# Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 07:03 pm GMT

| | | |
|---|---|---|
| PDB ID | : | 5OPT |
| EMDB ID | : | EMD-3844 |
| Title | : | Structure of KSRP in context of Trypanosoma cruzi 40S |
| Authors | : | Brito Querido, J.; Mancera-Martinez, E.; Vicens, Q.; Bochler, A.; Chicher, J.; Simonetti, A.; Hashem, Y. |
| Deposited on | : | 2017-08-10 |
| Resolution | : | 4.00 Å(reported) |

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

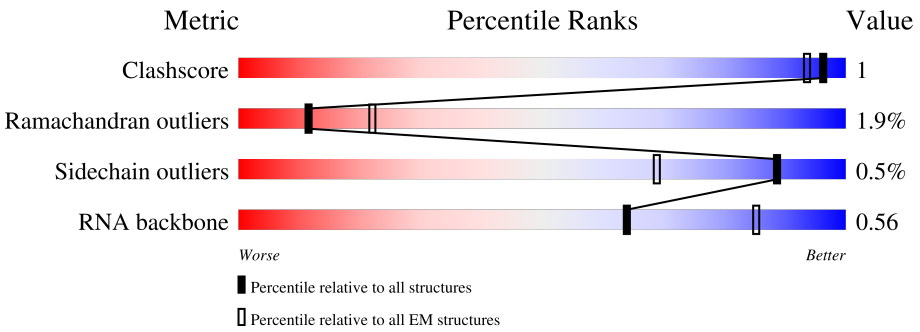
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.31.2 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.00 Å.

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




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |
| RNA backbone | 4643 | 859 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | p | 318 | 85% / 95% |
| 2 | q | 57 | 37% / 63% / 33% |
| 3 | r | 149 | 50% / 84% / 9% / 6% |
| 4 | t | 152 | 55% / 74% / 22% |
| 5 | u | 153 | 51% / 74% / 22% |
| 6 | L | 273 | 26% / 94% / 5% |
| 7 | M | 143 | 22% / 99% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 8 | O | 190 | 58% 95% 5% |
| 9 | Q | 211 | 22% 91% • 5% |
| 10 | R | 151 | 25% 92% •• 7% |
| 11 | S | 86 | 37% 93% •• 5% |
| 12 | T | 112 | 32% 93% 7% |
| 13 | U | 112 | 43% 60% • 39% |
| 14 | V | 144 | 33% 92% •• 6% |
| 15 | W | 261 | 21% 81% • 17% |
| 16 | X | 173 | 27% 84% • 14% |
| 17 | Y | 137 | 13% 90% 10% |
| 18 | Z | 221 | 15% 77% • 21% |
| 19 | b | 190 | 17% 85% • 14% |
| 20 | f | 245 | 23% 82% • 16% |
| 21 | d | 263 | 24% 84% • 15% |
| 22 | e | 130 | 19% 98% ••• |
| 23 | g | 236 | 11% 35% 65% |
| 24 | a | 110 | 40% 56% 7% 36% |
| 25 | i | 141 | 79% 82% • 14% |
| 26 | j | 150 | 35% 38% • • 57% |
| 27 | P | 250 | 27% 99% • |
| 28 | k | 196 | 32% 59% • 40% |
| 29 | l | 117 | 57% 85% 15% |
| 30 | m | 214 | 67% 88% 5% 7% |
| 31 | n | 161 | 41% 55% • 42% |
| 32 | o | 167 | 44% 79% • • 16% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 33 | c | 66 | 33% 86% 5% 9% |
| 34 | h | 257 | 47% 53% 10% • 33% |
| 35 | E | 2319 | 12% • 62% 20% • 13% |

# 2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 82219 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 protein called Activated protein kinase C receptor, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | p | 310 | 2405 | 1505 | 424 | 463 | 13 | 0 | 0 |

- Molecule 2 is a protein called Ribosomal protein S29, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | q | 38 | 311 | 191 | 64 | 52 | 4 | 0 | 0 |

- Molecule 3 is a protein called 40S ribosomal protein S16, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | r | 140 | 1113 | 706 | 212 | 192 | 3 | 0 | 0 |

- Molecule 4 is a protein called 40S ribosomal protein S15, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | t | 119 | 969 | 615 | 185 | 165 | 4 | 0 | 0 |

- Molecule 5 is a protein called 40S ribosomal protein S18, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | u | 120 | 981 | 614 | 194 | 169 | 4 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | L | 258 | 2038 | 1290 | 383 | 354 | 11 | 0 | 0 |

- Molecule 7 is a protein called 40S ribosomal protein S23, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 7 | M | 142 | 1116 | 706 | 220 | 188 | 2 | 0 | 0 |

- Molecule 8 is a protein called 40S ribosomal protein S5, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 8 | O | 190 | 1493 | 932 | 286 | 269 | 6 | 0 | 0 |

- Molecule 9 is a protein called Ribosomal protein S7, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 9 | Q | 200 | 1670 | 1063 | 324 | 277 | 6 | 0 | 0 |

- Molecule 10 is a protein called 40S ribosomal protein S13, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 10 | R | 141 | 1143 | 724 | 221 | 190 | 8 | 0 | 0 |

- Molecule 11 is a protein called 40S ribosomal protein S27, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 11 | S | 82 | 630 | 384 | 121 | 116 | 9 | 0 | 0 |

- Molecule 12 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 12 | T | 104 | 829 | 510 | 177 | 132 | 10 | 0 | 0 |

- Molecule 13 is a protein called 40S ribosomal protein S33, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 13 | U | 68 | 526 | 315 | 107 | 100 | 4 | 0 | 0 |

- Molecule 14 is a protein called 40S ribosomal protein S14, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 14 | V | 135 | 1011 | 620 | 195 | 187 | 9 | 0 | 0 |

- Molecule 15 is a protein called 40S ribosomal protein S3a-2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 15 | W | 217 | 1781 | 1124 | 337 | 313 | 7 | 0 | 0 |

- Molecule 16 is a protein called 40S ribosomal protein S11, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 16 | X | 148 | 1212 | 760 | 239 | 207 | 6 | 0 | 0 |

- Molecule 17 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 17 | Y | 123 | 989 | 628 | 194 | 165 | 2 | 0 | 0 |

- Molecule 18 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 18 | Z | 175 | 1404 | 885 | 283 | 233 | 3 | 0 | 0 |

- Molecule 19 is a protein called 40S ribosomal protein S9, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 19 | b | 164 | 1365 | 864 | 266 | 227 | 8 | 0 | 0 |

- Molecule 20 is a protein called 40S ribosomal protein SA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 20 | f | 207 | 1658 | 1060 | 299 | 288 | 11 | 0 | 0 |

- Molecule 21 is a protein called 40S ribosomal protein S2, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 21 | d | 223 | 1726 | 1098 | 304 | 314 | 10 | 0 | 0 |

- Molecule 22 is a protein called 40S ribosomal protein S15a, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 22 | e | 129 | 1019 | 647 | 188 | 176 | 8 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 23 | g | 83 | 635 | 395 | 116 | 122 | 2 | 0 | 0 |

- Molecule 24 is a protein called Ribosomal protein S25, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 24 | a | 70 | 553 | 356 | 97 | 97 | 3 | 0 | 0 |

- Molecule 25 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 25 | i | 121 | 958 | 594 | 174 | 185 | 5 | 0 | 0 |

- Molecule 26 is a protein called Ubiquitin/ribosomal protein S27a, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 26 | j | 64 | 518 | 324 | 98 | 90 | 6 | 0 | 0 |

- Molecule 27 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 27 | P | 249 | 1983 | 1244 | 402 | 333 | 4 | 0 | 0 |

- Molecule 28 is a protein called 40S ribosomal protein S17, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 28 | k | 118 | 972 | 610 | 187 | 170 | 5 | 0 | 0 |

- Molecule 29 is a protein called Ribosomal protein S20, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 29 | l | 99 | 784 | 497 | 144 | 140 | 3 | 0 | 0 |

- Molecule 30 is a protein called 40S ribosomal protein S3, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 30 | m | 200 | 1587 | 995 | 302 | 279 | 11 | 0 | 0 |

- Molecule 31 is a protein called 40S ribosomal protein S10, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 31 | n | 93 | 780 | 508 | 136 | 132 | 4 | 0 | 0 |

- Molecule 32 is a protein called Ribosomal protein S19, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 32 | o | 140 | 1116 | 702 | 221 | 185 | 8 | 0 | 0 |

- Molecule 33 is a protein called 40S ribosomal protein S30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 33 | c | 60 | 480 | 303 | 98 | 78 | 1 | 0 | 0 |

- Molecule 34 is a protein called RNA-binding protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 34 | h | 173 | 1358 | 862 | 259 | 234 | 3 | 0 | 0 |

- Molecule 35 is a RNA chain called 18S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 35 | E | 2022 | 43106 | 19268 | 7710 | 14111 | 2017 | 0 | 0 |

There are 5 discrepancies between the modelled and reference sequences:

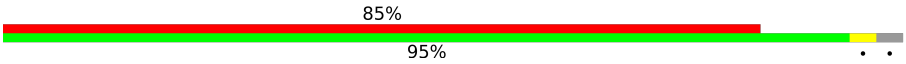
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| E | 143 | C | A | conflict | GB 320364483 |
| E | 805 | C | U | conflict | GB 320364483 |
| E | 2316 | U | - | insertion | GB 320364483 |
| E | 2317 | U | - | insertion | GB 320364483 |
| E | 2318 | U | - | insertion | GB 320364483 |

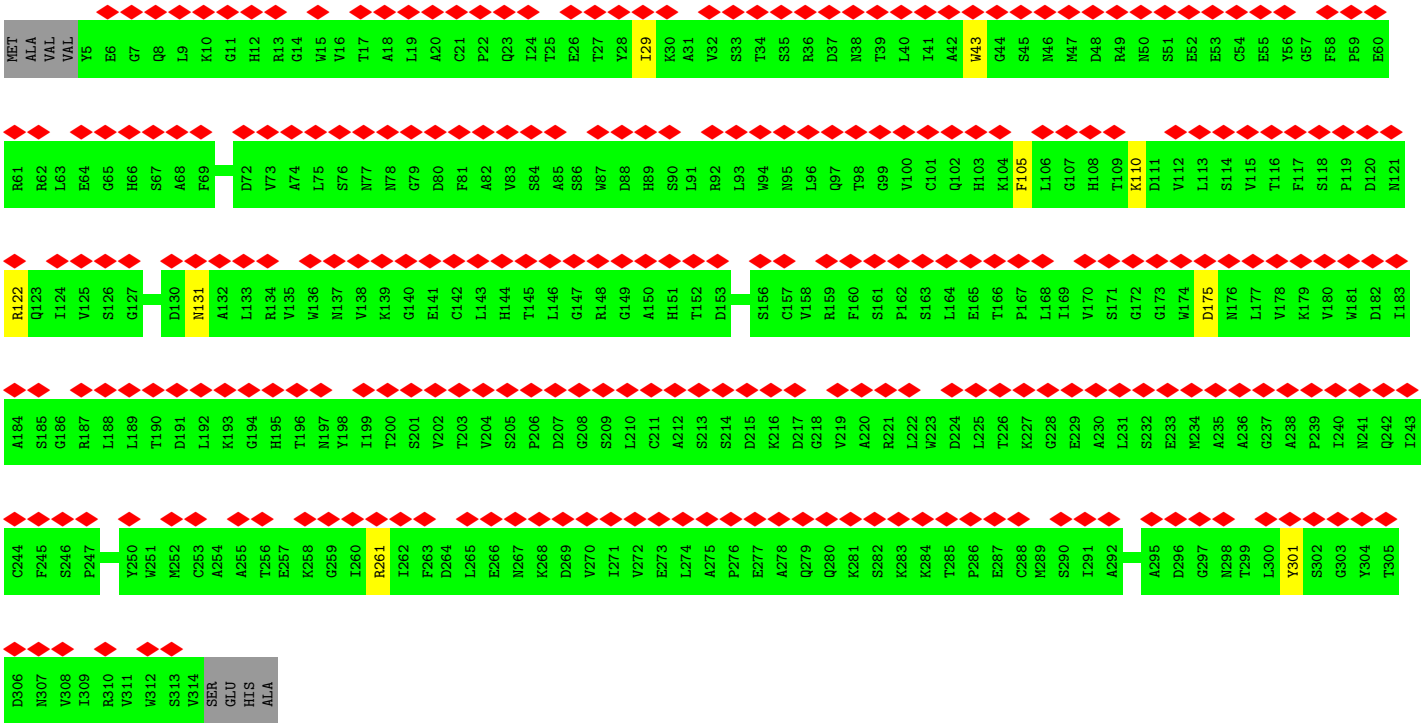
# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Activated protein kinase C receptor, putative

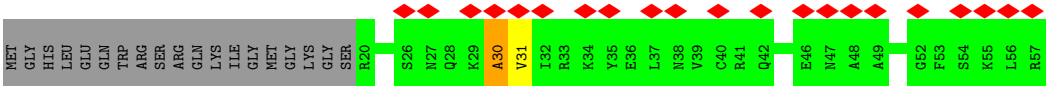
Chain p:



