99 | 110.70 |
| 22 | 23S1 | 2886 | A | C4-C5-C6 | 5.42 | 119.71 | 117.00 |
| 22 | 23S1 | 1503 | A | C4-C5-C6 | 5.42 | 119.71 | 117.00 |
| 22 | 23S1 | 1679 | A | N9-C4-C5 | 5.42 | 107.97 | 105.80 |
| 22 | 23S1 | 1690 | A | C4-C5-C6 | 5.42 | 119.71 | 117.00 |
| 22 | 23S1 | 2044 | C | C6-N1-C2 | -5.42 | 118.13 | 120.30 |
| 22 | 23S1 | 2184 | A | C4-C5-N7 | -5.42 | 107.99 | 110.70 |
| 23 | 05S1 | 57 | A | N9-C4-C5 | 5.42 | 107.97 | 105.80 |
| 22 | 23S1 | 1545 | A | N3-C4-N9 | 5.42 | 131.73 | 127.40 |
| 22 | 23S1 | 1819 | A | C5-C6-N1 | 5.42 | 120.41 | 117.70 |
| 1 | 16S1 | 495 | A | C4-C5-C6 | 5.41 | 119.71 | 117.00 |
| 1 | 16S1 | 712 | A | N9-C4-C5 | 5.41 | 107.97 | 105.80 |
| 1 | 16S1 | 1176 | A | N9-C4-C5 | 5.41 | 107.97 | 105.80 |
| 1 | 16S1 | 1319 | A | C4-C5-C6 | 5.41 | 119.71 | 117.00 |
| 22 | 23S1 | 104 | A | C5-C6-N1 | 5.41 | 120.41 | 117.70 |
| 22 | 23S1 | 911 | A | C5-N7-C8 | 5.41 | 106.61 | 103.90 |
| 22 | 23S1 | 2758 | A | C5-C6-N1 | 5.41 | 120.41 | 117.70 |
| 22 | 23S1 | 89 | A | C5-C6-N1 | 5.41 | 120.41 | 117.70 |
| 22 | 23S1 | 1641 | A | C4-C5-N7 | -5.41 | 107.99 | 110.70 |
| 22 | 23S1 | 2873 | A | C4-C5-N7 | -5.41 | 107.99 | 110.70 |
| 1 | 16S1 | 74 | A | C4-C5-C6 | 5.41 | 119.70 | 117.00 |
| 1 | 16S1 | 915 | A | N3-C4-N9 | 5.41 | 131.73 | 127.40 |
| 1 | 16S1 | 974 | A | C8-N9-C4 | 5.41 | 107.96 | 105.80 |
| 22 | 23S1 | 556 | A | N9-C4-C5 | 5.41 | 107.96 | 105.80 |
| 22 | 23S1 | 590 | A | C4-C5-N7 | -5.41 | 108.00 | 110.70 |
| 22 | 23S1 | 608 | A | C5-C6-N1 | 5.41 | 120.41 | 117.70 |
| 22 | 23S1 | 861 | A | C8-N9-C4 | 5.41 | 107.96 | 105.80 |
| 22 | 23S1 | 1230 | A | C8-N9-C4 | 5.41 | 107.96 | 105.80 |
| 22 | 23S1 | 1632 | A | C4-C5-N7 | -5.41 | 108.00 | 110.70 |
| 22 | 23S1 | 2679 | A | C5-C6-N1 | 5.41 | 120.41 | 117.70 |
| 22 | 23S1 | 2837 | A | C5-C6-N1 | 5.41 | 120.41 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 16S1 | 7 | A | C4-C5-C6 | 5.41 | 119.70 | 117.00 |
| 1 | 16S1 | 781 | A | C4-C5-C6 | 5.41 | 119.70 | 117.00 |
| 1 | 16S1 | 932 | C | C2-N1-C1' | 5.41 | 124.75 | 118.80 |
| 22 | 23S1 | 2309 | A | C4-C5-C6 | 5.41 | 119.70 | 117.00 |
| 22 | 23S1 | 2632 | A | N9-C4-C5 | 5.41 | 107.96 | 105.80 |
| 23 | 05S1 | 66 | A | C8-N9-C4 | 5.41 | 107.96 | 105.80 |
| 1 | 16S1 | 197 | A | C4-C5-N7 | -5.41 | 108.00 | 110.70 |
| 22 | 23S1 | 706 | A | N9-C4-C5 | 5.41 | 107.96 | 105.80 |
| 22 | 23S1 | 2406 | A | N3-C4-N9 | 5.41 | 131.73 | 127.40 |
| 1 | 16S1 | 600 | A | N9-C4-C5 | 5.41 | 107.96 | 105.80 |
| 1 | 16S1 | 1044 | A | N9-C4-C5 | 5.41 | 107.96 | 105.80 |
| 22 | 23S1 | 522 | A | C5-C6-N1 | 5.41 | 120.40 | 117.70 |
| 22 | 23S1 | 1385 | A | C4-C5-N7 | -5.41 | 108.00 | 110.70 |
| 22 | 23S1 | 1509 | A | C4-C5-N7 | -5.41 | 108.00 | 110.70 |
| 22 | 23S1 | 1829 | A | C5-C6-N1 | 5.41 | 120.40 | 117.70 |
| 1 | 16S1 | 101 | A | C5-C6-N1 | 5.40 | 120.40 | 117.70 |
| 1 | 16S1 | 459 | A | C8-N9-C4 | 5.40 | 107.96 | 105.80 |
| 22 | 23S1 | 176 | A | N9-C4-C5 | 5.40 | 107.96 | 105.80 |
| 22 | 23S1 | 310 | A | C4-C5-C6 | 5.40 | 119.70 | 117.00 |
| 22 | 23S1 | 675 | A | C5-C6-N1 | 5.40 | 120.40 | 117.70 |
| 22 | 23S1 | 896 | A | N9-C4-C5 | 5.40 | 107.96 | 105.80 |
| 22 | 23S1 | 917 | A | C4-C5-N7 | -5.40 | 108.00 | 110.70 |
| 22 | 23S1 | 1070 | A | C8-N9-C4 | 5.40 | 107.96 | 105.80 |
| 22 | 23S1 | 1916 | A | C5-C6-N1 | 5.40 | 120.40 | 117.70 |
| 22 | 23S1 | 2314 | A | N9-C4-C5 | 5.40 | 107.96 | 105.80 |
| 22 | 23S1 | 2412 | A | C8-N9-C4 | 5.40 | 107.96 | 105.80 |
| 22 | 23S1 | 2590 | A | N9-C4-C5 | 5.40 | 107.96 | 105.80 |
| 22 | 23S1 | 2734 | A | C4-C5-C6 | 5.40 | 119.70 | 117.00 |
| 22 | 23S1 | 2809 | A | N9-C4-C5 | 5.40 | 107.96 | 105.80 |
| 1 | 16S1 | 573 | A | C5-C6-N1 | 5.40 | 120.40 | 117.70 |
| 1 | 16S1 | 908 | A | N9-C4-C5 | 5.40 | 107.96 | 105.80 |
| 22 | 23S1 | 706 | A | C4-C5-N7 | -5.40 | 108.00 | 110.70 |
| 22 | 23S1 | 1630 | A | C5-C6-N1 | 5.40 | 120.40 | 117.70 |
| 22 | 23S1 | 1876 | A | C8-N9-C4 | 5.40 | 107.96 | 105.80 |
| 22 | 23S1 | 2005 | A | N3-C4-N9 | 5.40 | 131.72 | 127.40 |
| 22 | 23S1 | 2100 | G | C4-N9-C1' | 5.40 | 133.52 | 126.50 |
| 1 | 16S1 | 143 | A | C4-C5-C6 | 5.40 | 119.70 | 117.00 |
| 1 | 16S1 | 1507 | A | C5-C6-N1 | 5.40 | 120.40 | 117.70 |
| 22 | 23S1 | 2189 | U | C2-N3-C4 | 5.40 | 130.24 | 127.00 |
| 1 | 16S1 | 53 | A | C8-N9-C4 | 5.40 | 107.96 | 105.80 |
| 1 | 16S1 | 1287 | A | C5-C6-N1 | 5.40 | 120.40 | 117.70 |
| 22 | 23S1 | 160 | A | N3-C4-N9 | 5.40 | 131.72 | 127.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 320 | A | C8-N9-C4 | 5.40 | 107.96 | 105.80 |
| 22 | 23S1 | 368 | A | N9-C4-C5 | 5.40 | 107.96 | 105.80 |
| 22 | 23S1 | 631 | A | C4-C5-N7 | -5.40 | 108.00 | 110.70 |
| 22 | 23S1 | 637 | A | C4-C5-C6 | 5.40 | 119.70 | 117.00 |
| 22 | 23S1 | 2753 | A | C8-N9-C4 | 5.40 | 107.96 | 105.80 |
| 22 | 23S1 | 219 | A | C4-C5-C6 | 5.40 | 119.70 | 117.00 |
| 1 | 16S1 | 223 | A | C8-N9-C4 | 5.39 | 107.96 | 105.80 |
| 1 | 16S1 | 583 | A | C8-N9-C4 | 5.39 | 107.96 | 105.80 |
| 1 | 16S1 | 1067 | A | N3-C4-N9 | 5.39 | 131.72 | 127.40 |
| 22 | 23S1 | 563 | A | C4-C5-N7 | -5.39 | 108.00 | 110.70 |
| 22 | 23S1 | 1262 | A | C5-C6-N1 | 5.39 | 120.40 | 117.70 |
| 22 | 23S1 | 1597 | A | N3-C4-N9 | 5.39 | 131.72 | 127.40 |
| 22 | 23S1 | 1655 | A | C4-C5-N7 | -5.39 | 108.00 | 110.70 |
| 22 | 23S1 | 2369 | A | C5-N7-C8 | 5.39 | 106.60 | 103.90 |
| 22 | 23S1 | 2562 | U | N1-C2-O2 | 5.39 | 126.58 | 122.80 |
| 23 | 05S1 | 53 | A | N9-C4-C5 | 5.39 | 107.96 | 105.80 |
| 23 | 05S1 | 58 | A | N9-C4-C5 | 5.39 | 107.96 | 105.80 |
| 1 | 16S1 | 167 | A | C8-N9-C4 | 5.39 | 107.96 | 105.80 |
| 1 | 16S1 | 629 | A | C4-C5-N7 | -5.39 | 108.00 | 110.70 |
| 1 | 16S1 | 1093 | A | C5-C6-N1 | 5.39 | 120.40 | 117.70 |
| 22 | 23S1 | 1247 | A | N9-C4-C5 | 5.39 | 107.96 | 105.80 |
| 55 | PTR1 | 26 | A | C4-C5-C6 | 5.39 | 119.70 | 117.00 |
| 22 | 23S1 | 371 | A | C5-C6-N1 | 5.39 | 120.40 | 117.70 |
| 22 | 23S1 | 928 | A | C5-C6-N1 | 5.39 | 120.40 | 117.70 |
| 22 | 23S1 | 936 | A | C4-C5-C6 | 5.39 | 119.70 | 117.00 |
| 1 | 16S1 | 482 | A | C8-N9-C4 | 5.39 | 107.95 | 105.80 |
| 1 | 16S1 | 1150 | A | C5-C6-N1 | 5.39 | 120.39 | 117.70 |
| 22 | 23S1 | 878 | A | C5-C6-N1 | 5.39 | 120.39 | 117.70 |
| 22 | 23S1 | 1919 | A | C4-C5-C6 | 5.39 | 119.69 | 117.00 |
| 22 | 23S1 | 2298 | A | C4-C5-N7 | -5.39 | 108.00 | 110.70 |
| 22 | 23S1 | 2547 | A | N9-C4-C5 | 5.39 | 107.96 | 105.80 |
| 22 | 23S1 | 2820 | A | C4-C5-C6 | 5.39 | 119.69 | 117.00 |
| 1 | 16S1 | 694 | A | N9-C4-C5 | 5.39 | 107.95 | 105.80 |
| 1 | 16S1 | 1155 | A | C5-C6-N1 | 5.39 | 120.39 | 117.70 |
| 22 | 23S1 | 103 | A | C4-C5-N7 | -5.39 | 108.01 | 110.70 |
| 22 | 23S1 | 2033 | A | C5-C6-N1 | 5.39 | 120.39 | 117.70 |
| 22 | 23S1 | 2435 | A | N3-C4-N9 | 5.39 | 131.71 | 127.40 |
| 22 | 23S1 | 2448 | A | C4-C5-N7 | -5.39 | 108.01 | 110.70 |
| 22 | 23S1 | 2534 | A | C8-N9-C4 | 5.39 | 107.95 | 105.80 |
| 1 | 16S1 | 171 | A | C4-C5-N7 | -5.39 | 108.01 | 110.70 |
| 1 | 16S1 | 1329 | A | C4-C5-C6 | 5.39 | 119.69 | 117.00 |
| 22 | 23S1 | 216 | A | C5-C6-N1 | 5.39 | 120.39 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 346 | A | N9-C4-C5 | 5.39 | 107.95 | 105.80 |
| 22 | 23S1 | 478 | A | C5-C6-N1 | 5.39 | 120.39 | 117.70 |
| 22 | 23S1 | 1265 | A | C4-C5-N7 | -5.39 | 108.01 | 110.70 |
| 55 | PTR1 | 59 | A | C4-C5-N7 | -5.39 | 108.01 | 110.70 |
| 1 | 16S1 | 596 | A | C5-C6-N1 | 5.38 | 120.39 | 117.70 |
| 22 | 23S1 | 429 | A | C4-C5-N7 | -5.38 | 108.01 | 110.70 |
| 22 | 23S1 | 1637 | A | C4-C5-N7 | -5.38 | 108.01 | 110.70 |
| 55 | PTR1 | 42 | A | N9-C4-C5 | 5.38 | 107.95 | 105.80 |
| 22 | 23S1 | 270 | A | N3-C4-N9 | 5.38 | 131.71 | 127.40 |
| 22 | 23S1 | 844 | A | C5-C6-N1 | 5.38 | 120.39 | 117.70 |
| 22 | 23S1 | 1265 | A | C5-C6-N1 | 5.38 | 120.39 | 117.70 |
| 1 | 16S1 | 759 | A | N9-C4-C5 | 5.38 | 107.95 | 105.80 |
| 1 | 16S1 | 961 | U | C2-N3-C4 | -5.38 | 123.77 | 127.00 |
| 22 | 23S1 | 161 | A | C4-C5-N7 | -5.38 | 108.01 | 110.70 |
| 22 | 23S1 | 501 | A | N9-C4-C5 | 5.38 | 107.95 | 105.80 |
| 22 | 23S1 | 547 | A | N3-C4-N9 | 5.38 | 131.70 | 127.40 |
| 22 | 23S1 | 1084 | A | N9-C4-C5 | 5.38 | 107.95 | 105.80 |
| 22 | 23S1 | 1503 | A | C4-C5-N7 | -5.38 | 108.01 | 110.70 |
| 22 | 23S1 | 2154 | A | C5-C6-N1 | 5.38 | 120.39 | 117.70 |
| 22 | 23S1 | 156 | A | C8-N9-C4 | 5.38 | 107.95 | 105.80 |
| 22 | 23S1 | 2336 | A | C8-N9-C4 | 5.38 | 107.95 | 105.80 |
| 1 | 16S1 | 3 | A | C4-C5-N7 | -5.38 | 108.01 | 110.70 |
| 1 | 16S1 | 635 | A | C5-C6-N1 | 5.38 | 120.39 | 117.70 |
| 22 | 23S1 | 430 | A | C4-C5-N7 | -5.38 | 108.01 | 110.70 |
| 22 | 23S1 | 892 | A | N9-C4-C5 | 5.38 | 107.95 | 105.80 |
| 22 | 23S1 | 1354 | A | C5-C6-N1 | 5.38 | 120.39 | 117.70 |
| 22 | 23S1 | 1596 | A | C4-C5-C6 | 5.38 | 119.69 | 117.00 |
| 22 | 23S1 | 1700 | A | C4-C5-N7 | -5.38 | 108.01 | 110.70 |
| 22 | 23S1 | 2311 | A | C8-N9-C4 | 5.38 | 107.95 | 105.80 |
| 1 | 16S1 | 246 | A | C4-C5-N7 | -5.38 | 108.01 | 110.70 |
| 1 | 16S1 | 1408 | A | C4-C5-N7 | -5.38 | 108.01 | 110.70 |
| 22 | 23S1 | 294 | A | C4-C5-C6 | 5.38 | 119.69 | 117.00 |
| 22 | 23S1 | 1927 | A | C5-C6-N1 | 5.38 | 120.39 | 117.70 |
| 22 | 23S1 | 2377 | A | C4-C5-C6 | 5.38 | 119.69 | 117.00 |
| 22 | 23S1 | 2468 | A | C5-C6-N1 | 5.38 | 120.39 | 117.70 |
| 22 | 23S1 | 753 | A | C4-C5-N7 | -5.38 | 108.01 | 110.70 |
| 22 | 23S1 | 1348 | C | C6-N1-C2 | -5.38 | 118.15 | 120.30 |
| 22 | 23S1 | 2071 | A | C5-C6-N1 | 5.38 | 120.39 | 117.70 |
| 22 | 23S1 | 2829 | A | C4-C5-C6 | 5.38 | 119.69 | 117.00 |
| 1 | 16S1 | 223 | A | C5-C6-N1 | 5.37 | 120.39 | 117.70 |
| 1 | 16S1 | 1176 | A | C4-C5-N7 | -5.37 | 108.01 | 110.70 |
| 22 | 23S1 | 896 | A | C4-C5-C6 | 5.37 | 119.69 | 117.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 1039 | A | N9-C4-C5 | 5.37 | 107.95 | 105.80 |
| 22 | 23S1 | 1453 | A | C8-N9-C4 | 5.37 | 107.95 | 105.80 |
| 22 | 23S1 | 1525 | A | N3-C4-N9 | 5.37 | 131.70 | 127.40 |
| 22 | 23S1 | 1549 | A | N9-C4-C5 | 5.37 | 107.95 | 105.80 |
| 22 | 23S1 | 2134 | A | C4-C5-N7 | -5.37 | 108.01 | 110.70 |
| 1 | 16S1 | 937 | A | C4-C5-C6 | 5.37 | 119.69 | 117.00 |
| 22 | 23S1 | 13 | A | C4-C5-N7 | -5.37 | 108.01 | 110.70 |
| 22 | 23S1 | 126 | A | C4-C5-C6 | 5.37 | 119.69 | 117.00 |
| 22 | 23S1 | 182 | A | C5-C6-N1 | 5.37 | 120.39 | 117.70 |
| 22 | 23S1 | 603 | A | C4-C5-C6 | 5.37 | 119.69 | 117.00 |
| 22 | 23S1 | 1858 | A | C8-N9-C4 | 5.37 | 107.95 | 105.80 |
| 22 | 23S1 | 1937 | A | C4-C5-C6 | 5.37 | 119.69 | 117.00 |
| 22 | 23S1 | 2560 | A | C4-C5-N7 | -5.37 | 108.01 | 110.70 |
| 22 | 23S1 | 2679 | A | C8-N9-C4 | 5.37 | 107.95 | 105.80 |
| 22 | 23S1 | 2749 | A | C4-C5-C6 | 5.37 | 119.69 | 117.00 |
| 55 | PTR1 | 69 | A | C5-C6-N1 | 5.37 | 120.39 | 117.70 |
| 1 | 16S1 | 10 | A | C8-N9-C4 | 5.37 | 107.95 | 105.80 |
| 1 | 16S1 | 1117 | A | N3-C4-N9 | 5.37 | 131.70 | 127.40 |
| 22 | 23S1 | 2314 | A | C4-C5-N7 | -5.37 | 108.02 | 110.70 |
| 1 | 16S1 | 364 | A | C5-C6-N1 | 5.37 | 120.38 | 117.70 |
| 1 | 16S1 | 411 | A | C4-C5-C6 | 5.37 | 119.68 | 117.00 |
| 1 | 16S1 | 787 | A | C5-C6-N1 | 5.37 | 120.38 | 117.70 |
| 22 | 23S1 | 1545 | A | C4-C5-N7 | -5.37 | 108.02 | 110.70 |
| 22 | 23S1 | 1889 | A | C4-C5-N7 | -5.37 | 108.02 | 110.70 |
| 22 | 23S1 | 2135 | A | C8-N9-C4 | 5.37 | 107.95 | 105.80 |
| 22 | 23S1 | 1257 | C | C6-N1-C2 | -5.37 | 118.15 | 120.30 |
| 1 | 16S1 | 365 | U | C2-N3-C4 | 5.37 | 130.22 | 127.00 |
| 1 | 16S1 | 1176 | A | C8-N9-C4 | 5.37 | 107.95 | 105.80 |
| 22 | 23S1 | 716 | A | C4-C5-N7 | -5.37 | 108.02 | 110.70 |
| 22 | 23S1 | 988 | A | C8-N9-C4 | 5.37 | 107.95 | 105.80 |
| 22 | 23S1 | 1111 | A | C4-C5-N7 | -5.37 | 108.02 | 110.70 |
| 22 | 23S1 | 1809 | A | C4-C5-N7 | -5.37 | 108.02 | 110.70 |
| 22 | 23S1 | 2090 | A | C8-N9-C4 | 5.37 | 107.95 | 105.80 |
| 22 | 23S1 | 2247 | A | C5-C6-N1 | 5.37 | 120.38 | 117.70 |
| 1 | 16S1 | 199 | A | C4-C5-N7 | -5.36 | 108.02 | 110.70 |
| 1 | 16S1 | 810 | C | N1-C2-O2 | 5.36 | 122.12 | 118.90 |
| 1 | 16S1 | 831 | A | C4-C5-N7 | -5.36 | 108.02 | 110.70 |
| 1 | 16S1 | 1035 | A | C4-C5-N7 | -5.36 | 108.02 | 110.70 |
| 22 | 23S1 | 984 | A | C5-C6-N1 | 5.36 | 120.38 | 117.70 |
| 22 | 23S1 | 1129 | A | C4-C5-N7 | -5.36 | 108.02 | 110.70 |
| 22 | 23S1 | 1264 | A | C5-C6-N1 | 5.36 | 120.38 | 117.70 |
| 22 | 23S1 | 1330 | C | N3-C2-O2 | -5.36 | 118.15 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 1359 | A | C4-C5-N7 | -5.36 | 108.02 | 110.70 |
| 22 | 23S1 | 1431 | A | C5-C6-N1 | 5.36 | 120.38 | 117.70 |
| 22 | 23S1 | 1815 | A | N9-C4-C5 | 5.36 | 107.95 | 105.80 |
| 1 | 16S1 | 262 | A | N9-C4-C5 | 5.36 | 107.94 | 105.80 |
| 22 | 23S1 | 905 | A | C4-C5-C6 | 5.36 | 119.68 | 117.00 |
| 22 | 23S1 | 919 | U | N3-C2-O2 | -5.36 | 118.45 | 122.20 |
| 1 | 16S1 | 65 | A | C4-C5-C6 | 5.36 | 119.68 | 117.00 |
| 22 | 23S1 | 614 | A | N9-C4-C5 | 5.36 | 107.94 | 105.80 |
| 22 | 23S1 | 1307 | A | C8-N9-C4 | 5.36 | 107.94 | 105.80 |
| 22 | 23S1 | 2060 | A | C4-C5-N7 | -5.36 | 108.02 | 110.70 |
| 22 | 23S1 | 2297 | A | C8-N9-C4 | 5.36 | 107.94 | 105.80 |
| 22 | 23S1 | 2412 | A | C4-C5-N7 | -5.36 | 108.02 | 110.70 |
| 23 | 05S1 | 108 | A | C4-C5-C6 | 5.36 | 119.68 | 117.00 |
| 22 | 23S1 | 878 | A | N9-C4-C5 | 5.36 | 107.94 | 105.80 |
| 1 | 16S1 | 228 | A | N9-C4-C5 | 5.36 | 107.94 | 105.80 |
| 1 | 16S1 | 1110 | A | N3-C4-N9 | 5.36 | 131.69 | 127.40 |
| 1 | 16S1 | 1179 | A | C4-C5-C6 | 5.36 | 119.68 | 117.00 |
| 1 | 16S1 | 1340 | A | C4-C5-N7 | -5.36 | 108.02 | 110.70 |
| 22 | 23S1 | 1032 | A | C4-C5-N7 | -5.36 | 108.02 | 110.70 |
| 22 | 23S1 | 1658 | C | C6-N1-C2 | -5.36 | 118.16 | 120.30 |
| 22 | 23S1 | 2600 | A | C5-C6-N1 | 5.36 | 120.38 | 117.70 |
| 1 | 16S1 | 195 | A | N9-C4-C5 | 5.36 | 107.94 | 105.80 |
| 1 | 16S1 | 288 | A | C4-C5-N7 | -5.36 | 108.02 | 110.70 |
| 1 | 16S1 | 353 | A | N3-C4-N9 | 5.36 | 131.68 | 127.40 |
| 1 | 16S1 | 640 | A | N9-C4-C5 | 5.36 | 107.94 | 105.80 |
| 1 | 16S1 | 1146 | A | C8-N9-C4 | 5.36 | 107.94 | 105.80 |
| 22 | 23S1 | 299 | A | C5-C6-N1 | 5.36 | 120.38 | 117.70 |
| 22 | 23S1 | 507 | A | N9-C4-C5 | 5.36 | 107.94 | 105.80 |
| 22 | 23S1 | 1791 | A | N9-C4-C5 | 5.36 | 107.94 | 105.80 |
| 22 | 23S1 | 1890 | A | C4-C5-N7 | -5.36 | 108.02 | 110.70 |
| 22 | 23S1 | 2147 | A | C5-C6-N1 | 5.36 | 120.38 | 117.70 |
| 22 | 23S1 | 2278 | A | C5-C6-N1 | 5.36 | 120.38 | 117.70 |
| 1 | 16S1 | 16 | A | N3-C4-N9 | 5.35 | 131.68 | 127.40 |
| 22 | 23S1 | 1810 | A | C5-N7-C8 | 5.35 | 106.58 | 103.90 |
| 1 | 16S1 | 320 | A | C4-C5-C6 | 5.35 | 119.68 | 117.00 |
| 1 | 16S1 | 768 | A | C4-C5-C6 | 5.35 | 119.68 | 117.00 |
| 1 | 16S1 | 1333 | A | N3-C4-N9 | 5.35 | 131.68 | 127.40 |
| 22 | 23S1 | 143 | C | C2-N1-C1' | 5.35 | 124.69 | 118.80 |
| 22 | 23S1 | 216 | A | N9-C4-C5 | 5.35 | 107.94 | 105.80 |
| 22 | 23S1 | 917 | A | N9-C4-C5 | 5.35 | 107.94 | 105.80 |
| 22 | 23S1 | 2019 | A | C4-C5-N7 | -5.35 | 108.02 | 110.70 |
| 1 | 16S1 | 274 | A | C4-C5-N7 | -5.35 | 108.02 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 16S1 | 371 | A | C8-N9-C4 | 5.35 | 107.94 | 105.80 |
| 22 | 23S1 | 861 | A | C5-C6-N1 | 5.35 | 120.38 | 117.70 |
| 22 | 23S1 | 1353 | A | C4-C5-C6 | 5.35 | 119.67 | 117.00 |
| 22 | 23S1 | 95 | A | N3-C4-N9 | 5.35 | 131.68 | 127.40 |
| 22 | 23S1 | 2031 | A | C5-C6-N1 | 5.35 | 120.38 | 117.70 |
| 1 | 16S1 | 495 | A | N9-C4-C5 | 5.35 | 107.94 | 105.80 |
| 1 | 16S1 | 1201 | A | C4-C5-N7 | -5.35 | 108.03 | 110.70 |
| 1 | 16S1 | 1285 | A | C4-C5-C6 | 5.35 | 119.67 | 117.00 |
| 22 | 23S1 | 928 | A | N9-C4-C5 | 5.35 | 107.94 | 105.80 |
| 22 | 23S1 | 1780 | A | N9-C4-C5 | 5.35 | 107.94 | 105.80 |
| 22 | 23S1 | 2284 | A | N9-C4-C5 | 5.35 | 107.94 | 105.80 |
| 22 | 23S1 | 1385 | A | N3-C4-N9 | 5.35 | 131.68 | 127.40 |
| 22 | 23S1 | 2860 | A | N9-C4-C5 | 5.35 | 107.94 | 105.80 |
| 1 | 16S1 | 174 | A | C5-C6-N1 | 5.34 | 120.37 | 117.70 |
| 1 | 16S1 | 493 | A | C4-C5-C6 | 5.34 | 119.67 | 117.00 |
| 22 | 23S1 | 5 | A | C4-C5-N7 | -5.34 | 108.03 | 110.70 |
| 22 | 23S1 | 1090 | A | N3-C4-N9 | 5.34 | 131.68 | 127.40 |
| 22 | 23S1 | 1936 | A | O4'-C1'-N9 | 5.34 | 112.47 | 108.20 |
| 22 | 23S1 | 2632 | A | C5-C6-N1 | 5.34 | 120.37 | 117.70 |
| 1 | 16S1 | 958 | A | C4-C5-N7 | -5.34 | 108.03 | 110.70 |
| 1 | 16S1 | 1398 | A | C4-C5-N7 | -5.34 | 108.03 | 110.70 |
| 22 | 23S1 | 201 | C | N3-C2-O2 | -5.34 | 118.16 | 121.90 |
| 22 | 23S1 | 1308 | A | N3-C4-N9 | 5.34 | 131.67 | 127.40 |
| 22 | 23S1 | 1566 | A | C4-C5-C6 | 5.34 | 119.67 | 117.00 |
| 22 | 23S1 | 1775 | U | N3-C2-O2 | -5.34 | 118.46 | 122.20 |
| 22 | 23S1 | 2146 | C | P-O3'-C3' | 5.34 | 126.11 | 119.70 |
| 1 | 16S1 | 389 | A | C4-C5-N7 | -5.34 | 108.03 | 110.70 |
| 1 | 16S1 | 1368 | A | C4-C5-C6 | 5.34 | 119.67 | 117.00 |
| 22 | 23S1 | 190 | A | N9-C4-C5 | 5.34 | 107.94 | 105.80 |
| 22 | 23S1 | 1264 | A | C4-C5-C6 | 5.34 | 119.67 | 117.00 |
| 22 | 23S1 | 1384 | A | N3-C4-N9 | 5.34 | 131.67 | 127.40 |
| 1 | 16S1 | 408 | A | C5-C6-N1 | 5.34 | 120.37 | 117.70 |
| 1 | 16S1 | 1346 | A | N9-C4-C5 | 5.34 | 107.94 | 105.80 |
| 22 | 23S1 | 1815 | A | N3-C4-N9 | 5.34 | 131.67 | 127.40 |
| 1 | 16S1 | 131 | A | N3-C4-N9 | 5.34 | 131.67 | 127.40 |
| 1 | 16S1 | 959 | A | N9-C4-C5 | 5.34 | 107.94 | 105.80 |
| 22 | 23S1 | 181 | A | C4-C5-N7 | -5.34 | 108.03 | 110.70 |
| 22 | 23S1 | 613 | A | C8-N9-C4 | 5.34 | 107.94 | 105.80 |
| 22 | 23S1 | 1640 | A | C4-C5-N7 | -5.34 | 108.03 | 110.70 |
| 22 | 23S1 | 1928 | A | N3-C4-N9 | 5.34 | 131.67 | 127.40 |
| 22 | 23S1 | 2381 | A | C4-C5-C6 | 5.34 | 119.67 | 117.00 |
| 22 | 23S1 | 2741 | A | C8-N9-C4 | 5.34 | 107.94 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 2813 | A | C5-C6-N1 | 5.34 | 120.37 | 117.70 |
| 22 | 23S1 | 2154 | A | C4-C5-N7 | -5.33 | 108.03 | 110.70 |
| 1 | 16S1 | 1067 | A | N9-C4-C5 | 5.33 | 107.93 | 105.80 |
| 22 | 23S1 | 443 | A | C5-C6-N1 | 5.33 | 120.37 | 117.70 |
| 22 | 23S1 | 454 | A | N3-C4-N9 | 5.33 | 131.67 | 127.40 |
| 22 | 23S1 | 1336 | A | C8-N9-C4 | 5.33 | 107.93 | 105.80 |
| 1 | 16S1 | 238 | A | N9-C4-C5 | 5.33 | 107.93 | 105.80 |
| 1 | 16S1 | 435 | A | C5-C6-N1 | 5.33 | 120.37 | 117.70 |
| 1 | 16S1 | 1101 | A | C5-C6-N1 | 5.33 | 120.36 | 117.70 |
| 22 | 23S1 | 432 | A | C5-C6-N1 | 5.33 | 120.37 | 117.70 |
| 22 | 23S1 | 1237 | A | N3-C4-N9 | 5.33 | 131.66 | 127.40 |
| 22 | 23S1 | 1286 | A | N3-C4-N9 | 5.33 | 131.66 | 127.40 |
| 22 | 23S1 | 1548 | A | C8-N9-C4 | 5.33 | 107.93 | 105.80 |
| 22 | 23S1 | 2005 | A | C5-C6-N1 | 5.33 | 120.37 | 117.70 |
| 22 | 23S1 | 2241 | A | N9-C4-C5 | 5.33 | 107.93 | 105.80 |
| 22 | 23S1 | 2478 | A | N9-C4-C5 | 5.33 | 107.93 | 105.80 |
| 1 | 16S1 | 366 | A | C8-N9-C4 | 5.33 | 107.93 | 105.80 |
| 22 | 23S1 | 1032 | A | N3-C4-N9 | 5.33 | 131.66 | 127.40 |
| 22 | 23S1 | 1572 | A | C8-N9-C4 | 5.33 | 107.93 | 105.80 |
| 1 | 16S1 | 155 | A | C4-C5-N7 | -5.33 | 108.04 | 110.70 |
| 22 | 23S1 | 1069 | A | C4-C5-C6 | 5.33 | 119.66 | 117.00 |
| 22 | 23S1 | 1155 | A | C5-C6-N1 | 5.33 | 120.36 | 117.70 |
| 22 | 23S1 | 1285 | A | C4-C5-N7 | -5.33 | 108.04 | 110.70 |
| 22 | 23S1 | 1419 | A | N9-C4-C5 | 5.33 | 107.93 | 105.80 |
| 22 | 23S1 | 2059 | A | C8-N9-C4 | 5.33 | 107.93 | 105.80 |
| 22 | 23S1 | 2060 | A | N9-C4-C5 | 5.33 | 107.93 | 105.80 |
| 22 | 23S1 | 2328 | A | N9-C4-C5 | 5.33 | 107.93 | 105.80 |
| 23 | 05S1 | 78 | A | C4-C5-C6 | 5.33 | 119.66 | 117.00 |
| 15 | S151 | 89 | ARG | N-CA-C | 5.33 | 125.38 | 111.00 |
| 22 | 23S1 | 126 | A | C4-C5-N7 | -5.33 | 108.04 | 110.70 |
| 1 | 16S1 | 747 | A | C5-C6-N1 | 5.33 | 120.36 | 117.70 |
| 1 | 16S1 | 960 | U | N1-C2-O2 | 5.33 | 126.53 | 122.80 |
| 22 | 23S1 | 340 | A | N9-C4-C5 | 5.33 | 107.93 | 105.80 |
| 22 | 23S1 | 1054 | A | C5-C6-N1 | 5.33 | 120.36 | 117.70 |
| 22 | 23S1 | 1165 | A | C4-C5-C6 | 5.33 | 119.66 | 117.00 |
| 1 | 16S1 | 270 | A | N9-C4-C5 | 5.32 | 107.93 | 105.80 |
| 1 | 16S1 | 715 | A | N3-C4-N9 | 5.32 | 131.66 | 127.40 |
| 22 | 23S1 | 430 | A | C5-C6-N1 | 5.32 | 120.36 | 117.70 |
| 22 | 23S1 | 2225 | A | C5-C6-N1 | 5.32 | 120.36 | 117.70 |
| 55 | PTR1 | 73 | A | C4-C5-C6 | 5.32 | 119.66 | 117.00 |
| 1 | 16S1 | 10 | A | N9-C4-C5 | 5.32 | 107.93 | 105.80 |
| 1 | 16S1 | 95 | C | C6-N1-C2 | -5.32 | 118.17 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 16S1 | 363 | A | C4-C5-N7 | -5.32 | 108.04 | 110.70 |
| 1 | 16S1 | 415 | A | N9-C4-C5 | 5.32 | 107.93 | 105.80 |
| 1 | 16S1 | 906 | A | C5-C6-N1 | 5.32 | 120.36 | 117.70 |
| 1 | 16S1 | 1508 | A | C5-C6-N1 | 5.32 | 120.36 | 117.70 |
| 22 | 23S1 | 294 | A | C8-N9-C4 | 5.32 | 107.93 | 105.80 |
| 1 | 16S1 | 1431 | A | C4-C5-C6 | 5.32 | 119.66 | 117.00 |
| 1 | 16S1 | 1433 | A | C4-C5-N7 | -5.32 | 108.04 | 110.70 |
| 22 | 23S1 | 279 | A | C4-C5-N7 | -5.32 | 108.04 | 110.70 |
| 22 | 23S1 | 802 | A | C5-C6-N1 | 5.32 | 120.36 | 117.70 |
| 22 | 23S1 | 2541 | A | N9-C4-C5 | 5.32 | 107.93 | 105.80 |
| 1 | 16S1 | 1016 | A | C4-C5-C6 | 5.32 | 119.66 | 117.00 |
| 1 | 16S1 | 1410 | A | C4-C5-N7 | -5.32 | 108.04 | 110.70 |
| 22 | 23S1 | 95 | A | C4-C5-C6 | 5.32 | 119.66 | 117.00 |
| 22 | 23S1 | 443 | A | C4-C5-N7 | -5.32 | 108.04 | 110.70 |
| 22 | 23S1 | 675 | A | C4-C5-N7 | -5.32 | 108.04 | 110.70 |
| 22 | 23S1 | 2174 | C | N1-C2-O2 | 5.32 | 122.09 | 118.90 |
| 22 | 23S1 | 2314 | A | C8-N9-C4 | 5.32 | 107.93 | 105.80 |
| 1 | 16S1 | 781 | A | C5-C6-N1 | 5.32 | 120.36 | 117.70 |
| 1 | 16S1 | 1360 | A | C5-C6-N1 | 5.32 | 120.36 | 117.70 |
| 22 | 23S1 | 226 | A | C8-N9-C4 | 5.32 | 107.93 | 105.80 |
| 22 | 23S1 | 789 | A | C5-C6-N1 | 5.32 | 120.36 | 117.70 |
| 22 | 23S1 | 2639 | A | N9-C4-C5 | 5.32 | 107.93 | 105.80 |
| 22 | 23S1 | 2723 | C | C6-N1-C2 | -5.32 | 118.17 | 120.30 |
| 1 | 16S1 | 648 | A | C4-C5-N7 | -5.31 | 108.04 | 110.70 |
| 1 | 16S1 | 996 | A | C4-C5-N7 | -5.31 | 108.04 | 110.70 |
| 1 | 16S1 | 919 | A | C4-C5-N7 | -5.31 | 108.04 | 110.70 |
| 1 | 16S1 | 1377 | A | C4-C5-N7 | -5.31 | 108.04 | 110.70 |
| 1 | 16S1 | 1196 | A | C5-C6-N1 | 5.31 | 120.36 | 117.70 |
| 1 | 16S1 | 1254 | A | C5-C6-N1 | 5.31 | 120.36 | 117.70 |
| 2 | S021 | 129 | LEU | CA-CB-CG | 5.31 | 127.52 | 115.30 |
| 22 | 23S1 | 231 | A | C4-C5-N7 | -5.31 | 108.04 | 110.70 |
| 22 | 23S1 | 1654 | A | N9-C4-C5 | 5.31 | 107.92 | 105.80 |
| 1 | 16S1 | 119 | A | C4-C5-C6 | 5.31 | 119.66 | 117.00 |
| 1 | 16S1 | 282 | A | C5-C6-N1 | 5.31 | 120.35 | 117.70 |
| 22 | 23S1 | 320 | A | C5-C6-N1 | 5.31 | 120.35 | 117.70 |
| 22 | 23S1 | 538 | A | C4-C5-N7 | -5.31 | 108.05 | 110.70 |
| 22 | 23S1 | 2340 | A | C5-C6-N1 | 5.31 | 120.36 | 117.70 |
| 22 | 23S1 | 2733 | A | C4-C5-N7 | -5.31 | 108.05 | 110.70 |
| 22 | 23S1 | 294 | A | N9-C4-C5 | 5.31 | 107.92 | 105.80 |
| 22 | 23S1 | 608 | A | C8-N9-C4 | 5.31 | 107.92 | 105.80 |
| 22 | 23S1 | 655 | A | C4-C5-C6 | 5.31 | 119.65 | 117.00 |
| 22 | 23S1 | 1347 | A | C8-N9-C4 | 5.31 | 107.92 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 2183 | A | C4-C5-C6 | 5.31 | 119.65 | 117.00 |
| 22 | 23S1 | 2534 | A | C5-C6-N1 | 5.31 | 120.35 | 117.70 |
| 23 | 05S1 | 34 | A | C5-C6-N1 | 5.31 | 120.35 | 117.70 |
| 23 | 05S1 | 53 | A | C4-C5-C6 | 5.31 | 119.65 | 117.00 |
| 22 | 23S1 | 2184 | A | C5-C6-N1 | 5.31 | 120.35 | 117.70 |
| 1 | 16S1 | 1028 | C | C6-N1-C2 | -5.30 | 118.18 | 120.30 |
| 22 | 23S1 | 38 | A | C5-C6-N1 | 5.30 | 120.35 | 117.70 |
| 22 | 23S1 | 222 | A | C5-C6-N1 | 5.30 | 120.35 | 117.70 |
| 22 | 23S1 | 920 | A | C5-C6-N1 | 5.30 | 120.35 | 117.70 |
| 22 | 23S1 | 1603 | A | C5-C6-N1 | 5.30 | 120.35 | 117.70 |
| 22 | 23S1 | 244 | A | C5-C6-N1 | 5.30 | 120.35 | 117.70 |
| 1 | 16S1 | 298 | A | C4-C5-C6 | 5.30 | 119.65 | 117.00 |
| 1 | 16S1 | 602 | A | C4-C5-N7 | -5.30 | 108.05 | 110.70 |
| 22 | 23S1 | 127 | A | C4-C5-C6 | 5.30 | 119.65 | 117.00 |
| 1 | 16S1 | 1019 | A | C4-C5-C6 | 5.30 | 119.65 | 117.00 |
| 1 | 16S1 | 1197 | A | C8-N9-C4 | 5.30 | 107.92 | 105.80 |
| 22 | 23S1 | 1889 | A | N9-C4-C5 | 5.30 | 107.92 | 105.80 |
| 22 | 23S1 | 2882 | A | C5-C6-N1 | 5.30 | 120.35 | 117.70 |
| 1 | 16S1 | 119 | A | N3-C4-N9 | 5.30 | 131.64 | 127.40 |
| 1 | 16S1 | 794 | A | C5-C6-N1 | 5.30 | 120.35 | 117.70 |
| 22 | 23S1 | 1342 | A | N3-C4-N9 | 5.30 | 131.64 | 127.40 |
| 22 | 23S1 | 1365 | A | C4-C5-N7 | -5.30 | 108.05 | 110.70 |
| 22 | 23S1 | 1453 | A | C4-C5-N7 | -5.30 | 108.05 | 110.70 |
| 22 | 23S1 | 2043 | C | N1-C2-O2 | 5.30 | 122.08 | 118.90 |
| 22 | 23S1 | 2700 | A | C8-N9-C4 | 5.30 | 107.92 | 105.80 |
| 22 | 23S1 | 2761 | A | C4-C5-N7 | -5.30 | 108.05 | 110.70 |
| 22 | 23S1 | 2813 | A | C4-C5-N7 | -5.30 | 108.05 | 110.70 |
| 23 | 05S1 | 46 | A | C4-C5-C6 | 5.30 | 119.65 | 117.00 |
| 1 | 16S1 | 1036 | A | C4-C5-N7 | -5.29 | 108.05 | 110.70 |
| 22 | 23S1 | 943 | A | C8-N9-C4 | 5.29 | 107.92 | 105.80 |
| 22 | 23S1 | 1274 | A | N3-C4-N9 | 5.29 | 131.64 | 127.40 |
| 1 | 16S1 | 1111 | A | C8-N9-C4 | 5.29 | 107.92 | 105.80 |
| 1 | 16S1 | 1188 | A | C5-C6-N1 | 5.29 | 120.35 | 117.70 |
| 1 | 16S1 | 1377 | A | C5-C6-N1 | 5.29 | 120.35 | 117.70 |
| 1 | 16S1 | 1508 | A | N9-C4-C5 | 5.29 | 107.92 | 105.80 |
| 22 | 23S1 | 103 | A | N9-C4-C5 | 5.29 | 107.92 | 105.80 |
| 22 | 23S1 | 322 | A | N9-C4-C5 | 5.29 | 107.92 | 105.80 |
| 22 | 23S1 | 1241 | A | C8-N9-C4 | 5.29 | 107.92 | 105.80 |
| 22 | 23S1 | 1343 | G | C4-N9-C1' | 5.29 | 133.38 | 126.50 |
| 22 | 23S1 | 2726 | A | C5-C6-N1 | 5.29 | 120.35 | 117.70 |
| 22 | 23S1 | 2750 | A | C4-C5-N7 | -5.29 | 108.05 | 110.70 |
| 22 | 23S1 | 2820 | A | C5-C6-N1 | 5.29 | 120.35 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 16S1 | 155 | A | N9-C4-C5 | 5.29 | 107.92 | 105.80 |
| 1 | 16S1 | 167 | A | N9-C4-C5 | 5.29 | 107.92 | 105.80 |
| 1 | 16S1 | 382 | A | C5-C6-N1 | 5.29 | 120.35 | 117.70 |
| 1 | 16S1 | 845 | A | C5-C6-N1 | 5.29 | 120.35 | 117.70 |
| 22 | 23S1 | 53 | A | C4-C5-C6 | 5.29 | 119.65 | 117.00 |
| 22 | 23S1 | 223 | A | N9-C4-C5 | 5.29 | 107.92 | 105.80 |
| 22 | 23S1 | 1001 | A | N9-C4-C5 | 5.29 | 107.92 | 105.80 |
| 22 | 23S1 | 1967 | C | N3-C2-O2 | -5.29 | 118.20 | 121.90 |
| 22 | 23S1 | 2104 | C | C6-N1-C2 | -5.29 | 118.18 | 120.30 |
| 1 | 16S1 | 1179 | A | N3-C4-N9 | 5.29 | 131.63 | 127.40 |
| 22 | 23S1 | 748 | G | O4'-C1'-N9 | 5.29 | 112.43 | 108.20 |
| 22 | 23S1 | 2003 | A | C4-C5-N7 | -5.29 | 108.06 | 110.70 |
| 1 | 16S1 | 487 | A | C8-N9-C4 | 5.29 | 107.92 | 105.80 |
| 22 | 23S1 | 197 | A | C5-C6-N1 | 5.29 | 120.34 | 117.70 |
| 22 | 23S1 | 412 | A | C4-C5-N7 | -5.29 | 108.06 | 110.70 |
| 22 | 23S1 | 2146 | C | C6-N1-C2 | -5.29 | 118.18 | 120.30 |
| 22 | 23S1 | 2274 | A | N3-C4-N9 | 5.29 | 131.63 | 127.40 |
| 22 | 23S1 | 2820 | A | N3-C4-N9 | 5.29 | 131.63 | 127.40 |
| 22 | 23S1 | 2851 | A | N9-C4-C5 | 5.29 | 107.92 | 105.80 |
| 22 | 23S1 | 2434 | A | N3-C4-N9 | 5.29 | 131.63 | 127.40 |
| 1 | 16S1 | 503 | C | C5-C6-N1 | 5.29 | 123.64 | 121.00 |
| 1 | 16S1 | 825 | A | C4-C5-C6 | 5.29 | 119.64 | 117.00 |
| 22 | 23S1 | 222 | A | N9-C4-C5 | 5.29 | 107.92 | 105.80 |
| 22 | 23S1 | 817 | C | C6-N1-C2 | -5.29 | 118.19 | 120.30 |
| 22 | 23S1 | 1129 | A | C4-C5-C6 | 5.29 | 119.64 | 117.00 |
| 22 | 23S1 | 1204 | A | C4-C5-N7 | -5.29 | 108.06 | 110.70 |
| 22 | 23S1 | 1295 | C | N3-C2-O2 | -5.29 | 118.20 | 121.90 |
| 22 | 23S1 | 1579 | A | C5-C6-N1 | 5.29 | 120.34 | 117.70 |
| 22 | 23S1 | 1722 | A | C8-N9-C4 | 5.29 | 107.91 | 105.80 |
| 23 | 05S1 | 34 | A | N9-C4-C5 | 5.29 | 107.91 | 105.80 |
| 55 | PTR1 | 23 | A | C8-N9-C4 | 5.29 | 107.91 | 105.80 |
| 1 | 16S1 | 915 | A | C4-C5-N7 | -5.28 | 108.06 | 110.70 |
| 22 | 23S1 | 412 | A | N9-C4-C5 | 5.28 | 107.91 | 105.80 |
| 22 | 23S1 | 415 | A | C5-C6-N1 | 5.28 | 120.34 | 117.70 |
| 22 | 23S1 | 915 | C | C2-N1-C1' | 5.28 | 124.61 | 118.80 |
| 22 | 23S1 | 1960 | A | C4-C5-C6 | 5.28 | 119.64 | 117.00 |
| 22 | 23S1 | 2073 | C | C6-N1-C2 | -5.28 | 118.19 | 120.30 |
| 22 | 23S1 | 2247 | A | N9-C4-C5 | 5.28 | 107.91 | 105.80 |
| 22 | 23S1 | 1525 | A | C5-C6-N1 | 5.28 | 120.34 | 117.70 |
| 22 | 23S1 | 2758 | A | C8-N9-C4 | 5.28 | 107.91 | 105.80 |
| 1 | 16S1 | 1150 | A | N3-C4-N9 | 5.28 | 131.62 | 127.40 |
| 1 | 16S1 | 1362 | A | C8-N9-C4 | 5.28 | 107.91 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 311 | A | C8-N9-C4 | 5.28 | 107.91 | 105.80 |
| 22 | 23S1 | 1286 | A | C8-N9-C4 | 5.28 | 107.91 | 105.80 |
| 22 | 23S1 | 1304 | A | C5-C6-N1 | 5.28 | 120.34 | 117.70 |
| 22 | 23S1 | 1981 | A | N9-C4-C5 | 5.28 | 107.91 | 105.80 |
| 22 | 23S1 | 2327 | A | C5-C6-N1 | 5.28 | 120.34 | 117.70 |
| 1 | 16S1 | 1333 | A | C4-C5-C6 | 5.28 | 119.64 | 117.00 |
| 22 | 23S1 | 715 | A | C4-C5-N7 | -5.28 | 108.06 | 110.70 |
| 22 | 23S1 | 739 | A | C4-C5-N7 | -5.28 | 108.06 | 110.70 |
| 22 | 23S1 | 2800 | A | C4-C5-C6 | 5.28 | 119.64 | 117.00 |
| 1 | 16S1 | 607 | A | C8-N9-C4 | 5.28 | 107.91 | 105.80 |
| 22 | 23S1 | 226 | A | C4-C5-C6 | 5.28 | 119.64 | 117.00 |
| 22 | 23S1 | 670 | A | C4-C5-N7 | -5.28 | 108.06 | 110.70 |
| 22 | 23S1 | 981 | A | C8-N9-C4 | 5.28 | 107.91 | 105.80 |
| 22 | 23S1 | 1858 | A | N9-C4-C5 | 5.28 | 107.91 | 105.80 |
| 22 | 23S1 | 2814 | A | N9-C4-C5 | 5.28 | 107.91 | 105.80 |
| 23 | 05S1 | 91 | C | N1-C2-O2 | 5.28 | 122.07 | 118.90 |
| 1 | 16S1 | 120 | A | C5-C6-N1 | 5.28 | 120.34 | 117.70 |
| 1 | 16S1 | 1248 | A | C4-C5-C6 | 5.28 | 119.64 | 117.00 |
| 22 | 23S1 | 5 | A | N9-C4-C5 | 5.28 | 107.91 | 105.80 |
| 22 | 23S1 | 322 | A | C4-C5-N7 | -5.28 | 108.06 | 110.70 |
| 22 | 23S1 | 1213 | A | N9-C4-C5 | 5.28 | 107.91 | 105.80 |
| 22 | 23S1 | 2547 | A | C4-C5-N7 | -5.28 | 108.06 | 110.70 |
| 22 | 23S1 | 2660 | A | C4-C5-N7 | -5.28 | 108.06 | 110.70 |
| 1 | 16S1 | 1179 | A | C4-C5-N7 | -5.27 | 108.06 | 110.70 |
| 22 | 23S1 | 352 | A | N9-C4-C5 | 5.27 | 107.91 | 105.80 |
| 22 | 23S1 | 1505 | A | C4-C5-N7 | -5.27 | 108.06 | 110.70 |
| 22 | 23S1 | 74 | A | C5-C6-N1 | 5.27 | 120.34 | 117.70 |
| 22 | 23S1 | 817 | C | N3-C2-O2 | -5.27 | 118.21 | 121.90 |
| 22 | 23S1 | 1385 | A | C4-C5-C6 | 5.27 | 119.64 | 117.00 |
| 22 | 23S1 | 1395 | A | C4-C5-N7 | -5.27 | 108.06 | 110.70 |
| 22 | 23S1 | 2108 | A | C5-C6-N1 | 5.27 | 120.34 | 117.70 |
| 22 | 23S1 | 2602 | A | N9-C4-C5 | 5.27 | 107.91 | 105.80 |
| 1 | 16S1 | 1520 | C | N1-C2-O2 | 5.27 | 122.06 | 118.90 |
| 22 | 23S1 | 750 | A | C4-C5-C6 | 5.27 | 119.64 | 117.00 |
| 22 | 23S1 | 2015 | A | C5-C6-N1 | 5.27 | 120.34 | 117.70 |
| 1 | 16S1 | 336 | A | C8-N9-C4 | 5.27 | 107.91 | 105.80 |
| 22 | 23S1 | 402 | A | N3-C4-N9 | 5.27 | 131.62 | 127.40 |
| 22 | 23S1 | 740 | C | N3-C2-O2 | -5.27 | 118.21 | 121.90 |
| 22 | 23S1 | 897 | C | C5-C6-N1 | 5.27 | 123.63 | 121.00 |
| 22 | 23S1 | 2579 | C | N1-C2-O2 | 5.27 | 122.06 | 118.90 |
| 1 | 16S1 | 572 | A | N3-C4-N9 | 5.27 | 131.61 | 127.40 |
| 1 | 16S1 | 807 | A | C8-N9-C4 | 5.27 | 107.91 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 16S1 | 889 | A | C5-C6-N1 | 5.27 | 120.33 | 117.70 |
| 1 | 16S1 | 1257 | A | C5-C6-N1 | 5.27 | 120.33 | 117.70 |
| 22 | 23S1 | 142 | A | N9-C1'-C2' | -5.27 | 106.21 | 112.00 |
| 22 | 23S1 | 515 | A | C4-C5-N7 | -5.27 | 108.07 | 110.70 |
| 22 | 23S1 | 1665 | A | N9-C4-C5 | 5.27 | 107.91 | 105.80 |
| 1 | 16S1 | 706 | A | C4-C5-N7 | -5.27 | 108.07 | 110.70 |
| 22 | 23S1 | 262 | A | N3-C4-N9 | 5.27 | 131.61 | 127.40 |
| 1 | 16S1 | 1503 | A | C4-C5-N7 | -5.26 | 108.07 | 110.70 |
| 22 | 23S1 | 14 | A | C4-C5-C6 | 5.26 | 119.63 | 117.00 |
| 22 | 23S1 | 71 | A | C4-C5-N7 | -5.26 | 108.07 | 110.70 |
| 22 | 23S1 | 1366 | A | N9-C4-C5 | 5.26 | 107.91 | 105.80 |
| 22 | 23S1 | 2060 | A | C6-N1-C2 | 5.26 | 121.76 | 118.60 |
| 23 | 05S1 | 73 | A | C5-C6-N1 | 5.26 | 120.33 | 117.70 |
| 1 | 16S1 | 415 | A | C5-C6-N1 | 5.26 | 120.33 | 117.70 |
| 1 | 16S1 | 753 | A | C4-C5-N7 | -5.26 | 108.07 | 110.70 |
| 1 | 16S1 | 915 | A | C5-C6-N1 | 5.26 | 120.33 | 117.70 |
| 22 | 23S1 | 118 | A | N3-C4-N9 | 5.26 | 131.61 | 127.40 |
| 22 | 23S1 | 980 | A | N9-C4-C5 | 5.26 | 107.91 | 105.80 |
| 22 | 23S1 | 1503 | A | C8-N9-C4 | 5.26 | 107.91 | 105.80 |
| 22 | 23S1 | 2358 | A | C8-N9-C4 | 5.26 | 107.91 | 105.80 |
| 22 | 23S1 | 2560 | A | N9-C4-C5 | 5.26 | 107.91 | 105.80 |
| 1 | 16S1 | 306 | A | N9-C4-C5 | 5.26 | 107.91 | 105.80 |
| 1 | 16S1 | 996 | A | C5-C6-N1 | 5.26 | 120.33 | 117.70 |
| 22 | 23S1 | 637 | A | N3-C4-N9 | 5.26 | 131.61 | 127.40 |
| 22 | 23S1 | 2598 | A | C8-N9-C4 | 5.26 | 107.90 | 105.80 |
| 1 | 16S1 | 937 | A | C5-C6-N1 | 5.26 | 120.33 | 117.70 |
| 22 | 23S1 | 1165 | A | C5-C6-N1 | 5.26 | 120.33 | 117.70 |
| 22 | 23S1 | 2147 | A | C5-N7-C8 | 5.26 | 106.53 | 103.90 |
| 22 | 23S1 | 1098 | A | C8-N9-C4 | 5.26 | 107.90 | 105.80 |
| 22 | 23S1 | 1494 | A | C4-C5-N7 | -5.26 | 108.07 | 110.70 |
| 22 | 23S1 | 1889 | A | C5-C6-N1 | 5.26 | 120.33 | 117.70 |
| 1 | 16S1 | 130 | A | C5-C6-N1 | 5.26 | 120.33 | 117.70 |
| 1 | 16S1 | 315 | A | C4-C5-N7 | -5.26 | 108.07 | 110.70 |
| 1 | 16S1 | 1105 | A | C5-C6-N1 | 5.26 | 120.33 | 117.70 |
| 1 | 16S1 | 1246 | A | N9-C4-C5 | 5.26 | 107.90 | 105.80 |
| 22 | 23S1 | 2497 | A | C4-C5-N7 | -5.26 | 108.07 | 110.70 |
| 22 | 23S1 | 2821 | A | C5-C6-N1 | 5.26 | 120.33 | 117.70 |
| 1 | 16S1 | 8 | A | C4-C5-C6 | 5.25 | 119.63 | 117.00 |
| 1 | 16S1 | 8 | A | C5-C6-N1 | 5.25 | 120.33 | 117.70 |
| 1 | 16S1 | 149 | A | C4-C5-N7 | -5.25 | 108.07 | 110.70 |
| 22 | 23S1 | 752 | A | N3-C4-N9 | 5.25 | 131.60 | 127.40 |
| 22 | 23S1 | 1960 | A | C8-N9-C4 | 5.25 | 107.90 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 16S1 | 1246 | A | C8-N9-C4 | 5.25 | 107.90 | 105.80 |
| 22 | 23S1 | 1453 | A | C5-C6-N1 | 5.25 | 120.33 | 117.70 |
| 22 | 23S1 | 2882 | A | C4-C5-N7 | -5.25 | 108.07 | 110.70 |
| 1 | 16S1 | 129 | A | C4-C5-C6 | 5.25 | 119.62 | 117.00 |
| 22 | 23S1 | 141 | G | C4-N9-C1' | 5.25 | 133.33 | 126.50 |
| 22 | 23S1 | 223 | A | C4-C5-C6 | 5.25 | 119.63 | 117.00 |
| 22 | 23S1 | 877 | A | C4-C5-N7 | -5.25 | 108.07 | 110.70 |
| 22 | 23S1 | 1772 | A | C8-N9-C4 | 5.25 | 107.90 | 105.80 |
| 22 | 23S1 | 1780 | A | C4-C5-N7 | -5.25 | 108.07 | 110.70 |
| 23 | 05S1 | 46 | A | C8-N9-C4 | 5.25 | 107.90 | 105.80 |
| 1 | 16S1 | 3 | A | C4-C5-C6 | 5.25 | 119.62 | 117.00 |
| 1 | 16S1 | 907 | A | C5-C6-N1 | 5.25 | 120.33 | 117.70 |
| 22 | 23S1 | 1155 | A | C4-C5-N7 | -5.25 | 108.08 | 110.70 |
| 1 | 16S1 | 1092 | A | C4-C5-N7 | -5.25 | 108.08 | 110.70 |
| 22 | 23S1 | 241 | A | N3-C4-N9 | 5.25 | 131.60 | 127.40 |
| 22 | 23S1 | 415 | A | C8-N9-C4 | 5.25 | 107.90 | 105.80 |
| 22 | 23S1 | 1129 | A | N9-C4-C5 | 5.25 | 107.90 | 105.80 |
| 1 | 16S1 | 892 | A | C5-C6-N1 | 5.25 | 120.32 | 117.70 |
| 1 | 16S1 | 915 | A | N9-C4-C5 | 5.25 | 107.90 | 105.80 |
| 22 | 23S1 | 896 | A | N3-C4-N9 | 5.25 | 131.60 | 127.40 |
| 22 | 23S1 | 1354 | A | C8-N9-C4 | 5.25 | 107.90 | 105.80 |
| 1 | 16S1 | 1092 | A | C5-C6-N1 | 5.25 | 120.32 | 117.70 |
| 22 | 23S1 | 1634 | A | N3-C4-N9 | 5.25 | 131.60 | 127.40 |
| 22 | 23S1 | 1853 | A | C4-C5-N7 | -5.25 | 108.08 | 110.70 |
| 22 | 23S1 | 2434 | A | C4-C5-N7 | -5.25 | 108.08 | 110.70 |
| 1 | 16S1 | 706 | A | C5-C6-N1 | 5.24 | 120.32 | 117.70 |
| 22 | 23S1 | 575 | A | C8-N9-C4 | 5.24 | 107.90 | 105.80 |
| 22 | 23S1 | 1678 | A | N9-C4-C5 | 5.24 | 107.90 | 105.80 |
| 22 | 23S1 | 2005 | A | C4-C5-N7 | -5.24 | 108.08 | 110.70 |
| 22 | 23S1 | 2453 | A | C5-C6-N1 | 5.24 | 120.32 | 117.70 |
| 22 | 23S1 | 2564 | A | C8-N9-C4 | 5.24 | 107.90 | 105.80 |
| 1 | 16S1 | 243 | A | N9-C4-C5 | 5.24 | 107.90 | 105.80 |
| 22 | 23S1 | 300 | A | C5-C6-N1 | 5.24 | 120.32 | 117.70 |
| 22 | 23S1 | 718 | A | C8-N9-C4 | 5.24 | 107.90 | 105.80 |
| 22 | 23S1 | 899 | A | C4-C5-N7 | -5.24 | 108.08 | 110.70 |
| 1 | 16S1 | 1102 | A | C5-C6-N1 | 5.24 | 120.32 | 117.70 |
| 22 | 23S1 | 332 | A | C4-C5-N7 | -5.24 | 108.08 | 110.70 |
| 22 | 23S1 | 501 | A | C5-C6-N1 | 5.24 | 120.32 | 117.70 |
| 22 | 23S1 | 1089 | A | C5-C6-N1 | 5.24 | 120.32 | 117.70 |
| 22 | 23S1 | 1403 | A | C8-N9-C4 | 5.24 | 107.90 | 105.80 |
| 22 | 23S1 | 1590 | A | C8-N9-C4 | 5.24 | 107.90 | 105.80 |
| 22 | 23S1 | 1735 | A | C5-C6-N1 | 5.24 | 120.32 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 2019 | A | C5-C6-N1 | 5.24 | 120.32 | 117.70 |
| 22 | 23S1 | 2051 | A | N9-C4-C5 | 5.24 | 107.90 | 105.80 |
| 22 | 23S1 | 2147 | A | N3-C4-N9 | 5.24 | 131.59 | 127.40 |
| 22 | 23S1 | 2471 | A | C8-N9-C4 | 5.24 | 107.90 | 105.80 |
| 22 | 23S1 | 1014 | A | C4-C5-N7 | -5.24 | 108.08 | 110.70 |
| 22 | 23S1 | 1307 | A | C5-C6-N1 | 5.24 | 120.32 | 117.70 |
| 22 | 23S1 | 1330 | C | N1-C2-O2 | 5.24 | 122.04 | 118.90 |
| 22 | 23S1 | 2062 | A | C5-C6-N1 | 5.24 | 120.32 | 117.70 |
| 22 | 23S1 | 2531 | A | C8-N9-C4 | 5.24 | 107.89 | 105.80 |
| 22 | 23S1 | 2589 | A | C4-C5-N7 | -5.24 | 108.08 | 110.70 |
| 22 | 23S1 | 2820 | A | N9-C4-C5 | 5.24 | 107.89 | 105.80 |
| 22 | 23S1 | 2821 | A | C4-C5-N7 | -5.24 | 108.08 | 110.70 |
| 1 | 16S1 | 26 | A | N9-C4-C5 | 5.24 | 107.89 | 105.80 |
| 22 | 23S1 | 167 | A | C4-C5-N7 | -5.24 | 108.08 | 110.70 |
| 22 | 23S1 | 910 | A | C5-C6-N1 | 5.24 | 120.32 | 117.70 |
| 22 | 23S1 | 2749 | A | C8-N9-C4 | 5.24 | 107.89 | 105.80 |
| 22 | 23S1 | 2899 | A | C5-C6-N1 | 5.24 | 120.32 | 117.70 |
| 1 | 16S1 | 366 | A | N9-C4-C5 | 5.24 | 107.89 | 105.80 |
| 1 | 16S1 | 718 | A | C5-C6-N1 | 5.24 | 120.32 | 117.70 |
| 1 | 16S1 | 1499 | A | C4-C5-N7 | -5.24 | 108.08 | 110.70 |
| 1 | 16S1 | 1508 | A | C4-C5-N7 | -5.24 | 108.08 | 110.70 |
| 22 | 23S1 | 1308 | A | C8-N9-C4 | 5.24 | 107.89 | 105.80 |
| 22 | 23S1 | 1532 | A | C4-C5-N7 | -5.24 | 108.08 | 110.70 |
| 22 | 23S1 | 1644 | C | C6-N1-C2 | -5.24 | 118.20 | 120.30 |
| 22 | 23S1 | 2813 | A | C8-N9-C4 | 5.24 | 107.89 | 105.80 |
| 22 | 23S1 | 2835 | A | C5-C6-N1 | 5.24 | 120.32 | 117.70 |
| 22 | 23S1 | 1322 | A | N9-C4-C5 | 5.23 | 107.89 | 105.80 |
| 22 | 23S1 | 2435 | A | C4-C5-C6 | 5.23 | 119.62 | 117.00 |
| 23 | 05S1 | 59 | A | N9-C4-C5 | 5.23 | 107.89 | 105.80 |
| 1 | 16S1 | 914 | A | N3-C4-N9 | 5.23 | 131.59 | 127.40 |
| 1 | 16S1 | 993 | G | C4-N9-C1' | 5.23 | 133.30 | 126.50 |
| 1 | 16S1 | 1413 | A | C4-C5-C6 | 5.23 | 119.62 | 117.00 |
| 22 | 23S1 | 323 | C | C2-N1-C1' | 5.23 | 124.56 | 118.80 |
| 22 | 23S1 | 503 | A | N9-C4-C5 | 5.23 | 107.89 | 105.80 |
| 22 | 23S1 | 905 | A | C4-C5-N7 | -5.23 | 108.08 | 110.70 |
| 22 | 23S1 | 2636 | C | N3-C2-O2 | -5.23 | 118.24 | 121.90 |
| 55 | PTR1 | 62 | C | N3-C2-O2 | -5.23 | 118.24 | 121.90 |
| 1 | 16S1 | 787 | A | C4-C5-C6 | 5.23 | 119.62 | 117.00 |
| 1 | 16S1 | 1105 | A | N9-C4-C5 | 5.23 | 107.89 | 105.80 |
| 22 | 23S1 | 383 | C | N1-C2-O2 | 5.23 | 122.04 | 118.90 |
| 22 | 23S1 | 863 | A | C8-N9-C4 | 5.23 | 107.89 | 105.80 |
| 22 | 23S1 | 973 | A | C5-C6-N1 | 5.23 | 120.31 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 1126 | A | C4-C5-N7 | -5.23 | 108.08 | 110.70 |
| 22 | 23S1 | 1470 | A | N9-C4-C5 | 5.23 | 107.89 | 105.80 |
| 22 | 23S1 | 2058 | A | N9-C4-C5 | 5.23 | 107.89 | 105.80 |
| 22 | 23S1 | 13 | A | C5-C6-N1 | 5.23 | 120.31 | 117.70 |
| 22 | 23S1 | 574 | A | C5-C6-N1 | 5.23 | 120.31 | 117.70 |
| 22 | 23S1 | 1495 | A | C4-C5-N7 | -5.23 | 108.09 | 110.70 |
| 22 | 23S1 | 2019 | A | N9-C4-C5 | 5.23 | 107.89 | 105.80 |
| 1 | 16S1 | 1238 | A | C5-C6-N1 | 5.23 | 120.31 | 117.70 |
| 9 | S091 | 123 | ARG | C-N-CA | 5.23 | 134.77 | 121.70 |
| 22 | 23S1 | 309 | A | C4-C5-N7 | -5.23 | 108.09 | 110.70 |
| 22 | 23S1 | 793 | A | N9-C4-C5 | 5.23 | 107.89 | 105.80 |
| 22 | 23S1 | 941 | A | C5-C6-N1 | 5.23 | 120.31 | 117.70 |
| 22 | 23S1 | 1117 | C | N1-C2-O2 | 5.23 | 122.04 | 118.90 |
| 22 | 23S1 | 2435 | A | C8-N9-C4 | 5.23 | 107.89 | 105.80 |
| 22 | 23S1 | 675 | A | C4-C5-C6 | 5.22 | 119.61 | 117.00 |
| 22 | 23S1 | 1552 | A | C5-C6-N1 | 5.22 | 120.31 | 117.70 |
| 22 | 23S1 | 2800 | A | N3-C4-N9 | 5.22 | 131.58 | 127.40 |
| 1 | 16S1 | 60 | A | C8-N9-C4 | 5.22 | 107.89 | 105.80 |
| 1 | 16S1 | 155 | A | C8-N9-C4 | 5.22 | 107.89 | 105.80 |
| 1 | 16S1 | 784 | A | N9-C4-C5 | 5.22 | 107.89 | 105.80 |
| 1 | 16S1 | 864 | A | N9-C4-C5 | 5.22 | 107.89 | 105.80 |
| 1 | 16S1 | 978 | A | C4-C5-C6 | 5.22 | 119.61 | 117.00 |
| 22 | 23S1 | 201 | C | C6-N1-C2 | -5.22 | 118.21 | 120.30 |
| 22 | 23S1 | 432 | A | C8-N9-C4 | 5.22 | 107.89 | 105.80 |
| 22 | 23S1 | 685 | A | C4-C5-C6 | 5.22 | 119.61 | 117.00 |
| 22 | 23S1 | 896 | A | C8-N9-C4 | 5.22 | 107.89 | 105.80 |
| 22 | 23S1 | 1848 | A | N9-C4-C5 | 5.22 | 107.89 | 105.80 |
| 1 | 16S1 | 630 | A | C4-C5-N7 | -5.22 | 108.09 | 110.70 |
| 22 | 23S1 | 979 | A | C5-C6-N1 | 5.22 | 120.31 | 117.70 |
| 22 | 23S1 | 1586 | A | C5-C6-N1 | 5.22 | 120.31 | 117.70 |
| 22 | 23S1 | 1745 | A | C8-N9-C4 | 5.22 | 107.89 | 105.80 |
| 1 | 16S1 | 655 | A | C4-C5-N7 | -5.22 | 108.09 | 110.70 |
| 12 | S121 | 103 | ASP | CB-CG-OD1 | 5.22 | 123.00 | 118.30 |
| 22 | 23S1 | 270 | A | C5-C6-N1 | 5.22 | 120.31 | 117.70 |
| 22 | 23S1 | 309 | A | N9-C4-C5 | 5.22 | 107.89 | 105.80 |
| 22 | 23S1 | 547 | A | C4-C5-C6 | 5.22 | 119.61 | 117.00 |
| 22 | 23S1 | 838 | C | C6-N1-C2 | -5.22 | 118.21 | 120.30 |
| 22 | 23S1 | 1005 | C | N3-C2-O2 | -5.22 | 118.25 | 121.90 |
| 22 | 23S1 | 1312 | U | N3-C4-O4 | -5.22 | 115.75 | 119.40 |
| 22 | 23S1 | 2639 | A | C4-C5-C6 | 5.22 | 119.61 | 117.00 |
| 1 | 16S1 | 139 | A | C5-C6-N1 | 5.22 | 120.31 | 117.70 |
| 1 | 16S1 | 1130 | A | N3-C4-N9 | 5.22 | 131.57 | 127.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 16S1 | 1180 | A | C4-C5-N7 | -5.22 | 108.09 | 110.70 |
| 22 | 23S1 | 781 | A | C8-N9-C4 | 5.22 | 107.89 | 105.80 |
| 22 | 23S1 | 782 | A | C5-C6-N1 | 5.22 | 120.31 | 117.70 |
| 22 | 23S1 | 996 | A | C5-C6-N1 | 5.22 | 120.31 | 117.70 |
| 22 | 23S1 | 1253 | A | C5-N7-C8 | 5.22 | 106.51 | 103.90 |
| 1 | 16S1 | 1141 | C | C6-N1-C2 | -5.22 | 118.21 | 120.30 |
| 1 | 16S1 | 1306 | A | C5-C6-N1 | 5.22 | 120.31 | 117.70 |
| 22 | 23S1 | 348 | A | C4-C5-N7 | -5.22 | 108.09 | 110.70 |
| 22 | 23S1 | 497 | A | C4-C5-C6 | 5.22 | 119.61 | 117.00 |
| 22 | 23S1 | 941 | A | N9-C4-C5 | 5.22 | 107.89 | 105.80 |
| 22 | 23S1 | 2006 | C | C6-N1-C2 | -5.22 | 118.21 | 120.30 |
| 22 | 23S1 | 2615 | U | N1-C2-O2 | 5.22 | 126.45 | 122.80 |
| 1 | 16S1 | 205 | A | C4-C5-N7 | -5.21 | 108.09 | 110.70 |
| 1 | 16S1 | 790 | A | C5-C6-N1 | 5.21 | 120.31 | 117.70 |
| 22 | 23S1 | 330 | A | N9-C4-C5 | 5.21 | 107.89 | 105.80 |
| 22 | 23S1 | 896 | A | C4-C5-N7 | -5.21 | 108.09 | 110.70 |
| 22 | 23S1 | 1260 | A | C4-C5-N7 | -5.21 | 108.09 | 110.70 |
| 22 | 23S1 | 1609 | A | N9-C4-C5 | 5.21 | 107.89 | 105.80 |
| 1 | 16S1 | 488 | C | C2-N1-C1' | 5.21 | 124.53 | 118.80 |
| 22 | 23S1 | 118 | A | N9-C4-C5 | 5.21 | 107.89 | 105.80 |
| 22 | 23S1 | 550 | C | N1-C2-O2 | 5.21 | 122.03 | 118.90 |
| 22 | 23S1 | 1611 | C | N1-C2-O2 | 5.21 | 122.03 | 118.90 |
| 1 | 16S1 | 1225 | A | C4-C5-N7 | -5.21 | 108.09 | 110.70 |
| 9 | S091 | 63 | LEU | CA-CB-CG | 5.21 | 127.29 | 115.30 |
| 22 | 23S1 | 217 | A | C8-N9-C4 | 5.21 | 107.89 | 105.80 |
| 22 | 23S1 | 265 | A | N9-C4-C5 | 5.21 | 107.89 | 105.80 |
| 22 | 23S1 | 310 | A | N3-C4-N9 | 5.21 | 131.57 | 127.40 |
| 22 | 23S1 | 1786 | A | C5-C6-N1 | 5.21 | 120.31 | 117.70 |
| 22 | 23S1 | 2335 | A | C8-N9-C4 | 5.21 | 107.89 | 105.80 |
| 22 | 23S1 | 2879 | A | C8-N9-C4 | 5.21 | 107.89 | 105.80 |
| 22 | 23S1 | 756 | A | C4-C5-N7 | -5.21 | 108.09 | 110.70 |
| 22 | 23S1 | 840 | C | C6-N1-C2 | -5.21 | 118.22 | 120.30 |
| 22 | 23S1 | 1635 | A | C4-C5-N7 | -5.21 | 108.09 | 110.70 |