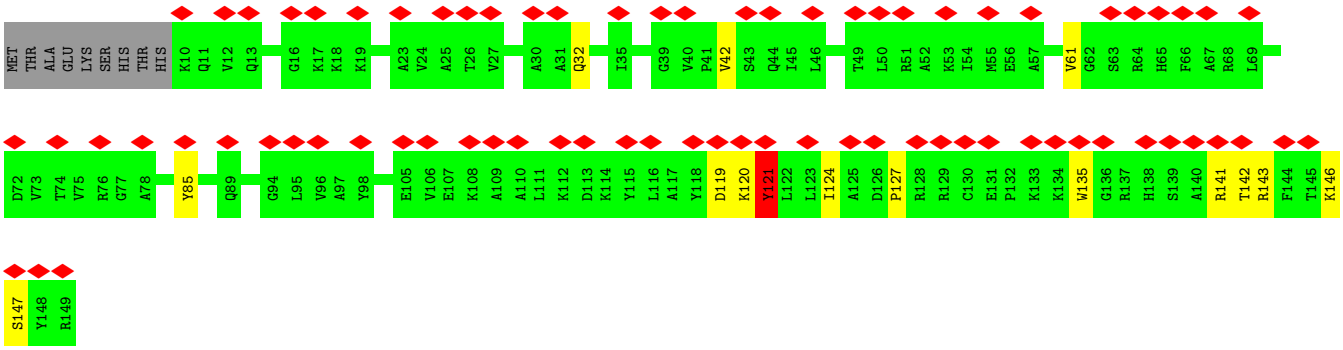

- Molecule 2: Ribosomal protein S29, putative

Chain q:



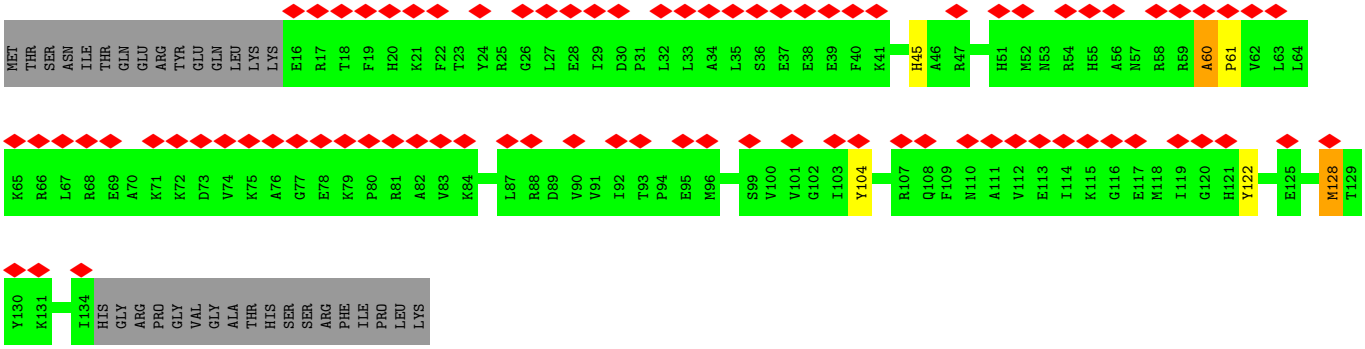

- Molecule 3: 40S ribosomal protein S16, putative

Chain r:



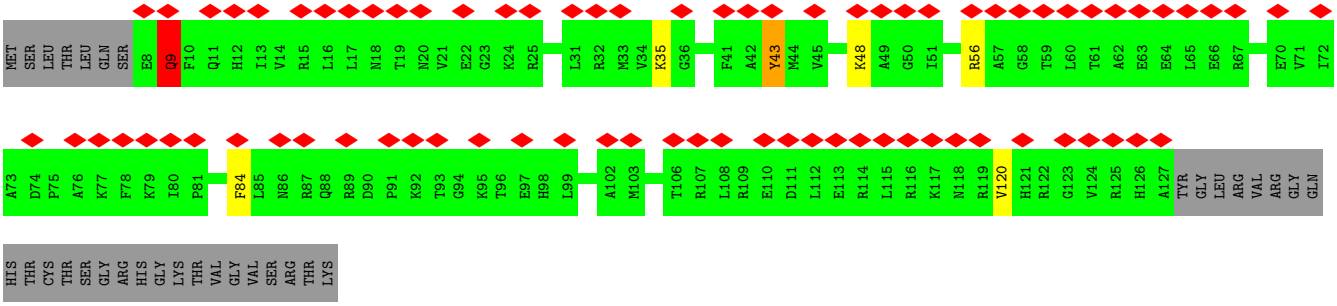

- Molecule 4: 40S ribosomal protein S15, putative

Chain t:



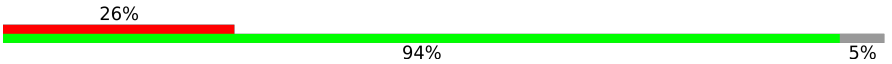

- Molecule 5: 40S ribosomal protein S18, putative

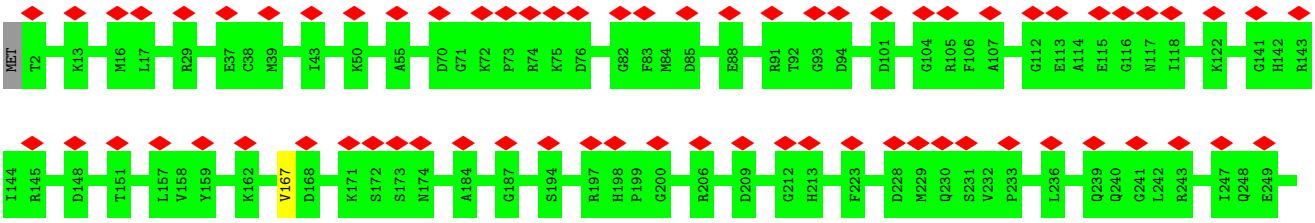
Chain u:

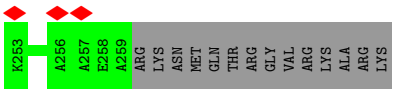



- Molecule 6: 40S ribosomal protein S4

Chain L:

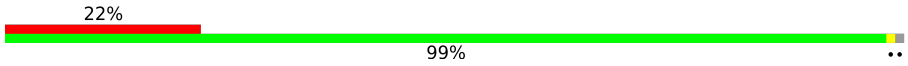


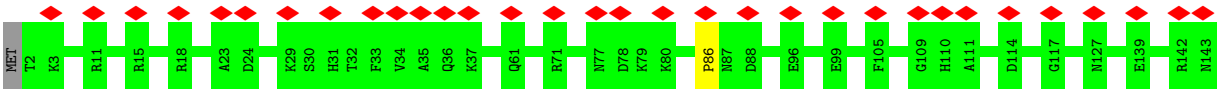






- Molecule 7: 40S ribosomal protein S23, putative

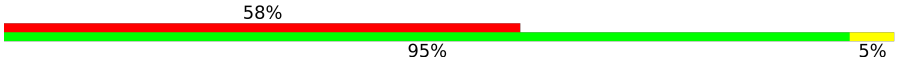
Chain M:

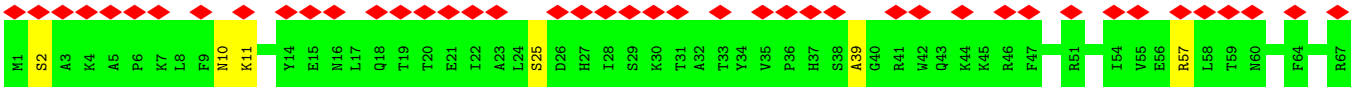


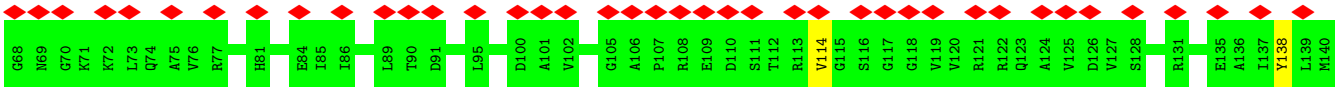



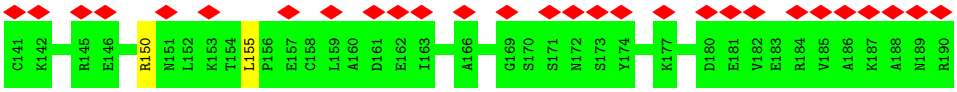

- Molecule 8: 40S ribosomal protein S5, putative

Chain O:



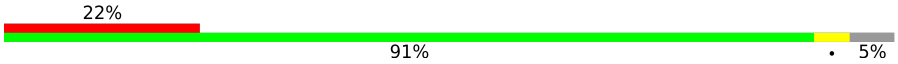



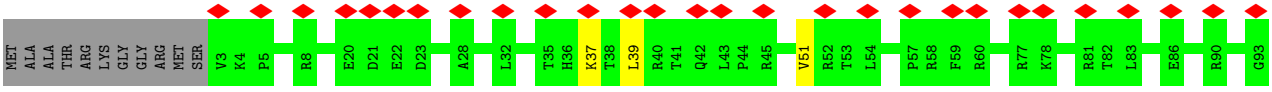



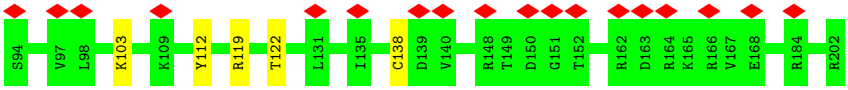




- Molecule 9: Ribosomal protein S7, putative

Chain Q:

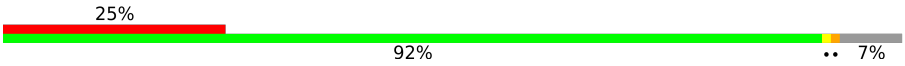


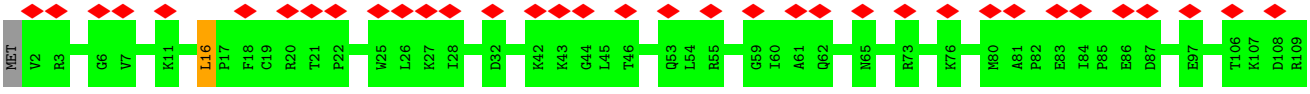



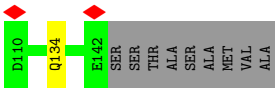




- Molecule 10: 40S ribosomal protein S13, putative

Chain R:

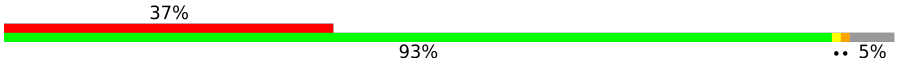


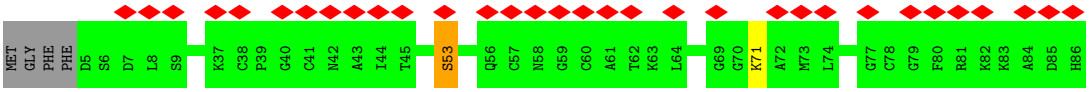




- Molecule 11: 40S ribosomal protein S27, putative

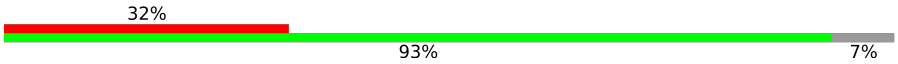
Chain S:

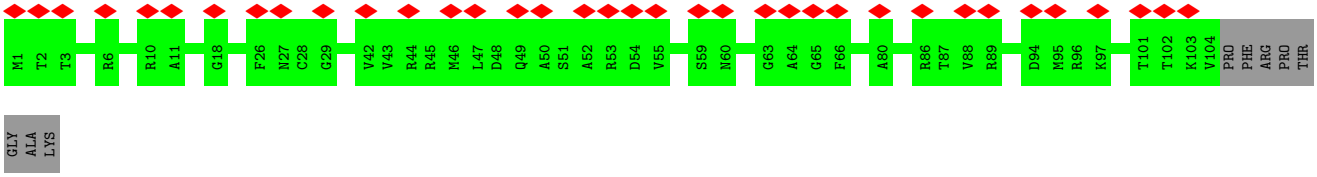



- Molecule 12: 40S ribosomal protein S26

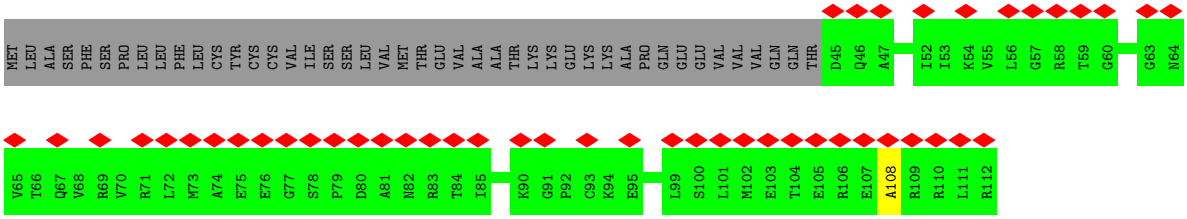
Chain T:



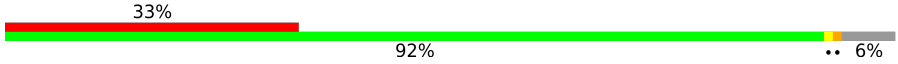

- Molecule 13: 40S ribosomal protein S33, putative

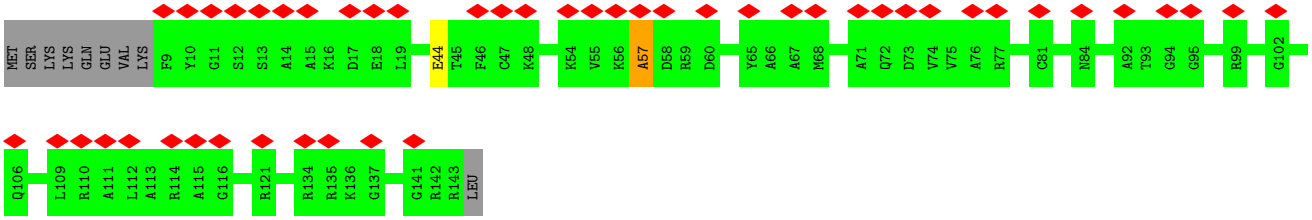
Chain U:




- Molecule 14: 40S ribosomal protein S14, putative

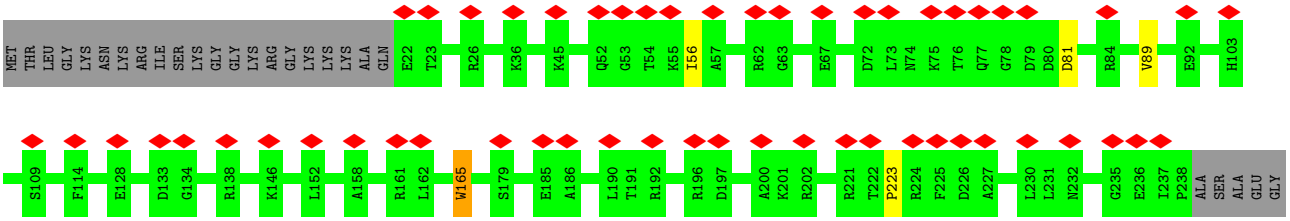
Chain V:

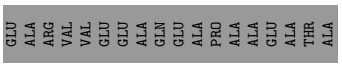



- Molecule 15: 40S ribosomal protein S3a-2

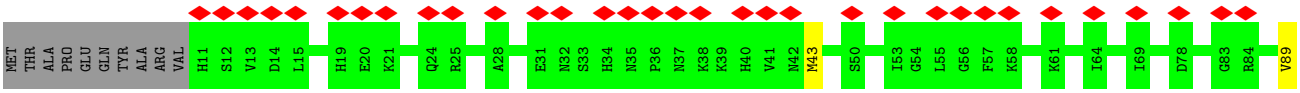
Chain W:

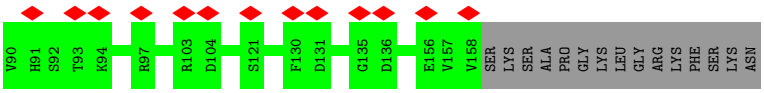





• Molecule 16: 40S ribosomal protein S11, putative

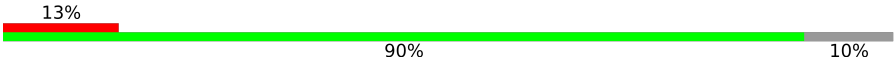
Chain X:

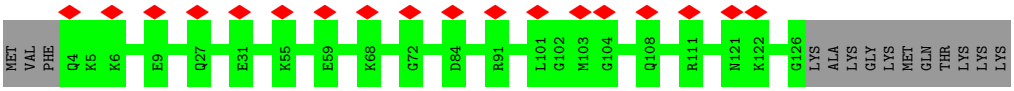



• Molecule 17: 40S ribosomal protein S24

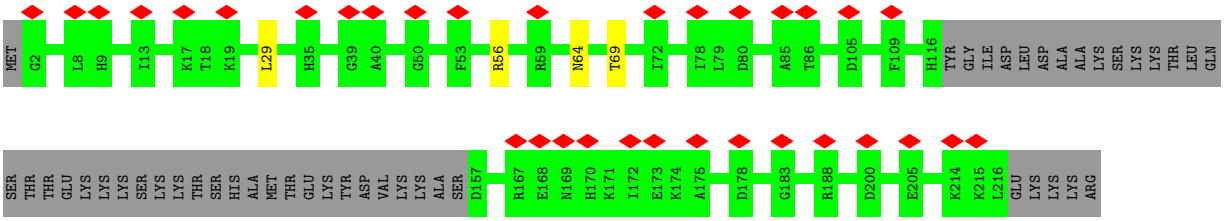
Chain Y:



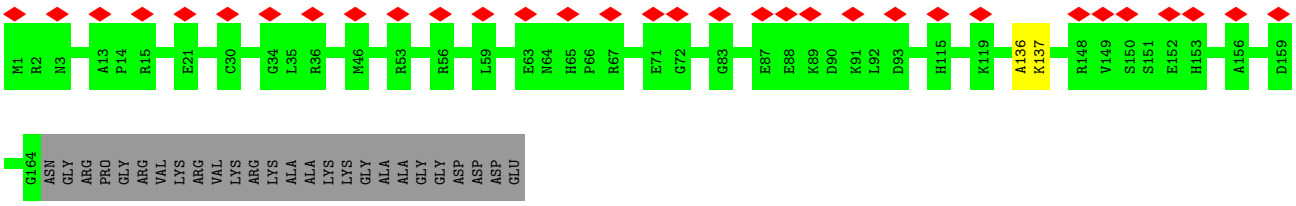

• Molecule 18: 40S ribosomal protein S8

Chain Z:



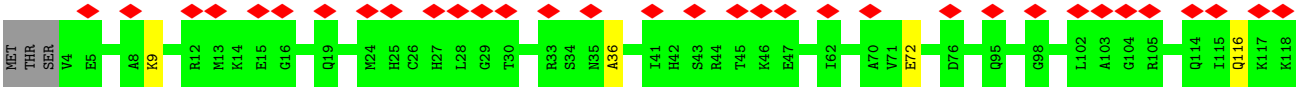

• Molecule 19: 40S ribosomal protein S9, putative

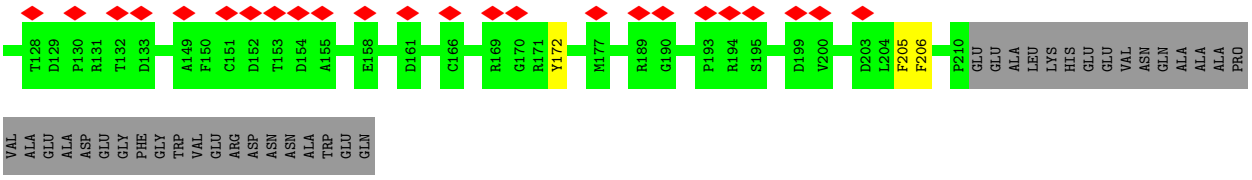
Chain b:




• Molecule 20: 40S ribosomal protein SA

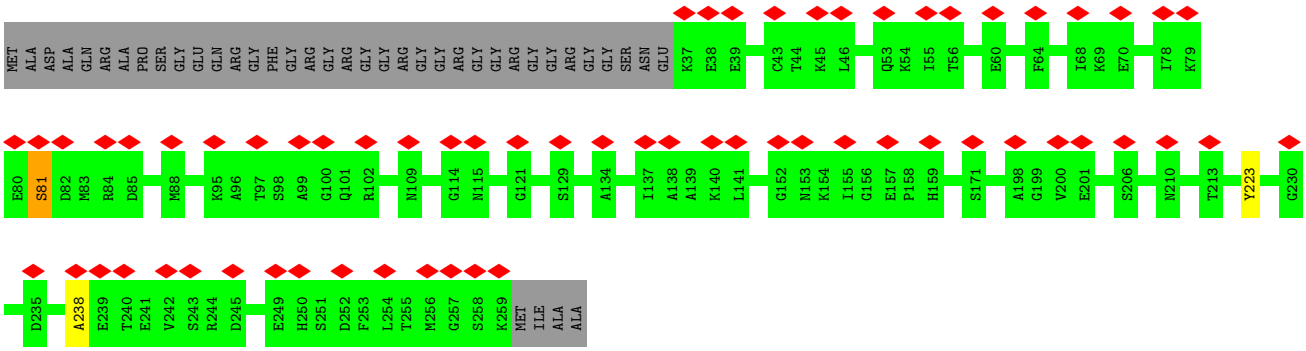
Chain f:





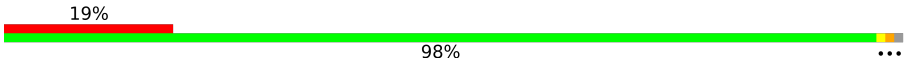

- Molecule 21: 40S ribosomal protein S2, putative

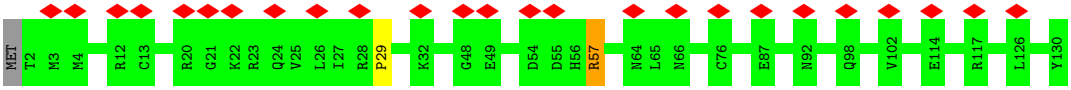
Chain d:




- Molecule 22: 40S ribosomal protein S15a, putative

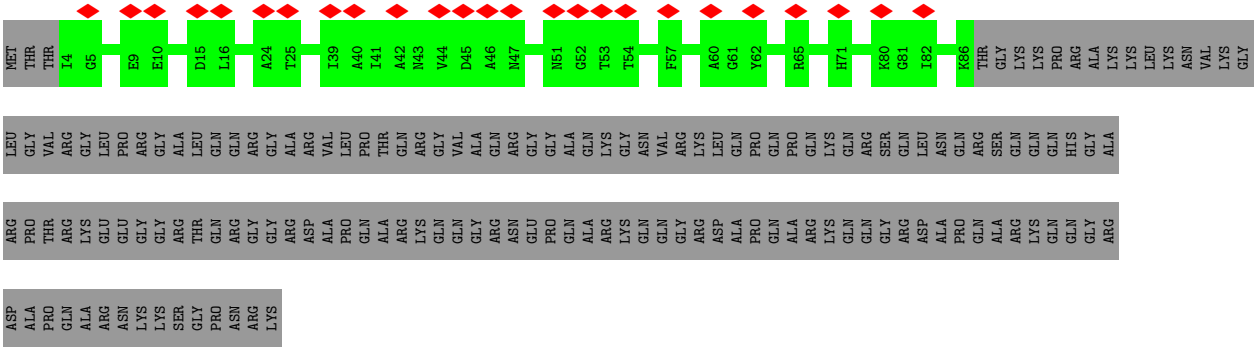
Chain e:



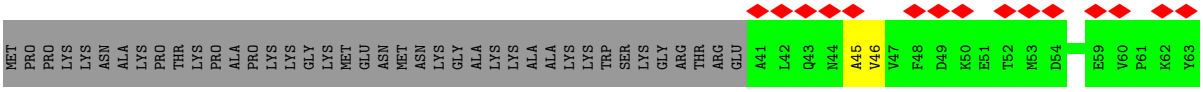

- Molecule 23: 40S ribosomal protein S21, putative

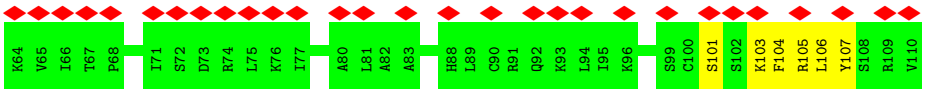
Chain g:




- Molecule 24: Ribosomal protein S25, putative

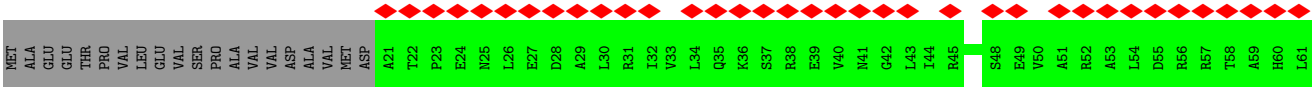
Chain a:

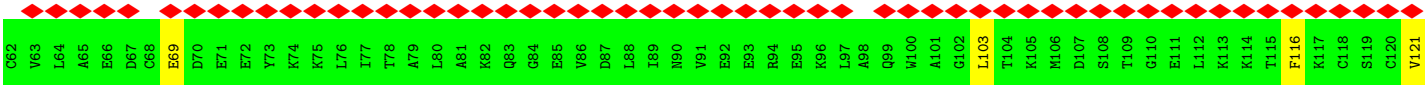


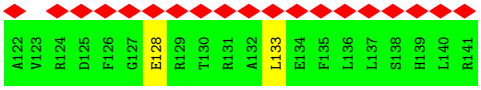



- Molecule 25: 40S ribosomal protein S12

Chain i:

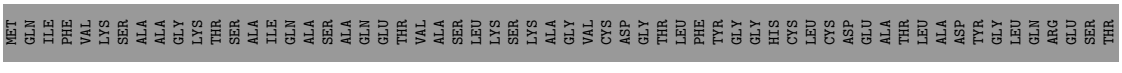


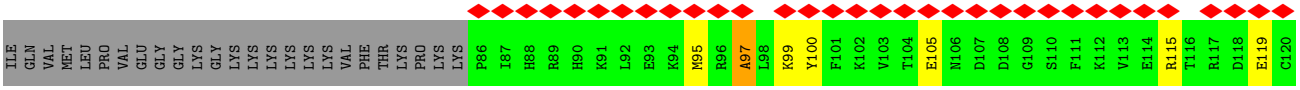



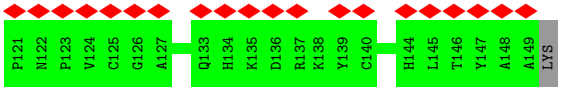




- Molecule 26: Ubiquitin/ribosomal protein S27a, putative

Chain j:

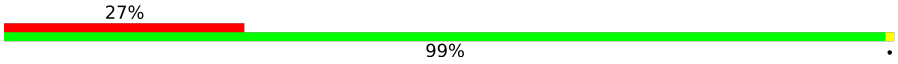


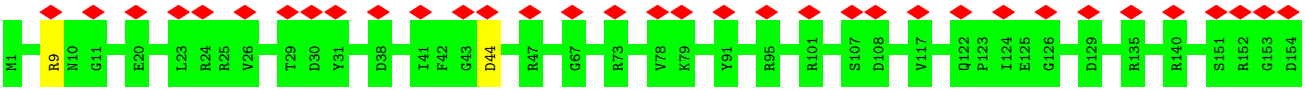



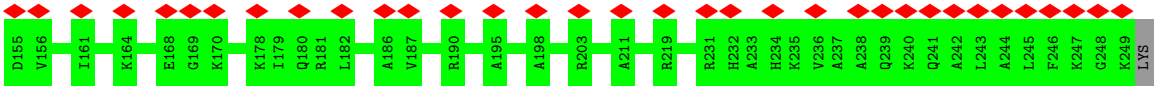




- Molecule 27: 40S ribosomal protein S6

Chain P:

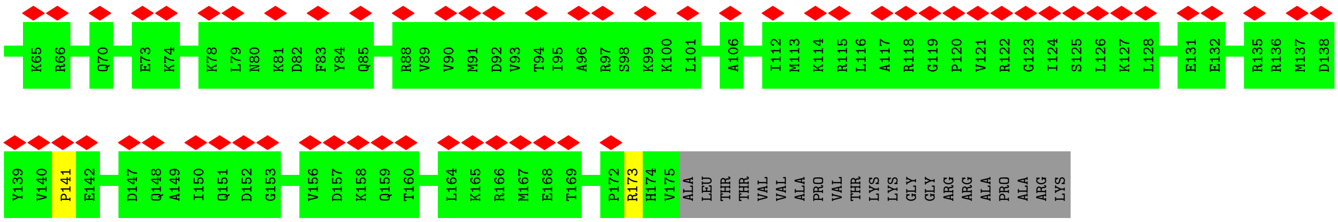


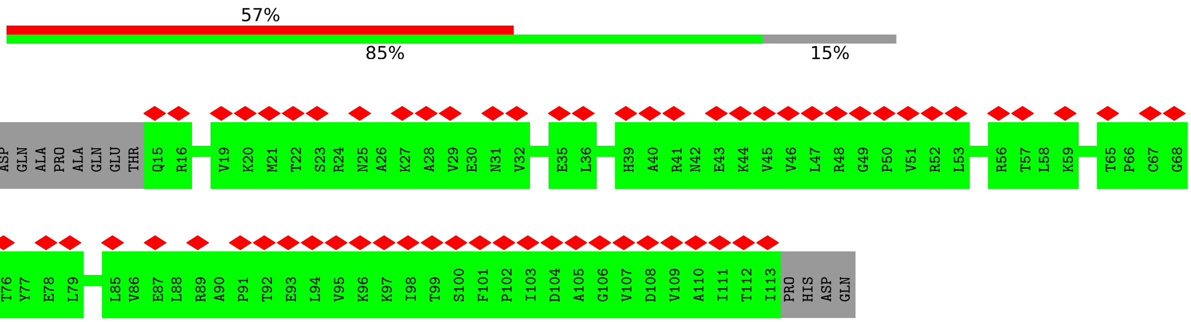

- Molecule 28: 40S ribosomal protein S17, putative

Chain k:



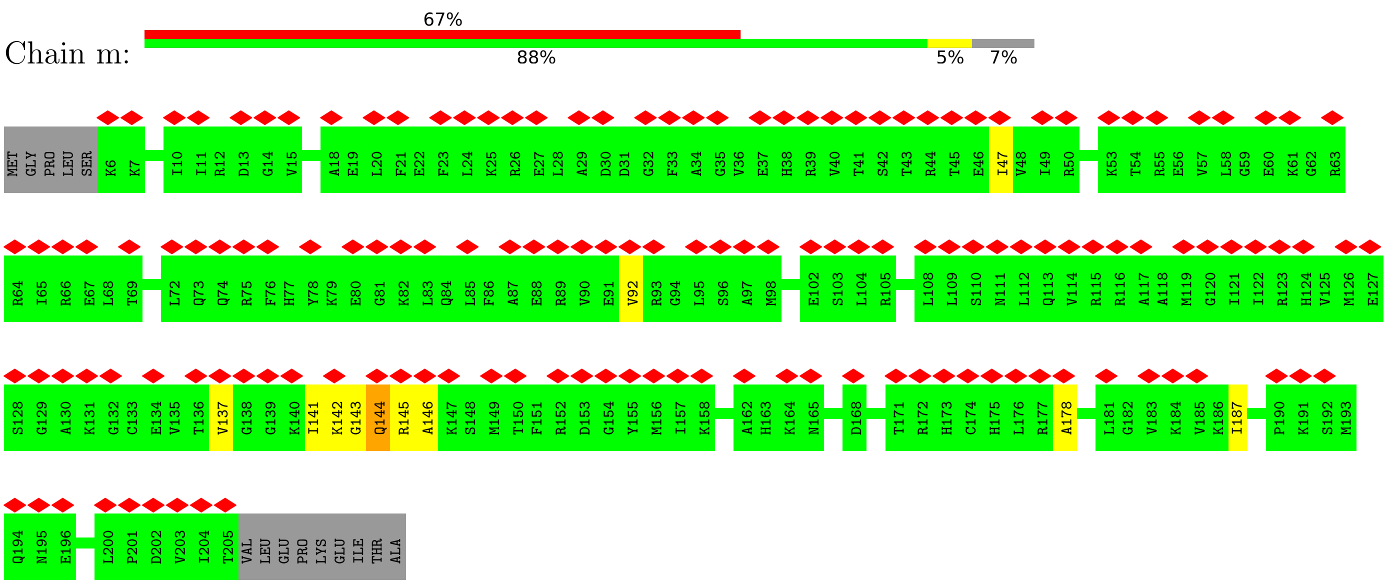

• Molecule 29: Ribosomal protein S20, putative

Chain l:



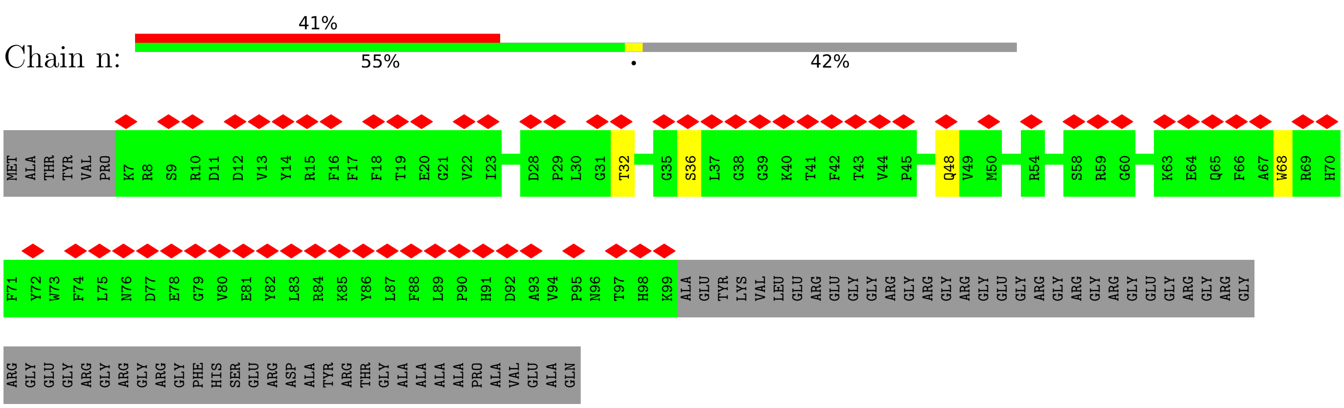

• Molecule 30: 40S ribosomal protein S3, putative

Chain m:



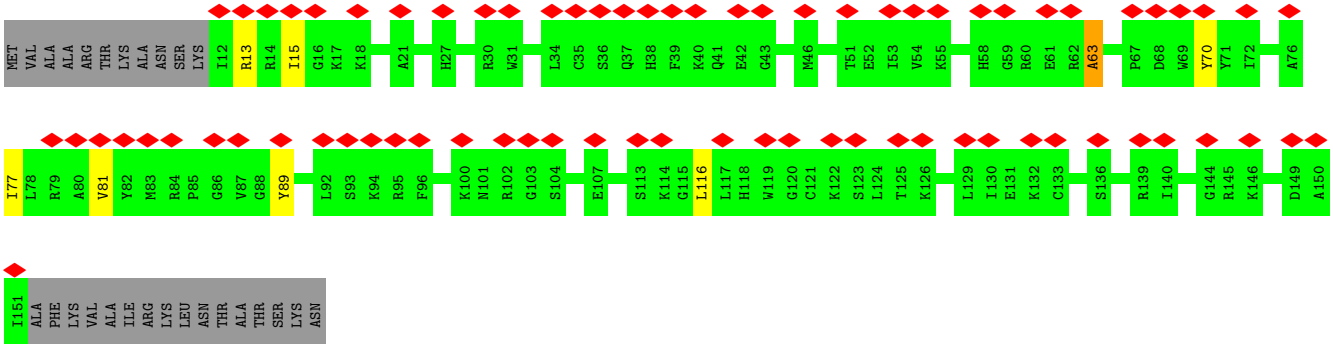

• Molecule 31: 40S ribosomal protein S10, putative

Chain n:



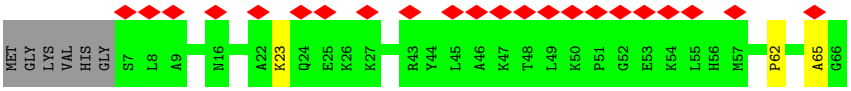
- Molecule 32: Ribosomal protein S19, putative

Chain o:



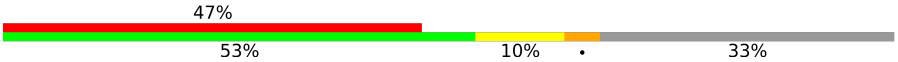

- Molecule 33: 40S ribosomal protein S30

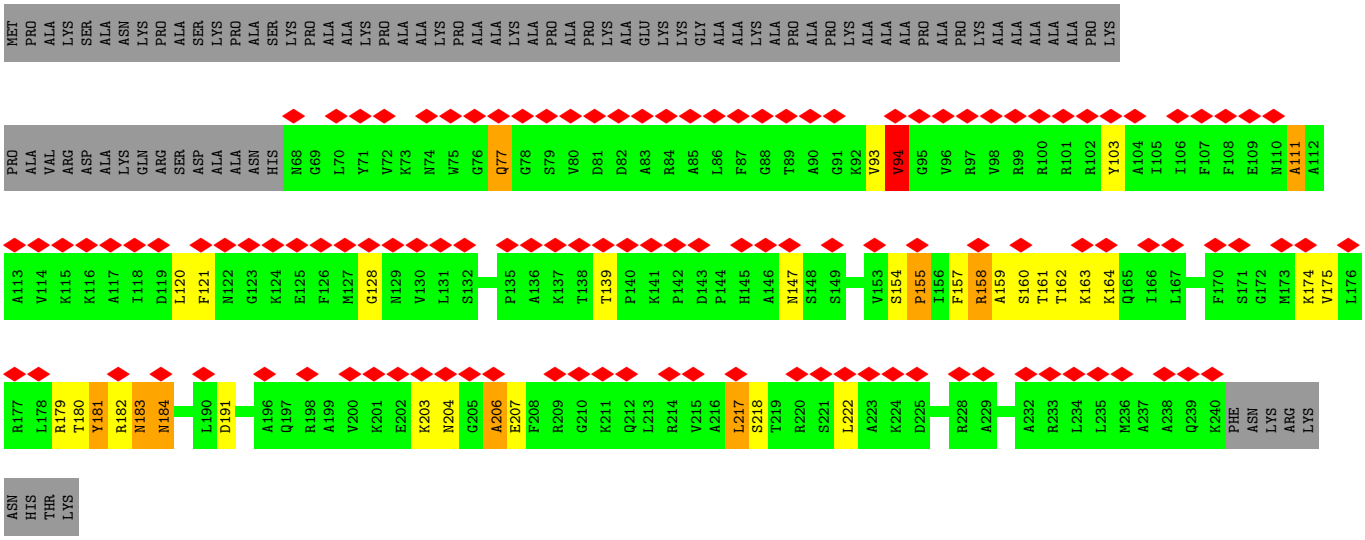
Chain c:




- Molecule 34: RNA-binding protein, putative

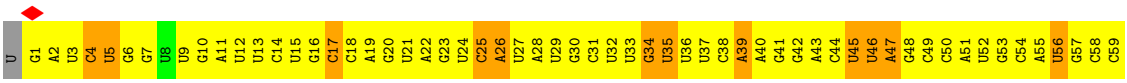
Chain h:

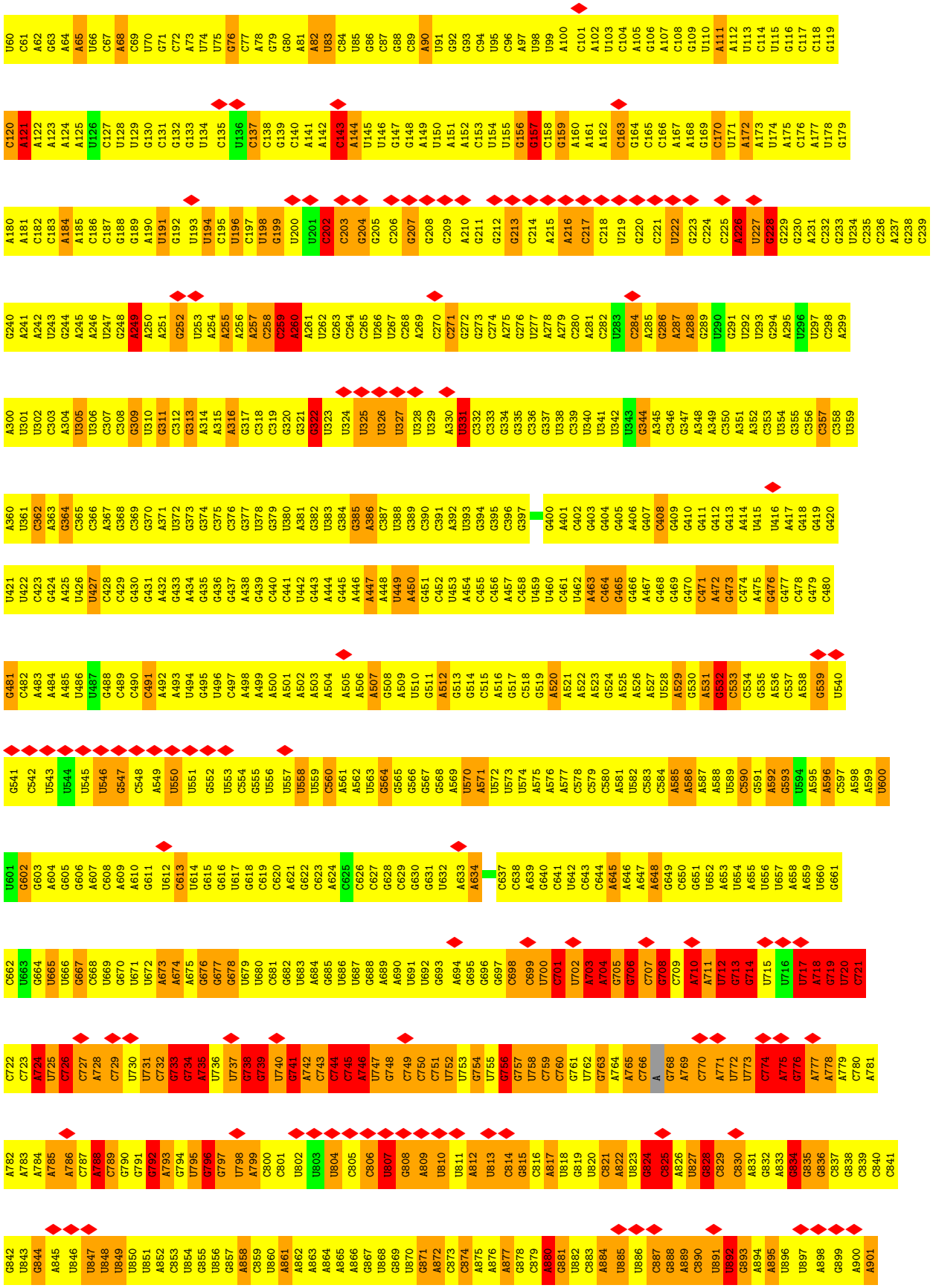


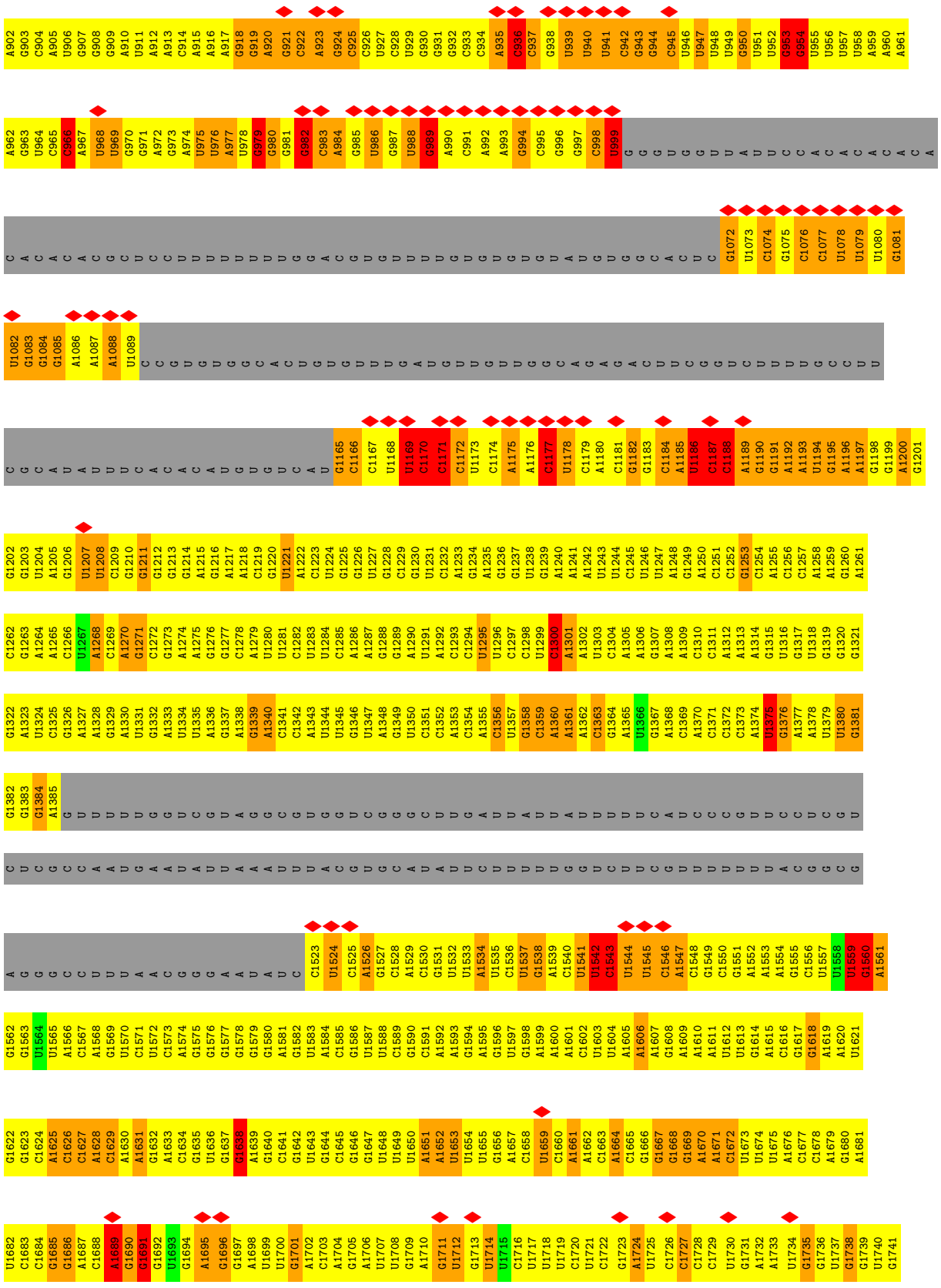



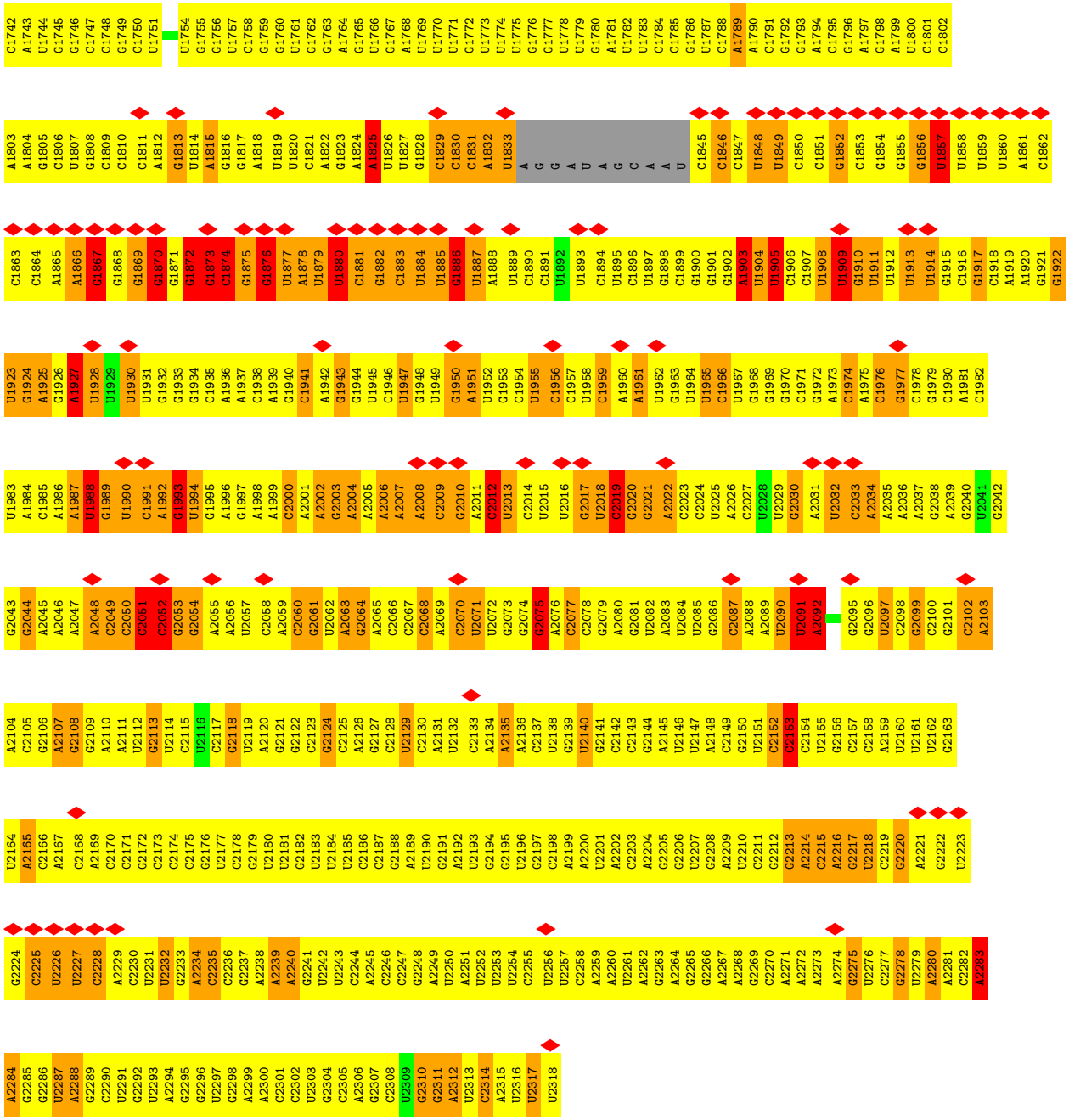

- Molecule 35: 18S rRNA

Chain E:




U60 C61 A62 G63 A64 A65 U66 C67 A68 C69 U70 G71 C72 A73 U74 U75 G76 C77 A78 G79 G80 A81 A82 U83 C84 U85 G86 C87 G88 C89 A90 U91 G92 G93 C94 U95 C96 A97 U98 U99 A100 C101 A102 U103 C104 A105 G106 A107 C108 G109 U110 A111 A112 U113 C114 U115 G116 C117 C118 G119
C120 A121 A122 A123 A124 A125 U126 C127 U128 U129 G130 C131 G132 G133 U134 C135 U136 C137 C138 G139 C140 A141 A142 C143 A144 U145 U146 G147 G148 A149 U150 A151 A152 C153 U154 U155 G156 G157 C158 G159 A160 A161 A162 C163 G164 C165 C166 A167 A168 G169 C170 U171 A172 A173 U174 A175 C176 A177 U178 G179
A180 A181 C182 C183 A184 A185 C186 C187 G188 G189 A190 U191 G192 U193 U194 C195 U196 C197 U198 G199 U200 U201 G202 C203 G204 G205 C206 G207 G208 C209 A210 G211 G212 G213 C214 A215 A216 C217 C218 U219 G220 C221 U222 G223 C224 C225 A226 U227 G228 G229 G230 A231 C232 G233 U234 C235 C236 A237 G238 C239
G240 A241 A242 U243 G244 A245 A246 U247 G248 A249 A250 A251 G252 U253 A254 A255 A256 A257 C258 C259 A260 A261 U262 G263 C264 C265 U266 U267 C268 A269 C270 C271 G272 G273 C274 A275 G276 U277 A278 A279 C280 A281 C282 U283 C284 A285 G286 A287 A288 G289 U290 G291 U292 U293 G294 A295 U296 U297 C298 A299
A300 U301 U302 C303 A304 U305 U306 C307 C308 G309 U310 G311 C312 G313 A314 A315 A316 G317 C318 C319 G320 G321 G322 U323 U324 U325 U326 U327 U328 U329 A330 U331 C332 C333 G334 G335 C336 G337 U338 C339 U340 U341 U342 U343 G344 A345 C346 G347 A348 A349 C350 A351 A352 C353 U354 G355 C356 C357 C358 U359
A360 U361 C362 A363 G364 C365 C366 A367 G368 C369 G370 A371 U372 G373 G374 C375 C376 G377 U378 G379 U380 A381 G382 U383 G384 U385 A386 C387 U388 G389 C390 U391 A392 U393 G394 G395 C396 G397 G400 A401 C402 G403 G404 G405 A406 G407 C408 G409 G410 G411 G412 G413 A414 U415 U416 A417 G418 G419 G420
U421 U422 C423 G424 A425 U426 U427 C428 C429 G430 G431 A432 G433 A434 G435 G436 G437 A438 G439 C440 C441 U442 G443 A444 G445 A446 A447 A448 U449 A450 G451 C452 U453 A454 C455 C456 A457 C458 U459 U460 C461 U462 A463 C464 G465 G466 A467 G468 G469 G470 C471 A472 G473 C474 A475 G476 G477 C478 G479 C480
G481 C482 A483 A484 A485 U486 U487 G488 C489 C490 C491 A492 A493 U494 G495 U496 C497 A498 A499 A500 A501 A502 A503 A504 A505 A506 A507 G508 A509 U510 G511 A512 G513 G514 C515 A516 G517 C518 U519 A520 A521 A522 A523 G524 A525 A526 A527 U528 A529 G530 A531 G532 C533 C534 G535 A536 C537 A538 G539 U540
G541 C542 U543 U544 U545 U546 G547 C548 A549 U550 U551 G552 U553 C554 G555 U556 U557 U558 U559 C560 A561 A562 U563 G564 G565 G566 G567 G568 A569 U570 A571 U572 U573 U574 A575 A576 A577 C578 C579 C580 A581 U582 C583 C584 A585 A586 A587 A588 U589 C590 G591 A592 G593 U594 A595 A596 C597 A598 A599 U600
U601 G602 G603 A604 G605 G606 A607 C608 A609 A610 G611 U612 C613 U614 G615 G616 U617 G618 C619 C620 A621 G622 A623 A624 C625 C626 C627 G628 G629 G630 G631 U632 A633 A634 C637 C638 A639 G640 C641 U642 C643 C644 A645 A646 A647 A648 G649 G650 G651 U652 A653 U654 A655 U656 U657 A658 A659 U660 G661
C662 U663 G664 U665 U666 G667 C668 U669 G670 U671 U672 A673 A674 A675 G676 G677 G678 U679 U680 C681 G682 U683 A684 G685 U686 U687 G688 A689 A690 U691 U692 G693 A694 G695 G696 G697 C698 C699 U700 C701 U702 A703 A704 G705 G706 C707 G708 C709 A710 A711 U712 G713 G714 U715 U716 U717 A718 G719 U720 C721
C722 C723 A724 U725 C726 C727 A728 C729 G730 U731 C732 G733 G734 A735 U736 U737 G738 G739 U740 G741 A742 C743 C744 C745 A746 U747 G748 C749 C750 C751 U752 U753 G754 U755 G756 G757 U758 C759 C760 G761 U762 G763 A764 A765 C766 A G768 A769 C770 A771 U772 U773 C774 A775 G776 A777 A778 A779 C780 A781
A782 A783 A784 A785 A786 C787 A788 C789 G790 G791 G792 A793 G794 U795 G796 G797 U798 A799 C800 C801 U802 U803 U804 C805 C806 U807 G808 A809 U810 U811 A812 U813 C814 G815 C816 A817 U818 G819 U820 C821 A822 U823 G824 C825 A826 U827 G828 C829 C830 A831 G832 A833 G834 G835 G836 C837 G838 C839 C840 C841
G842 U843 G844 A845 U846 U847 U848 U849 U850 U851 A852 C853 U854 G855 U856 G857 A858 C859 U860 A861 A862 A863 A864 A865 A866 G867 U868 G869 U870 G871 A872 C873 C874 A875 A876 A877 G878 C879 A880 G881 U882 C883 A884 U885 U886 C887 G888 A889 C890 U891 U892 G893 A894 A895 U896 U897 A898 C899 A900 A901