| 22 | 23S1 | 1890 | A | C4-C5-C6 | 5.21 | 119.61 | 117.00 |
| 1 | 16S1 | 336 | A | C5-C6-N1 | 5.21 | 120.30 | 117.70 |
| 1 | 16S1 | 487 | A | C5-C6-N1 | 5.21 | 120.30 | 117.70 |
| 1 | 16S1 | 676 | A | N9-C4-C5 | 5.21 | 107.88 | 105.80 |
| 1 | 16S1 | 1092 | A | C4-C5-C6 | 5.21 | 119.61 | 117.00 |
| 1 | 16S1 | 1287 | A | N9-C4-C5 | 5.21 | 107.88 | 105.80 |
| 22 | 23S1 | 49 | A | C8-N9-C4 | 5.21 | 107.88 | 105.80 |
| 22 | 23S1 | 1787 | A | N9-C4-C5 | 5.21 | 107.88 | 105.80 |
| 22 | 23S1 | 1960 | A | C4-C5-N7 | -5.21 | 108.10 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 16S1 | 704 | A | C4-C5-N7 | -5.21 | 108.10 | 110.70 |
| 1 | 16S1 | 1228 | C | C6-N1-C2 | -5.21 | 118.22 | 120.30 |
| 22 | 23S1 | 481 | G | O4'-C1'-N9 | 5.21 | 112.37 | 108.20 |
| 22 | 23S1 | 676 | A | C8-N9-C4 | 5.21 | 107.88 | 105.80 |
| 22 | 23S1 | 1367 | A | N9-C4-C5 | 5.21 | 107.88 | 105.80 |
| 22 | 23S1 | 1634 | A | C4-C5-C6 | 5.21 | 119.60 | 117.00 |
| 22 | 23S1 | 1678 | A | N3-C4-N9 | 5.21 | 131.56 | 127.40 |
| 22 | 23S1 | 2020 | A | N9-C4-C5 | 5.21 | 107.88 | 105.80 |
| 22 | 23S1 | 2740 | A | C4-C5-N7 | -5.21 | 108.10 | 110.70 |
| 1 | 16S1 | 1082 | A | C4-C5-N7 | -5.21 | 108.10 | 110.70 |
| 22 | 23S1 | 322 | A | N3-C4-N9 | 5.21 | 131.56 | 127.40 |
| 22 | 23S1 | 668 | A | N9-C4-C5 | 5.21 | 107.88 | 105.80 |
| 22 | 23S1 | 1142 | A | C8-N9-C4 | 5.21 | 107.88 | 105.80 |
| 1 | 16S1 | 498 | A | C4-C5-N7 | -5.20 | 108.10 | 110.70 |
| 1 | 16S1 | 777 | A | C4-C5-N7 | -5.20 | 108.10 | 110.70 |
| 1 | 16S1 | 1145 | A | N9-C4-C5 | 5.20 | 107.88 | 105.80 |
| 22 | 23S1 | 915 | C | N3-C2-O2 | -5.20 | 118.26 | 121.90 |
| 22 | 23S1 | 2736 | A | C5-C6-N1 | 5.20 | 120.30 | 117.70 |
| 1 | 16S1 | 109 | A | C8-N9-C4 | 5.20 | 107.88 | 105.80 |
| 22 | 23S1 | 203 | A | N9-C4-C5 | 5.20 | 107.88 | 105.80 |
| 1 | 16S1 | 19 | A | C5-C6-N1 | 5.20 | 120.30 | 117.70 |
| 1 | 16S1 | 1434 | A | N9-C4-C5 | 5.20 | 107.88 | 105.80 |
| 22 | 23S1 | 1039 | A | C8-N9-C4 | 5.20 | 107.88 | 105.80 |
| 22 | 23S1 | 1194 | A | C8-N9-C4 | 5.20 | 107.88 | 105.80 |
| 22 | 23S1 | 1387 | A | N9-C4-C5 | 5.20 | 107.88 | 105.80 |
| 22 | 23S1 | 2009 | A | N9-C4-C5 | 5.20 | 107.88 | 105.80 |
| 1 | 16S1 | 197 | A | N9-C4-C5 | 5.20 | 107.88 | 105.80 |
| 1 | 16S1 | 946 | A | N9-C4-C5 | 5.20 | 107.88 | 105.80 |
| 21 | S211 | 21 | ARG | NE-CZ-NH1 | 5.20 | 122.90 | 120.30 |
| 22 | 23S1 | 706 | A | C4-C5-C6 | 5.20 | 119.60 | 117.00 |
| 22 | 23S1 | 959 | A | N9-C4-C5 | 5.20 | 107.88 | 105.80 |
| 22 | 23S1 | 1144 | A | N9-C4-C5 | 5.20 | 107.88 | 105.80 |
| 22 | 23S1 | 1304 | A | N3-C4-N9 | 5.20 | 131.56 | 127.40 |
| 22 | 23S1 | 1572 | A | C5-C6-N1 | 5.20 | 120.30 | 117.70 |
| 22 | 23S1 | 2388 | A | N9-C4-C5 | 5.20 | 107.88 | 105.80 |
| 1 | 16S1 | 409 | U | N3-C2-O2 | -5.20 | 118.56 | 122.20 |
| 1 | 16S1 | 937 | A | C4-C5-N7 | -5.20 | 108.10 | 110.70 |
| 22 | 23S1 | 322 | A | C4-C5-C6 | 5.20 | 119.60 | 117.00 |
| 22 | 23S1 | 2781 | A | N3-C4-N9 | 5.20 | 131.56 | 127.40 |
| 1 | 16S1 | 510 | A | C8-N9-C4 | 5.20 | 107.88 | 105.80 |
| 1 | 16S1 | 1081 | A | N9-C4-C5 | 5.20 | 107.88 | 105.80 |
| 22 | 23S1 | 899 | A | C5-C6-N1 | 5.20 | 120.30 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22 | 23S1 | 1088 | A | C4-C5-N7 | -5.20 | 108.10 | 110.70 |
| 1 | 16S1 | 958 | A | C8-N9-C4 | 5.19 | 107.88 | 105.80 |
| 22 | 23S1 | 282 | A | C8-N9-C4 | 5.19 | 107.88 | 105.80 |
| 22 | 23S1 | 1244 | A | C5-C6-N1 | 5.19 | 120.30 | 117.70 |
| 22 | 23S1 | 1569 | A | N3-C4-N9 | 5.19 | 131.56 | 127.40 |
| 22 | 23S1 | 2882 | A | N9-C4-C5 | 5.19 | 107.88 | 105.80 |
| 1 | 16S1 | 129 | A | C4-C5-N7 | -5.19 | 108.10 | 110.70 |
| 1 | 16S1 | 1493 | A | N3-C4-N9 | 5.19 | 131.56 | 127.40 |
| 22 | 23S1 | 332 | A | C5-C6-N1 | 5.19 | 120.30 | 117.70 |
| 22 | 23S1 | 457 | A | C4-C5-N7 | -5.19 | 108.10 | 110.70 |
| 22 | 23S1 | 582 | A | N9-C4-C5 | 5.19 | 107.88 | 105.80 |
| 22 | 23S1 | 1885 | A | C4-C5-C6 | 5.19 | 119.60 | 117.00 |
| 1 | 16S1 | 1155 | A | N9-C4-C5 | 5.19 | 107.88 | 105.80 |
| 1 | 16S1 | 1368 | A | C4-C5-N7 | -5.19 | 108.11 | 110.70 |
| 22 | 23S1 | 63 | A | C5-C6-N1 | 5.19 | 120.30 | 117.70 |
| 22 | 23S1 | 1073 | A | N9-C4-C5 | 5.19 | 107.88 | 105.80 |
| 22 | 23S1 | 1384 | A | C4-C5-C6 | 5.19 | 119.59 | 117.00 |
| 22 | 23S1 | 2766 | A | C5-N7-C8 | 5.19 | 106.50 | 103.90 |
| 1 | 16S1 | 4 | U | O4'-C1'-N1 | 5.19 | 112.35 | 108.20 |
| 1 | 16S1 | 1117 | A | C4-C5-C6 | 5.19 | 119.59 | 117.00 |
| 22 | 23S1 | 2100 | G | C8-N9-C1' | -5.19 | 120.25 | 127.00 |
| 1 | 16S1 | 263 | A | C5-C6-N1 | 5.19 | 120.29 | 117.70 |
| 22 | 23S1 | 2278 | A | C4-C5-N7 | -5.19 | 108.11 | 110.70 |
| 22 | 23S1 | 2572 | A | C5-C6-N1 | 5.19 | 120.29 | 117.70 |
| 22 | 23S1 | 2850 | A | C4-C5-N7 | -5.19 | 108.11 | 110.70 |
| 55 | PTR1 | 23 | A | C4-C5-C6 | 5.19 | 119.59 | 117.00 |
| 1 | 16S1 | 889 | A | C4-C5-N7 | -5.19 | 108.11 | 110.70 |
| 22 | 23S1 | 231 | A | C8-N9-C4 | 5.19 | 107.88 | 105.80 |
| 22 | 23S1 | 671 | C | N1-C2-O2 | 5.19 | 122.01 | 118.90 |
| 1 | 16S1 | 197 | A | N3-C4-N9 | 5.18 | 131.55 | 127.40 |
| 1 | 16S1 | 546 | A | C5-C6-N1 | 5.18 | 120.29 | 117.70 |
| 1 | 16S1 | 547 | A | N9-C4-C5 | 5.18 | 107.87 | 105.80 |
| 1 | 16S1 | 1492 | A | C4-C5-N7 | -5.18 | 108.11 | 110.70 |
| 1 | 16S1 | 1500 | A | C6-N1-C2 | 5.18 | 121.71 | 118.60 |
| 22 | 23S1 | 330 | A | C5-C6-N1 | 5.18 | 120.29 | 117.70 |
| 22 | 23S1 | 1010 | A | N9-C4-C5 | 5.18 | 107.87 | 105.80 |
| 22 | 23S1 | 1272 | A | C4-C5-C6 | 5.18 | 119.59 | 117.00 |
| 22 | 23S1 | 2741 | A | C4-C5-C6 | 5.18 | 119.59 | 117.00 |
| 23 | 05S1 | 104 | A | N9-C4-C5 | 5.18 | 107.87 | 105.80 |
| 1 | 16S1 | 430 | A | C8-N9-C4 | 5.18 | 107.87 | 105.80 |
| 22 | 23S1 | 2274 | A | N9-C4-C5 | 5.18 | 107.87 | 105.80 |
| 22 | 23S1 | 2778 | A | C4-C5-N7 | -5.18 | 108.11 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23 | 05S1 | 53 | A | C4-C5-N7 | -5.18 | 108.11 | 110.70 |
| 22 | 23S1 | 111 | A | N9-C4-C5 | 5.18 | 107.87 | 105.80 |
| 1 | 16S1 | 532 | A | C8-N9-C4 | 5.18 | 107.87 | 105.80 |
| 22 | 23S1 | 118 | A | C4-C5-N7 | -5.18 | 108.11 | 110.70 |
| 22 | 23S1 | 526 | A | N9-C4-C5 | 5.18 | 107.87 | 105.80 |
| 22 | 23S1 | 784 | G | C3'-C2'-C1' | 5.18 | 105.64 | 101.50 |
| 22 | 23S1 | 1077 | A | N9-C4-C5 | 5.18 | 107.87 | 105.80 |
| 1 | 16S1 | 414 | A | C4-C5-C6 | 5.18 | 119.59 | 117.00 |
| 1 | 16S1 | 1019 | A | C5-C6-N1 | 5.18 | 120.29 | 117.70 |
| 22 | 23S1 | 226 | A | N9-C4-C5 | 5.18 | 107.87 | 105.80 |
| 22 | 23S1 | 792 | A | C5-C6-N1 | 5.18 | 120.29 | 117.70 |
| 22 | 23S1 | 1073 | A | C4-C5-N7 | -5.18 | 108.11 | 110.70 |
| 22 | 23S1 | 2100 | G | N3-C4-C5 | -5.18 | 126.01 | 128.60 |
| 1 | 16S1 | 238 | A | C4-C5-N7 | -5.17 | 108.11 | 110.70 |
| 1 | 16S1 | 892 | A | C4-C5-N7 | -5.17 | 108.11 | 110.70 |
| 22 | 23S1 | 702 | U | C2-N1-C1' | 5.17 | 123.91 | 117.70 |
| 22 | 23S1 | 1077 | A | N3-C4-N9 | 5.17 | 131.54 | 127.40 |
| 22 | 23S1 | 1776 | G | C4-N9-C1' | 5.17 | 133.23 | 126.50 |
| 22 | 23S1 | 2274 | A | C6-N1-C2 | 5.17 | 121.70 | 118.60 |
| 22 | 23S1 | 2531 | A | C4-C5-N7 | -5.17 | 108.11 | 110.70 |
| 22 | 23S1 | 2886 | A | C5-C6-N1 | 5.17 | 120.29 | 117.70 |
| 22 | 23S1 | 76 | C | N1-C2-O2 | 5.17 | 122.00 | 118.90 |
| 22 | 23S1 | 996 | A | N9-C4-C5 | 5.17 | 107.87 | 105.80 |
| 23 | 05S1 | 39 | A | C5-C6-N1 | 5.17 | 120.29 | 117.70 |
| 1 | 16S1 | 572 | A | C4-C5-N7 | -5.17 | 108.11 | 110.70 |
| 1 | 16S1 | 815 | A | N9-C4-C5 | 5.17 | 107.87 | 105.80 |
| 22 | 23S1 | 28 | A | C5-C6-N1 | 5.17 | 120.29 | 117.70 |
| 22 | 23S1 | 522 | A | C8-N9-C4 | 5.17 | 107.87 | 105.80 |
| 22 | 23S1 | 927 | A | C8-N9-C4 | 5.17 | 107.87 | 105.80 |
| 22 | 23S1 | 1583 | A | C5-C6-N1 | 5.17 | 120.29 | 117.70 |
| 22 | 23S1 | 1749 | A | C8-N9-C4 | 5.17 | 107.87 | 105.80 |
| 22 | 23S1 | 2241 | A | C5-C6-N1 | 5.17 | 120.29 | 117.70 |
| 22 | 23S1 | 2376 | A | C4-C5-N7 | -5.17 | 108.11 | 110.70 |
| 1 | 16S1 | 1004 | A | C8-N9-C4 | 5.17 | 107.87 | 105.80 |
| 1 | 16S1 | 1319 | A | N9-C4-C5 | 5.17 | 107.87 | 105.80 |
| 22 | 23S1 | 981 | A | N9-C4-C5 | 5.17 | 107.87 | 105.80 |
| 22 | 23S1 | 1134 | A | C5-C6-N1 | 5.17 | 120.28 | 117.70 |
| 22 | 23S1 | 1783 | A | C8-N9-C4 | 5.17 | 107.87 | 105.80 |
| 22 | 23S1 | 2733 | A | C8-N9-C4 | 5.17 | 107.87 | 105.80 |
| 23 | 05S1 | 53 | A | N3-C4-N9 | 5.17 | 131.53 | 127.40 |
| 1 | 16S1 | 7 | A | N9-C4-C5 | 5.17 | 107.87 | 105.80 |
| 1 | 16S1 | 409 | U | C2-N1-C1' | 5.17 | 123.90 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 16S1 | 459 | A | C5-C6-N1 | 5.17 | 120.28 | 117.70 |
| 1 | 16S1 | 676 | A | C8-N9-C4 | 5.17 | 107.87 | 105.80 |
| 1 | 16S1 | 729 | A | C5-C6-N1 | 5.17 | 120.28 | 117.70 |
| 1 | 16S1 | 782 | A | C5-C6-N1 | 5.17 | 120.28 | 117.70 |
| 22 | 23S1 | 278 | A | N9-C4-C5 | 5.17 | 107.87 | 105.80 |
| 22 | 23S1 | 753 | A | N9-C4-C5 | 5.17 | 107.87 | 105.80 |
| 22 | 23S1 | 1383 | A | C4-C5-N7 | -5.17 | 108.12 | 110.70 |
| 22 | 23S1 | 1403 | A | N9-C4-C5 | 5.17 | 107.87 | 105.80 |
| 22 | 23S1 | 1632 | A | C5-C6-N1 | 5.17 | 120.28 | 117.70 |
| 22 | 23S1 | 2482 | A | C8-N9-C4 | 5.17 | 107.87 | 105.80 |
| 22 | 23S1 | 2682 | A | C4-C5-C6 | 5.17 | 119.58 | 117.00 |
| 23 | 05S1 | 94 | A | C8-N9-C4 | 5.17 | 107.87 | 105.80 |
| 1 | 16S1 | 1368 | A | C5-C6-N1 | 5.17 | 120.28 | 117.70 |
| 22 | 23S1 | 216 | A | C4-C5-C6 | 5.17 | 119.58 | 117.00 |
| 1 | 16S1 | 535 | A | C4-C5-N7 | -5.16 | 108.12 | 110.70 |
| 1 | 16S1 | 781 | A | C4-C5-N7 | -5.16 | 108.12 | 110.70 |
| 1 | 16S1 | 1180 | A | C5-C6-N1 | 5.16 | 120.28 | 117.70 |
| 22 | 23S1 | 146 | A | C4-C5-N7 | -5.16 | 108.12 | 110.70 |
| 22 | 23S1 | 172 | A | C4-C5-N7 | -5.16 | 108.12 | 110.70 |
| 22 | 23S1 | 2632 | A | C4-C5-C6 | 5.16 | 119.58 | 117.00 |
| 1 | 16S1 | 303 | A | C5-C6-N1 | 5.16 | 120.28 | 117.70 |
| 22 | 23S1 | 1057 | A | C4-C5-N7 | -5.16 | 108.12 | 110.70 |
| 22 | 23S1 | 2577 | A | N9-C4-C5 | 5.16 | 107.86 | 105.80 |
| 1 | 16S1 | 630 | A | N9-C4-C5 | 5.16 | 107.86 | 105.80 |
| 1 | 16S1 | 695 | A | N9-C4-C5 | 5.16 | 107.86 | 105.80 |
| 1 | 16S1 | 949 | A | C5-C6-N1 | 5.16 | 120.28 | 117.70 |
| 22 | 23S1 | 983 | A | C4-C5-C6 | 5.16 | 119.58 | 117.00 |
| 22 | 23S1 | 1779 | U | N1-C2-O2 | 5.16 | 126.41 | 122.80 |
| 22 | 23S1 | 2381 | A | N9-C4-C5 | 5.16 | 107.86 | 105.80 |
| 1 | 16S1 | 119 | A | C5-C6-N1 | 5.16 | 120.28 | 117.70 |
| 1 | 16S1 | 595 | A | N9-C4-C5 | 5.16 | 107.86 | 105.80 |
| 22 | 23S1 | 2134 | A | C5-C6-N1 | 5.16 | 120.28 | 117.70 |
| 1 | 16S1 | 172 | A | C8-N9-C4 | 5.16 | 107.86 | 105.80 |
| 1 | 16S1 | 579 | A | C5-C6-N1 | 5.16 | 120.28 | 117.70 |
| 22 | 23S1 | 1749 | A | N9-C4-C5 | 5.16 | 107.86 | 105.80 |
| 1 | 16S1 | 7 | A | C4-C5-N7 | -5.16 | 108.12 | 110.70 |
| 1 | 16S1 | 630 | A | C8-N9-C4 | 5.16 | 107.86 | 105.80 |
| 22 | 23S1 | 482 | A | C8-N9-C4 | 5.16 | 107.86 | 105.80 |
| 22 | 23S1 | 1327 | A | C5-C6-N1 | 5.16 | 120.28 | 117.70 |
| 22 | 23S1 | 1805 | A | C5-C6-N1 | 5.16 | 120.28 | 117.70 |
| 22 | 23S1 | 2070 | A | C4-C5-N7 | -5.16 | 108.12 | 110.70 |
| 22 | 23S1 | 2366 | A | C4-C5-N7 | -5.16 | 108.12 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 2406 | A | C4-C5-N7 | -5.16 | 108.12 | 110.70 |
| 22 | 23S1 | 654 | A | C5-C6-N1 | 5.15 | 120.28 | 117.70 |
| 22 | 23S1 | 2377 | A | C5-C6-N1 | 5.15 | 120.28 | 117.70 |
| 1 | 16S1 | 253 | A | N9-C4-C5 | 5.15 | 107.86 | 105.80 |
| 1 | 16S1 | 300 | A | N7-C8-N9 | -5.15 | 111.22 | 113.80 |
| 1 | 16S1 | 456 | A | N3-C4-N9 | 5.15 | 131.52 | 127.40 |
| 22 | 23S1 | 2328 | A | C5-C6-N1 | 5.15 | 120.28 | 117.70 |
| 22 | 23S1 | 2856 | A | N9-C4-C5 | 5.15 | 107.86 | 105.80 |
| 1 | 16S1 | 715 | A | C4-C5-C6 | 5.15 | 119.58 | 117.00 |
| 1 | 16S1 | 749 | A | C4-C5-C6 | 5.15 | 119.58 | 117.00 |
| 22 | 23S1 | 478 | A | N9-C4-C5 | 5.15 | 107.86 | 105.80 |
| 22 | 23S1 | 959 | A | C4-C5-N7 | -5.15 | 108.12 | 110.70 |
| 22 | 23S1 | 1773 | A | C4-C5-N7 | -5.15 | 108.12 | 110.70 |
| 22 | 23S1 | 1952 | A | C4-C5-N7 | -5.15 | 108.12 | 110.70 |
| 22 | 23S1 | 878 | A | C4-C5-C6 | 5.15 | 119.58 | 117.00 |
| 22 | 23S1 | 1155 | A | C4-C5-C6 | 5.15 | 119.58 | 117.00 |
| 1 | 16S1 | 746 | A | C4-C5-N7 | -5.15 | 108.13 | 110.70 |
| 1 | 16S1 | 857 | C | N3-C2-O2 | -5.15 | 118.30 | 121.90 |
| 1 | 16S1 | 865 | A | N9-C4-C5 | 5.15 | 107.86 | 105.80 |
| 22 | 23S1 | 666 | A | C5-C6-N1 | 5.15 | 120.27 | 117.70 |
| 22 | 23S1 | 1204 | A | N3-C4-N9 | 5.15 | 131.52 | 127.40 |
| 22 | 23S1 | 1802 | A | C8-N9-C4 | 5.15 | 107.86 | 105.80 |
| 22 | 23S1 | 2475 | C | C6-N1-C2 | -5.15 | 118.24 | 120.30 |
| 1 | 16S1 | 1456 | A | C4-C5-N7 | -5.15 | 108.13 | 110.70 |
| 6 | S061 | 72 | ASP | CB-CG-OD1 | 5.15 | 122.93 | 118.30 |
| 22 | 23S1 | 497 | A | N3-C4-N9 | 5.15 | 131.52 | 127.40 |
| 22 | 23S1 | 905 | A | N9-C4-C5 | 5.15 | 107.86 | 105.80 |
| 22 | 23S1 | 990 | A | C5-C6-N1 | 5.15 | 120.27 | 117.70 |
| 1 | 16S1 | 192 | A | C4-C5-N7 | -5.14 | 108.13 | 110.70 |
| 1 | 16S1 | 533 | A | N9-C4-C5 | 5.14 | 107.86 | 105.80 |
| 1 | 16S1 | 1246 | A | C4-C5-N7 | -5.14 | 108.13 | 110.70 |
| 22 | 23S1 | 990 | A | N9-C4-C5 | 5.14 | 107.86 | 105.80 |
| 22 | 23S1 | 1583 | A | N3-C4-N9 | 5.14 | 131.52 | 127.40 |
| 22 | 23S1 | 1808 | A | N3-C4-N9 | 5.14 | 131.51 | 127.40 |
| 1 | 16S1 | 906 | A | N9-C4-C5 | 5.14 | 107.86 | 105.80 |
| 22 | 23S1 | 2358 | A | N9-C4-C5 | 5.14 | 107.86 | 105.80 |
| 22 | 23S1 | 2679 | A | C4-C5-N7 | -5.14 | 108.13 | 110.70 |
| 22 | 23S1 | 2738 | A | N3-C4-N9 | 5.14 | 131.51 | 127.40 |
| 22 | 23S1 | 2749 | A | C5-C6-N1 | 5.14 | 120.27 | 117.70 |
| 1 | 16S1 | 309 | A | N9-C4-C5 | 5.14 | 107.86 | 105.80 |
| 1 | 16S1 | 825 | A | N9-C4-C5 | 5.14 | 107.86 | 105.80 |
| 22 | 23S1 | 1001 | A | C8-N9-C4 | 5.14 | 107.86 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 2750 | A | C5-C6-N1 | 5.14 | 120.27 | 117.70 |
| 1 | 16S1 | 10 | A | C4-C5-N7 | -5.14 | 108.13 | 110.70 |
| 1 | 16S1 | 160 | A | N9-C4-C5 | 5.14 | 107.86 | 105.80 |
| 1 | 16S1 | 560 | A | C4-C5-N7 | -5.14 | 108.13 | 110.70 |
| 1 | 16S1 | 1150 | A | C4-C5-N7 | -5.14 | 108.13 | 110.70 |
| 22 | 23S1 | 199 | A | C5-C6-N1 | 5.14 | 120.27 | 117.70 |
| 22 | 23S1 | 497 | A | C4-C5-N7 | -5.14 | 108.13 | 110.70 |
| 22 | 23S1 | 609 | A | C5-C6-N1 | 5.14 | 120.27 | 117.70 |
| 22 | 23S1 | 1744 | A | C8-N9-C4 | 5.14 | 107.86 | 105.80 |
| 22 | 23S1 | 2033 | A | N3-C4-N9 | 5.14 | 131.51 | 127.40 |
| 22 | 23S1 | 1194 | A | C4-C5-C6 | 5.14 | 119.57 | 117.00 |
| 22 | 23S1 | 1439 | A | C4-C5-C6 | 5.14 | 119.57 | 117.00 |
| 22 | 23S1 | 1670 | C | N3-C2-O2 | -5.14 | 118.30 | 121.90 |
| 1 | 16S1 | 1395 | C | N1-C2-O2 | 5.14 | 121.98 | 118.90 |
| 22 | 23S1 | 21 | A | C4-C5-N7 | -5.14 | 108.13 | 110.70 |
| 22 | 23S1 | 160 | A | C4-C5-C6 | 5.14 | 119.57 | 117.00 |
| 22 | 23S1 | 165 | A | N3-C4-N9 | 5.14 | 131.51 | 127.40 |
| 22 | 23S1 | 1342 | A | C4-C5-N7 | -5.14 | 108.13 | 110.70 |
| 22 | 23S1 | 1420 | A | C4-C5-N7 | -5.14 | 108.13 | 110.70 |
| 22 | 23S1 | 1532 | A | C5-C6-N1 | 5.14 | 120.27 | 117.70 |
| 22 | 23S1 | 2071 | A | C8-N9-C4 | 5.14 | 107.86 | 105.80 |
| 22 | 23S1 | 2366 | A | C8-N9-C4 | 5.14 | 107.86 | 105.80 |
| 23 | 05S1 | 52 | A | C4-C5-N7 | -5.14 | 108.13 | 110.70 |
| 1 | 16S1 | 325 | A | C5-C6-N1 | 5.13 | 120.27 | 117.70 |
| 1 | 16S1 | 681 | A | N9-C4-C5 | 5.13 | 107.85 | 105.80 |
| 1 | 16S1 | 1042 | A | C5-C6-N1 | 5.13 | 120.27 | 117.70 |
| 22 | 23S1 | 91 | A | N3-C4-N9 | 5.13 | 131.51 | 127.40 |
| 1 | 16S1 | 50 | A | C5-C6-N1 | 5.13 | 120.27 | 117.70 |
| 1 | 16S1 | 574 | A | C4-C5-C6 | 5.13 | 119.57 | 117.00 |
| 22 | 23S1 | 1952 | A | C4-C5-C6 | 5.13 | 119.57 | 117.00 |
| 22 | 23S1 | 2260 | C | N3-C2-O2 | -5.13 | 118.31 | 121.90 |
| 22 | 23S1 | 2797 | U | N3-C2-O2 | -5.13 | 118.61 | 122.20 |
| 22 | 23S1 | 1664 | A | N9-C4-C5 | 5.13 | 107.85 | 105.80 |
| 22 | 23S1 | 1789 | A | C8-N9-C4 | 5.13 | 107.85 | 105.80 |
| 55 | PTR1 | 59 | A | N9-C4-C5 | 5.13 | 107.85 | 105.80 |
| 1 | 16S1 | 1016 | A | C5-C6-N1 | 5.13 | 120.27 | 117.70 |
| 1 | 16S1 | 1035 | A | C8-N9-C4 | 5.13 | 107.85 | 105.80 |
| 55 | PTR1 | 73 | A | C5-C6-N1 | 5.13 | 120.27 | 117.70 |
| 1 | 16S1 | 1430 | A | C5-C6-N1 | 5.13 | 120.26 | 117.70 |
| 22 | 23S1 | 547 | A | C4-C5-N7 | -5.13 | 108.14 | 110.70 |
| 22 | 23S1 | 918 | A | N9-C4-C5 | 5.13 | 107.85 | 105.80 |
| 22 | 23S1 | 1640 | A | C4-C5-C6 | 5.13 | 119.56 | 117.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 1876 | A | N9-C4-C5 | 5.13 | 107.85 | 105.80 |
| 1 | 16S1 | 197 | A | C4-C5-C6 | 5.13 | 119.56 | 117.00 |
| 1 | 16S1 | 468 | A | C4-C5-C6 | 5.13 | 119.56 | 117.00 |
| 22 | 23S1 | 1439 | A | C5-C6-N1 | 5.13 | 120.26 | 117.70 |
| 22 | 23S1 | 2154 | A | N9-C4-C5 | 5.13 | 107.85 | 105.80 |
| 1 | 16S1 | 1465 | A | C4-C5-N7 | -5.12 | 108.14 | 110.70 |
| 22 | 23S1 | 352 | A | C4-C5-N7 | -5.12 | 108.14 | 110.70 |
| 22 | 23S1 | 941 | A | C8-N9-C4 | 5.12 | 107.85 | 105.80 |
| 1 | 16S1 | 766 | A | C5-C6-N1 | 5.12 | 120.26 | 117.70 |
| 1 | 16S1 | 1044 | A | C8-N9-C4 | 5.12 | 107.85 | 105.80 |
| 1 | 16S1 | 1318 | A | C5-C6-N1 | 5.12 | 120.26 | 117.70 |
| 1 | 16S1 | 1502 | A | C4-C5-C6 | 5.12 | 119.56 | 117.00 |
| 22 | 23S1 | 270 | A | N9-C4-C5 | 5.12 | 107.85 | 105.80 |
| 22 | 23S1 | 677 | A | C8-N9-C4 | 5.12 | 107.85 | 105.80 |
| 22 | 23S1 | 877 | A | C5-C6-N1 | 5.12 | 120.26 | 117.70 |
| 22 | 23S1 | 988 | A | C4-C5-N7 | -5.12 | 108.14 | 110.70 |
| 22 | 23S1 | 1664 | A | C4-C5-N7 | -5.12 | 108.14 | 110.70 |
| 22 | 23S1 | 1815 | A | C5-C6-N1 | 5.12 | 120.26 | 117.70 |
| 22 | 23S1 | 2733 | A | C5-C6-N1 | 5.12 | 120.26 | 117.70 |
| 1 | 16S1 | 60 | A | N3-C4-N9 | 5.12 | 131.50 | 127.40 |
| 1 | 16S1 | 482 | A | C5-C6-N1 | 5.12 | 120.26 | 117.70 |
| 1 | 16S1 | 1201 | A | C8-N9-C4 | 5.12 | 107.85 | 105.80 |
| 1 | 16S1 | 1201 | A | N9-C4-C5 | 5.12 | 107.85 | 105.80 |
| 22 | 23S1 | 563 | A | C5-C6-N1 | 5.12 | 120.26 | 117.70 |
| 22 | 23S1 | 1552 | A | N9-C4-C5 | 5.12 | 107.85 | 105.80 |
| 22 | 23S1 | 1610 | A | N3-C4-N9 | 5.12 | 131.50 | 127.40 |
| 22 | 23S1 | 1890 | A | N3-C4-N9 | 5.12 | 131.50 | 127.40 |
| 22 | 23S1 | 1991 | U | N3-C2-O2 | -5.12 | 118.61 | 122.20 |
| 1 | 16S1 | 101 | A | N9-C4-C5 | 5.12 | 107.85 | 105.80 |
| 22 | 23S1 | 1787 | A | C5-C6-N1 | 5.12 | 120.26 | 117.70 |
| 22 | 23S1 | 2369 | A | C5-C6-N1 | 5.12 | 120.26 | 117.70 |
| 1 | 16S1 | 1080 | A | N9-C4-C5 | 5.12 | 107.85 | 105.80 |
| 1 | 16S1 | 1324 | A | N9-C4-C5 | 5.12 | 107.85 | 105.80 |
| 22 | 23S1 | 21 | A | C8-N9-C4 | 5.12 | 107.85 | 105.80 |
| 22 | 23S1 | 176 | A | C4-C5-N7 | -5.12 | 108.14 | 110.70 |
| 22 | 23S1 | 1244 | A | C4-C5-N7 | -5.12 | 108.14 | 110.70 |
| 22 | 23S1 | 1427 | A | N3-C4-N9 | 5.12 | 131.50 | 127.40 |
| 22 | 23S1 | 2173 | A | C4-C5-N7 | -5.12 | 108.14 | 110.70 |
| 22 | 23S1 | 2882 | A | C4-C5-C6 | 5.12 | 119.56 | 117.00 |
| 1 | 16S1 | 1254 | A | N9-C4-C5 | 5.12 | 107.85 | 105.80 |
| 22 | 23S1 | 1698 | A | C5-C6-N1 | 5.12 | 120.26 | 117.70 |
| 1 | 16S1 | 539 | A | C5-C6-N1 | 5.12 | 120.26 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22 | 23S1 | 439 | A | N9-C4-C5 | 5.12 | 107.85 | 105.80 |
| 22 | 23S1 | 644 | A | C8-N9-C4 | 5.12 | 107.85 | 105.80 |
| 22 | 23S1 | 1876 | A | C4-C5-N7 | -5.12 | 108.14 | 110.70 |
| 22 | 23S1 | 2433 | A | C8-N9-C4 | 5.12 | 107.85 | 105.80 |
| 22 | 23S1 | 2758 | A | C4-C5-N7 | -5.12 | 108.14 | 110.70 |
| 22 | 23S1 | 374 | A | C5-C6-N1 | 5.11 | 120.26 | 117.70 |
| 22 | 23S1 | 548 | G | N3-C4-C5 | -5.11 | 126.04 | 128.60 |
| 22 | 23S1 | 909 | A | C4-C5-C6 | 5.11 | 119.56 | 117.00 |
| 22 | 23S1 | 1608 | A | C5-C6-N1 | 5.11 | 120.26 | 117.70 |
| 22 | 23S1 | 2749 | A | N9-C4-C5 | 5.11 | 107.84 | 105.80 |
| 1 | 16S1 | 486 | U | N3-C2-O2 | -5.11 | 118.62 | 122.20 |
| 1 | 16S1 | 768 | A | C5-C6-N1 | 5.11 | 120.26 | 117.70 |
| 1 | 16S1 | 937 | A | C8-N9-C4 | 5.11 | 107.84 | 105.80 |
| 22 | 23S1 | 2657 | A | C6-N1-C2 | 5.11 | 121.67 | 118.60 |
| 1 | 16S1 | 243 | A | C4-C5-N7 | -5.11 | 108.14 | 110.70 |
| 1 | 16S1 | 488 | C | C6-N1-C2 | -5.11 | 118.26 | 120.30 |
| 1 | 16S1 | 1331 | G | O4'-C1'-N9 | 5.11 | 112.29 | 108.20 |
| 1 | 16S1 | 1428 | A | C8-N9-C4 | 5.11 | 107.84 | 105.80 |
| 22 | 23S1 | 345 | A | C4-C5-N7 | -5.11 | 108.14 | 110.70 |
| 22 | 23S1 | 391 | A | C5-C6-N1 | 5.11 | 120.25 | 117.70 |
| 22 | 23S1 | 1328 | A | C8-N9-C4 | 5.11 | 107.84 | 105.80 |
| 22 | 23S1 | 1494 | A | N3-C4-N9 | 5.11 | 131.49 | 127.40 |
| 22 | 23S1 | 1759 | A | C8-N9-C4 | 5.11 | 107.84 | 105.80 |
| 1 | 16S1 | 706 | A | C8-N9-C4 | 5.11 | 107.84 | 105.80 |
| 1 | 16S1 | 1410 | A | C8-N9-C4 | 5.11 | 107.84 | 105.80 |
| 22 | 23S1 | 1089 | A | N9-C4-C5 | 5.11 | 107.84 | 105.80 |
| 22 | 23S1 | 2322 | A | C5-C6-N1 | 5.11 | 120.25 | 117.70 |
| 22 | 23S1 | 2851 | A | C4-C5-N7 | -5.11 | 108.15 | 110.70 |
| 22 | 23S1 | 28 | A | C4-C5-C6 | 5.11 | 119.55 | 117.00 |
| 22 | 23S1 | 216 | A | C4-C5-N7 | -5.11 | 108.15 | 110.70 |
| 22 | 23S1 | 256 | A | C4-C5-N7 | -5.11 | 108.15 | 110.70 |
| 22 | 23S1 | 311 | A | C4-C5-N7 | -5.11 | 108.15 | 110.70 |
| 22 | 23S1 | 740 | C | N1-C2-O2 | 5.11 | 121.96 | 118.90 |
| 22 | 23S1 | 752 | A | C5-C6-N1 | 5.11 | 120.25 | 117.70 |
| 22 | 23S1 | 1342 | A | C4-C5-C6 | 5.11 | 119.55 | 117.00 |
| 22 | 23S1 | 1853 | A | N3-C4-N9 | 5.11 | 131.49 | 127.40 |
| 22 | 23S1 | 1985 | C | N3-C2-O2 | -5.11 | 118.33 | 121.90 |
| 1 | 16S1 | 189 | A | N9-C4-C5 | 5.11 | 107.84 | 105.80 |
| 1 | 16S1 | 1250 | A | C5-C6-N1 | 5.11 | 120.25 | 117.70 |
| 22 | 23S1 | 1262 | A | C8-N9-C4 | 5.11 | 107.84 | 105.80 |
| 22 | 23S1 | 1754 | A | C4-C5-C6 | 5.11 | 119.55 | 117.00 |
| 22 | 23S1 | 2211 | A | C5-C6-N1 | 5.11 | 120.25 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 16S1 | 211 | G | C6-N1-C2 | -5.10 | 122.04 | 125.10 |
| 1 | 16S1 | 236 | A | C5-C6-N1 | 5.10 | 120.25 | 117.70 |
| 1 | 16S1 | 1082 | A | C5-C6-N1 | 5.10 | 120.25 | 117.70 |
| 1 | 16S1 | 1269 | A | C4-C5-N7 | -5.10 | 108.15 | 110.70 |
| 1 | 16S1 | 1429 | A | C4-C5-N7 | -5.10 | 108.15 | 110.70 |
| 22 | 23S1 | 1014 | A | N9-C4-C5 | 5.10 | 107.84 | 105.80 |
| 23 | 05S1 | 68 | C | N1-C2-O2 | 5.10 | 121.96 | 118.90 |
| 1 | 16S1 | 28 | A | N9-C4-C5 | 5.10 | 107.84 | 105.80 |
| 1 | 16S1 | 1101 | A | N3-C4-N9 | 5.10 | 131.48 | 127.40 |
| 22 | 23S1 | 172 | A | N9-C4-C5 | 5.10 | 107.84 | 105.80 |
| 22 | 23S1 | 734 | A | C5-C6-N1 | 5.10 | 120.25 | 117.70 |
| 22 | 23S1 | 802 | A | C8-N9-C4 | 5.10 | 107.84 | 105.80 |
| 22 | 23S1 | 2169 | A | N9-C4-C5 | 5.10 | 107.84 | 105.80 |
| 1 | 16S1 | 1492 | A | C5-C6-N1 | 5.10 | 120.25 | 117.70 |
| 22 | 23S1 | 734 | A | C4-C5-N7 | -5.10 | 108.15 | 110.70 |
| 22 | 23S1 | 1005 | C | N1-C2-O2 | 5.10 | 121.96 | 118.90 |
| 1 | 16S1 | 649 | A | C8-N9-C4 | 5.10 | 107.84 | 105.80 |
| 22 | 23S1 | 42 | A | N9-C4-C5 | 5.10 | 107.84 | 105.80 |
| 22 | 23S1 | 383 | C | N3-C2-O2 | -5.10 | 118.33 | 121.90 |
| 55 | PTR1 | 51 | A | C5-C6-N1 | 5.10 | 120.25 | 117.70 |
| 1 | 16S1 | 807 | A | C4-C5-N7 | -5.10 | 108.15 | 110.70 |
| 22 | 23S1 | 190 | A | C4-C5-N7 | -5.10 | 108.15 | 110.70 |
| 22 | 23S1 | 204 | A | N3-C4-N9 | 5.10 | 131.48 | 127.40 |
| 22 | 23S1 | 64 | A | C5-C6-N1 | 5.09 | 120.25 | 117.70 |
| 22 | 23S1 | 1304 | A | C4-C5-C6 | 5.09 | 119.55 | 117.00 |
| 22 | 23S1 | 1525 | A | C8-N9-C4 | 5.09 | 107.84 | 105.80 |
| 22 | 23S1 | 2009 | A | C4-C5-C6 | 5.09 | 119.55 | 117.00 |
| 22 | 23S1 | 1598 | A | C8-N9-C4 | 5.09 | 107.84 | 105.80 |
| 1 | 16S1 | 715 | A | N9-C4-C5 | 5.09 | 107.84 | 105.80 |
| 22 | 23S1 | 894 | U | N1-C2-O2 | 5.09 | 126.36 | 122.80 |
| 22 | 23S1 | 897 | C | N1-C2-O2 | 5.09 | 121.95 | 118.90 |
| 22 | 23S1 | 1363 | C | N3-C2-O2 | -5.09 | 118.34 | 121.90 |
| 22 | 23S1 | 1744 | A | N9-C4-C5 | 5.09 | 107.84 | 105.80 |
| 1 | 16S1 | 364 | A | C4-C5-C6 | 5.09 | 119.54 | 117.00 |
| 1 | 16S1 | 456 | A | C4-C5-C6 | 5.09 | 119.54 | 117.00 |
| 1 | 16S1 | 488 | C | N3-C2-O2 | -5.09 | 118.34 | 121.90 |
| 22 | 23S1 | 988 | A | N9-C4-C5 | 5.09 | 107.84 | 105.80 |
| 22 | 23S1 | 1650 | A | C5-C6-N1 | 5.09 | 120.25 | 117.70 |
| 22 | 23S1 | 1774 | C | N1-C2-O2 | 5.09 | 121.95 | 118.90 |
| 22 | 23S1 | 2135 | A | C4-C5-N7 | -5.09 | 108.16 | 110.70 |
| 22 | 23S1 | 2531 | A | N9-C4-C5 | 5.09 | 107.84 | 105.80 |
| 1 | 16S1 | 1196 | A | N9-C4-C5 | 5.09 | 107.83 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 635 | C | N3-C2-O2 | -5.09 | 118.34 | 121.90 |
| 22 | 23S1 | 984 | A | C4-C5-N7 | -5.09 | 108.16 | 110.70 |
| 1 | 16S1 | 560 | A | C8-N9-C4 | 5.09 | 107.83 | 105.80 |
| 22 | 23S1 | 783 | A | C5-C6-N1 | 5.09 | 120.24 | 117.70 |
| 22 | 23S1 | 1784 | A | C5-C6-N1 | 5.09 | 120.24 | 117.70 |
| 22 | 23S1 | 2366 | A | N9-C4-C5 | 5.09 | 107.83 | 105.80 |
| 22 | 23S1 | 2710 | C | C6-N1-C2 | -5.09 | 118.27 | 120.30 |
| 1 | 16S1 | 131 | A | C4-C5-N7 | -5.08 | 108.16 | 110.70 |
| 1 | 16S1 | 356 | A | C4-C5-N7 | -5.08 | 108.16 | 110.70 |
| 1 | 16S1 | 1251 | A | C4-C5-N7 | -5.08 | 108.16 | 110.70 |
| 22 | 23S1 | 310 | A | C4-C5-N7 | -5.08 | 108.16 | 110.70 |
| 22 | 23S1 | 1433 | A | C4-C5-N7 | -5.08 | 108.16 | 110.70 |
| 1 | 16S1 | 243 | A | N3-C4-N9 | 5.08 | 131.47 | 127.40 |
| 1 | 16S1 | 759 | A | C8-N9-C4 | 5.08 | 107.83 | 105.80 |
| 22 | 23S1 | 507 | A | C5-C6-N1 | 5.08 | 120.24 | 117.70 |
| 22 | 23S1 | 1785 | A | C5-C6-N1 | 5.08 | 120.24 | 117.70 |
| 22 | 23S1 | 2162 | G | P-O3'-C3' | 5.08 | 125.80 | 119.70 |
| 22 | 23S1 | 2725 | A | C8-N9-C4 | 5.08 | 107.83 | 105.80 |
| 1 | 16S1 | 411 | A | OP1-P-O3' | 5.08 | 116.38 | 105.20 |
| 1 | 16S1 | 487 | A | C4-C5-N7 | -5.08 | 108.16 | 110.70 |
| 1 | 16S1 | 595 | A | C4-C5-N7 | -5.08 | 108.16 | 110.70 |
| 22 | 23S1 | 609 | A | C4-C5-N7 | -5.08 | 108.16 | 110.70 |
| 22 | 23S1 | 668 | A | C4-C5-N7 | -5.08 | 108.16 | 110.70 |
| 22 | 23S1 | 1214 | A | C4-C5-N7 | -5.08 | 108.16 | 110.70 |
| 55 | PTR1 | 62 | C | C5-C6-N1 | 5.08 | 123.54 | 121.00 |
| 1 | 16S1 | 702 | A | N3-C4-N9 | 5.08 | 131.46 | 127.40 |
| 22 | 23S1 | 621 | A | C5-C6-N1 | 5.08 | 120.24 | 117.70 |
| 22 | 23S1 | 1241 | A | C4-C5-N7 | -5.08 | 108.16 | 110.70 |
| 23 | 05S1 | 104 | A | C4-C5-N7 | -5.08 | 108.16 | 110.70 |
| 1 | 16S1 | 454 | G | N1-C2-N2 | -5.08 | 111.63 | 116.20 |
| 1 | 16S1 | 878 | A | C4-C5-N7 | -5.08 | 108.16 | 110.70 |
| 1 | 16S1 | 975 | A | C6-N1-C2 | 5.08 | 121.65 | 118.60 |
| 22 | 23S1 | 84 | A | C6-N1-C2 | 5.08 | 121.65 | 118.60 |
| 22 | 23S1 | 223 | A | C8-N9-C4 | 5.08 | 107.83 | 105.80 |
| 22 | 23S1 | 715 | A | C5-C6-N1 | 5.08 | 120.24 | 117.70 |
| 22 | 23S1 | 972 | A | C5-C6-N1 | 5.08 | 120.24 | 117.70 |
| 22 | 23S1 | 1089 | A | C4-C5-N7 | -5.08 | 108.16 | 110.70 |
| 1 | 16S1 | 607 | A | N9-C4-C5 | 5.08 | 107.83 | 105.80 |
| 1 | 16S1 | 1197 | A | C5-C6-N1 | 5.08 | 120.24 | 117.70 |
| 22 | 23S1 | 582 | A | C4-C5-N7 | -5.08 | 108.16 | 110.70 |
| 22 | 23S1 | 1070 | A | N9-C4-C5 | 5.08 | 107.83 | 105.80 |
| 22 | 23S1 | 1322 | A | N3-C4-N9 | 5.08 | 131.46 | 127.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 16S1 | 596 | A | N9-C4-C5 | 5.08 | 107.83 | 105.80 |
| 1 | 16S1 | 1032 | G | C4-N9-C1' | 5.08 | 133.10 | 126.50 |
| 1 | 16S1 | 1430 | A | C4-C5-N7 | -5.08 | 108.16 | 110.70 |
| 22 | 23S1 | 781 | A | C4-C5-N7 | -5.08 | 108.16 | 110.70 |
| 22 | 23S1 | 906 | U | O4'-C1'-N1 | 5.08 | 112.26 | 108.20 |
| 22 | 23S1 | 1046 | A | C4-C5-N7 | -5.08 | 108.16 | 110.70 |
| 22 | 23S1 | 1548 | A | C4-C5-N7 | -5.08 | 108.16 | 110.70 |
| 22 | 23S1 | 2009 | A | C5-C6-N1 | 5.08 | 120.24 | 117.70 |
| 22 | 23S1 | 2443 | C | N3-C2-O2 | -5.08 | 118.35 | 121.90 |
| 22 | 23S1 | 2823 | A | C4-C5-C6 | 5.08 | 119.54 | 117.00 |
| 22 | 23S1 | 2829 | A | C5-C6-N1 | 5.08 | 120.24 | 117.70 |
| 23 | 05S1 | 24 | G | N3-C4-C5 | -5.08 | 126.06 | 128.60 |
| 1 | 16S1 | 270 | A | C4-C5-N7 | -5.07 | 108.16 | 110.70 |
| 1 | 16S1 | 288 | A | C8-N9-C4 | 5.07 | 107.83 | 105.80 |
| 1 | 16S1 | 1021 | A | C4-C5-N7 | -5.07 | 108.16 | 110.70 |
| 22 | 23S1 | 49 | A | N9-C4-C5 | 5.07 | 107.83 | 105.80 |
| 22 | 23S1 | 225 | C | C6-N1-C2 | -5.07 | 118.27 | 120.30 |
| 22 | 23S1 | 345 | A | C5-C6-N1 | 5.07 | 120.24 | 117.70 |
| 22 | 23S1 | 685 | A | C4-C5-N7 | -5.07 | 108.16 | 110.70 |
| 22 | 23S1 | 2307 | G | C5-C6-O6 | -5.07 | 125.56 | 128.60 |
| 23 | 05S1 | 15 | A | C4-C5-N7 | -5.07 | 108.16 | 110.70 |
| 22 | 23S1 | 94 | A | C5-C6-N1 | 5.07 | 120.24 | 117.70 |
| 22 | 23S1 | 423 | A | C4-C5-N7 | -5.07 | 108.16 | 110.70 |
| 22 | 23S1 | 1754 | A | C6-N1-C2 | 5.07 | 121.64 | 118.60 |
| 1 | 16S1 | 330 | C | N3-C2-O2 | -5.07 | 118.35 | 121.90 |
| 22 | 23S1 | 443 | A | C4-C5-C6 | 5.07 | 119.54 | 117.00 |
| 22 | 23S1 | 453 | A | C5-C6-N1 | 5.07 | 120.24 | 117.70 |
| 22 | 23S1 | 1654 | A | C5-C6-N1 | 5.07 | 120.23 | 117.70 |
| 22 | 23S1 | 1774 | C | N3-C2-O2 | -5.07 | 118.35 | 121.90 |
| 1 | 16S1 | 8 | A | C4-C5-N7 | -5.07 | 108.17 | 110.70 |
| 22 | 23S1 | 64 | A | C4-C5-N7 | -5.07 | 108.17 | 110.70 |
| 22 | 23S1 | 1819 | A | C4-C5-N7 | -5.07 | 108.17 | 110.70 |
| 22 | 23S1 | 2716 | C | N3-C2-O2 | -5.07 | 118.35 | 121.90 |
| 1 | 16S1 | 573 | A | C4-C5-N7 | -5.07 | 108.17 | 110.70 |
| 1 | 16S1 | 649 | A | C5-C6-N1 | 5.07 | 120.23 | 117.70 |
| 1 | 16S1 | 702 | A | C4-C5-C6 | 5.07 | 119.53 | 117.00 |
| 1 | 16S1 | 712 | A | C4-C5-N7 | -5.07 | 108.17 | 110.70 |
| 22 | 23S1 | 1384 | A | C8-N9-C4 | 5.07 | 107.83 | 105.80 |
| 22 | 23S1 | 2173 | A | N9-C4-C5 | 5.07 | 107.83 | 105.80 |
| 1 | 16S1 | 309 | A | C4-C5-C6 | 5.07 | 119.53 | 117.00 |
| 1 | 16S1 | 889 | A | N3-C4-N9 | 5.07 | 131.45 | 127.40 |
| 1 | 16S1 | 1067 | A | C4-C5-N7 | -5.07 | 108.17 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 16S1 | 1493 | A | C5-C6-N1 | 5.07 | 120.23 | 117.70 |
| 22 | 23S1 | 996 | A | C4-C5-N7 | -5.07 | 108.17 | 110.70 |
| 22 | 23S1 | 1272 | A | N3-C4-N9 | 5.07 | 131.45 | 127.40 |
| 22 | 23S1 | 2268 | A | N9-C4-C5 | 5.07 | 107.83 | 105.80 |
| 22 | 23S1 | 2564 | A | N3-C4-N9 | 5.07 | 131.45 | 127.40 |
| 1 | 16S1 | 98 | A | C4-C5-N7 | -5.06 | 108.17 | 110.70 |
| 1 | 16S1 | 777 | A | C8-N9-C4 | 5.06 | 107.83 | 105.80 |
| 1 | 16S1 | 857 | C | C6-N1-C2 | -5.06 | 118.28 | 120.30 |
| 22 | 23S1 | 118 | A | C4-C5-C6 | 5.06 | 119.53 | 117.00 |
| 22 | 23S1 | 983 | A | N9-C4-C5 | 5.06 | 107.83 | 105.80 |
| 22 | 23S1 | 1928 | A | C4-C5-N7 | -5.06 | 108.17 | 110.70 |
| 1 | 16S1 | 1275 | A | C4-C5-N7 | -5.06 | 108.17 | 110.70 |
| 22 | 23S1 | 1654 | A | C4-C5-N7 | -5.06 | 108.17 | 110.70 |
| 22 | 23S1 | 2098 | U | N3-C2-O2 | -5.06 | 118.66 | 122.20 |
| 22 | 23S1 | 2107 | G | C5-C6-O6 | 5.06 | 131.64 | 128.60 |
| 22 | 23S1 | 1569 | A | N9-C4-C5 | 5.06 | 107.82 | 105.80 |
| 22 | 23S1 | 2317 | A | N9-C4-C5 | 5.06 | 107.82 | 105.80 |
| 22 | 23S1 | 2358 | A | C5-C6-N1 | 5.06 | 120.23 | 117.70 |
| 1 | 16S1 | 383 | A | C5-C6-N6 | 5.06 | 127.75 | 123.70 |
| 22 | 23S1 | 603 | A | N9-C4-C5 | 5.06 | 107.82 | 105.80 |
| 22 | 23S1 | 1677 | A | N9-C4-C5 | 5.06 | 107.82 | 105.80 |
| 22 | 23S1 | 2868 | A | C5-C6-N1 | 5.06 | 120.23 | 117.70 |
| 22 | 23S1 | 802 | A | C4-C5-N7 | -5.06 | 108.17 | 110.70 |
| 22 | 23S1 | 1151 | A | C8-N9-C4 | 5.06 | 107.82 | 105.80 |
| 22 | 23S1 | 1268 | A | C5-C6-N1 | 5.06 | 120.23 | 117.70 |
| 22 | 23S1 | 1780 | A | C8-N9-C4 | 5.06 | 107.82 | 105.80 |
| 22 | 23S1 | 1858 | A | C4-C5-N7 | -5.06 | 108.17 | 110.70 |
| 22 | 23S1 | 2317 | A | C4-C5-N7 | -5.06 | 108.17 | 110.70 |
| 22 | 23S1 | 2321 | U | C2-N1-C1' | 5.06 | 123.77 | 117.70 |
| 22 | 23S1 | 483 | A | C5-C6-N1 | 5.06 | 120.23 | 117.70 |
| 22 | 23S1 | 1793 | C | C6-N1-C2 | -5.06 | 118.28 | 120.30 |
| 1 | 16S1 | 166 | U | N3-C2-O2 | -5.05 | 118.66 | 122.20 |
| 1 | 16S1 | 222 | C | N1-C2-O2 | 5.05 | 121.93 | 118.90 |
| 1 | 16S1 | 1288 | A | C5-C6-N1 | 5.05 | 120.23 | 117.70 |
| 1 | 16S1 | 1318 | A | C8-N9-C4 | 5.05 | 107.82 | 105.80 |
| 1 | 16S1 | 1499 | A | C4-C5-C6 | 5.05 | 119.53 | 117.00 |
| 22 | 23S1 | 5 | A | C8-N9-C4 | 5.05 | 107.82 | 105.80 |
| 22 | 23S1 | 1079 | C | N3-C2-O2 | -5.05 | 118.36 | 121.90 |
| 23 | 05S1 | 24 | G | N3-C4-N9 | 5.05 | 129.03 | 126.00 |
| 1 | 16S1 | 1152 | A | C5-C6-N1 | 5.05 | 120.23 | 117.70 |
| 1 | 16S1 | 1430 | A | C8-N9-C4 | 5.05 | 107.82 | 105.80 |
| 22 | 23S1 | 311 | A | N9-C4-C5 | 5.05 | 107.82 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 565 | C | N3-C2-O2 | -5.05 | 118.36 | 121.90 |
| 22 | 23S1 | 742 | A | N9-C4-C5 | 5.05 | 107.82 | 105.80 |
| 22 | 23S1 | 1609 | A | C8-N9-C4 | 5.05 | 107.82 | 105.80 |
| 1 | 16S1 | 349 | A | C4-C5-C6 | 5.05 | 119.53 | 117.00 |
| 1 | 16S1 | 715 | A | C5-C6-N1 | 5.05 | 120.22 | 117.70 |
| 1 | 16S1 | 1408 | A | C5-C6-N1 | 5.05 | 120.22 | 117.70 |
| 1 | 16S1 | 1413 | A | N3-C4-N9 | 5.05 | 131.44 | 127.40 |
| 1 | 16S1 | 1534 | A | C4-C5-N7 | -5.05 | 108.17 | 110.70 |
| 22 | 23S1 | 1276 | A | C5-C6-N1 | 5.05 | 120.22 | 117.70 |
| 22 | 23S1 | 1350 | C | N1-C2-O2 | 5.05 | 121.93 | 118.90 |
| 22 | 23S1 | 1413 | A | C5-C6-N1 | 5.05 | 120.23 | 117.70 |
| 22 | 23S1 | 2433 | A | C4-C5-N7 | -5.05 | 108.17 | 110.70 |
| 22 | 23S1 | 2813 | A | C4-C5-C6 | 5.05 | 119.53 | 117.00 |
| 1 | 16S1 | 108 | G | C4-N9-C1' | 5.05 | 133.06 | 126.50 |
| 1 | 16S1 | 196 | A | C4-C5-C6 | 5.05 | 119.53 | 117.00 |
| 22 | 23S1 | 670 | A | N9-C4-C5 | 5.05 | 107.82 | 105.80 |
| 22 | 23S1 | 866 | A | C4-C5-N7 | -5.05 | 108.18 | 110.70 |
| 22 | 23S1 | 1084 | A | C8-N9-C4 | 5.05 | 107.82 | 105.80 |
| 22 | 23S1 | 1286 | A | C4-C5-N7 | -5.05 | 108.18 | 110.70 |
| 22 | 23S1 | 2579 | C | C6-N1-C2 | -5.05 | 118.28 | 120.30 |
| 1 | 16S1 | 195 | A | C8-N9-C4 | 5.05 | 107.82 | 105.80 |
| 1 | 16S1 | 321 | A | N9-C4-C5 | 5.05 | 107.82 | 105.80 |
| 1 | 16S1 | 456 | A | C5-C6-N1 | 5.05 | 120.22 | 117.70 |
| 22 | 23S1 | 131 | A | C8-N9-C4 | 5.05 | 107.82 | 105.80 |
| 22 | 23S1 | 204 | A | C4-C5-N7 | -5.05 | 108.18 | 110.70 |
| 22 | 23S1 | 946 | C | N3-C2-O2 | -5.05 | 118.37 | 121.90 |
| 22 | 23S1 | 1054 | A | C8-N9-C4 | 5.05 | 107.82 | 105.80 |
| 22 | 23S1 | 1133 | A | C4-C5-N7 | -5.05 | 108.18 | 110.70 |
| 22 | 23S1 | 1373 | A | N9-C4-C5 | 5.05 | 107.82 | 105.80 |
| 22 | 23S1 | 1580 | A | C4-C5-N7 | -5.05 | 108.18 | 110.70 |
| 22 | 23S1 | 1690 | A | C5-C6-N1 | 5.05 | 120.22 | 117.70 |
| 22 | 23S1 | 125 | A | C4-C5-N7 | -5.04 | 108.18 | 110.70 |
| 22 | 23S1 | 265 | A | C4-C5-N7 | -5.04 | 108.18 | 110.70 |
| 22 | 23S1 | 1754 | A | C8-N9-C4 | 5.04 | 107.82 | 105.80 |
| 22 | 23S1 | 2346 | A | C4-C5-N7 | -5.04 | 108.18 | 110.70 |
| 23 | 05S1 | 58 | A | C5-C6-N1 | 5.04 | 120.22 | 117.70 |
| 1 | 16S1 | 523 | A | C5-C6-N1 | 5.04 | 120.22 | 117.70 |
| 22 | 23S1 | 64 | A | N9-C4-C5 | 5.04 | 107.82 | 105.80 |
| 22 | 23S1 | 207 | A | C4-C5-C6 | 5.04 | 119.52 | 117.00 |
| 22 | 23S1 | 592 | A | C5-C6-N1 | 5.04 | 120.22 | 117.70 |
| 22 | 23S1 | 1067 | A | N9-C4-C5 | 5.04 | 107.82 | 105.80 |
| 22 | 23S1 | 2205 | A | C5-C6-N1 | 5.04 | 120.22 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 563 | A | C8-N9-C4 | 5.04 | 107.82 | 105.80 |
| 22 | 23S1 | 2199 | A | C5-C6-N1 | 5.04 | 120.22 | 117.70 |
| 1 | 16S1 | 192 | A | C5-C6-N1 | 5.04 | 120.22 | 117.70 |
| 1 | 16S1 | 238 | A | C5-C6-N1 | 5.04 | 120.22 | 117.70 |
| 1 | 16S1 | 327 | A | C5-C6-N1 | 5.04 | 120.22 | 117.70 |
| 22 | 23S1 | 632 | A | C5-C6-N1 | 5.04 | 120.22 | 117.70 |
| 22 | 23S1 | 1284 | A | C5-C6-N1 | 5.04 | 120.22 | 117.70 |
| 22 | 23S1 | 2284 | A | C8-N9-C4 | 5.04 | 107.81 | 105.80 |
| 22 | 23S1 | 2753 | A | N3-C4-N9 | 5.04 | 131.43 | 127.40 |
| 23 | 05S1 | 71 | C | N3-C2-O2 | -5.04 | 118.37 | 121.90 |
| 22 | 23S1 | 614 | A | C5-C6-N1 | 5.04 | 120.22 | 117.70 |
| 1 | 16S1 | 539 | A | C8-N9-C4 | 5.04 | 107.81 | 105.80 |
| 22 | 23S1 | 182 | A | C8-N9-C4 | 5.04 | 107.81 | 105.80 |
| 22 | 23S1 | 515 | A | C8-N9-C4 | 5.04 | 107.81 | 105.80 |
| 22 | 23S1 | 1117 | C | N3-C2-O2 | -5.04 | 118.38 | 121.90 |
| 22 | 23S1 | 1308 | A | C5-C6-N1 | 5.04 | 120.22 | 117.70 |
| 22 | 23S1 | 2602 | A | C5-C6-N1 | 5.04 | 120.22 | 117.70 |
| 22 | 23S1 | 2893 | A | C5-C6-N1 | 5.04 | 120.22 | 117.70 |
| 1 | 16S1 | 274 | A | C4-C5-C6 | 5.03 | 119.52 | 117.00 |
| 1 | 16S1 | 536 | C | N3-C2-O2 | -5.03 | 118.38 | 121.90 |
| 1 | 16S1 | 1340 | A | C4-C5-C6 | 5.03 | 119.52 | 117.00 |
| 22 | 23S1 | 2635 | A | C8-N9-C4 | 5.03 | 107.81 | 105.80 |
| 1 | 16S1 | 687 | A | C4-C5-N7 | -5.03 | 108.18 | 110.70 |
| 1 | 16S1 | 1196 | A | C4-C5-N7 | -5.03 | 108.18 | 110.70 |
| 22 | 23S1 | 142 | A | C5-C6-N1 | 5.03 | 120.22 | 117.70 |
| 22 | 23S1 | 671 | C | N3-C2-O2 | -5.03 | 118.38 | 121.90 |
| 1 | 16S1 | 642 | A | C8-N9-C4 | 5.03 | 107.81 | 105.80 |
| 22 | 23S1 | 217 | A | N9-C4-C5 | 5.03 | 107.81 | 105.80 |
| 22 | 23S1 | 1932 | A | C4-C5-C6 | 5.03 | 119.52 | 117.00 |
| 22 | 23S1 | 2003 | A | N9-C4-C5 | 5.03 | 107.81 | 105.80 |
| 22 | 23S1 | 2307 | G | C8-N9-C4 | 5.03 | 108.41 | 106.40 |
| 22 | 23S1 | 2369 | A | N9-C4-C5 | 5.03 | 107.81 | 105.80 |
| 22 | 23S1 | 2435 | A | C5-C6-N1 | 5.03 | 120.22 | 117.70 |
| 1 | 16S1 | 253 | A | C4-C5-N7 | -5.03 | 108.19 | 110.70 |
| 1 | 16S1 | 784 | A | C4-C5-N7 | -5.03 | 108.19 | 110.70 |
| 1 | 16S1 | 900 | A | C4-C5-N7 | -5.03 | 108.19 | 110.70 |
| 22 | 23S1 | 127 | A | N3-C4-N9 | 5.03 | 131.42 | 127.40 |
| 22 | 23S1 | 1394 | U | C6-N1-C1' | 5.03 | 128.24 | 121.20 |
| 22 | 23S1 | 402 | A | C4-C5-N7 | -5.03 | 108.19 | 110.70 |
| 22 | 23S1 | 1494 | A | C8-N9-C4 | 5.03 | 107.81 | 105.80 |
| 22 | 23S1 | 2005 | A | N9-C4-C5 | 5.03 | 107.81 | 105.80 |
| 22 | 23S1 | 2176 | A | N9-C4-C5 | 5.03 | 107.81 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 16S1 | 493 | A | C8-N9-C4 | 5.03 | 107.81 | 105.80 |
| 1 | 16S1 | 1250 | A | N3-C4-N9 | 5.03 | 131.42 | 127.40 |
| 22 | 23S1 | 1021 | A | C4-C5-N7 | -5.03 | 108.19 | 110.70 |
| 1 | 16S1 | 440 | C | C6-N1-C2 | -5.02 | 118.29 | 120.30 |
| 1 | 16S1 | 816 | A | C8-N9-C4 | 5.02 | 107.81 | 105.80 |
| 1 | 16S1 | 1289 | A | C4-C5-C6 | 5.02 | 119.51 | 117.00 |
| 22 | 23S1 | 945 | A | C4-C5-N7 | -5.02 | 108.19 | 110.70 |
| 22 | 23S1 | 1866 | A | C4-C5-N7 | -5.02 | 108.19 | 110.70 |
| 22 | 23S1 | 1912 | A | C5-C6-N1 | 5.02 | 120.21 | 117.70 |
| 22 | 23S1 | 2776 | A | N3-C4-N9 | 5.02 | 131.42 | 127.40 |
| 1 | 16S1 | 816 | A | N9-C4-C5 | 5.02 | 107.81 | 105.80 |
| 1 | 16S1 | 1044 | A | C4-C5-N7 | -5.02 | 108.19 | 110.70 |
| 22 | 23S1 | 182 | A | N9-C4-C5 | 5.02 | 107.81 | 105.80 |
| 22 | 23S1 | 556 | A | C4-C5-N7 | -5.02 | 108.19 | 110.70 |
| 22 | 23S1 | 572 | A | C5-C6-N1 | 5.02 | 120.21 | 117.70 |
| 22 | 23S1 | 1608 | A | C4-C5-N7 | -5.02 | 108.19 | 110.70 |
| 22 | 23S1 | 1669 | A | C4-C5-N7 | -5.02 | 108.19 | 110.70 |
| 22 | 23S1 | 1805 | A | C8-N9-C4 | 5.02 | 107.81 | 105.80 |
| 1 | 16S1 | 1196 | A | C4-C5-C6 | 5.02 | 119.51 | 117.00 |
| 22 | 23S1 | 223 | A | N3-C4-N9 | 5.02 | 131.42 | 127.40 |
| 22 | 23S1 | 1384 | A | C5-C6-N1 | 5.02 | 120.21 | 117.70 |
| 22 | 23S1 | 1535 | A | C8-N9-C4 | 5.02 | 107.81 | 105.80 |
| 22 | 23S1 | 2547 | A | C8-N9-C4 | 5.02 | 107.81 | 105.80 |
| 1 | 16S1 | 489 | C | O4'-C1'-N1 | 5.02 | 112.22 | 108.20 |
| 1 | 16S1 | 759 | A | C4-C5-N7 | -5.02 | 108.19 | 110.70 |
| 22 | 23S1 | 981 | A | N3-C4-N9 | 5.02 | 131.41 | 127.40 |
| 22 | 23S1 | 1427 | A | C8-N9-C4 | 5.02 | 107.81 | 105.80 |
| 22 | 23S1 | 2636 | C | N1-C2-O2 | 5.02 | 121.91 | 118.90 |
| 23 | 05S1 | 70 | C | C6-N1-C2 | -5.02 | 118.29 | 120.30 |
| 1 | 16S1 | 574 | A | C4-C5-N7 | -5.02 | 108.19 | 110.70 |
| 1 | 16S1 | 622 | A | C8-N9-C4 | 5.02 | 107.81 | 105.80 |
| 22 | 23S1 | 783 | A | C4-C5-N7 | -5.02 | 108.19 | 110.70 |
| 22 | 23S1 | 833 | A | C4-C5-C6 | 5.02 | 119.51 | 117.00 |
| 22 | 23S1 | 1378 | A | N3-C4-N9 | 5.02 | 131.41 | 127.40 |
| 22 | 23S1 | 2425 | A | C4-C5-N7 | -5.02 | 108.19 | 110.70 |
| 1 | 16S1 | 1227 | A | N3-C4-N9 | 5.02 | 131.41 | 127.40 |
| 22 | 23S1 | 352 | A | C4-C5-C6 | 5.02 | 119.51 | 117.00 |
| 22 | 23S1 | 655 | A | C4-C5-N7 | -5.02 | 108.19 | 110.70 |
| 1 | 16S1 | 460 | A | C8-N9-C4 | 5.01 | 107.81 | 105.80 |
| 22 | 23S1 | 155 | A | C4-C5-N7 | -5.01 | 108.19 | 110.70 |
| 22 | 23S1 | 216 | A | C8-N9-C4 | 5.01 | 107.81 | 105.80 |
| 22 | 23S1 | 330 | A | C4-C5-N7 | -5.01 | 108.19 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 344 | A | C4-C5-N7 | -5.01 | 108.19 | 110.70 |
| 22 | 23S1 | 532 | A | C4-C5-N7 | -5.01 | 108.19 | 110.70 |
| 22 | 23S1 | 1403 | A | C4-C5-N7 | -5.01 | 108.19 | 110.70 |
| 22 | 23S1 | 1679 | A | C5-C6-N1 | 5.01 | 120.21 | 117.70 |
| 22 | 23S1 | 1515 | A | C4-C5-N7 | -5.01 | 108.19 | 110.70 |
| 1 | 16S1 | 152 | A | C5-N7-C8 | 5.01 | 106.41 | 103.90 |
| 1 | 16S1 | 313 | A | C5-C6-N1 | 5.01 | 120.20 | 117.70 |
| 1 | 16S1 | 916 | U | N3-C2-O2 | -5.01 | 118.69 | 122.20 |
| 1 | 16S1 | 949 | A | N9-C4-C5 | 5.01 | 107.80 | 105.80 |
| 22 | 23S1 | 52 | A | C8-N9-C4 | 5.01 | 107.81 | 105.80 |
| 22 | 23S1 | 508 | A | C4-C5-N7 | -5.01 | 108.19 | 110.70 |
| 22 | 23S1 | 2758 | A | N3-C4-N9 | 5.01 | 131.41 | 127.40 |
| 1 | 16S1 | 415 | A | C8-N9-C4 | 5.01 | 107.80 | 105.80 |
| 1 | 16S1 | 495 | A | C4-C5-N7 | -5.01 | 108.19 | 110.70 |
| 1 | 16S1 | 802 | A | C4-C5-C6 | 5.01 | 119.50 | 117.00 |
| 1 | 16S1 | 807 | A | N9-C4-C5 | 5.01 | 107.80 | 105.80 |
| 22 | 23S1 | 294 | A | C5-C6-N1 | 5.01 | 120.20 | 117.70 |
| 22 | 23S1 | 378 | C | C6-N1-C2 | -5.01 | 118.30 | 120.30 |
| 22 | 23S1 | 582 | A | C8-N9-C4 | 5.01 | 107.80 | 105.80 |
| 22 | 23S1 | 1754 | A | N9-C4-C5 | 5.01 | 107.80 | 105.80 |
| 22 | 23S1 | 126 | A | C5-C6-N1 | 5.01 | 120.20 | 117.70 |
| 22 | 23S1 | 541 | A | C8-N9-C4 | 5.01 | 107.80 | 105.80 |
| 22 | 23S1 | 1189 | A | C4-C5-N7 | -5.01 | 108.20 | 110.70 |
| 22 | 23S1 | 294 | A | C4-C5-N7 | -5.01 | 108.20 | 110.70 |
| 22 | 23S1 | 439 | A | C8-N9-C4 | 5.01 | 107.80 | 105.80 |
| 22 | 23S1 | 512 | G | C5-N7-C8 | -5.01 | 101.80 | 104.30 |
| 22 | 23S1 | 781 | A | N9-C4-C5 | 5.01 | 107.80 | 105.80 |
| 22 | 23S1 | 986 | C | C6-N1-C2 | -5.01 | 118.30 | 120.30 |
| 22 | 23S1 | 2513 | A | C5-C6-N1 | 5.01 | 120.20 | 117.70 |
| 22 | 23S1 | 2741 | A | N3-C4-N9 | 5.01 | 131.41 | 127.40 |
| 55 | PTR1 | 20 | U | C4-C5-C6 | -5.01 | 116.70 | 119.70 |
| 1 | 16S1 | 648 | A | C8-N9-C4 | 5.00 | 107.80 | 105.80 |
| 1 | 16S1 | 1005 | A | C4-C5-N7 | -5.00 | 108.20 | 110.70 |
| 1 | 16S1 | 1513 | A | C5-C6-N1 | 5.00 | 120.20 | 117.70 |
| 22 | 23S1 | 22 | C | OP1-P-O3' | -5.00 | 94.19 | 105.20 |
| 22 | 23S1 | 423 | A | N3-C4-N9 | 5.00 | 131.40 | 127.40 |
| 22 | 23S1 | 1515 | A | C8-N9-C4 | 5.00 | 107.80 | 105.80 |
| 22 | 23S1 | 2530 | A | C5-C6-N1 | 5.00 | 120.20 | 117.70 |
| 55 | PTR1 | 23 | A | C4-C5-N7 | -5.00 | 108.20 | 110.70 |
| 1 | 16S1 | 777 | A | C5-C6-N1 | 5.00 | 120.20 | 117.70 |
| 1 | 16S1 | 908 | A | C4-C5-N7 | -5.00 | 108.20 | 110.70 |
| 22 | 23S1 | 91 | A | C4-C5-N7 | -5.00 | 108.20 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 22 | 23S1 | 1398 | C | N1-C2-O2 | 5.00 | 121.90 | 118.90 |
| 1 | 16S1 | 1408 | A | N3-C4-N9 | 5.00 | 131.40 | 127.40 |
| 22 | 23S1 | 197 | A | C4-C5-N7 | -5.00 | 108.20 | 110.70 |
| 22 | 23S1 | 529 | A | N3-C4-N9 | 5.00 | 131.40 | 127.40 |
| 22 | 23S1 | 793 | A | C4-C5-N7 | -5.00 | 108.20 | 110.70 |
| 22 | 23S1 | 793 | A | C5-C6-N1 | 5.00 | 120.20 | 117.70 |
| 22 | 23S1 | 1067 | A | C8-N9-C4 | 5.00 | 107.80 | 105.80 |
| 22 | 23S1 | 1095 | A | C5-C6-N1 | 5.00 | 120.20 | 117.70 |
| 22 | 23S1 | 1504 | A | C5-C6-N1 | 5.00 | 120.20 | 117.70 |
| 22 | 23S1 | 1872 | A | N7-C8-N9 | -5.00 | 111.30 | 113.80 |
| 22 | 23S1 | 2058 | A | C5-C6-N1 | 5.00 | 120.20 | 117.70 |