A902 G903 C904 A905 U906 G907 G908 G909 A910 U911 A912 A913 C914 A915 A916 A917 G918 G919 A920 G921 C922 A923 G924 C925 C926 U927 C928 U929 G930 G931 G932 C933 C934 A935 C936 C937 G938 U939 U940 U941 C942 G943 G944 C945 U946 U947 U948 U949 G950 U951 U952 G953 G954 U955 U956 U957 U958 A959 A960 A961
A962 G963 U964 C965 C966 A967 U968 U969 G970 G971 A972 G973 A974 U975 U976 A977 U978 G979 G980 G981 G982 C983 A984 G985 U986 G987 U988 G989 A990 C991 A992 A993 G994 C995 G996 G997 C998 U999 G G G U C U A U U C C A C A C A C A
C A C A C A C G G C U C C U U U U U U U U U U G G A C G G U U G U U U U U G U U G U U G U G U G G A C U U C G1072 U1073 C1074 G1075 C1076 C1077 U1078 U1079 U1080 G1081
U1082 G1083 G1084 G1085 A1086 A1087 A1088 U1089 C C G U G U G C A C U G U U G G U U U U G A U G U U G U U G U U G U G U U G U G U G


C1742 A1743 U1744 G1745 G1746 C1747 C1748 G1749 C1750 U1751
U1754 G1755 G1756 U1757 C1758 G1759 G1760 U1761 G1762 G1763 A1764 G1765 U1766 G1767 A1768 U1769 U1770 U1771 G1772 U1773 U1774 U1775 G1776 G1777 U1778 U1779 G1780 A1781 U1782 U1783 C1784 C1785 G1786 U1787 C1788 A1789 A1790 C1791 G1792 G1793 A1794 C1795 G1796 A1797 G1798 A1799 U1800 C1801 C1802
A1803 A1804 G1805 C1806 U1807 G1808 C1809 C1810 C1811 A1812 G1813 U1814 A1815 G1816 G1817 A1818 U1819 U1820 C1821 A1822 G1823 A1824 A1825 U1826 U1827 G1828 C1829 C1830 C1831 A1832 U1833 A G G A U A G C A A U C1845 C1846 C1847 U1848 U1849 C1850 C1851 G1852 C1853 C1854 G1855 G1856 U1857 U1858 U1859 U1860 A1861 C1862
C1863 C1864 A1865 A1866 G1867 G1868 G1869 G1870 G1871 G1872 G1873 C1874 G1875 G1876 U1877 A1878 U1879 U1880 C1881 G1882 C1883 U1884 U1885 G1886 U1887 A1888 U1889 C1890 C1891 U1892 U1893 C1894 U1895 C1896 U1897 G1898 C1899 G1900 G1901 G1902 A1903 U1904 U1905 C1906 C1907 U1908 U1909 G1910 U1911 U1912 U1913 U1914 G1915 C1916 G1917 C1918 A1919 A1920 G1921 G1922
U1923 G1924 A1925 G1926 A1927 U1928 U1929 U1930 U1931 G1932 G1933 G1934 C1935 A1936 G1937 C1938 A1939 G1940 C1941 A1942 G1943 C1944 U1945 C1946 U1947 G1948 U1949 G1950 A1951 U1952 G1953 C1954 U1955 C1956 C1957 U1958 C1959 A1960 A1961 U1962 G1963 U1964 U1965 C1966 U1967 G1968 G1969 G1970 C1971 G1972 A1973 C1974 A1975 C1976 G1977 C1978 G1979 C1980 A1981 C1982
U1983 A1984 C1985 A1986 A1987 U1988 G1989 U1990 C1991 A1992 G1993 U1994 G1995 A1996 G1997 A1998 A1999 C2000 A2001 A2002 G2003 A2004 A2005 A2006 A2007 A2008 C2009 G2010 A2011 C2012 U2013 C2014 U2015 U2016 G2017 U2018 C2019 G2020 G2021 A2022 C2023 C2024 U2025 A2026 C2027 U2028 U2029 G2030 A2031 U2032 C2033 A2034 A2035 A2036 A2037 G2038 A2039 G2040 U2041 G2042
G2043 G2044 A2045 A2046 A2047 A2048 C2049 C2050 C2051 C2052 G2053 G2054 A2055 A2056 U2057 C2058 A2059 C2060 G2061 U2062 A2063 G2064 A2065 C2066 C2067 C2068 A2069 C2070 U2071 U2072 G2073 G2074 G2075 A2076 C2077 C2078 G2079 A2080 G2081 U2082 A2083 U2084 U2085 G2086 C2087 A2088 A2089 U2090 U2091 A2092 G2095 G2096 U2097 C2098 G2099 C2100 C2101 C2102 A2103
A2104 C2105 G2106 A2107 G2108 G2109 A2110 A2111 U2112 G2113 U2114 C2115 U2116 C2117 G2118 U2119 A2120 G2121 G2122 C2123 G2124 C2125 A2126 G2127 C2128 U2129 C2130 A2131 U2132 C2133 A2134 A2135 A2136 C2137 U2138 G2139 U2140 G2141 C2142 C2143 G2144 A2145 U2146 U2147 A2148 C2149 G2150 U2151 C2152 C2153 C2154 U2155 G2156 C2157 C2158 A2159 U2160 U2161 U2162 G2163
U2164 A2165 C2166 A2167 C2168 A2169 C2170 C2171 G2172 C2173 C2174 C2175 G2176 U2177 C2178 G2179 U2180 U2181 G2182 U2183 U2184 U2185 C2186 C2187 G2188 A2189 U2190 G2191 A2192 U2193 G2194 G2195 U2196 G2197 C2198 A2199 A2200 U2201 A2202 C2203 A2204 G2205 G2206 U2207 G2208 A2209 U2210 C2211 G2212 G2213 A2214 C2215 A2216 G2217 U2218 C2219 G2220 A2221 G2222 U2223
G2224 C2225 U2226 U2227 C2228 A2229 C2230 U2231 U2232 G2233 A2234 C2235 C2236 G2237 A2238 A2239 A2240 G2241 U2242 U2243 G2244 A2245 C2246 C2247 G2248 A2249 U2250 A2251 U2252 U2253 U2254 C2255 U2256 U2257 C2258 A2259 A2260 U2261 A2262 G2263 A2264 G2265 G2266 A2267 A2268 G2269 C2270 A2271 A2272 A2273 A2274 G2275 U2276 C2277 G2278 U2279 A2280 A2281 C2282 A2283
A2284 G2285 G2286 U2287 A2288 G2289 C2290 U2291 G2292 U2293 A2294 G2295 G2296 U2297 G2298 A2299 A2300 C2301 C2302 U2303 G2304 C2305 A2306 G2307 C2308 U2309 G2310 G2311 A2312 U2313 C2314 A2315 U2316 U2317 U2318

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 86000 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 2.2 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | FEI FALCON II (4k x 4k) | Depositor |
| Maximum map value | 0.257 | Depositor |
| Minimum map value | -0.132 | Depositor |
| Average map value | -0.000 | Depositor |
| Map value standard deviation | 0.017 | Depositor |
| Recommended contour level | 0.0549 | Depositor |
| Map size (Å) | 499.19998, 499.19998, 499.19998 | wwPDB |
| Map dimensions | 320, 320, 320 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.56, 1.56, 1.56 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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 | p | 0.94 | 0/2461 | 1.01 | 3/3347 (0.1%) |
| 2 | q | 1.09 | 0/314 | 1.04 | 1/416 (0.2%) |
| 3 | r | 1.02 | 0/1131 | 1.11 | 5/1520 (0.3%) |
| 4 | t | 1.02 | 0/988 | 1.05 | 3/1325 (0.2%) |
| 5 | u | 1.05 | 0/996 | 1.10 | 5/1334 (0.4%) |
| 6 | L | 0.99 | 0/2073 | 0.98 | 0/2787 |
| 7 | M | 0.97 | 0/1137 | 0.94 | 0/1520 |
| 8 | O | 0.99 | 0/1515 | 0.96 | 0/2034 |
| 9 | Q | 1.06 | 0/1703 | 1.01 | 0/2290 |
| 10 | R | 1.00 | 0/1164 | 0.96 | 0/1559 |
| 11 | S | 0.99 | 0/641 | 1.01 | 1/858 (0.1%) |
| 12 | T | 1.13 | 0/845 | 1.00 | 0/1129 |
| 13 | U | 1.13 | 0/527 | 1.04 | 0/702 |
| 14 | V | 1.04 | 0/1026 | 1.02 | 1/1376 (0.1%) |
| 15 | W | 1.03 | 0/1809 | 1.01 | 1/2437 (0.0%) |
| 16 | X | 1.02 | 0/1238 | 0.96 | 0/1662 |
| 17 | Y | 1.01 | 0/1004 | 0.98 | 0/1335 |
| 18 | Z | 1.06 | 0/1424 | 1.01 | 0/1904 |
| 19 | b | 1.03 | 0/1394 | 0.95 | 0/1874 |
| 20 | f | 0.97 | 0/1693 | 1.01 | 5/2290 (0.2%) |
| 21 | d | 0.94 | 0/1760 | 1.03 | 2/2376 (0.1%) |
| 22 | e | 1.00 | 0/1037 | 1.03 | 0/1391 |
| 23 | g | 0.92 | 0/644 | 0.89 | 0/875 |
| 24 | a | 0.92 | 0/559 | 1.03 | 1/748 (0.1%) |
| 25 | i | 0.98 | 0/966 | 0.97 | 2/1295 (0.2%) |
| 26 | j | 0.98 | 0/530 | 1.10 | 3/707 (0.4%) |
| 27 | P | 1.09 | 0/2008 | 0.98 | 0/2678 |
| 28 | k | 1.00 | 0/985 | 0.98 | 0/1313 |
| 29 | l | 0.99 | 0/794 | 1.06 | 0/1076 |
| 30 | m | 1.03 | 0/1606 | 1.02 | 4/2141 (0.2%) |
| 31 | n | 0.98 | 0/804 | 0.99 | 0/1082 |
| 32 | o | 1.00 | 0/1140 | 1.09 | 2/1524 (0.1%) |
| 33 | c | 0.98 | 0/488 | 0.97 | 0/644 |
| 34 | h | 1.06 | 0/1381 | 1.22 | 4/1857 (0.2%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 35 | E | 1.63 | 86/48215 (0.2%) | 2.51 | 5573/75140 (7.4%) |
| All | All | 1.38 | 86/88000 (0.1%) | 2.03 | 5616/128546 (4.4%) |

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 |
|---|---|---|---|
| 1 | p | 0 | 3 |
| 3 | r | 0 | 7 |
| 4 | t | 0 | 2 |
| 5 | u | 0 | 4 |
| 8 | O | 0 | 3 |
| 9 | Q | 0 | 3 |
| 15 | W | 0 | 1 |
| 18 | Z | 0 | 1 |
| 22 | e | 0 | 1 |
| 24 | a | 0 | 2 |
| 26 | j | 0 | 1 |
| 27 | P | 0 | 2 |
| 28 | k | 0 | 1 |
| 30 | m | 0 | 2 |
| 32 | o | 0 | 2 |
| 33 | c | 0 | 2 |
| 34 | h | 0 | 22 |
| 35 | E | 4 | 121 |
| All | All | 4 | 180 |

All (86) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 35 | E | 724 | A | N9-C4 | -14.62 | 1.29 | 1.37 |
| 35 | E | 734 | G | N9-C4 | -13.56 | 1.27 | 1.38 |
| 35 | E | 711 | A | N9-C4 | -10.05 | 1.31 | 1.37 |
| 35 | E | 718 | A | N9-C4 | -9.61 | 1.32 | 1.37 |
| 35 | E | 738 | G | N9-C4 | -8.96 | 1.30 | 1.38 |
| 35 | E | 746 | A | N9-C4 | -8.02 | 1.33 | 1.37 |
| 35 | E | 733 | G | N1-C2 | 8.02 | 1.44 | 1.37 |
| 35 | E | 724 | A | N3-C4 | -7.54 | 1.30 | 1.34 |
| 35 | E | 724 | A | N7-C5 | -7.52 | 1.34 | 1.39 |
| 35 | E | 1873 | G | C6-N1 | 6.76 | 1.44 | 1.39 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 35 | E | 953 | G | N1-C2 | 6.71 | 1.43 | 1.37 |
| 35 | E | 162 | A | N7-C5 | -6.59 | 1.35 | 1.39 |
| 35 | E | 746 | A | N7-C5 | -6.45 | 1.35 | 1.39 |
| 35 | E | 172 | A | N7-C5 | -6.44 | 1.35 | 1.39 |
| 35 | E | 2189 | A | N7-C5 | -6.42 | 1.35 | 1.39 |
| 35 | E | 1600 | A | N7-C5 | -6.35 | 1.35 | 1.39 |
| 35 | E | 1327 | A | N7-C5 | -6.30 | 1.35 | 1.39 |
| 35 | E | 1305 | A | N7-C5 | -6.29 | 1.35 | 1.39 |
| 35 | E | 1852 | G | N1-C2 | 6.11 | 1.42 | 1.37 |
| 35 | E | 711 | A | N7-C5 | -6.09 | 1.35 | 1.39 |
| 35 | E | 2104 | A | N7-C5 | -6.07 | 1.35 | 1.39 |
| 35 | E | 1593 | A | N7-C5 | -6.06 | 1.35 | 1.39 |
| 35 | E | 1082 | U | C2'-C1' | -6.01 | 1.46 | 1.53 |
| 35 | E | 1768 | A | N7-C5 | -6.00 | 1.35 | 1.39 |
| 35 | E | 1872 | G | C2'-C1' | -5.95 | 1.46 | 1.53 |
| 35 | E | 256 | A | N7-C5 | -5.94 | 1.35 | 1.39 |
| 35 | E | 954 | G | N1-C2 | 5.85 | 1.42 | 1.37 |
| 35 | E | 1083 | G | C2'-C1' | -5.82 | 1.47 | 1.53 |
| 35 | E | 2264 | A | N7-C5 | -5.75 | 1.35 | 1.39 |
| 35 | E | 1554 | A | N7-C5 | -5.73 | 1.35 | 1.39 |
| 35 | E | 1348 | A | N7-C5 | -5.66 | 1.35 | 1.39 |
| 35 | E | 1328 | A | N7-C5 | -5.60 | 1.35 | 1.39 |
| 35 | E | 1872 | G | C2-N3 | 5.58 | 1.37 | 1.32 |
| 35 | E | 97 | A | N7-C5 | -5.54 | 1.35 | 1.39 |
| 35 | E | 1384 | G | N1-C2 | 5.50 | 1.42 | 1.37 |
| 35 | E | 1873 | G | N1-C2 | 5.50 | 1.42 | 1.37 |
| 35 | E | 1185 | A | N7-C5 | -5.49 | 1.35 | 1.39 |
| 35 | E | 734 | G | N1-C2 | 5.46 | 1.42 | 1.37 |
| 35 | E | 40 | A | N7-C5 | -5.46 | 1.35 | 1.39 |
| 35 | E | 952 | U | C2-N3 | 5.46 | 1.41 | 1.37 |
| 35 | E | 1634 | C | N3-C4 | 5.44 | 1.37 | 1.33 |
| 35 | E | 2120 | A | N7-C5 | -5.41 | 1.36 | 1.39 |
| 35 | E | 833 | A | C2'-C1' | -5.40 | 1.47 | 1.53 |
| 35 | E | 895 | A | N7-C5 | -5.38 | 1.36 | 1.39 |
| 35 | E | 734 | G | C6-N1 | 5.36 | 1.43 | 1.39 |
| 35 | E | 259 | C | N3-C4 | 5.33 | 1.37 | 1.33 |
| 35 | E | 1876 | G | N1-C2 | 5.31 | 1.42 | 1.37 |
| 35 | E | 1186 | U | C2-N3 | 5.30 | 1.41 | 1.37 |
| 35 | E | 1601 | A | N7-C5 | -5.28 | 1.36 | 1.39 |
| 35 | E | 90 | A | N7-C5 | -5.27 | 1.36 | 1.39 |
| 35 | E | 953 | G | N9-C4 | -5.26 | 1.33 | 1.38 |
| 35 | E | 725 | U | C2-N3 | 5.24 | 1.41 | 1.37 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 35 | E | 2113 | G | N1-C2 | 5.23 | 1.42 | 1.37 |
| 35 | E | 1625 | A | N7-C5 | -5.21 | 1.36 | 1.39 |
| 35 | E | 2134 | A | N7-C5 | -5.21 | 1.36 | 1.39 |
| 35 | E | 1730 | U | C2-N3 | 5.20 | 1.41 | 1.37 |
| 35 | E | 260 | A | N7-C5 | -5.20 | 1.36 | 1.39 |
| 35 | E | 175 | A | N7-C5 | -5.18 | 1.36 | 1.39 |
| 35 | E | 738 | G | N1-C2 | 5.18 | 1.41 | 1.37 |
| 35 | E | 51 | A | N7-C5 | -5.17 | 1.36 | 1.39 |
| 35 | E | 2214 | A | N7-C5 | -5.17 | 1.36 | 1.39 |
| 35 | E | 1675 | U | C2-N3 | 5.17 | 1.41 | 1.37 |
| 35 | E | 2204 | A | N7-C5 | -5.17 | 1.36 | 1.39 |
| 35 | E | 2145 | A | N7-C5 | -5.15 | 1.36 | 1.39 |
| 35 | E | 1599 | A | N7-C5 | -5.13 | 1.36 | 1.39 |
| 35 | E | 446 | A | N7-C5 | -5.12 | 1.36 | 1.39 |
| 35 | E | 777 | A | N7-C5 | -5.12 | 1.36 | 1.39 |
| 35 | E | 202 | C | N3-C4 | 5.12 | 1.37 | 1.33 |
| 35 | E | 807 | U | O3'-P | -5.11 | 1.55 | 1.61 |
| 35 | E | 1233 | A | N7-C5 | -5.11 | 1.36 | 1.39 |
| 35 | E | 1773 | U | C2-N3 | 5.09 | 1.41 | 1.37 |
| 35 | E | 710 | A | N7-C5 | -5.08 | 1.36 | 1.39 |
| 35 | E | 774 | C | O3'-P | -5.08 | 1.55 | 1.61 |
| 35 | E | 2152 | C | N3-C4 | 5.08 | 1.37 | 1.33 |
| 35 | E | 979 | G | C2-N3 | 5.07 | 1.36 | 1.32 |
| 35 | E | 1553 | A | N7-C5 | -5.06 | 1.36 | 1.39 |
| 35 | E | 757 | G | C2-N3 | 5.06 | 1.36 | 1.32 |
| 35 | E | 834 | G | C2-N3 | 5.06 | 1.36 | 1.32 |
| 35 | E | 909 | G | C2-N3 | 5.06 | 1.36 | 1.32 |
| 35 | E | 592 | A | N7-C5 | -5.05 | 1.36 | 1.39 |
| 35 | E | 756 | G | N1-C2 | 5.04 | 1.41 | 1.37 |
| 35 | E | 722 | C | N1-C2 | -5.04 | 1.35 | 1.40 |
| 35 | E | 1825 | A | N7-C5 | -5.03 | 1.36 | 1.39 |
| 35 | E | 1899 | C | N3-C4 | 5.03 | 1.37 | 1.33 |
| 35 | E | 363 | A | N7-C5 | -5.03 | 1.36 | 1.39 |
| 35 | E | 718 | A | N7-C5 | -5.01 | 1.36 | 1.39 |