There are no chirality outliers.

All (23) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 26 | L041 | 152 | GLU | Peptide |
| 29 | L091 | 104 | THR | Peptide |
| 29 | L091 | 108 | VAL | Peptide |
| 29 | L091 | 145 | ASN | Peptide |
| 29 | L091 | 41 | LYS | Peptide |
| 29 | L091 | 66 | ASN | Peptide |
| 33 | L151 | 35 | HIS | Peptide |
| 30 | L311 | 53 | THR | Peptide |
| 51 | L351 | 31 | HIS | Peptide |
| 2 | S021 | 128 | LYS | Peptide |
| 2 | S021 | 5 | SER | Peptide |
| 3 | S031 | 85 | GLU | Peptide |
| 10 | S101 | 27 | GLU | Peptide |
| 10 | S101 | 56 | HIS | Peptide |
| 10 | S101 | 57 | VAL | Mainchain |
| 10 | S101 | 82 | LYS | Peptide |
| 10 | S101 | 92 | LEU | Peptide |
| 13 | S131 | 11 | ASP | Peptide |
| 13 | S131 | 45 | ILE | Peptide |
| 13 | S131 | 65 | VAL | Peptide |
| 19 | S191 | 27 | ASP | Peptide |
| 19 | S191 | 28 | LYS | Peptide |
| 19 | S191 | 81 | ARG | Mainchain |

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 16S1 | 32930 | 0 | 0 | 0 | 0 |
| 2 | S021 | 1753 | 0 | 0 | 0 | 0 |
| 3 | S031 | 1624 | 0 | 0 | 0 | 0 |
| 4 | S041 | 1643 | 0 | 0 | 0 | 0 |
| 5 | S051 | 1144 | 0 | 0 | 0 | 0 |
| 6 | S061 | 862 | 0 | 0 | 0 | 0 |
| 7 | S071 | 1181 | 0 | 0 | 0 | 0 |
| 8 | S081 | 979 | 0 | 0 | 0 | 0 |
| 9 | S091 | 1022 | 0 | 0 | 0 | 0 |
| 10 | S101 | 795 | 0 | 0 | 0 | 0 |
| 11 | S111 | 877 | 0 | 0 | 0 | 0 |
| 12 | S121 | 957 | 0 | 0 | 0 | 0 |
| 13 | S131 | 883 | 0 | 0 | 0 | 0 |
| 14 | S141 | 799 | 0 | 0 | 0 | 0 |
| 15 | S151 | 714 | 0 | 0 | 0 | 0 |
| 16 | S161 | 649 | 0 | 0 | 0 | 0 |
| 17 | S171 | 648 | 0 | 0 | 0 | 0 |
| 18 | S181 | 455 | 0 | 0 | 0 | 0 |
| 19 | S191 | 656 | 0 | 0 | 0 | 0 |
| 20 | S201 | 670 | 0 | 0 | 0 | 0 |
| 21 | S211 | 465 | 0 | 0 | 0 | 0 |
| 22 | 23S1 | 62209 | 0 | 0 | 0 | 0 |
| 23 | 05S1 | 2569 | 0 | 0 | 0 | 0 |
| 24 | L021 | 2082 | 0 | 0 | 0 | 0 |
| 25 | L031 | 1566 | 0 | 0 | 0 | 0 |
| 26 | L041 | 1552 | 0 | 0 | 0 | 0 |
| 27 | L051 | 1410 | 0 | 0 | 0 | 0 |
| 28 | L061 | 1323 | 0 | 0 | 0 | 0 |
| 29 | L091 | 1110 | 0 | 0 | 0 | 0 |
| 30 | L311 | 522 | 0 | 0 | 0 | 0 |
| 31 | L131 | 1129 | 0 | 0 | 0 | 0 |
| 32 | L141 | 946 | 0 | 0 | 0 | 0 |
| 33 | L151 | 1053 | 0 | 0 | 0 | 0 |
| 34 | L161 | 1075 | 0 | 0 | 0 | 0 |
| 35 | L171 | 945 | 0 | 0 | 0 | 0 |
| 36 | L181 | 900 | 0 | 0 | 0 | 0 |
| 37 | L191 | 917 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 38 | L201 | 947 | 0 | 0 | 0 | 0 |
| 39 | L211 | 816 | 0 | 0 | 0 | 0 |
| 40 | L221 | 857 | 0 | 0 | 0 | 0 |
| 41 | L231 | 738 | 0 | 0 | 0 | 0 |
| 42 | L241 | 779 | 0 | 0 | 0 | 0 |
| 43 | L251 | 753 | 0 | 0 | 0 | 0 |
| 44 | L271 | 580 | 0 | 0 | 0 | 0 |
| 45 | L281 | 625 | 0 | 0 | 0 | 0 |
| 46 | L291 | 501 | 0 | 0 | 0 | 0 |
| 47 | L301 | 449 | 0 | 0 | 0 | 0 |
| 48 | L321 | 444 | 0 | 0 | 0 | 0 |
| 49 | L331 | 414 | 0 | 0 | 0 | 0 |
| 50 | L341 | 377 | 0 | 0 | 0 | 0 |
| 51 | L351 | 504 | 0 | 0 | 0 | 0 |
| 52 | L361 | 302 | 0 | 0 | 0 | 0 |
| 53 | SPE1 | 300 | 0 | 0 | 0 | 0 |
| 54 | MRN1 | 146 | 0 | 0 | 0 | 0 |
| 55 | PTR1 | 1627 | 0 | 0 | 0 | 0 |
| 56 | 16S1 | 87 | 0 | 0 | 0 | 0 |
| 56 | 23S1 | 249 | 0 | 0 | 0 | 0 |
| 56 | L231 | 1 | 0 | 0 | 0 | 0 |
| 56 | PTR1 | 1 | 0 | 0 | 0 | 0 |
| 56 | SPE1 | 1 | 0 | 0 | 0 | 0 |
| 57 | 05S1 | 1 | 0 | 0 | 0 | 0 |
| 57 | 16S1 | 39 | 0 | 0 | 0 | 0 |
| 57 | 23S1 | 106 | 0 | 0 | 0 | 0 |
| 57 | L031 | 1 | 0 | 0 | 0 | 0 |
| 58 | 05S1 | 9 | 0 | 0 | 0 | 0 |
| 58 | 16S1 | 145 | 0 | 0 | 0 | 0 |
| 58 | 23S1 | 908 | 0 | 0 | 0 | 0 |
| 58 | L021 | 26 | 0 | 0 | 0 | 0 |
| 58 | L031 | 17 | 0 | 0 | 0 | 0 |
| 58 | L041 | 11 | 0 | 0 | 0 | 0 |
| 58 | L131 | 6 | 0 | 0 | 0 | 0 |
| 58 | L141 | 6 | 0 | 0 | 0 | 0 |
| 58 | L151 | 5 | 0 | 0 | 0 | 0 |
| 58 | L161 | 5 | 0 | 0 | 0 | 0 |
| 58 | L171 | 5 | 0 | 0 | 0 | 0 |
| 58 | L181 | 1 | 0 | 0 | 0 | 0 |
| 58 | L191 | 4 | 0 | 0 | 0 | 0 |
| 58 | L201 | 3 | 0 | 0 | 0 | 0 |
| 58 | L211 | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 58 | L221 | 8 | 0 | 0 | 0 | 0 |
| 58 | L231 | 1 | 0 | 0 | 0 | 0 |
| 58 | L241 | 2 | 0 | 0 | 0 | 0 |
| 58 | L251 | 1 | 0 | 0 | 0 | 0 |
| 58 | L271 | 3 | 0 | 0 | 0 | 0 |
| 58 | L281 | 2 | 0 | 0 | 0 | 0 |
| 58 | L321 | 3 | 0 | 0 | 0 | 0 |
| 58 | L331 | 1 | 0 | 0 | 0 | 0 |
| 58 | L341 | 8 | 0 | 0 | 0 | 0 |
| 58 | L351 | 3 | 0 | 0 | 0 | 0 |
| 58 | MRN1 | 1 | 0 | 0 | 0 | 0 |
| 58 | PTR1 | 2 | 0 | 0 | 0 | 0 |
| 58 | S021 | 1 | 0 | 0 | 0 | 0 |
| 58 | S031 | 1 | 0 | 0 | 0 | 0 |
| 58 | S081 | 1 | 0 | 0 | 0 | 0 |
| 58 | S091 | 1 | 0 | 0 | 0 | 0 |
| 58 | S111 | 2 | 0 | 0 | 0 | 0 |
| 58 | S131 | 1 | 0 | 0 | 0 | 0 |
| 58 | S171 | 1 | 0 | 0 | 0 | 0 |
| 58 | SPE1 | 6 | 0 | 0 | 0 | 0 |
| 59 | L311 | 1 | 0 | 0 | 0 | 0 |
| 59 | L361 | 1 | 0 | 0 | 0 | 0 |
| 59 | S021 | 1 | 0 | 0 | 0 | 0 |
| 60 | 23S1 | 9 | 0 | 0 | 0 | 0 |
| 61 | 16S1 | 167 | 0 | 0 | 0 | 0 |
| 61 | 23S1 | 619 | 0 | 0 | 0 | 0 |
| 61 | L021 | 3 | 0 | 0 | 0 | 0 |
| 61 | L031 | 2 | 0 | 0 | 0 | 0 |
| 61 | L151 | 2 | 0 | 0 | 0 | 0 |
| 61 | L171 | 2 | 0 | 0 | 0 | 0 |
| 61 | S111 | 1 | 0 | 0 | 0 | 0 |
| 61 | S131 | 2 | 0 | 0 | 0 | 0 |
| 61 | S141 | 1 | 0 | 0 | 0 | 0 |
| 61 | S171 | 1 | 0 | 0 | 0 | 0 |
| All | All | 146672 | 0 | 0 | 0 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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 | S021 | 222/241 (92%) | 208 (94%) | 13 (6%) | 1 (0%) | 25 | 49 |
| 3 | S031 | 204/233 (88%) | 193 (95%) | 11 (5%) | 0 | 100 | 100 |
| 4 | S041 | 203/206 (98%) | 200 (98%) | 3 (2%) | 0 | 100 | 100 |
| 5 | S051 | 153/167 (92%) | 144 (94%) | 9 (6%) | 0 | 100 | 100 |
| 6 | S061 | 104/135 (77%) | 102 (98%) | 2 (2%) | 0 | 100 | 100 |
| 7 | S071 | 149/179 (83%) | 139 (93%) | 10 (7%) | 0 | 100 | 100 |
| 8 | S081 | 127/130 (98%) | 125 (98%) | 2 (2%) | 0 | 100 | 100 |
| 9 | S091 | 125/130 (96%) | 115 (92%) | 10 (8%) | 0 | 100 | 100 |
| 10 | S101 | 97/103 (94%) | 91 (94%) | 5 (5%) | 1 (1%) | 13 | 33 |
| 11 | S111 | 115/129 (89%) | 106 (92%) | 9 (8%) | 0 | 100 | 100 |
| 12 | S121 | 120/124 (97%) | 113 (94%) | 7 (6%) | 0 | 100 | 100 |
| 13 | S131 | 112/118 (95%) | 105 (94%) | 6 (5%) | 1 (1%) | 14 | 35 |
| 14 | S141 | 99/102 (97%) | 85 (86%) | 13 (13%) | 1 (1%) | 13 | 33 |
| 15 | S151 | 86/89 (97%) | 83 (96%) | 3 (4%) | 0 | 100 | 100 |
| 16 | S161 | 80/82 (98%) | 75 (94%) | 4 (5%) | 1 (1%) | 10 | 26 |
| 17 | S171 | 78/84 (93%) | 76 (97%) | 2 (3%) | 0 | 100 | 100 |
| 18 | S181 | 53/75 (71%) | 52 (98%) | 1 (2%) | 0 | 100 | 100 |
| 19 | S191 | 80/92 (87%) | 76 (95%) | 4 (5%) | 0 | 100 | 100 |
| 20 | S201 | 84/87 (97%) | 81 (96%) | 3 (4%) | 0 | 100 | 100 |
| 21 | S211 | 54/71 (76%) | 54 (100%) | 0 | 0 | 100 | 100 |
| 24 | L021 | 269/273 (98%) | 263 (98%) | 6 (2%) | 0 | 100 | 100 |
| 25 | L031 | 206/209 (99%) | 200 (97%) | 5 (2%) | 1 (0%) | 25 | 49 |
| 26 | L041 | 199/201 (99%) | 196 (98%) | 3 (2%) | 0 | 100 | 100 |
| 27 | L051 | 175/179 (98%) | 167 (95%) | 8 (5%) | 0 | 100 | 100 |
| 28 | L061 | 174/177 (98%) | 171 (98%) | 3 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 29 | L091 | 147/149 (99%) | 129 (88%) | 17 (12%) | 1 (1%) | 19 | 42 |
| 30 | L311 | 64/70 (91%) | 57 (89%) | 7 (11%) | 0 | 100 | 100 |
| 31 | L131 | 140/142 (99%) | 138 (99%) | 2 (1%) | 0 | 100 | 100 |
| 32 | L141 | 121/123 (98%) | 119 (98%) | 2 (2%) | 0 | 100 | 100 |
| 33 | L151 | 142/144 (99%) | 136 (96%) | 5 (4%) | 1 (1%) | 19 | 42 |
| 34 | L161 | 133/136 (98%) | 132 (99%) | 1 (1%) | 0 | 100 | 100 |
| 35 | L171 | 116/127 (91%) | 111 (96%) | 5 (4%) | 0 | 100 | 100 |
| 36 | L181 | 115/117 (98%) | 112 (97%) | 3 (3%) | 0 | 100 | 100 |
| 37 | L191 | 112/115 (97%) | 109 (97%) | 3 (3%) | 0 | 100 | 100 |
| 38 | L201 | 115/118 (98%) | 115 (100%) | 0 | 0 | 100 | 100 |
| 39 | L211 | 101/103 (98%) | 97 (96%) | 4 (4%) | 0 | 100 | 100 |
| 40 | L221 | 108/110 (98%) | 108 (100%) | 0 | 0 | 100 | 100 |
| 41 | L231 | 91/100 (91%) | 87 (96%) | 4 (4%) | 0 | 100 | 100 |
| 42 | L241 | 100/104 (96%) | 94 (94%) | 6 (6%) | 0 | 100 | 100 |
| 43 | L251 | 92/94 (98%) | 92 (100%) | 0 | 0 | 100 | 100 |
| 44 | L271 | 74/85 (87%) | 72 (97%) | 2 (3%) | 0 | 100 | 100 |
| 45 | L281 | 75/78 (96%) | 75 (100%) | 0 | 0 | 100 | 100 |
| 46 | L291 | 60/63 (95%) | 59 (98%) | 1 (2%) | 0 | 100 | 100 |
| 47 | L301 | 56/59 (95%) | 55 (98%) | 1 (2%) | 0 | 100 | 100 |
| 48 | L321 | 54/57 (95%) | 54 (100%) | 0 | 0 | 100 | 100 |
| 49 | L331 | 49/55 (89%) | 49 (100%) | 0 | 0 | 100 | 100 |
| 50 | L341 | 44/46 (96%) | 42 (96%) | 2 (4%) | 0 | 100 | 100 |
| 51 | L351 | 62/65 (95%) | 59 (95%) | 2 (3%) | 1 (2%) | 8 | 21 |
| 52 | L361 | 36/38 (95%) | 36 (100%) | 0 | 0 | 100 | 100 |
| 53 | SPE1 | 32/34 (94%) | 32 (100%) | 0 | 0 | 100 | 100 |
| All | All | 5607/5948 (94%) | 5389 (96%) | 209 (4%) | 9 (0%) | 45 | 68 |

All (9) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | S101 | 57 | VAL |
| 25 | L031 | 149 | ASN |
| 51 | L351 | 32 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | S131 | 66 | GLU |
| 14 | S141 | 54 | ASP |
| 16 | S161 | 45 | GLU |
| 29 | L091 | 45 | GLU |
| 33 | L151 | 36 | LYS |
| 2 | S021 | 127 | ASP |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 | S021 | 186/199 (94%) | 184 (99%) | 2 (1%) | 70 | 87 |
| 3 | S031 | 170/190 (90%) | 169 (99%) | 1 (1%) | 84 | 94 |
| 4 | S041 | 172/173 (99%) | 169 (98%) | 3 (2%) | 56 | 81 |
| 5 | S051 | 118/126 (94%) | 117 (99%) | 1 (1%) | 79 | 91 |
| 6 | S061 | 92/116 (79%) | 92 (100%) | 0 | 100 | 100 |
| 7 | S071 | 124/147 (84%) | 123 (99%) | 1 (1%) | 79 | 91 |
| 8 | S081 | 104/105 (99%) | 104 (100%) | 0 | 100 | 100 |
| 9 | S091 | 105/107 (98%) | 102 (97%) | 3 (3%) | 37 | 67 |
| 10 | S101 | 87/90 (97%) | 87 (100%) | 0 | 100 | 100 |
| 11 | S111 | 90/99 (91%) | 90 (100%) | 0 | 100 | 100 |
| 12 | S121 | 102/103 (99%) | 100 (98%) | 2 (2%) | 50 | 78 |
| 13 | S131 | 92/96 (96%) | 91 (99%) | 1 (1%) | 70 | 87 |
| 14 | S141 | 79/84 (94%) | 78 (99%) | 1 (1%) | 65 | 85 |
| 15 | S151 | 76/77 (99%) | 75 (99%) | 1 (1%) | 65 | 85 |
| 16 | S161 | 65/65 (100%) | 64 (98%) | 1 (2%) | 60 | 83 |
| 17 | S171 | 74/78 (95%) | 74 (100%) | 0 | 100 | 100 |
| 18 | S181 | 48/65 (74%) | 46 (96%) | 2 (4%) | 25 | 53 |
| 19 | S191 | 71/79 (90%) | 71 (100%) | 0 | 100 | 100 |
| 20 | S201 | 65/66 (98%) | 65 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 21 | S211 | 48/61 (79%) | 47 (98%) | 1 (2%) | 48 | 76 |
| 24 | L021 | 216/218 (99%) | 215 (100%) | 1 (0%) | 86 | 95 |
| 25 | L031 | 163/163 (100%) | 161 (99%) | 2 (1%) | 67 | 86 |
| 26 | L041 | 165/165 (100%) | 163 (99%) | 2 (1%) | 67 | 86 |
| 27 | L051 | 148/150 (99%) | 145 (98%) | 3 (2%) | 50 | 78 |
| 28 | L061 | 137/138 (99%) | 136 (99%) | 1 (1%) | 81 | 93 |
| 29 | L091 | 114/114 (100%) | 112 (98%) | 2 (2%) | 54 | 80 |
| 30 | L311 | 59/62 (95%) | 59 (100%) | 0 | 100 | 100 |
| 31 | L131 | 116/116 (100%) | 116 (100%) | 0 | 100 | 100 |
| 32 | L141 | 104/104 (100%) | 104 (100%) | 0 | 100 | 100 |
| 33 | L151 | 103/103 (100%) | 102 (99%) | 1 (1%) | 73 | 89 |
| 34 | L161 | 108/108 (100%) | 108 (100%) | 0 | 100 | 100 |
| 35 | L171 | 98/103 (95%) | 97 (99%) | 1 (1%) | 73 | 89 |
| 36 | L181 | 87/87 (100%) | 87 (100%) | 0 | 100 | 100 |
| 37 | L191 | 99/100 (99%) | 99 (100%) | 0 | 100 | 100 |
| 38 | L201 | 89/90 (99%) | 88 (99%) | 1 (1%) | 70 | 87 |
| 39 | L211 | 84/84 (100%) | 84 (100%) | 0 | 100 | 100 |
| 40 | L221 | 93/93 (100%) | 92 (99%) | 1 (1%) | 70 | 87 |
| 41 | L231 | 80/84 (95%) | 80 (100%) | 0 | 100 | 100 |
| 42 | L241 | 83/85 (98%) | 83 (100%) | 0 | 100 | 100 |
| 43 | L251 | 78/78 (100%) | 78 (100%) | 0 | 100 | 100 |
| 44 | L271 | 57/63 (90%) | 57 (100%) | 0 | 100 | 100 |
| 45 | L281 | 67/68 (98%) | 65 (97%) | 2 (3%) | 36 | 65 |
| 46 | L291 | 54/55 (98%) | 54 (100%) | 0 | 100 | 100 |
| 47 | L301 | 48/49 (98%) | 48 (100%) | 0 | 100 | 100 |
| 48 | L321 | 47/48 (98%) | 46 (98%) | 1 (2%) | 48 | 76 |
| 49 | L331 | 45/49 (92%) | 45 (100%) | 0 | 100 | 100 |
| 50 | L341 | 38/38 (100%) | 37 (97%) | 1 (3%) | 41 | 70 |
| 51 | L351 | 51/52 (98%) | 51 (100%) | 0 | 100 | 100 |
| 52 | L361 | 34/34 (100%) | 33 (97%) | 1 (3%) | 37 | 67 |
| 53 | SPE1 | 31/31 (100%) | 28 (90%) | 3 (10%) | 6 | 17 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|-------------|
| All | All | 4664/4858 (96%) | 4621 (99%) | 43 (1%) | 74 90 |

All (43) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | S021 | 37 | LYS |
| 2 | S021 | 112 | LYS |
| 3 | S031 | 107 | ARG |
| 4 | S041 | 26 | ARG |
| 4 | S041 | 56 | ARG |
| 4 | S041 | 188 | ARG |
| 5 | S051 | 69 | ARG |
| 7 | S071 | 5 | ARG |
| 9 | S091 | 59 | GLU |
| 9 | S091 | 106 | ARG |
| 9 | S091 | 113 | ARG |
| 12 | S121 | 86 | ARG |
| 12 | S121 | 120 | LYS |
| 13 | S131 | 107 | ARG |
| 14 | S141 | 61 | ARG |
| 15 | S151 | 89 | ARG |
| 16 | S161 | 5 | ARG |
| 18 | S181 | 57 | ARG |
| 18 | S181 | 73 | ARG |
| 21 | S211 | 7 | ARG |
| 24 | L021 | 80 | ARG |
| 25 | L031 | 13 | ARG |
| 25 | L031 | 33 | ARG |
| 26 | L041 | 21 | ARG |
| 26 | L041 | 44 | ARG |
| 27 | L051 | 48 | LYS |
| 27 | L051 | 102 | ARG |
| 27 | L051 | 150 | ARG |
| 28 | L061 | 175 | LYS |
| 29 | L091 | 57 | LYS |
| 29 | L091 | 71 | LYS |
| 33 | L151 | 78 | ARG |
| 35 | L171 | 2 | ARG |
| 38 | L201 | 51 | ARG |
| 40 | L221 | 92 | ARG |
| 45 | L281 | 27 | ARG |
| 45 | L281 | 72 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48 | L321 | 40 | ARG |
| 50 | L341 | 39 | ARG |
| 52 | L361 | 12 | ARG |
| 53 | SPE1 | 4 | ASN |
| 53 | SPE1 | 12 | ARG |
| 53 | SPE1 | 32 | ASN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | 16S1 | 1530/1534 (99%) | 175 (11%) | 1 (0%) |
| 22 | 23S1 | 2890/2897 (99%) | 292 (10%) | 18 (0%) |
| 23 | 05S1 | 119/120 (99%) | 8 (6%) | 0 |
| 54 | MRN1 | 6/7 (85%) | 3 (50%) | 1 (16%) |
| 55 | PTR1 | 73/76 (96%) | 12 (16%) | 1 (1%) |
| All | All | 4618/4634 (99%) | 490 (10%) | 21 (0%) |

All (490) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 16S1 | 4 | U |
| 1 | 16S1 | 7 | A |
| 1 | 16S1 | 9 | G |
| 1 | 16S1 | 32 | A |
| 1 | 16S1 | 39 | G |
| 1 | 16S1 | 47 | C |
| 1 | 16S1 | 48 | C |
| 1 | 16S1 | 50 | A |
| 1 | 16S1 | 51 | A |
| 1 | 16S1 | 71 | A |
| 1 | 16S1 | 72 | A |
| 1 | 16S1 | 75 | G |
| 1 | 16S1 | 76 | G |
| 1 | 16S1 | 78 | A |
| 1 | 16S1 | 79 | G |
| 1 | 16S1 | 83 | C |
| 1 | 16S1 | 84 | U |
| 1 | 16S1 | 85 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 16S1 | 86 | G |
| 1 | 16S1 | 87 | C |
| 1 | 16S1 | 88 | U |
| 1 | 16S1 | 89 | U |
| 1 | 16S1 | 95 | C |
| 1 | 16S1 | 98 | A |
| 1 | 16S1 | 116 | A |
| 1 | 16S1 | 130 | A |
| 1 | 16S1 | 131 | A |
| 1 | 16S1 | 164 | G |
| 1 | 16S1 | 181 | A |
| 1 | 16S1 | 197 | A |
| 1 | 16S1 | 210 | C |
| 1 | 16S1 | 226 | G |
| 1 | 16S1 | 245 | U |
| 1 | 16S1 | 247 | G |
| 1 | 16S1 | 251 | G |
| 1 | 16S1 | 266 | G |
| 1 | 16S1 | 267 | C |
| 1 | 16S1 | 289 | G |
| 1 | 16S1 | 306 | A |
| 1 | 16S1 | 321 | A |
| 1 | 16S1 | 328 | C |
| 1 | 16S1 | 352 | C |
| 1 | 16S1 | 354 | G |
| 1 | 16S1 | 367 | U |
| 1 | 16S1 | 372 | C |
| 1 | 16S1 | 373 | A |
| 1 | 16S1 | 384 | G |
| 1 | 16S1 | 392 | C |
| 1 | 16S1 | 397 | A |
| 1 | 16S1 | 406 | G |
| 1 | 16S1 | 413 | G |
| 1 | 16S1 | 414 | A |
| 1 | 16S1 | 429 | U |
| 1 | 16S1 | 435 | A |
| 1 | 16S1 | 439 | U |
| 1 | 16S1 | 467 | U |
| 1 | 16S1 | 468 | A |
| 1 | 16S1 | 478 | A |
| 1 | 16S1 | 479 | U |
| 1 | 16S1 | 481 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 16S1 | 484 | G |
| 1 | 16S1 | 486 | U |
| 1 | 16S1 | 497 | G |
| 1 | 16S1 | 509 | A |
| 1 | 16S1 | 511 | C |
| 1 | 16S1 | 513 | C |
| 1 | 16S1 | 516 | PSU |
| 1 | 16S1 | 518 | C |
| 1 | 16S1 | 527 | G7M |
| 1 | 16S1 | 528 | C |
| 1 | 16S1 | 532 | A |
| 1 | 16S1 | 547 | A |
| 1 | 16S1 | 559 | A |
| 1 | 16S1 | 572 | A |
| 1 | 16S1 | 573 | A |
| 1 | 16S1 | 576 | C |
| 1 | 16S1 | 577 | G |
| 1 | 16S1 | 579 | A |
| 1 | 16S1 | 633 | G |
| 1 | 16S1 | 650 | G |
| 1 | 16S1 | 653 | U |
| 1 | 16S1 | 665 | A |
| 1 | 16S1 | 718 | A |
| 1 | 16S1 | 721 | G |
| 1 | 16S1 | 722 | G |
| 1 | 16S1 | 734 | G |
| 1 | 16S1 | 748 | G |
| 1 | 16S1 | 755 | G |
| 1 | 16S1 | 777 | A |
| 1 | 16S1 | 793 | U |
| 1 | 16S1 | 794 | A |
| 1 | 16S1 | 815 | A |
| 1 | 16S1 | 817 | C |
| 1 | 16S1 | 821 | G |
| 1 | 16S1 | 828 | U |
| 1 | 16S1 | 832 | G |
| 1 | 16S1 | 841 | C |
| 1 | 16S1 | 842 | U |
| 1 | 16S1 | 843 | U |
| 1 | 16S1 | 846 | G |
| 1 | 16S1 | 926 | G |
| 1 | 16S1 | 934 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 16S1 | 942 | G |
| 1 | 16S1 | 960 | U |
| 1 | 16S1 | 966 | 2MG |
| 1 | 16S1 | 969 | A |
| 1 | 16S1 | 975 | A |
| 1 | 16S1 | 976 | G |
| 1 | 16S1 | 977 | A |
| 1 | 16S1 | 993 | G |
| 1 | 16S1 | 1004 | A |
| 1 | 16S1 | 1005 | A |
| 1 | 16S1 | 1019 | A |
| 1 | 16S1 | 1020 | G |
| 1 | 16S1 | 1026 | G |
| 1 | 16S1 | 1028 | C |
| 1 | 16S1 | 1029 | U |
| 1 | 16S1 | 1030 | U |
| 1 | 16S1 | 1032 | G |
| 1 | 16S1 | 1045 | C |
| 1 | 16S1 | 1053 | G |
| 1 | 16S1 | 1065 | U |
| 1 | 16S1 | 1094 | G |
| 1 | 16S1 | 1095 | U |
| 1 | 16S1 | 1101 | A |
| 1 | 16S1 | 1132 | C |
| 1 | 16S1 | 1139 | G |
| 1 | 16S1 | 1140 | C |
| 1 | 16S1 | 1141 | C |
| 1 | 16S1 | 1157 | A |
| 1 | 16S1 | 1158 | C |
| 1 | 16S1 | 1159 | U |
| 1 | 16S1 | 1169 | A |
| 1 | 16S1 | 1184 | G |
| 1 | 16S1 | 1196 | A |
| 1 | 16S1 | 1197 | A |
| 1 | 16S1 | 1212 | U |
| 1 | 16S1 | 1213 | A |
| 1 | 16S1 | 1225 | A |
| 1 | 16S1 | 1226 | C |
| 1 | 16S1 | 1227 | A |
| 1 | 16S1 | 1238 | A |
| 1 | 16S1 | 1256 | A |
| 1 | 16S1 | 1257 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 16S1 | 1258 | G |
| 1 | 16S1 | 1260 | G |
| 1 | 16S1 | 1280 | A |
| 1 | 16S1 | 1285 | A |
| 1 | 16S1 | 1299 | A |
| 1 | 16S1 | 1300 | G |
| 1 | 16S1 | 1302 | C |
| 1 | 16S1 | 1317 | C |
| 1 | 16S1 | 1318 | A |
| 1 | 16S1 | 1320 | C |
| 1 | 16S1 | 1340 | A |
| 1 | 16S1 | 1346 | A |
| 1 | 16S1 | 1353 | G |
| 1 | 16S1 | 1363 | A |
| 1 | 16S1 | 1364 | U |
| 1 | 16S1 | 1370 | G |
| 1 | 16S1 | 1419 | G |
| 1 | 16S1 | 1429 | A |
| 1 | 16S1 | 1432 | G |
| 1 | 16S1 | 1441 | A |
| 1 | 16S1 | 1487 | G |
| 1 | 16S1 | 1492 | A |
| 1 | 16S1 | 1493 | A |
| 1 | 16S1 | 1497 | G |
| 1 | 16S1 | 1499 | A |
| 1 | 16S1 | 1502 | A |
| 1 | 16S1 | 1503 | A |
| 1 | 16S1 | 1506 | U |
| 1 | 16S1 | 1517 | G |
| 1 | 16S1 | 1529 | G |
| 1 | 16S1 | 1530 | G |
| 22 | 23S1 | 23 | G |
| 22 | 23S1 | 34 | U |
| 22 | 23S1 | 61 | C |
| 22 | 23S1 | 71 | A |
| 22 | 23S1 | 74 | A |
| 22 | 23S1 | 75 | G |
| 22 | 23S1 | 84 | A |
| 22 | 23S1 | 101 | A |
| 22 | 23S1 | 103 | A |
| 22 | 23S1 | 118 | A |
| 22 | 23S1 | 119 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | 23S1 | 120 | U |
| 22 | 23S1 | 163 | C |
| 22 | 23S1 | 165 | A |
| 22 | 23S1 | 181 | A |
| 22 | 23S1 | 196 | A |
| 22 | 23S1 | 215 | G |
| 22 | 23S1 | 216 | A |
| 22 | 23S1 | 221 | A |
| 22 | 23S1 | 222 | A |
| 22 | 23S1 | 233 | A |
| 22 | 23S1 | 248 | G |
| 22 | 23S1 | 265 | A |
| 22 | 23S1 | 276 | U |
| 22 | 23S1 | 278 | A |
| 22 | 23S1 | 302 | C |
| 22 | 23S1 | 303 | G |
| 22 | 23S1 | 311 | A |
| 22 | 23S1 | 330 | A |
| 22 | 23S1 | 386 | G |
| 22 | 23S1 | 396 | G |
| 22 | 23S1 | 411 | G |
| 22 | 23S1 | 467 | G |
| 22 | 23S1 | 481 | G |
| 22 | 23S1 | 491 | G |
| 22 | 23S1 | 505 | A |
| 22 | 23S1 | 509 | C |
| 22 | 23S1 | 529 | A |
| 22 | 23S1 | 530 | G |
| 22 | 23S1 | 531 | C |
| 22 | 23S1 | 532 | A |
| 22 | 23S1 | 544 | C |
| 22 | 23S1 | 546 | U |
| 22 | 23S1 | 547 | A |
| 22 | 23S1 | 548 | G |
| 22 | 23S1 | 549 | G |
| 22 | 23S1 | 563 | A |
| 22 | 23S1 | 573 | U |
| 22 | 23S1 | 575 | A |
| 22 | 23S1 | 586 | A |
| 22 | 23S1 | 603 | A |
| 22 | 23S1 | 613 | A |
| 22 | 23S1 | 614 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | 23S1 | 637 | A |
| 22 | 23S1 | 645 | C |
| 22 | 23S1 | 647 | G |
| 22 | 23S1 | 653 | U |
| 22 | 23S1 | 654 | A |
| 22 | 23S1 | 655 | A |
| 22 | 23S1 | 686 | U |
| 22 | 23S1 | 717 | C |
| 22 | 23S1 | 730 | A |
| 22 | 23S1 | 747 | 5MU |
| 22 | 23S1 | 765 | C |
| 22 | 23S1 | 775 | G |
| 22 | 23S1 | 776 | G |
| 22 | 23S1 | 782 | A |
| 22 | 23S1 | 784 | G |
| 22 | 23S1 | 789 | A |
| 22 | 23S1 | 805 | G |
| 22 | 23S1 | 812 | C |
| 22 | 23S1 | 827 | U |
| 22 | 23S1 | 828 | U |
| 22 | 23S1 | 829 | A |
| 22 | 23S1 | 846 | U |
| 22 | 23S1 | 847 | U |
| 22 | 23S1 | 858 | G |
| 22 | 23S1 | 859 | G |
| 22 | 23S1 | 884 | U |
| 22 | 23S1 | 896 | A |
| 22 | 23S1 | 910 | A |
| 22 | 23S1 | 931 | U |
| 22 | 23S1 | 946 | C |
| 22 | 23S1 | 961 | C |
| 22 | 23S1 | 974 | G |
| 22 | 23S1 | 983 | A |
| 22 | 23S1 | 996 | A |
| 22 | 23S1 | 1005 | C |
| 22 | 23S1 | 1012 | U |
| 22 | 23S1 | 1013 | C |
| 22 | 23S1 | 1022 | G |
| 22 | 23S1 | 1026 | G |
| 22 | 23S1 | 1033 | U |
| 22 | 23S1 | 1054 | A |
| 22 | 23S1 | 1070 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | 23S1 | 1088 | A |
| 22 | 23S1 | 1112 | G |
| 22 | 23S1 | 1130 | U |
| 22 | 23S1 | 1132 | U |
| 22 | 23S1 | 1133 | A |
| 22 | 23S1 | 1135 | C |
| 22 | 23S1 | 1142 | A |
| 22 | 23S1 | 1173 | U |
| 22 | 23S1 | 1174 | U |
| 22 | 23S1 | 1175 | A |
| 22 | 23S1 | 1176 | U |
| 22 | 23S1 | 1212 | G |
| 22 | 23S1 | 1250 | G |
| 22 | 23S1 | 1253 | A |
| 22 | 23S1 | 1256 | G |
| 22 | 23S1 | 1271 | G |
| 22 | 23S1 | 1272 | A |
| 22 | 23S1 | 1300 | G |
| 22 | 23S1 | 1301 | A |
| 22 | 23S1 | 1329 | U |
| 22 | 23S1 | 1352 | U |
| 22 | 23S1 | 1365 | A |
| 22 | 23S1 | 1379 | U |
| 22 | 23S1 | 1383 | A |
| 22 | 23S1 | 1403 | A |
| 22 | 23S1 | 1416 | G |
| 22 | 23S1 | 1420 | A |
| 22 | 23S1 | 1428 | C |
| 22 | 23S1 | 1452 | G |
| 22 | 23S1 | 1453 | A |
| 22 | 23S1 | 1482 | G |
| 22 | 23S1 | 1508 | A |
| 22 | 23S1 | 1509 | A |
| 22 | 23S1 | 1515 | A |
| 22 | 23S1 | 1566 | A |
| 22 | 23S1 | 1569 | A |
| 22 | 23S1 | 1578 | U |
| 22 | 23S1 | 1606 | C |
| 22 | 23S1 | 1608 | A |
| 22 | 23S1 | 1610 | A |
| 22 | 23S1 | 1617 | C |
| 22 | 23S1 | 1647 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | 23S1 | 1648 | U |
| 22 | 23S1 | 1649 | G |
| 22 | 23S1 | 1674 | G |
| 22 | 23S1 | 1729 | U |
| 22 | 23S1 | 1730 | C |
| 22 | 23S1 | 1732 | C |
| 22 | 23S1 | 1738 | G |
| 22 | 23S1 | 1757 | A |
| 22 | 23S1 | 1758 | U |
| 22 | 23S1 | 1764 | C |
| 22 | 23S1 | 1773 | A |
| 22 | 23S1 | 1782 | U |
| 22 | 23S1 | 1800 | C |
| 22 | 23S1 | 1801 | A |
| 22 | 23S1 | 1802 | A |
| 22 | 23S1 | 1808 | A |
| 22 | 23S1 | 1811 | G |
| 22 | 23S1 | 1816 | C |
| 22 | 23S1 | 1829 | A |
| 22 | 23S1 | 1871 | A |
| 22 | 23S1 | 1872 | A |
| 22 | 23S1 | 1873 | G |
| 22 | 23S1 | 1906 | G |
| 22 | 23S1 | 1914 | C |
| 22 | 23S1 | 1929 | G |
| 22 | 23S1 | 1930 | G |
| 22 | 23S1 | 1937 | A |
| 22 | 23S1 | 1938 | A |
| 22 | 23S1 | 1939 | 5MU |
| 22 | 23S1 | 1955 | U |
| 22 | 23S1 | 1967 | C |
| 22 | 23S1 | 1970 | A |
| 22 | 23S1 | 1971 | U |
| 22 | 23S1 | 1972 | G |
| 22 | 23S1 | 1991 | U |
| 22 | 23S1 | 1993 | U |
| 22 | 23S1 | 2020 | A |
| 22 | 23S1 | 2023 | C |
| 22 | 23S1 | 2027 | G |
| 22 | 23S1 | 2031 | A |
| 22 | 23S1 | 2033 | A |
| 22 | 23S1 | 2043 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | 23S1 | 2055 | C |
| 22 | 23S1 | 2056 | G |
| 22 | 23S1 | 2060 | A |
| 22 | 23S1 | 2061 | G |
| 22 | 23S1 | 2069 | G7M |
| 22 | 23S1 | 2093 | G |
| 22 | 23S1 | 2101 | A |
| 22 | 23S1 | 2110 | G |
| 22 | 23S1 | 2111 | U |
| 22 | 23S1 | 2112 | G |
| 22 | 23S1 | 2113 | U |
| 22 | 23S1 | 2115 | G |
| 22 | 23S1 | 2116 | G |
| 22 | 23S1 | 2117 | A |
| 22 | 23S1 | 2118 | U |
| 22 | 23S1 | 2119 | A |
| 22 | 23S1 | 2124 | G |
| 22 | 23S1 | 2125 | G |
| 22 | 23S1 | 2126 | A |
| 22 | 23S1 | 2127 | G |
| 22 | 23S1 | 2128 | G |
| 22 | 23S1 | 2131 | U |
| 22 | 23S1 | 2132 | U |
| 22 | 23S1 | 2133 | G |
| 22 | 23S1 | 2137 | U |
| 22 | 23S1 | 2142 | A |
| 22 | 23S1 | 2146 | C |
| 22 | 23S1 | 2147 | A |
| 22 | 23S1 | 2157 | G |
| 22 | 23S1 | 2158 | A |
| 22 | 23S1 | 2159 | G |
| 22 | 23S1 | 2163 | A |
| 22 | 23S1 | 2164 | C |
| 22 | 23S1 | 2165 | C |
| 22 | 23S1 | 2171 | A |
| 22 | 23S1 | 2172 | U |
| 22 | 23S1 | 2173 | A |
| 22 | 23S1 | 2182 | U |
| 22 | 23S1 | 2183 | A |
| 22 | 23S1 | 2188 | U |
| 22 | 23S1 | 2189 | U |
| 22 | 23S1 | 2190 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | 23S1 | 2195 | U |
| 22 | 23S1 | 2198 | A |
| 22 | 23S1 | 2204 | G |
| 22 | 23S1 | 2211 | A |
| 22 | 23S1 | 2225 | A |
| 22 | 23S1 | 2238 | G |
| 22 | 23S1 | 2239 | G |
| 22 | 23S1 | 2252 | G |
| 22 | 23S1 | 2283 | C |
| 22 | 23S1 | 2287 | A |
| 22 | 23S1 | 2288 | A |
| 22 | 23S1 | 2305 | U |
| 22 | 23S1 | 2308 | G |
| 22 | 23S1 | 2325 | G |
| 22 | 23S1 | 2333 | A |
| 22 | 23S1 | 2336 | A |
| 22 | 23S1 | 2345 | G |
| 22 | 23S1 | 2347 | C |
| 22 | 23S1 | 2350 | C |
| 22 | 23S1 | 2368 | C |
| 22 | 23S1 | 2383 | G |
| 22 | 23S1 | 2385 | C |
| 22 | 23S1 | 2402 | U |
| 22 | 23S1 | 2406 | A |
| 22 | 23S1 | 2425 | A |
| 22 | 23S1 | 2429 | G |
| 22 | 23S1 | 2435 | A |
| 22 | 23S1 | 2441 | U |
| 22 | 23S1 | 2448 | A |
| 22 | 23S1 | 2476 | A |
| 22 | 23S1 | 2478 | A |
| 22 | 23S1 | 2491 | U |
| 22 | 23S1 | 2502 | G |
| 22 | 23S1 | 2504 | PSU |
| 22 | 23S1 | 2505 | G |
| 22 | 23S1 | 2518 | A |
| 22 | 23S1 | 2529 | G |
| 22 | 23S1 | 2547 | A |
| 22 | 23S1 | 2566 | A |
| 22 | 23S1 | 2567 | G |
| 22 | 23S1 | 2573 | C |
| 22 | 23S1 | 2578 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | 23S1 | 2582 | G |
| 22 | 23S1 | 2602 | A |
| 22 | 23S1 | 2609 | U |
| 22 | 23S1 | 2613 | U |
| 22 | 23S1 | 2615 | U |
| 22 | 23S1 | 2629 | U |
| 22 | 23S1 | 2646 | C |
| 22 | 23S1 | 2663 | G |
| 22 | 23S1 | 2689 | U |
| 22 | 23S1 | 2690 | U |
| 22 | 23S1 | 2714 | G |
| 22 | 23S1 | 2726 | A |
| 22 | 23S1 | 2733 | A |
| 22 | 23S1 | 2744 | G |
| 22 | 23S1 | 2748 | A |
| 22 | 23S1 | 2757 | A |
| 22 | 23S1 | 2765 | A |
| 22 | 23S1 | 2778 | A |
| 22 | 23S1 | 2791 | G |
| 22 | 23S1 | 2820 | A |
| 22 | 23S1 | 2821 | A |
| 22 | 23S1 | 2835 | A |
| 22 | 23S1 | 2861 | U |
| 22 | 23S1 | 2873 | A |
| 22 | 23S1 | 2880 | C |
| 22 | 23S1 | 2883 | A |
| 22 | 23S1 | 2884 | U |
| 22 | 23S1 | 2885 | G |
| 22 | 23S1 | 2891 | U |
| 23 | 05S1 | 35 | C |
| 23 | 05S1 | 44 | G |
| 23 | 05S1 | 56 | G |
| 23 | 05S1 | 68 | C |
| 23 | 05S1 | 89 | U |
| 23 | 05S1 | 90 | C |
| 23 | 05S1 | 105 | G |
| 23 | 05S1 | 109 | A |
| 54 | MRN1 | 4 | C |
| 54 | MRN1 | 6 | U |
| 54 | MRN1 | 7 | U |
| 55 | PTR1 | 16 | C |
| 55 | PTR1 | 17 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 55 | PTR1 | 17(A) | G |
| 55 | PTR1 | 19 | A |
| 55 | PTR1 | 20 | U |
| 55 | PTR1 | 31 | G |
| 55 | PTR1 | 46 | G7M |
| 55 | PTR1 | 54 | 5MU |
| 55 | PTR1 | 57 | G |
| 55 | PTR1 | 59 | A |
| 55 | PTR1 | 63 | U |
| 55 | PTR1 | 76 | A |

All (21) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 16S1 | 1225 | A |
| 22 | 23S1 | 125 | A |
| 22 | 23S1 | 199 | A |
| 22 | 23S1 | 685 | A |
| 22 | 23S1 | 764 | A |
| 22 | 23S1 | 784 | G |
| 22 | 23S1 | 984 | A |
| 22 | 23S1 | 1142 | A |
| 22 | 23S1 | 1508 | A |
| 22 | 23S1 | 1608 | A |
| 22 | 23S1 | 1970 | A |
| 22 | 23S1 | 2146 | C |
| 22 | 23S1 | 2162 | G |
| 22 | 23S1 | 2188 | U |
| 22 | 23S1 | 2189 | U |
| 22 | 23S1 | 2251 | OMG |
| 22 | 23S1 | 2518 | A |
| 22 | 23S1 | 2756 | U |
| 22 | 23S1 | 2873 | A |
| 54 | MRN1 | 5 | G |
| 55 | PTR1 | 19 | A |

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

44 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 |
| 1 | MA6 | 16S1 | 1519 | 1 | 18,26,27 | 1.25 | 1 (5%) | 19,38,41 | 3.26 | 3 (15%) |
| 1 | 4OC | 16S1 | 1402 | 1,56 | 20,23,24 | 2.94 | 8 (40%) | 26,32,35 | 1.11 | 2 (7%) |
| 1 | 5MC | 16S1 | 1407 | 1 | 18,22,23 | 3.30 | 7 (38%) | 26,32,35 | 0.99 | 3 (11%) |
| 1 | MA6 | 16S1 | 1518 | 1 | 18,26,27 | 1.30 | 2 (11%) | 19,38,41 | 3.20 | 2 (10%) |
| 22 | PSU | 23S1 | 2504 | 22,57 | 18,21,22 | 4.06 | 7 (38%) | 22,30,33 | 1.76 | 4 (18%) |
| 22 | PSU | 23S1 | 1917 | 22 | 18,21,22 | 4.09 | 7 (38%) | 22,30,33 | 1.62 | 4 (18%) |
| 22 | 2MG | 23S1 | 1835 | 22 | 18,26,27 | 2.25 | 7 (38%) | 16,38,41 | 1.51 | 4 (25%) |
| 22 | 3TD | 23S1 | 1915 | 22 | 18,22,23 | 3.99 | 8 (44%) | 22,32,35 | 1.56 | 2 (9%) |
| 1 | 2MG | 16S1 | 1516 | 1 | 18,26,27 | 2.28 | 7 (38%) | 16,38,41 | 1.58 | 4 (25%) |
| 25 | MEQ | L031 | 150 | 25 | 8,9,10 | 1.58 | 2 (25%) | 5,10,12 | 1.80 | 1 (20%) |
| 34 | 4D4 | L161 | 81 | 34 | 9,11,12 | 2.51 | 4 (44%) | 8,13,15 | 1.14 | 1 (12%) |
| 22 | PSU | 23S1 | 2604 | 22 | 18,21,22 | 3.98 | 7 (38%) | 22,30,33 | 1.75 | 4 (18%) |
| 1 | G7M | 16S1 | 527 | 1,57 | 20,26,27 | 2.36 | 6 (30%) | 17,39,42 | 1.20 | 2 (11%) |
| 22 | PSU | 23S1 | 2605 | 22 | 18,21,22 | 4.03 | 7 (38%) | 22,30,33 | 1.70 | 4 (18%) |
| 1 | 5MC | 16S1 | 967 | 1 | 18,22,23 | 3.35 | 7 (38%) | 26,32,35 | 1.13 | 2 (7%) |
| 1 | 2MG | 16S1 | 1207 | 1,57 | 18,26,27 | 2.38 | 7 (38%) | 16,38,41 | 1.41 | 4 (25%) |
| 53 | FME | SPE1 | 1 | 53 | 8,9,10 | 1.00 | 1 (12%) | 7,9,11 | 0.98 | 0 |
| 55 | 2MG | PTR1 | 37 | 55 | 18,26,27 | 2.36 | 7 (38%) | 16,38,41 | 1.37 | 4 (25%) |
| 55 | RSP | PTR1 | 32 | 55 | 17,21,22 | 3.96 | 6 (35%) | 22,30,33 | 1.23 | 2 (9%) |
| 22 | OMG | 23S1 | 2251 | 55,22,57 | 18,26,27 | 2.41 | 8 (44%) | 19,38,41 | 1.92 | 7 (36%) |
| 22 | OMC | 23S1 | 2498 | 22,56 | 19,22,23 | 2.77 | 8 (42%) | 26,31,34 | 1.00 | 1 (3%) |
| 55 | PSU | PTR1 | 55 | 55 | 18,21,22 | 4.22 | 7 (38%) | 22,30,33 | 1.92 | 5 (22%) |
| 22 | 2MA | 23S1 | 2503 | 22,56,57 | 19,25,26 | 3.21 | 6 (31%) | 21,37,40 | 1.72 | 3 (14%) |
| 22 | PSU | 23S1 | 1911 | 22 | 18,21,22 | 4.13 | 7 (38%) | 22,30,33 | 1.94 | 5 (22%) |
| 22 | 6MZ | 23S1 | 1618 | 22 | 18,25,26 | 2.89 | 4 (22%) | 16,36,39 | 2.30 | 3 (18%) |
| 1 | UR3 | 16S1 | 1498 | 1 | 19,22,23 | 2.98 | 8 (42%) | 26,32,35 | 1.43 | 2 (7%) |
| 22 | 5MU | 23S1 | 747 | 22 | 19,22,23 | 0.92 | 2 (10%) | 28,32,35 | 1.31 | 3 (10%) |
| 22 | 5MC | 23S1 | 1962 | 22,57 | 18,22,23 | 3.26 | 7 (38%) | 26,32,35 | 1.00 | 2 (7%) |
| 22 | 2MG | 23S1 | 2445 | 22 | 18,26,27 | 2.31 | 7 (38%) | 16,38,41 | 1.56 | 4 (25%) |
| 22 | 5MU | 23S1 | 1939 | 22,57 | 19,22,23 | 0.70 | 0 | 28,32,35 | 1.27 | 4 (14%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 22 | PSU | 23S1 | 2457 | 22 | 18,21,22 | 4.03 | 7 (38%) | 22,30,33 | 2.05 | 6 (27%) |
| 55 | 4SU | PTR1 | 8 | 55 | 18,21,22 | 3.48 | 8 (44%) | 26,30,33 | 1.80 | 5 (19%) |
| 55 | G7M | PTR1 | 46 | 55 | 20,26,27 | 2.51 | 7 (35%) | 17,39,42 | 1.20 | 2 (11%) |
| 22 | OMU | 23S1 | 2552 | 22,56 | 19,22,23 | 2.77 | 7 (36%) | 26,31,34 | 1.84 | 5 (19%) |
| 22 | PSU | 23S1 | 2580 | 22,57 | 18,21,22 | 4.03 | 7 (38%) | 22,30,33 | 2.14 | 6 (27%) |
| 22 | 1MG | 23S1 | 745 | 22 | 18,26,27 | 2.47 | 6 (33%) | 19,39,42 | 1.44 | 4 (21%) |
| 1 | PSU | 16S1 | 516 | 1,56 | 18,21,22 | 4.03 | 8 (44%) | 22,30,33 | 1.74 | 6 (27%) |
| 22 | 6MZ | 23S1 | 2030 | 22 | 18,25,26 | 2.86 | 5 (27%) | 16,36,39 | 2.93 | 4 (25%) |
| 22 | PSU | 23S1 | 746 | 22,56 | 18,21,22 | 3.99 | 7 (38%) | 22,30,33 | 1.96 | 5 (22%) |
| 1 | 2MG | 16S1 | 966 | 1 | 18,26,27 | 2.45 | 7 (38%) | 16,38,41 | 1.39 | 3 (18%) |
| 12 | D2T | S121 | 89 | 12 | 7,9,10 | 1.03 | 0 | 6,11,13 | 2.27 | 3 (50%) |
| 55 | 5MU | PTR1 | 54 | 55 | 19,22,23 | 0.98 | 2 (10%) | 28,32,35 | 1.21 | 4 (14%) |
| 22 | G7M | 23S1 | 2069 | 22,57 | 20,26,27 | 2.24 | 6 (30%) | 17,39,42 | 1.25 | 3 (17%) |
| 22 | PSU | 23S1 | 955 | 22 | 18,21,22 | 3.99 | 7 (38%) | 22,30,33 | 1.92 | 4 (18%) |

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 |
|-----|------|-------|------|-------|---------|------------|---------|
| 1 | MA6 | 16S1 | 1519 | 1 | - | 3/7/29/30 | 0/3/3/3 |
| 1 | 4OC | 16S1 | 1402 | 1,56 | - | 1/9/29/30 | 0/2/2/2 |
| 1 | 5MC | 16S1 | 1407 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | MA6 | 16S1 | 1518 | 1 | - | 0/7/29/30 | 0/3/3/3 |
| 22 | PSU | 23S1 | 2504 | 22,57 | - | 2/7/25/26 | 0/2/2/2 |
| 22 | PSU | 23S1 | 1917 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | 2MG | 23S1 | 1835 | 22 | - | 0/5/27/28 | 0/3/3/3 |
| 22 | 3TD | 23S1 | 1915 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 2MG | 16S1 | 1516 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 25 | MEQ | L031 | 150 | 25 | - | 2/8/9/11 | - |
| 34 | 4D4 | L161 | 81 | 34 | - | 3/11/12/14 | - |
| 22 | PSU | 23S1 | 2604 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | G7M | 16S1 | 527 | 1,57 | - | 2/3/25/26 | 0/3/3/3 |
| 22 | PSU | 23S1 | 2605 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MC | 16S1 | 967 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 2MG | 16S1 | 1207 | 1,57 | - | 0/5/27/28 | 0/3/3/3 |
| 53 | FME | SPE1 | 1 | 53 | - | 4/7/9/11 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|----------|---------|-----------|---------|
| 55 | 2MG | PTR1 | 37 | 55 | - | 0/5/27/28 | 0/3/3/3 |
| 55 | RSP | PTR1 | 32 | 55 | - | 2/7/25/26 | 0/2/2/2 |
| 22 | OMG | 23S1 | 2251 | 55,22,57 | - | 1/5/27/28 | 0/3/3/3 |
| 22 | OMC | 23S1 | 2498 | 22,56 | - | 0/9/27/28 | 0/2/2/2 |
| 55 | PSU | PTR1 | 55 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | 2MA | 23S1 | 2503 | 22,56,57 | - | 2/3/25/26 | 0/3/3/3 |
| 22 | PSU | 23S1 | 1911 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | 6MZ | 23S1 | 1618 | 22 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | UR3 | 16S1 | 1498 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | 5MU | 23S1 | 747 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | 5MC | 23S1 | 1962 | 22,57 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | 2MG | 23S1 | 2445 | 22 | - | 1/5/27/28 | 0/3/3/3 |
| 22 | 5MU | 23S1 | 1939 | 22,57 | - | 2/7/25/26 | 0/2/2/2 |
| 22 | PSU | 23S1 | 2457 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 55 | 4SU | PTR1 | 8 | 55 | - | 1/7/25/26 | 0/2/2/2 |
| 55 | G7M | PTR1 | 46 | 55 | - | 1/3/25/26 | 0/3/3/3 |
| 22 | OMU | 23S1 | 2552 | 22,56 | - | 0/9/27/28 | 0/2/2/2 |
| 22 | PSU | 23S1 | 2580 | 22,57 | - | 1/7/25/26 | 0/2/2/2 |
| 22 | 1MG | 23S1 | 745 | 22 | - | 0/3/25/26 | 0/3/3/3 |
| 1 | PSU | 16S1 | 516 | 1,56 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | 6MZ | 23S1 | 2030 | 22 | - | 2/5/27/28 | 0/3/3/3 |
| 22 | PSU | 23S1 | 746 | 22,56 | - | 1/7/25/26 | 0/2/2/2 |
| 1 | 2MG | 16S1 | 966 | 1 | - | 2/5/27/28 | 0/3/3/3 |
| 12 | D2T | S121 | 89 | 12 | - | 1/7/12/14 | - |
| 55 | 5MU | PTR1 | 54 | 55 | - | 2/7/25/26 | 0/2/2/2 |
| 22 | G7M | 23S1 | 2069 | 22,57 | - | 2/3/25/26 | 0/3/3/3 |
| 22 | PSU | 23S1 | 955 | 22 | - | 0/7/25/26 | 0/2/2/2 |

All (256) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 55 | PTR1 | 32 | RSP | C2-N3 | 12.27 | 1.49 | 1.36 |
| 22 | 23S1 | 1915 | 3TD | C6-C5 | 11.53 | 1.48 | 1.35 |
| 22 | 23S1 | 2504 | PSU | C6-C5 | 11.20 | 1.48 | 1.35 |
| 55 | PTR1 | 55 | PSU | C6-C5 | 11.19 | 1.48 | 1.35 |
| 22 | 23S1 | 1911 | PSU | C6-C5 | 11.08 | 1.48 | 1.35 |
| 22 | 23S1 | 1917 | PSU | C6-C5 | 11.08 | 1.48 | 1.35 |
| 22 | 23S1 | 2457 | PSU | C6-C5 | 10.98 | 1.48 | 1.35 |
| 22 | 23S1 | 2605 | PSU | C6-C5 | 10.91 | 1.48 | 1.35 |
| 22 | 23S1 | 955 | PSU | C6-C5 | 10.83 | 1.47 | 1.35 |
| 22 | 23S1 | 1618 | 6MZ | C6-N6 | 10.83 | 1.52 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 2580 | PSU | C6-C5 | 10.77 | 1.47 | 1.35 |
| 22 | 23S1 | 2604 | PSU | C6-C5 | 10.71 | 1.47 | 1.35 |
| 1 | 16S1 | 516 | PSU | C6-C5 | 10.68 | 1.47 | 1.35 |
| 22 | 23S1 | 746 | PSU | C6-C5 | 10.65 | 1.47 | 1.35 |
| 22 | 23S1 | 2030 | 6MZ | C6-N6 | 10.54 | 1.52 | 1.35 |
| 22 | 23S1 | 1911 | PSU | C2-N1 | 9.38 | 1.49 | 1.36 |
| 55 | PTR1 | 55 | PSU | C2-N1 | 9.36 | 1.49 | 1.36 |
| 22 | 23S1 | 1917 | PSU | C2-N1 | 9.13 | 1.49 | 1.36 |
| 22 | 23S1 | 2605 | PSU | C2-N1 | 9.11 | 1.49 | 1.36 |
| 1 | 16S1 | 516 | PSU | C2-N1 | 9.09 | 1.49 | 1.36 |
| 22 | 23S1 | 2604 | PSU | C2-N1 | 8.98 | 1.48 | 1.36 |
| 22 | 23S1 | 2457 | PSU | C2-N1 | 8.90 | 1.48 | 1.36 |
| 22 | 23S1 | 746 | PSU | C2-N1 | 8.83 | 1.48 | 1.36 |
| 1 | 16S1 | 1407 | 5MC | C6-C5 | 8.73 | 1.48 | 1.34 |
| 22 | 23S1 | 2504 | PSU | C2-N1 | 8.72 | 1.48 | 1.36 |
| 22 | 23S1 | 2580 | PSU | C2-N1 | 8.68 | 1.48 | 1.36 |
| 22 | 23S1 | 955 | PSU | C2-N1 | 8.58 | 1.48 | 1.36 |
| 1 | 16S1 | 967 | 5MC | C6-C5 | 8.53 | 1.48 | 1.34 |
| 22 | 23S1 | 1962 | 5MC | C6-C5 | 8.44 | 1.48 | 1.34 |
| 22 | 23S1 | 1915 | 3TD | C2-N1 | 8.24 | 1.47 | 1.37 |
| 22 | 23S1 | 2503 | 2MA | C4-N3 | 8.09 | 1.48 | 1.35 |
| 1 | 16S1 | 1498 | UR3 | C2-N1 | 8.05 | 1.50 | 1.38 |
| 55 | PTR1 | 55 | PSU | C2-N3 | 7.20 | 1.49 | 1.37 |
| 22 | 23S1 | 2503 | 2MA | C2-N3 | 7.04 | 1.46 | 1.34 |
| 55 | PTR1 | 8 | 4SU | C4-N3 | 7.02 | 1.45 | 1.37 |
| 22 | 23S1 | 2580 | PSU | C2-N3 | 6.78 | 1.49 | 1.37 |
| 22 | 23S1 | 2504 | PSU | C2-N3 | 6.74 | 1.49 | 1.37 |
| 22 | 23S1 | 1911 | PSU | C2-N3 | 6.74 | 1.49 | 1.37 |
| 22 | 23S1 | 955 | PSU | C2-N3 | 6.70 | 1.49 | 1.37 |
| 22 | 23S1 | 1917 | PSU | C2-N3 | 6.60 | 1.48 | 1.37 |
| 55 | PTR1 | 8 | 4SU | C2-N1 | 6.58 | 1.49 | 1.38 |
| 22 | 23S1 | 746 | PSU | C2-N3 | 6.56 | 1.48 | 1.37 |
| 22 | 23S1 | 2605 | PSU | C2-N3 | 6.50 | 1.48 | 1.37 |
| 1 | 16S1 | 516 | PSU | C2-N3 | 6.49 | 1.48 | 1.37 |
| 22 | 23S1 | 2457 | PSU | C2-N3 | 6.45 | 1.48 | 1.37 |
| 55 | PTR1 | 8 | 4SU | C2-N3 | 6.41 | 1.49 | 1.38 |
| 22 | 23S1 | 2604 | PSU | C2-N3 | 6.29 | 1.48 | 1.37 |
| 22 | 23S1 | 2552 | OMU | C2-N1 | 6.28 | 1.48 | 1.38 |
| 1 | 16S1 | 1402 | 4OC | C4-N3 | 6.16 | 1.43 | 1.32 |
| 22 | 23S1 | 745 | 1MG | C2-N3 | 6.15 | 1.45 | 1.34 |
| 1 | 16S1 | 967 | 5MC | C4-N3 | 6.15 | 1.44 | 1.34 |
| 1 | 16S1 | 1402 | 4OC | C6-C5 | 6.00 | 1.49 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 22 | 23S1 | 2503 | 2MA | C2-N1 | 5.90 | 1.44 | 1.34 |
| 22 | 23S1 | 2552 | OMU | C2-N3 | 5.90 | 1.48 | 1.38 |
| 22 | 23S1 | 1962 | 5MC | C4-N3 | 5.87 | 1.44 | 1.34 |
| 55 | PTR1 | 32 | RSP | C6-C5 | 5.80 | 1.48 | 1.35 |
| 34 | L161 | 81 | 4D4 | CZ-NE | 5.77 | 1.44 | 1.33 |
| 1 | 16S1 | 967 | 5MC | C2-N3 | 5.66 | 1.47 | 1.36 |
| 22 | 23S1 | 2498 | OMC | C6-C5 | 5.65 | 1.48 | 1.35 |
| 1 | 16S1 | 1498 | UR3 | C6-C5 | 5.63 | 1.48 | 1.35 |
| 22 | 23S1 | 1962 | 5MC | C2-N3 | 5.60 | 1.47 | 1.36 |
| 1 | 16S1 | 1402 | 4OC | C2-N3 | 5.52 | 1.47 | 1.36 |
| 55 | PTR1 | 8 | 4SU | C6-C5 | 5.50 | 1.47 | 1.35 |
| 22 | 23S1 | 2498 | OMC | C2-N3 | 5.50 | 1.47 | 1.36 |
| 1 | 16S1 | 1407 | 5MC | C2-N3 | 5.45 | 1.47 | 1.36 |
| 55 | PTR1 | 46 | G7M | C2-N3 | 5.44 | 1.46 | 1.33 |
| 1 | 16S1 | 1407 | 5MC | C4-N3 | 5.38 | 1.43 | 1.34 |
| 1 | 16S1 | 527 | G7M | C2-N3 | 5.38 | 1.46 | 1.33 |
| 1 | 16S1 | 966 | 2MG | C2-N2 | 5.26 | 1.45 | 1.33 |
| 22 | 23S1 | 2552 | OMU | C6-C5 | 5.16 | 1.47 | 1.35 |
| 55 | PTR1 | 32 | RSP | C4-N4 | 5.11 | 1.46 | 1.33 |
| 55 | PTR1 | 32 | RSP | C4-N3 | 5.10 | 1.44 | 1.34 |
| 55 | PTR1 | 37 | 2MG | C2-N2 | 5.03 | 1.44 | 1.33 |
| 22 | 23S1 | 745 | 1MG | C4-N3 | 4.98 | 1.49 | 1.37 |
| 22 | 23S1 | 1915 | 3TD | C6-N1 | 4.97 | 1.44 | 1.36 |
| 1 | 16S1 | 1207 | 2MG | C2-N2 | 4.94 | 1.44 | 1.33 |
| 55 | PTR1 | 46 | G7M | C4-N3 | 4.89 | 1.49 | 1.37 |
| 55 | PTR1 | 55 | PSU | C6-N1 | 4.87 | 1.44 | 1.36 |
| 22 | 23S1 | 2251 | OMG | C2-N3 | 4.85 | 1.45 | 1.33 |
| 1 | 16S1 | 966 | 2MG | C4-N3 | 4.82 | 1.49 | 1.37 |
| 22 | 23S1 | 2503 | 2MA | C6-N1 | 4.80 | 1.42 | 1.33 |
| 1 | 16S1 | 527 | G7M | C4-N3 | 4.78 | 1.49 | 1.37 |
| 1 | 16S1 | 1516 | 2MG | C2-N2 | 4.78 | 1.44 | 1.33 |
| 55 | PTR1 | 46 | G7M | C6-N1 | 4.76 | 1.45 | 1.37 |
| 22 | 23S1 | 2445 | 2MG | C2-N2 | 4.76 | 1.43 | 1.33 |
| 1 | 16S1 | 516 | PSU | C6-N1 | 4.75 | 1.44 | 1.36 |
| 22 | 23S1 | 2069 | G7M | C2-N3 | 4.71 | 1.44 | 1.33 |
| 22 | 23S1 | 1917 | PSU | C6-N1 | 4.68 | 1.44 | 1.36 |
| 1 | 16S1 | 966 | 2MG | C2-N1 | 4.67 | 1.44 | 1.36 |
| 1 | 16S1 | 1498 | UR3 | C2-N3 | 4.64 | 1.48 | 1.39 |
| 22 | 23S1 | 1911 | PSU | C6-N1 | 4.62 | 1.43 | 1.36 |
| 22 | 23S1 | 2251 | OMG | C4-N3 | 4.59 | 1.48 | 1.37 |
| 22 | 23S1 | 1915 | 3TD | C1'-C5 | -4.59 | 1.39 | 1.50 |
| 22 | 23S1 | 1835 | 2MG | C2-N2 | 4.58 | 1.43 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | 23S1 | 746 | PSU | C6-N1 | 4.56 | 1.43 | 1.36 |
| 1 | 16S1 | 1207 | 2MG | C4-N3 | 4.50 | 1.48 | 1.37 |
| 55 | PTR1 | 8 | 4SU | C4-S4 | -4.50 | 1.59 | 1.68 |
| 1 | 16S1 | 1407 | 5MC | C6-N1 | 4.49 | 1.45 | 1.38 |
| 55 | PTR1 | 37 | 2MG | C2-N1 | 4.49 | 1.43 | 1.36 |
| 1 | 16S1 | 527 | G7M | C6-N1 | 4.46 | 1.44 | 1.37 |
| 1 | 16S1 | 1207 | 2MG | C2-N1 | 4.45 | 1.43 | 1.36 |
| 22 | 23S1 | 2069 | G7M | C4-N3 | 4.45 | 1.48 | 1.37 |
| 22 | 23S1 | 2069 | G7M | C6-N1 | 4.45 | 1.44 | 1.37 |
| 22 | 23S1 | 2604 | PSU | C6-N1 | 4.44 | 1.43 | 1.36 |
| 22 | 23S1 | 2498 | OMC | C2-N1 | 4.44 | 1.49 | 1.40 |
| 22 | 23S1 | 2457 | PSU | C6-N1 | 4.44 | 1.43 | 1.36 |
| 22 | 23S1 | 2498 | OMC | C4-N4 | 4.42 | 1.44 | 1.33 |
| 22 | 23S1 | 745 | 1MG | C2-N2 | 4.41 | 1.42 | 1.34 |
| 22 | 23S1 | 2605 | PSU | C6-N1 | 4.41 | 1.43 | 1.36 |
| 55 | PTR1 | 37 | 2MG | C4-N3 | 4.39 | 1.48 | 1.37 |
| 22 | 23S1 | 955 | PSU | C6-N1 | 4.34 | 1.43 | 1.36 |
| 22 | 23S1 | 2504 | PSU | C6-N1 | 4.34 | 1.43 | 1.36 |
| 22 | 23S1 | 2498 | OMC | C4-N3 | 4.33 | 1.43 | 1.34 |
| 1 | 16S1 | 1498 | UR3 | O4-C4 | -4.33 | 1.14 | 1.23 |
| 1 | 16S1 | 1516 | 2MG | C4-N3 | 4.32 | 1.47 | 1.37 |
| 22 | 23S1 | 2251 | OMG | C2-N2 | 4.31 | 1.44 | 1.34 |
| 22 | 23S1 | 2580 | PSU | C6-N1 | 4.29 | 1.43 | 1.36 |
| 55 | PTR1 | 8 | 4SU | C5-C4 | 4.28 | 1.48 | 1.42 |
| 22 | 23S1 | 2445 | 2MG | C4-N3 | 4.20 | 1.47 | 1.37 |
| 22 | 23S1 | 1915 | 3TD | C2-N3 | 4.20 | 1.47 | 1.38 |
| 22 | 23S1 | 1835 | 2MG | C4-N3 | 4.12 | 1.47 | 1.37 |
| 1 | 16S1 | 1516 | 2MG | C2-N1 | 4.11 | 1.43 | 1.36 |
| 1 | 16S1 | 967 | 5MC | C4-N4 | 4.10 | 1.44 | 1.34 |
| 1 | 16S1 | 1402 | 4OC | C4-N4 | 4.06 | 1.44 | 1.35 |
| 22 | 23S1 | 1835 | 2MG | C2-N1 | 4.02 | 1.43 | 1.36 |
| 1 | 16S1 | 967 | 5MC | C6-N1 | 3.98 | 1.44 | 1.38 |
| 55 | PTR1 | 46 | G7M | C2-N2 | 3.92 | 1.43 | 1.34 |
| 22 | 23S1 | 2445 | 2MG | C2-N1 | 3.90 | 1.43 | 1.36 |
| 1 | 16S1 | 967 | 5MC | C2-N1 | 3.90 | 1.48 | 1.40 |
| 1 | 16S1 | 1407 | 5MC | C4-N4 | 3.90 | 1.44 | 1.34 |
| 1 | 16S1 | 1402 | 4OC | C2-N1 | 3.88 | 1.48 | 1.40 |
| 22 | 23S1 | 1962 | 5MC | C4-N4 | 3.88 | 1.44 | 1.34 |
| 22 | 23S1 | 1962 | 5MC | C6-N1 | 3.83 | 1.44 | 1.38 |
| 55 | PTR1 | 55 | PSU | C4-N3 | 3.77 | 1.45 | 1.38 |
| 22 | 23S1 | 2069 | G7M | C2-N2 | 3.73 | 1.43 | 1.34 |
| 1 | 16S1 | 527 | G7M | C2-N2 | 3.71 | 1.43 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 22 | 23S1 | 2552 | OMU | O4-C4 | -3.62 | 1.17 | 1.24 |
| 1 | 16S1 | 1402 | 4OC | O2-C2 | -3.59 | 1.17 | 1.23 |
| 55 | PTR1 | 46 | G7M | C5-C6 | 3.58 | 1.54 | 1.45 |
| 1 | 16S1 | 1402 | 4OC | C5-C4 | 3.57 | 1.48 | 1.40 |
| 22 | 23S1 | 1962 | 5MC | C2-N1 | 3.56 | 1.47 | 1.40 |
| 22 | 23S1 | 2445 | 2MG | C5-C4 | -3.51 | 1.34 | 1.43 |
| 1 | 16S1 | 1407 | 5MC | C2-N1 | 3.48 | 1.47 | 1.40 |
| 55 | PTR1 | 32 | RSP | C6-N1 | 3.47 | 1.46 | 1.38 |
| 1 | 16S1 | 966 | 2MG | C6-N1 | 3.46 | 1.43 | 1.37 |
| 1 | 16S1 | 1207 | 2MG | C6-N1 | 3.45 | 1.43 | 1.37 |
| 22 | 23S1 | 1911 | PSU | C4-N3 | 3.45 | 1.45 | 1.38 |
| 22 | 23S1 | 955 | PSU | C4-N3 | 3.44 | 1.45 | 1.38 |
| 22 | 23S1 | 2552 | OMU | C4-N3 | 3.43 | 1.44 | 1.38 |
| 22 | 23S1 | 1917 | PSU | C4-N3 | 3.41 | 1.45 | 1.38 |
| 22 | 23S1 | 2504 | PSU | C4-N3 | 3.39 | 1.45 | 1.38 |
| 1 | 16S1 | 516 | PSU | C4-N3 | 3.37 | 1.45 | 1.38 |
| 1 | 16S1 | 527 | G7M | C5-C6 | 3.36 | 1.54 | 1.45 |
| 22 | 23S1 | 1835 | 2MG | C5-C4 | -3.32 | 1.34 | 1.43 |
| 22 | 23S1 | 2580 | PSU | C4-N3 | 3.29 | 1.44 | 1.38 |
| 22 | 23S1 | 2604 | PSU | C4-N3 | 3.28 | 1.44 | 1.38 |
| 1 | 16S1 | 1516 | 2MG | C5-C4 | -3.28 | 1.34 | 1.43 |
| 22 | 23S1 | 1835 | 2MG | C6-N1 | 3.23 | 1.42 | 1.37 |
| 25 | L031 | 150 | MEQ | OE1-CD | -3.20 | 1.16 | 1.23 |
| 1 | 16S1 | 1407 | 5MC | O2-C2 | -3.20 | 1.17 | 1.23 |
| 55 | PTR1 | 37 | 2MG | C6-N1 | 3.20 | 1.42 | 1.37 |
| 22 | 23S1 | 2605 | PSU | C4-N3 | 3.16 | 1.44 | 1.38 |
| 55 | PTR1 | 32 | RSP | C2-S2 | -3.15 | 1.59 | 1.67 |
| 34 | L161 | 81 | 4D4 | CZ-NH2 | 3.15 | 1.44 | 1.32 |
| 22 | 23S1 | 2251 | OMG | C5-C4 | -3.15 | 1.35 | 1.43 |
| 22 | 23S1 | 1962 | 5MC | O2-C2 | -3.13 | 1.17 | 1.23 |
| 22 | 23S1 | 2069 | G7M | C5-C6 | 3.13 | 1.53 | 1.45 |
| 22 | 23S1 | 2498 | OMC | O2-C2 | -3.13 | 1.17 | 1.23 |
| 1 | 16S1 | 1518 | MA6 | C5-C4 | -3.09 | 1.32 | 1.40 |
| 22 | 23S1 | 745 | 1MG | C5-C4 | -3.09 | 1.35 | 1.43 |
| 22 | 23S1 | 746 | PSU | C4-N3 | 3.08 | 1.44 | 1.38 |
| 1 | 16S1 | 1519 | MA6 | C5-C4 | -3.06 | 1.32 | 1.40 |
| 22 | 23S1 | 2457 | PSU | C4-N3 | 3.02 | 1.44 | 1.38 |
| 1 | 16S1 | 1207 | 2MG | C5-C4 | -3.01 | 1.35 | 1.43 |
| 1 | 16S1 | 1498 | UR3 | O2-C2 | -3.00 | 1.17 | 1.22 |
| 1 | 16S1 | 1498 | UR3 | C5-C4 | 3.00 | 1.51 | 1.43 |
| 22 | 23S1 | 2445 | 2MG | C6-N1 | 2.98 | 1.42 | 1.37 |
| 55 | PTR1 | 37 | 2MG | C5-C4 | -2.97 | 1.35 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22 | 23S1 | 2552 | OMU | O2-C2 | -2.97 | 1.17 | 1.23 |
| 1 | 16S1 | 1402 | 4OC | C6-N1 | 2.97 | 1.45 | 1.38 |
| 22 | 23S1 | 2251 | OMG | C6-N1 | 2.94 | 1.42 | 1.37 |
| 22 | 23S1 | 2445 | 2MG | O6-C6 | -2.93 | 1.17 | 1.23 |
| 1 | 16S1 | 967 | 5MC | O2-C2 | -2.92 | 1.18 | 1.23 |
| 1 | 16S1 | 1207 | 2MG | C5-C6 | 2.91 | 1.53 | 1.47 |
| 22 | 23S1 | 1618 | 6MZ | C2-N3 | 2.90 | 1.36 | 1.32 |
| 1 | 16S1 | 966 | 2MG | C5-C4 | -2.87 | 1.35 | 1.43 |
| 55 | PTR1 | 8 | 4SU | C6-N1 | 2.86 | 1.44 | 1.38 |
| 22 | 23S1 | 2030 | 6MZ | C2-N3 | 2.86 | 1.36 | 1.32 |
| 22 | 23S1 | 2580 | PSU | O4-C4 | -2.85 | 1.18 | 1.23 |
| 55 | PTR1 | 37 | 2MG | C5-C6 | 2.84 | 1.53 | 1.47 |
| 1 | 16S1 | 1516 | 2MG | C6-N1 | 2.84 | 1.42 | 1.37 |
| 22 | 23S1 | 2498 | OMC | C6-N1 | 2.83 | 1.44 | 1.38 |
| 55 | PTR1 | 54 | 5MU | C2-N1 | 2.77 | 1.42 | 1.38 |
| 22 | 23S1 | 2503 | 2MA | C6-C5 | 2.76 | 1.53 | 1.43 |
| 22 | 23S1 | 2457 | PSU | O4-C4 | -2.74 | 1.18 | 1.23 |
| 22 | 23S1 | 1835 | 2MG | O6-C6 | -2.72 | 1.17 | 1.23 |
| 22 | 23S1 | 2030 | 6MZ | C5-C4 | -2.71 | 1.33 | 1.40 |
| 1 | 16S1 | 1516 | 2MG | C5-C6 | 2.70 | 1.52 | 1.47 |
| 22 | 23S1 | 2445 | 2MG | C5-C6 | 2.69 | 1.52 | 1.47 |
| 22 | 23S1 | 2580 | PSU | O4'-C1' | -2.69 | 1.40 | 1.43 |
| 22 | 23S1 | 2251 | OMG | O6-C6 | -2.68 | 1.17 | 1.23 |
| 22 | 23S1 | 1915 | 3TD | O2-C2 | -2.62 | 1.18 | 1.23 |
| 22 | 23S1 | 1618 | 6MZ | C5-C4 | -2.62 | 1.34 | 1.40 |
| 22 | 23S1 | 745 | 1MG | O6-C6 | -2.61 | 1.17 | 1.22 |
| 1 | 16S1 | 1516 | 2MG | O6-C6 | -2.59 | 1.18 | 1.23 |
| 22 | 23S1 | 1618 | 6MZ | C9-N6 | 2.58 | 1.49 | 1.45 |
| 22 | 23S1 | 2604 | PSU | O4-C4 | -2.58 | 1.18 | 1.23 |
| 22 | 23S1 | 2251 | OMG | C5-C6 | 2.57 | 1.52 | 1.47 |
| 55 | PTR1 | 46 | G7M | C2-N1 | 2.57 | 1.44 | 1.37 |
| 22 | 23S1 | 955 | PSU | O4-C4 | -2.55 | 1.18 | 1.23 |
| 1 | 16S1 | 966 | 2MG | O6-C6 | -2.54 | 1.18 | 1.23 |
| 22 | 23S1 | 746 | PSU | O4-C4 | -2.53 | 1.18 | 1.23 |
| 1 | 16S1 | 527 | G7M | C2-N1 | 2.53 | 1.43 | 1.37 |
| 22 | 23S1 | 2605 | PSU | O4-C4 | -2.53 | 1.18 | 1.23 |
| 1 | 16S1 | 966 | 2MG | C5-C6 | 2.50 | 1.52 | 1.47 |
| 22 | 23S1 | 2503 | 2MA | C6-N6 | -2.48 | 1.24 | 1.34 |
| 1 | 16S1 | 1207 | 2MG | O6-C6 | -2.44 | 1.18 | 1.23 |
| 55 | PTR1 | 46 | G7M | O4'-C1' | -2.44 | 1.37 | 1.41 |
| 34 | L161 | 81 | 4D4 | CZ-NH1 | -2.43 | 1.24 | 1.34 |
| 22 | 23S1 | 2504 | PSU | O4-C4 | -2.42 | 1.19 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 55 | PTR1 | 37 | 2MG | O6-C6 | -2.40 | 1.18 | 1.23 |
| 55 | PTR1 | 8 | 4SU | O2-C2 | -2.38 | 1.18 | 1.23 |
| 22 | 23S1 | 2552 | OMU | C6-N1 | 2.38 | 1.43 | 1.38 |
| 1 | 16S1 | 1498 | UR3 | C6-N1 | 2.37 | 1.43 | 1.38 |
| 22 | 23S1 | 747 | 5MU | C5M-C5 | -2.36 | 1.44 | 1.50 |
| 22 | 23S1 | 2030 | 6MZ | C9-N6 | 2.35 | 1.49 | 1.45 |
| 22 | 23S1 | 1915 | 3TD | C4-N3 | 2.33 | 1.45 | 1.40 |
| 22 | 23S1 | 746 | PSU | O4'-C1' | -2.33 | 1.40 | 1.43 |
| 22 | 23S1 | 1835 | 2MG | C5-C6 | 2.32 | 1.52 | 1.47 |
| 1 | 16S1 | 516 | PSU | O4-C4 | -2.32 | 1.19 | 1.23 |
| 22 | 23S1 | 1911 | PSU | O4-C4 | -2.30 | 1.19 | 1.23 |
| 22 | 23S1 | 1917 | PSU | O4-C4 | -2.29 | 1.19 | 1.23 |
| 22 | 23S1 | 2069 | G7M | C2-N1 | 2.29 | 1.43 | 1.37 |
| 22 | 23S1 | 1917 | PSU | C1'-C5 | 2.29 | 1.55 | 1.50 |
| 1 | 16S1 | 516 | PSU | O4'-C1' | -2.27 | 1.40 | 1.43 |
| 22 | 23S1 | 2605 | PSU | C1'-C5 | 2.23 | 1.55 | 1.50 |
| 25 | L031 | 150 | MEQ | CD-NE2 | 2.23 | 1.44 | 1.34 |
| 22 | 23S1 | 2504 | PSU | C1'-C5 | 2.20 | 1.55 | 1.50 |
| 55 | PTR1 | 55 | PSU | C1'-C5 | 2.18 | 1.55 | 1.50 |
| 22 | 23S1 | 2251 | OMG | C2-N1 | 2.17 | 1.43 | 1.37 |
| 55 | PTR1 | 55 | PSU | O4-C4 | -2.14 | 1.19 | 1.23 |
| 1 | 16S1 | 1518 | MA6 | C4-N3 | -2.14 | 1.32 | 1.35 |
| 22 | 23S1 | 2498 | OMC | C5-C4 | 2.13 | 1.47 | 1.42 |
| 22 | 23S1 | 2604 | PSU | C1'-C5 | 2.12 | 1.55 | 1.50 |
| 1 | 16S1 | 1498 | UR3 | C3U-N3 | -2.11 | 1.43 | 1.47 |
| 22 | 23S1 | 745 | 1MG | C5-C6 | 2.11 | 1.53 | 1.47 |
| 22 | 23S1 | 747 | 5MU | C2-N1 | 2.10 | 1.41 | 1.38 |
| 22 | 23S1 | 2457 | PSU | O4'-C1' | -2.08 | 1.41 | 1.43 |
| 22 | 23S1 | 1915 | 3TD | O4-C4 | -2.08 | 1.18 | 1.23 |
| 22 | 23S1 | 2030 | 6MZ | C6-N1 | -2.07 | 1.31 | 1.34 |
| 22 | 23S1 | 955 | PSU | C1'-C5 | 2.06 | 1.54 | 1.50 |
| 22 | 23S1 | 1911 | PSU | C1'-C5 | 2.05 | 1.54 | 1.50 |
| 1 | 16S1 | 516 | PSU | C1'-C5 | 2.04 | 1.54 | 1.50 |
| 55 | PTR1 | 54 | 5MU | C2-N3 | 2.04 | 1.41 | 1.38 |
| 53 | SPE1 | 1 | FME | CA-N | -2.02 | 1.43 | 1.46 |
| 34 | L161 | 81 | 4D4 | OB-CB | -2.01 | 1.39 | 1.43 |

All (151) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 16S1 | 1519 | MA6 | N1-C6-N6 | -12.35 | 104.06 | 117.06 |
| 1 | 16S1 | 1518 | MA6 | N1-C6-N6 | -12.19 | 104.23 | 117.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 23S1 | 2030 | 6MZ | C9-N6-C6 | -7.60 | 116.33 | 122.87 |
| 1 | 16S1 | 1519 | MA6 | N3-C2-N1 | -6.34 | 118.78 | 128.68 |
| 22 | 23S1 | 2503 | 2MA | C2-N3-C4 | 6.17 | 120.53 | 115.52 |
| 1 | 16S1 | 1518 | MA6 | N3-C2-N1 | -6.09 | 119.17 | 128.68 |
| 22 | 23S1 | 1618 | 6MZ | N3-C2-N1 | -6.07 | 119.19 | 128.68 |
| 22 | 23S1 | 2030 | 6MZ | N3-C2-N1 | -5.86 | 119.51 | 128.68 |
| 22 | 23S1 | 2552 | OMU | C4-N3-C2 | -5.86 | 118.85 | 126.58 |
| 55 | PTR1 | 8 | 4SU | C4-N3-C2 | -5.62 | 121.88 | 127.34 |
| 1 | 16S1 | 1498 | UR3 | C4-N3-C2 | -5.30 | 119.57 | 124.56 |
| 22 | 23S1 | 2030 | 6MZ | C2-N1-C6 | 5.27 | 121.11 | 116.59 |
| 22 | 23S1 | 2580 | PSU | C4-N3-C2 | -5.09 | 119.01 | 126.34 |
| 22 | 23S1 | 1915 | 3TD | N1-C2-N3 | 5.09 | 120.15 | 116.14 |
| 22 | 23S1 | 2457 | PSU | N1-C2-N3 | 5.07 | 120.88 | 115.13 |
| 22 | 23S1 | 2580 | PSU | N1-C2-N3 | 5.01 | 120.81 | 115.13 |
| 22 | 23S1 | 746 | PSU | C4-N3-C2 | -5.00 | 119.14 | 126.34 |
| 22 | 23S1 | 1911 | PSU | C4-N3-C2 | -4.98 | 119.17 | 126.34 |
| 22 | 23S1 | 2457 | PSU | C4-N3-C2 | -4.79 | 119.44 | 126.34 |
| 55 | PTR1 | 55 | PSU | C4-N3-C2 | -4.78 | 119.45 | 126.34 |
| 22 | 23S1 | 955 | PSU | C4-N3-C2 | -4.78 | 119.46 | 126.34 |
| 22 | 23S1 | 746 | PSU | N1-C2-N3 | 4.77 | 120.54 | 115.13 |
| 22 | 23S1 | 955 | PSU | N1-C2-N3 | 4.66 | 120.41 | 115.13 |
| 22 | 23S1 | 1911 | PSU | N1-C2-N3 | 4.63 | 120.38 | 115.13 |
| 22 | 23S1 | 1618 | 6MZ | C9-N6-C6 | -4.57 | 118.94 | 122.87 |
| 55 | PTR1 | 8 | 4SU | C5-C4-N3 | 4.57 | 118.93 | 114.69 |
| 22 | 23S1 | 2605 | PSU | C4-N3-C2 | -4.46 | 119.91 | 126.34 |
| 22 | 23S1 | 2604 | PSU | C4-N3-C2 | -4.43 | 119.96 | 126.34 |
| 55 | PTR1 | 55 | PSU | N1-C2-N3 | 4.32 | 120.03 | 115.13 |
| 1 | 16S1 | 516 | PSU | C4-N3-C2 | -4.26 | 120.19 | 126.34 |
| 22 | 23S1 | 2504 | PSU | N1-C2-N3 | 4.26 | 119.96 | 115.13 |
| 22 | 23S1 | 2504 | PSU | C4-N3-C2 | -4.24 | 120.22 | 126.34 |
| 22 | 23S1 | 1618 | 6MZ | C2-N1-C6 | 4.21 | 120.20 | 116.59 |
| 22 | 23S1 | 2604 | PSU | N1-C2-N3 | 4.15 | 119.83 | 115.13 |
| 22 | 23S1 | 745 | 1MG | C5-C6-N1 | 4.12 | 120.09 | 113.90 |
| 22 | 23S1 | 2552 | OMU | N3-C2-N1 | 4.08 | 120.30 | 114.89 |
| 22 | 23S1 | 1917 | PSU | C4-N3-C2 | -3.91 | 120.70 | 126.34 |
| 22 | 23S1 | 2605 | PSU | N1-C2-N3 | 3.87 | 119.52 | 115.13 |
| 22 | 23S1 | 2445 | 2MG | C5-C6-N1 | 3.82 | 120.70 | 113.95 |
| 1 | 16S1 | 516 | PSU | N1-C2-N3 | 3.82 | 119.46 | 115.13 |
| 1 | 16S1 | 1516 | 2MG | C5-C6-N1 | 3.76 | 120.59 | 113.95 |
| 22 | 23S1 | 1915 | 3TD | C4-N3-C2 | -3.76 | 120.53 | 124.61 |
| 22 | 23S1 | 2552 | OMU | C5-C4-N3 | 3.76 | 120.46 | 114.84 |
| 22 | 23S1 | 2251 | OMG | O3'-C3'-C2' | 3.67 | 121.58 | 111.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | 23S1 | 747 | 5MU | C6-C5-C4 | 3.65 | 121.08 | 118.03 |
| 22 | 23S1 | 1917 | PSU | N1-C2-N3 | 3.64 | 119.25 | 115.13 |
| 12 | S121 | 89 | D2T | CB1-SB-CB | 3.63 | 109.00 | 102.44 |
| 1 | 16S1 | 966 | 2MG | C5-C6-N1 | 3.54 | 120.21 | 113.95 |
| 22 | 23S1 | 2457 | PSU | C6-N1-C2 | -3.54 | 119.06 | 122.68 |
| 22 | 23S1 | 2251 | OMG | C5-C6-N1 | 3.49 | 120.12 | 113.95 |
| 25 | L031 | 150 | MEQ | CG-CD-NE2 | 3.49 | 121.13 | 116.29 |
| 22 | 23S1 | 1835 | 2MG | C5-C6-N1 | 3.46 | 120.07 | 113.95 |
| 22 | 23S1 | 2030 | 6MZ | C1'-N9-C4 | -3.46 | 120.56 | 126.64 |
| 22 | 23S1 | 1962 | 5MC | C5-C6-N1 | -3.41 | 119.83 | 123.34 |
| 22 | 23S1 | 955 | PSU | C6-N1-C2 | -3.40 | 119.21 | 122.68 |
| 1 | 16S1 | 1207 | 2MG | C5-C6-N1 | 3.40 | 119.95 | 113.95 |
| 22 | 23S1 | 2504 | PSU | C6-N1-C2 | -3.34 | 119.27 | 122.68 |
| 22 | 23S1 | 2580 | PSU | C6-C5-C4 | 3.33 | 120.53 | 118.20 |
| 22 | 23S1 | 2580 | PSU | C6-N1-C2 | -3.26 | 119.35 | 122.68 |
| 55 | PTR1 | 37 | 2MG | C5-C6-N1 | 3.25 | 119.70 | 113.95 |
| 55 | PTR1 | 54 | 5MU | C4-N3-C2 | -3.20 | 123.20 | 127.35 |
| 22 | 23S1 | 746 | PSU | C6-N1-C2 | -3.18 | 119.43 | 122.68 |
| 55 | PTR1 | 55 | PSU | O2-C2-N1 | -3.15 | 119.32 | 122.79 |
| 22 | 23S1 | 1917 | PSU | C6-N1-C2 | -3.14 | 119.48 | 122.68 |
| 22 | 23S1 | 2457 | PSU | C6-C5-C4 | 3.13 | 120.39 | 118.20 |
| 22 | 23S1 | 2580 | PSU | O2-C2-N1 | -3.13 | 119.35 | 122.79 |
| 55 | PTR1 | 32 | RSP | S2-C2-N3 | -3.11 | 116.09 | 121.49 |
| 12 | S121 | 89 | D2T | OD2-CG-CB | 3.10 | 119.85 | 113.15 |
| 22 | 23S1 | 1939 | 5MU | C4-N3-C2 | -3.08 | 123.37 | 127.35 |
| 22 | 23S1 | 746 | PSU | C6-C5-C4 | 3.07 | 120.34 | 118.20 |
| 1 | 16S1 | 967 | 5MC | C5-C6-N1 | -3.07 | 120.18 | 123.34 |
| 22 | 23S1 | 747 | 5MU | C4-N3-C2 | -3.03 | 123.42 | 127.35 |
| 55 | PTR1 | 55 | PSU | C6-C5-C4 | 3.03 | 120.32 | 118.20 |
| 22 | 23S1 | 2552 | OMU | O4-C4-C5 | -3.02 | 119.85 | 125.16 |
| 55 | PTR1 | 8 | 4SU | N3-C2-N1 | 3.00 | 118.87 | 114.89 |
| 1 | 16S1 | 1516 | 2MG | CM2-N2-C2 | -2.98 | 117.28 | 123.86 |
| 22 | 23S1 | 955 | PSU | O2-C2-N1 | -2.94 | 119.55 | 122.79 |
| 22 | 23S1 | 1911 | PSU | C6-C5-C4 | 2.93 | 120.25 | 118.20 |
| 1 | 16S1 | 1402 | 4OC | O2-C2-N3 | -2.93 | 117.57 | 122.33 |
| 55 | PTR1 | 8 | 4SU | C5-C4-S4 | -2.89 | 120.74 | 124.47 |
| 22 | 23S1 | 1911 | PSU | C6-N1-C2 | -2.89 | 119.73 | 122.68 |
| 22 | 23S1 | 2445 | 2MG | CM2-N2-C2 | -2.87 | 117.52 | 123.86 |
| 22 | 23S1 | 2251 | OMG | C2-N1-C6 | -2.87 | 119.81 | 125.10 |
| 22 | 23S1 | 1835 | 2MG | CM2-N2-C2 | -2.87 | 117.53 | 123.86 |
| 22 | 23S1 | 1939 | 5MU | C6-C5-C4 | 2.85 | 120.42 | 118.03 |
| 1 | 16S1 | 516 | PSU | C6-C5-C4 | 2.85 | 120.19 | 118.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 23S1 | 2503 | 2MA | N3-C2-N1 | -2.85 | 120.53 | 125.73 |
| 1 | 16S1 | 527 | G7M | C2-N1-C6 | -2.83 | 119.89 | 125.10 |
| 22 | 23S1 | 2498 | OMC | O2-C2-N3 | -2.83 | 117.73 | 122.33 |
| 22 | 23S1 | 2251 | OMG | O3'-C3'-C4' | 2.82 | 119.20 | 111.05 |
| 22 | 23S1 | 2069 | G7M | N2-C2-N1 | 2.79 | 122.66 | 116.71 |
| 22 | 23S1 | 745 | 1MG | C8-N7-C5 | 2.79 | 108.30 | 102.99 |
| 22 | 23S1 | 2604 | PSU | C6-N1-C2 | -2.76 | 119.86 | 122.68 |
| 22 | 23S1 | 746 | PSU | O2-C2-N1 | -2.73 | 119.79 | 122.79 |
| 22 | 23S1 | 2445 | 2MG | C8-N7-C5 | 2.71 | 108.16 | 102.99 |
| 55 | PTR1 | 32 | RSP | C1'-N1-C2 | 2.71 | 124.44 | 118.44 |
| 22 | 23S1 | 2251 | OMG | C8-N7-C5 | 2.69 | 108.12 | 102.99 |
| 1 | 16S1 | 516 | PSU | C6-N1-C2 | -2.68 | 119.95 | 122.68 |
| 1 | 16S1 | 966 | 2MG | O6-C6-C5 | -2.67 | 119.15 | 124.37 |
| 55 | PTR1 | 46 | G7M | C2-N1-C6 | -2.64 | 120.23 | 125.10 |
| 55 | PTR1 | 55 | PSU | C6-N1-C2 | -2.64 | 119.99 | 122.68 |
| 1 | 16S1 | 1516 | 2MG | C8-N7-C5 | 2.64 | 108.01 | 102.99 |
| 55 | PTR1 | 54 | 5MU | C6-C5-C4 | 2.63 | 120.23 | 118.03 |
| 22 | 23S1 | 2457 | PSU | O2-C2-N1 | -2.63 | 119.90 | 122.79 |
| 22 | 23S1 | 1835 | 2MG | C8-N7-C5 | 2.60 | 107.93 | 102.99 |
| 22 | 23S1 | 1835 | 2MG | O6-C6-C5 | -2.59 | 119.31 | 124.37 |
| 22 | 23S1 | 2069 | G7M | C2-N1-C6 | -2.58 | 120.36 | 125.10 |
| 1 | 16S1 | 967 | 5MC | CM5-C5-C6 | -2.56 | 119.44 | 122.85 |
| 55 | PTR1 | 37 | 2MG | C8-N7-C5 | 2.55 | 107.86 | 102.99 |
| 22 | 23S1 | 2605 | PSU | C6-N1-C2 | -2.53 | 120.09 | 122.68 |
| 22 | 23S1 | 1939 | 5MU | C5-C6-N1 | -2.53 | 120.74 | 123.34 |
| 1 | 16S1 | 1207 | 2MG | C8-N7-C5 | 2.49 | 107.74 | 102.99 |
| 1 | 16S1 | 1402 | 4OC | C6-C5-C4 | 2.49 | 120.01 | 116.96 |
| 1 | 16S1 | 1407 | 5MC | C5-C6-N1 | -2.47 | 120.79 | 123.34 |
| 1 | 16S1 | 1498 | UR3 | C6-N1-C2 | -2.45 | 119.59 | 121.79 |
| 34 | L161 | 81 | 4D4 | CG-CD-NE | -2.42 | 104.87 | 111.87 |
| 22 | 23S1 | 2580 | PSU | O4'-C1'-C2' | 2.42 | 108.55 | 105.14 |
| 1 | 16S1 | 966 | 2MG | C8-N7-C5 | 2.38 | 107.53 | 102.99 |
| 1 | 16S1 | 1207 | 2MG | CM2-N2-C2 | -2.38 | 118.61 | 123.86 |
| 55 | PTR1 | 37 | 2MG | CM2-N2-C2 | -2.37 | 118.63 | 123.86 |
| 22 | 23S1 | 2251 | OMG | C3'-C2'-C1' | -2.34 | 98.50 | 102.89 |
| 1 | 16S1 | 1516 | 2MG | O6-C6-C5 | -2.32 | 119.84 | 124.37 |
| 22 | 23S1 | 2503 | 2MA | C1'-N9-C4 | 2.24 | 130.58 | 126.64 |
| 22 | 23S1 | 2504 | PSU | O2-C2-N1 | -2.24 | 120.32 | 122.79 |
| 22 | 23S1 | 1962 | 5MC | CM5-C5-C6 | -2.24 | 119.86 | 122.85 |
| 22 | 23S1 | 1911 | PSU | O2-C2-N1 | -2.24 | 120.33 | 122.79 |
| 22 | 23S1 | 2445 | 2MG | O6-C6-C5 | -2.24 | 120.00 | 124.37 |
| 22 | 23S1 | 2604 | PSU | C6-C5-C4 | 2.23 | 119.75 | 118.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 23S1 | 1939 | 5MU | C5-C4-N3 | 2.18 | 117.17 | 115.31 |
| 1 | 16S1 | 1407 | 5MC | C5-C4-N3 | -2.18 | 119.33 | 121.67 |
| 22 | 23S1 | 2069 | G7M | N1-C2-N3 | -2.15 | 119.29 | 123.32 |
| 55 | PTR1 | 8 | 4SU | C1'-N1-C2 | 2.15 | 121.46 | 117.57 |
| 1 | 16S1 | 1407 | 5MC | O2-C2-N3 | -2.12 | 118.89 | 122.33 |
| 22 | 23S1 | 2552 | OMU | O2-C2-N1 | -2.11 | 119.98 | 122.79 |
| 1 | 16S1 | 1207 | 2MG | O6-C6-C5 | -2.11 | 120.25 | 124.37 |
| 22 | 23S1 | 745 | 1MG | O6-C6-C5 | -2.10 | 120.47 | 124.19 |
| 1 | 16S1 | 527 | G7M | N2-C2-N1 | 2.10 | 121.18 | 116.71 |
| 22 | 23S1 | 2251 | OMG | O6-C6-C5 | -2.08 | 120.30 | 124.37 |
| 55 | PTR1 | 54 | 5MU | C5M-C5-C6 | -2.05 | 120.11 | 122.85 |
| 22 | 23S1 | 2457 | PSU | O4'-C1'-C2' | 2.05 | 108.03 | 105.14 |
| 1 | 16S1 | 1519 | MA6 | C1'-N9-C4 | -2.04 | 123.06 | 126.64 |
| 12 | S121 | 89 | D2T | OD2-CG-OD1 | -2.04 | 119.46 | 124.09 |
| 22 | 23S1 | 1917 | PSU | C6-C5-C4 | 2.04 | 119.62 | 118.20 |
| 55 | PTR1 | 46 | G7M | N2-C2-N1 | 2.04 | 121.05 | 116.71 |
| 22 | 23S1 | 2605 | PSU | C6-C5-C4 | 2.03 | 119.62 | 118.20 |
| 55 | PTR1 | 54 | 5MU | C5-C4-N3 | 2.02 | 117.04 | 115.31 |
| 1 | 16S1 | 516 | PSU | O4'-C1'-C2' | 2.02 | 108.00 | 105.14 |
| 55 | PTR1 | 37 | 2MG | O6-C6-C5 | -2.01 | 120.44 | 124.37 |
| 22 | 23S1 | 745 | 1MG | CM1-N1-C6 | 2.01 | 120.30 | 117.55 |
| 1 | 16S1 | 516 | PSU | O2-C2-N1 | -2.01 | 120.58 | 122.79 |
| 22 | 23S1 | 747 | 5MU | C5-C6-N1 | -2.01 | 121.28 | 123.34 |

There are no chirality outliers.

All (38) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 1 | 16S1 | 527 | G7M | O4'-C4'-C5'-O5' |
| 1 | 16S1 | 527 | G7M | C3'-C4'-C5'-O5' |
| 1 | 16S1 | 966 | 2MG | O4'-C4'-C5'-O5' |
| 1 | 16S1 | 966 | 2MG | C3'-C4'-C5'-O5' |
| 1 | 16S1 | 1519 | MA6 | O4'-C4'-C5'-O5' |
| 25 | L031 | 150 | MEQ | N-CA-CB-CG |
| 25 | L031 | 150 | MEQ | C-CA-CB-CG |
| 53 | SPE1 | 1 | FME | C-CA-CB-CG |
| 55 | PTR1 | 32 | RSP | C3'-C4'-C5'-O5' |
| 55 | PTR1 | 54 | 5MU | C3'-C4'-C5'-O5' |
| 22 | 23S1 | 2030 | 6MZ | O4'-C4'-C5'-O5' |
| 22 | 23S1 | 2504 | PSU | O4'-C4'-C5'-O5' |
| 1 | 16S1 | 1519 | MA6 | C3'-C4'-C5'-O5' |
| 22 | 23S1 | 2030 | 6MZ | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 22 | 23S1 | 2504 | PSU | C3'-C4'-C5'-O5' |
| 55 | PTR1 | 32 | RSP | O4'-C4'-C5'-O5' |
| 53 | SPE1 | 1 | FME | N-CA-CB-CG |
| 55 | PTR1 | 54 | 5MU | O4'-C4'-C5'-O5' |
| 34 | L161 | 81 | 4D4 | OB-CB-CG-CD |
| 22 | 23S1 | 1939 | 5MU | C3'-C4'-C5'-O5' |
| 22 | 23S1 | 1939 | 5MU | O4'-C4'-C5'-O5' |
| 55 | PTR1 | 46 | G7M | C4'-C5'-O5'-P |
| 12 | S121 | 89 | D2T | CG-CB-SB-CB1 |
| 22 | 23S1 | 2445 | 2MG | C3'-C4'-C5'-O5' |
| 1 | 16S1 | 1402 | 4OC | O4'-C4'-C5'-O5' |
| 34 | L161 | 81 | 4D4 | CA-CB-CG-CD |
| 22 | 23S1 | 2069 | G7M | C4'-C5'-O5'-P |
| 53 | SPE1 | 1 | FME | CA-CB-CG-SD |
| 22 | 23S1 | 2069 | G7M | O4'-C4'-C5'-O5' |
| 22 | 23S1 | 2503 | 2MA | C4'-C5'-O5'-P |
| 1 | 16S1 | 1519 | MA6 | C5-C6-N6-C10 |
| 55 | PTR1 | 8 | 4SU | O4'-C4'-C5'-O5' |
| 22 | 23S1 | 2251 | OMG | C1'-C2'-O2'-CM2 |
| 22 | 23S1 | 2580 | PSU | O4'-C4'-C5'-O5' |
| 22 | 23S1 | 746 | PSU | O4'-C1'-C5-C6 |
| 22 | 23S1 | 2503 | 2MA | O4'-C4'-C5'-O5' |
| 34 | L161 | 81 | 4D4 | O-C-CA-CB |
| 53 | SPE1 | 1 | FME | CB-CG-SD-CE |

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1691 ligands modelled in this entry, 489 are monoatomic and 1201 are unknown - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 60 | ORN | 23S1 | 3001 | - | 7,8,8 | 0.76 | 0 | 8,9,9 | 0.70 | 0 |

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 |
|-----|------|-------|------|------|---------|----------|-------|
| 60 | ORN | 23S1 | 3001 | - | - | 2/8/8/8 | - |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|------------|
| 60 | 23S1 | 3001 | ORN | N-CA-CB-CG |
| 60 | 23S1 | 3001 | ORN | C-CA-CB-CG |

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](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 22 | 23S1 | 2 |
| 55 | PTR1 | 1 |
| 10 | S101 | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | 23S1 | 885:C | O3' | 892:A | P | 13.12 |
| 1 | PTR1 | 46:G7M | O3' | 48:C | P | 5.31 |
| 1 | 23S1 | 2099:U | O3' | 2100:G | P | 4.47 |
| 1 | S101 | 53:ILE | C | 54:SER | N | 1.18 |