All (5616) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 774 | C | P-O3'-C3' | 37.91 | 165.19 | 119.70 |
| 35 | E | 1187 | C | P-O3'-C3' | 33.90 | 160.37 | 119.70 |
| 35 | E | 976 | U | O5'-P-OP2 | -24.56 | 81.23 | 110.70 |
| 35 | E | 976 | U | O5'-P-OP1 | -24.39 | 81.44 | 110.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 703 | A | P-O3'-C3' | 23.77 | 148.22 | 119.70 |
| 35 | E | 531 | A | P-O3'-C3' | 22.35 | 146.52 | 119.70 |
| 35 | E | 1904 | U | P-O3'-C3' | 21.62 | 145.65 | 119.70 |
| 35 | E | 807 | U | P-O3'-C3' | 20.81 | 144.67 | 119.70 |
| 35 | E | 769 | A | P-O3'-C3' | 20.03 | 143.74 | 119.70 |
| 35 | E | 998 | C | P-O3'-C3' | 18.73 | 142.18 | 119.70 |
| 35 | E | 1546 | C | P-O3'-C3' | 18.58 | 141.99 | 119.70 |
| 35 | E | 1191 | G | P-O3'-C3' | 18.57 | 141.98 | 119.70 |
| 35 | E | 2048 | A | P-O3'-C3' | 18.40 | 141.78 | 119.70 |
| 35 | E | 2049 | C | P-O3'-C3' | 17.14 | 140.26 | 119.70 |
| 35 | E | 939 | U | P-O3'-C3' | 16.81 | 139.87 | 119.70 |
| 35 | E | 756 | G | P-O3'-C3' | 16.39 | 139.37 | 119.70 |
| 35 | E | 808 | G | P-O3'-C3' | 16.26 | 139.21 | 119.70 |
| 35 | E | 227 | U | P-O3'-C3' | 16.06 | 138.97 | 119.70 |
| 35 | E | 701 | C | P-O3'-C3' | 15.68 | 138.51 | 119.70 |
| 35 | E | 711 | A | N1-C6-N6 | 15.56 | 127.94 | 118.60 |
| 35 | E | 918 | G | P-O3'-C3' | 15.32 | 138.08 | 119.70 |
| 35 | E | 810 | U | P-O3'-C3' | 15.11 | 137.83 | 119.70 |
| 35 | E | 724 | A | N1-C6-N6 | 15.06 | 127.64 | 118.60 |
| 35 | E | 275 | A | N1-C6-N6 | 14.90 | 127.54 | 118.60 |
| 35 | E | 279 | A | N1-C6-N6 | 14.80 | 127.48 | 118.60 |
| 35 | E | 697 | G | P-O3'-C3' | 14.59 | 137.21 | 119.70 |
| 35 | E | 1088 | A | N1-C6-N6 | 14.56 | 127.34 | 118.60 |
| 35 | E | 795 | U | P-O3'-C3' | 14.56 | 137.17 | 119.70 |
| 35 | E | 975 | U | O3'-P-O5' | 14.46 | 131.48 | 104.00 |
| 35 | E | 890 | C | P-O3'-C3' | 14.46 | 137.05 | 119.70 |
| 35 | E | 175 | A | N1-C6-N6 | 14.43 | 127.26 | 118.60 |
| 35 | E | 765 | A | P-O3'-C3' | 14.34 | 136.91 | 119.70 |
| 35 | E | 727 | C | P-O3'-C3' | 14.27 | 136.82 | 119.70 |
| 35 | E | 1639 | A | N1-C6-N6 | 14.23 | 127.14 | 118.60 |
| 35 | E | 705 | G | P-O3'-C3' | 14.04 | 136.54 | 119.70 |
| 35 | E | 1607 | A | N1-C6-N6 | 13.97 | 126.98 | 118.60 |
| 35 | E | 962 | A | N1-C6-N6 | 13.96 | 126.97 | 118.60 |
| 35 | E | 1534 | A | N1-C6-N6 | 13.92 | 126.95 | 118.60 |
| 35 | E | 260 | A | N1-C6-N6 | 13.88 | 126.93 | 118.60 |
| 35 | E | 1200 | A | N1-C6-N6 | 13.84 | 126.90 | 118.60 |
| 35 | E | 942 | C | P-O3'-C3' | 13.78 | 136.24 | 119.70 |
| 35 | E | 2136 | A | N1-C6-N6 | 13.76 | 126.85 | 118.60 |
| 35 | E | 536 | A | N1-C6-N6 | 13.74 | 126.84 | 118.60 |
| 35 | E | 738 | G | N1-C6-O6 | 13.65 | 128.09 | 119.90 |
| 35 | E | 777 | A | P-O3'-C3' | 13.64 | 136.07 | 119.70 |
| 35 | E | 813 | U | P-O3'-C3' | 13.63 | 136.05 | 119.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 210 | A | N1-C6-N6 | 13.57 | 126.74 | 118.60 |
| 35 | E | 734 | G | N1-C6-O6 | 13.57 | 128.04 | 119.90 |
| 35 | E | 984 | A | N1-C6-N6 | 13.55 | 126.73 | 118.60 |
| 35 | E | 1554 | A | N1-C6-N6 | 13.54 | 126.73 | 118.60 |
| 35 | E | 1903 | A | P-O3'-C3' | 13.47 | 135.86 | 119.70 |
| 35 | E | 2306 | A | N1-C6-N6 | 13.42 | 126.65 | 118.60 |
| 35 | E | 2281 | A | N1-C6-N6 | 13.39 | 126.64 | 118.60 |
| 35 | E | 746 | A | N1-C6-N6 | 13.35 | 126.61 | 118.60 |
| 35 | E | 1593 | A | N1-C6-N6 | 13.35 | 126.61 | 118.60 |
| 35 | E | 561 | A | N1-C6-N6 | 13.25 | 126.55 | 118.60 |
| 35 | E | 1287 | A | N1-C6-N6 | 13.25 | 126.55 | 118.60 |
| 35 | E | 483 | A | N1-C6-N6 | 13.25 | 126.55 | 118.60 |
| 35 | E | 261 | A | N1-C6-N6 | 13.24 | 126.54 | 118.60 |
| 35 | E | 1998 | A | N1-C6-N6 | 13.23 | 126.54 | 118.60 |
| 35 | E | 920 | A | N1-C6-N6 | 13.21 | 126.52 | 118.60 |
| 35 | E | 2280 | A | N1-C6-N6 | 13.20 | 126.52 | 118.60 |
| 35 | E | 2092 | A | N1-C6-N6 | 13.20 | 126.52 | 118.60 |
| 35 | E | 646 | A | N1-C6-N6 | 13.15 | 126.49 | 118.60 |
| 35 | E | 2217 | G | P-O3'-C3' | 13.14 | 135.47 | 119.70 |
| 35 | E | 2229 | A | N1-C6-N6 | 13.13 | 126.48 | 118.60 |
| 35 | E | 1374 | A | N1-C6-N6 | 13.12 | 126.47 | 118.60 |
| 35 | E | 1193 | A | N1-C6-N6 | 13.09 | 126.46 | 118.60 |
| 35 | E | 2245 | A | N1-C6-N6 | 13.09 | 126.45 | 118.60 |
| 35 | E | 1981 | A | N1-C6-N6 | 13.05 | 126.43 | 118.60 |
| 35 | E | 434 | A | N1-C6-N6 | 13.05 | 126.43 | 118.60 |
| 35 | E | 2268 | A | N1-C6-N6 | 13.04 | 126.43 | 118.60 |
| 35 | E | 889 | A | N1-C6-N6 | 13.04 | 126.42 | 118.60 |
| 35 | E | 1652 | A | N1-C6-N6 | 13.04 | 126.42 | 118.60 |
| 35 | E | 910 | A | N1-C6-N6 | 13.03 | 126.42 | 118.60 |
| 35 | E | 1986 | A | N1-C6-N6 | 13.02 | 126.41 | 118.60 |
| 35 | E | 1790 | A | N1-C6-N6 | 13.00 | 126.40 | 118.60 |
| 35 | E | 1218 | A | N1-C6-N6 | 13.00 | 126.40 | 118.60 |
| 35 | E | 892 | U | P-O3'-C3' | 12.98 | 135.27 | 119.70 |
| 35 | E | 1866 | A | N1-C6-N6 | 12.96 | 126.38 | 118.60 |
| 35 | E | 1799 | A | N1-C6-N6 | 12.95 | 126.37 | 118.60 |
| 35 | E | 2022 | A | N1-C6-N6 | 12.94 | 126.37 | 118.60 |
| 35 | E | 1925 | A | N1-C6-N6 | 12.94 | 126.36 | 118.60 |
| 35 | E | 1268 | A | N1-C6-N6 | 12.93 | 126.36 | 118.60 |
| 35 | E | 1301 | A | N1-C6-N6 | 12.92 | 126.35 | 118.60 |
| 35 | E | 1804 | A | N1-C6-N6 | 12.92 | 126.35 | 118.60 |
| 35 | E | 864 | A | N1-C6-N6 | 12.91 | 126.35 | 118.60 |
| 35 | E | 492 | A | N1-C6-N6 | 12.89 | 126.33 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 2080 | A | N1-C6-N6 | 12.89 | 126.33 | 118.60 |
| 35 | E | 2251 | A | N1-C6-N6 | 12.88 | 126.33 | 118.60 |
| 35 | E | 923 | A | N1-C6-N6 | 12.88 | 126.33 | 118.60 |
| 35 | E | 1240 | A | N1-C6-N6 | 12.87 | 126.32 | 118.60 |
| 35 | E | 538 | A | N1-C6-N6 | 12.86 | 126.32 | 118.60 |
| 35 | E | 1595 | A | N1-C6-N6 | 12.86 | 126.32 | 118.60 |
| 35 | E | 2264 | A | N1-C6-N6 | 12.86 | 126.31 | 118.60 |
| 35 | E | 2059 | A | N1-C6-N6 | 12.85 | 126.31 | 118.60 |
| 35 | E | 278 | A | N1-C6-N6 | 12.82 | 126.30 | 118.60 |
| 35 | E | 457 | A | N1-C6-N6 | 12.79 | 126.28 | 118.60 |
| 35 | E | 1973 | A | N1-C6-N6 | 12.79 | 126.28 | 118.60 |
| 35 | E | 526 | A | N1-C6-N6 | 12.78 | 126.27 | 118.60 |
| 35 | E | 645 | A | N1-C6-N6 | 12.78 | 126.27 | 118.60 |
| 35 | E | 1615 | A | N1-C6-N6 | 12.77 | 126.26 | 118.60 |
| 35 | E | 1360 | A | N1-C6-N6 | 12.76 | 126.26 | 118.60 |
| 35 | E | 160 | A | N1-C6-N6 | 12.76 | 126.25 | 118.60 |
| 35 | E | 2004 | A | N1-C6-N6 | 12.75 | 126.25 | 118.60 |
| 35 | E | 976 | U | OP1-P-OP2 | 12.74 | 138.71 | 119.60 |
| 35 | E | 2002 | A | N1-C6-N6 | 12.74 | 126.25 | 118.60 |
| 35 | E | 1290 | A | N1-C6-N6 | 12.74 | 126.24 | 118.60 |
| 35 | E | 1815 | A | N1-C6-N6 | 12.73 | 126.24 | 118.60 |
| 35 | E | 702 | U | P-O3'-C3' | 12.72 | 134.97 | 119.70 |
| 35 | E | 22 | A | N1-C6-N6 | 12.72 | 126.23 | 118.60 |
| 35 | E | 1702 | A | N1-C6-N6 | 12.72 | 126.23 | 118.60 |
| 35 | E | 549 | A | N1-C6-N6 | 12.71 | 126.22 | 118.60 |
| 35 | E | 1261 | A | N1-C6-N6 | 12.71 | 126.22 | 118.60 |
| 35 | E | 1082 | U | P-O3'-C3' | 12.70 | 134.94 | 119.70 |
| 35 | E | 2221 | A | N1-C6-N6 | 12.70 | 126.22 | 118.60 |
| 35 | E | 450 | A | N1-C6-N6 | 12.69 | 126.21 | 118.60 |
| 35 | E | 1336 | A | N1-C6-N6 | 12.69 | 126.21 | 118.60 |
| 35 | E | 2209 | A | N1-C6-N6 | 12.69 | 126.21 | 118.60 |
| 35 | E | 414 | A | N1-C6-N6 | 12.68 | 126.21 | 118.60 |
| 35 | E | 1628 | A | N1-C6-N6 | 12.67 | 126.20 | 118.60 |
| 35 | E | 1196 | A | N1-C6-N6 | 12.64 | 126.19 | 118.60 |
| 35 | E | 1302 | A | N1-C6-N6 | 12.64 | 126.19 | 118.60 |
| 35 | E | 604 | A | N1-C6-N6 | 12.64 | 126.18 | 118.60 |
| 35 | E | 658 | A | N1-C6-N6 | 12.62 | 126.17 | 118.60 |
| 35 | E | 202 | C | P-O3'-C3' | 12.62 | 134.84 | 119.70 |
| 35 | E | 226 | A | N1-C6-N6 | 12.61 | 126.17 | 118.60 |
| 35 | E | 1309 | A | N1-C6-N6 | 12.61 | 126.17 | 118.60 |
| 35 | E | 73 | A | N1-C6-N6 | 12.60 | 126.16 | 118.60 |
| 35 | E | 1235 | A | N1-C6-N6 | 12.60 | 126.16 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 105 | A | N1-C6-N6 | 12.60 | 126.16 | 118.60 |
| 35 | E | 1818 | A | N1-C6-N6 | 12.58 | 126.14 | 118.60 |
| 35 | E | 2234 | A | N1-C6-N6 | 12.56 | 126.14 | 118.60 |
| 35 | E | 144 | A | N1-C6-N6 | 12.56 | 126.13 | 118.60 |
| 35 | E | 1355 | A | N1-C6-N6 | 12.55 | 126.13 | 118.60 |
| 35 | E | 1222 | A | N1-C6-N6 | 12.55 | 126.13 | 118.60 |
| 35 | E | 281 | A | N1-C6-N6 | 12.54 | 126.12 | 118.60 |
| 35 | E | 121 | A | N1-C6-N6 | 12.53 | 126.12 | 118.60 |
| 35 | E | 1275 | A | N1-C6-N6 | 12.53 | 126.12 | 118.60 |
| 35 | E | 1679 | A | N1-C6-N6 | 12.53 | 126.12 | 118.60 |
| 35 | E | 62 | A | N1-C6-N6 | 12.53 | 126.12 | 118.60 |
| 35 | E | 111 | A | N1-C6-N6 | 12.52 | 126.11 | 118.60 |
| 35 | E | 1188 | C | P-O5'-C5' | 12.52 | 140.94 | 120.90 |
| 35 | E | 2047 | A | N1-C6-N6 | 12.51 | 126.11 | 118.60 |
| 35 | E | 1241 | A | N1-C6-N6 | 12.51 | 126.11 | 118.60 |
| 35 | E | 2234 | A | P-O3'-C3' | 12.50 | 134.70 | 119.70 |
| 35 | E | 814 | C | P-O3'-C3' | 12.50 | 134.70 | 119.70 |
| 35 | E | 1185 | A | N1-C6-N6 | 12.49 | 126.10 | 118.60 |
| 35 | E | 78 | A | N1-C6-N6 | 12.49 | 126.09 | 118.60 |
| 35 | E | 1951 | A | N1-C6-N6 | 12.49 | 126.09 | 118.60 |
| 35 | E | 1308 | A | N1-C6-N6 | 12.48 | 126.09 | 118.60 |
| 35 | E | 1657 | A | N1-C6-N6 | 12.48 | 126.09 | 118.60 |
| 35 | E | 1732 | A | N1-C6-N6 | 12.48 | 126.09 | 118.60 |
| 35 | E | 1681 | A | N1-C6-N6 | 12.47 | 126.08 | 118.60 |
| 35 | E | 381 | A | N1-C6-N6 | 12.47 | 126.08 | 118.60 |
| 35 | E | 2200 | A | N1-C6-N6 | 12.47 | 126.08 | 118.60 |
| 35 | E | 392 | A | N1-C6-N6 | 12.47 | 126.08 | 118.60 |
| 35 | E | 472 | A | N1-C6-N6 | 12.46 | 126.08 | 118.60 |
| 35 | E | 2288 | A | N1-C6-N6 | 12.45 | 126.07 | 118.60 |
| 35 | E | 1286 | A | N1-C6-N6 | 12.45 | 126.07 | 118.60 |
| 35 | E | 2001 | A | N1-C6-N6 | 12.45 | 126.07 | 118.60 |
| 35 | E | 251 | A | N1-C6-N6 | 12.44 | 126.06 | 118.60 |
| 35 | E | 1314 | A | N1-C6-N6 | 12.44 | 126.06 | 118.60 |
| 35 | E | 935 | A | P-O3'-C3' | 12.44 | 134.62 | 119.70 |
| 35 | E | 505 | A | N1-C6-N6 | 12.43 | 126.06 | 118.60 |
| 35 | E | 1279 | A | N1-C6-N6 | 12.43 | 126.06 | 118.60 |
| 35 | E | 799 | A | N1-C6-N6 | 12.42 | 126.05 | 118.60 |
| 35 | E | 1609 | A | N1-C6-N6 | 12.42 | 126.05 | 118.60 |
| 35 | E | 1574 | A | N1-C6-N6 | 12.42 | 126.05 | 118.60 |
| 35 | E | 1553 | A | N1-C6-N6 | 12.41 | 126.05 | 118.60 |
| 35 | E | 2145 | A | N1-C6-N6 | 12.40 | 126.04 | 118.60 |
| 35 | E | 2202 | A | N1-C6-N6 | 12.40 | 126.04 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 852 | A | N1-C6-N6 | 12.40 | 126.04 | 118.60 |
| 35 | E | 581 | A | N1-C6-N6 | 12.40 | 126.04 | 118.60 |
| 35 | E | 475 | A | N1-C6-N6 | 12.39 | 126.04 | 118.60 |
| 35 | E | 588 | A | N1-C6-N6 | 12.39 | 126.04 | 118.60 |
| 35 | E | 1086 | A | N1-C6-N6 | 12.38 | 126.03 | 118.60 |
| 35 | E | 1706 | A | N1-C6-N6 | 12.37 | 126.02 | 118.60 |
| 35 | E | 123 | A | N1-C6-N6 | 12.36 | 126.02 | 118.60 |
| 35 | E | 349 | A | N1-C6-N6 | 12.36 | 126.02 | 118.60 |
| 35 | E | 2088 | A | N1-C6-N6 | 12.36 | 126.01 | 118.60 |
| 35 | E | 1192 | A | P-O3'-C3' | 12.35 | 134.52 | 119.70 |
| 35 | E | 1710 | A | N1-C6-N6 | 12.35 | 126.01 | 118.60 |
| 35 | E | 1936 | A | N1-C6-N6 | 12.35 | 126.01 | 118.60 |
| 35 | E | 831 | A | N1-C6-N6 | 12.34 | 126.00 | 118.60 |
| 35 | E | 639 | A | N1-C6-N6 | 12.34 | 126.00 | 118.60 |
| 35 | E | 509 | A | N1-C6-N6 | 12.34 | 126.00 | 118.60 |
| 35 | E | 215 | A | N1-C6-N6 | 12.33 | 126.00 | 118.60 |
| 35 | E | 406 | A | N1-C6-N6 | 12.33 | 126.00 | 118.60 |
| 35 | E | 1330 | A | N1-C6-N6 | 12.33 | 126.00 | 118.60 |
| 35 | E | 785 | A | N1-C6-N6 | 12.33 | 126.00 | 118.60 |
| 35 | E | 704 | A | N1-C6-N6 | 12.32 | 125.99 | 118.60 |
| 35 | E | 190 | A | N1-C6-N6 | 12.31 | 125.98 | 118.60 |
| 35 | E | 287 | A | N1-C6-N6 | 12.30 | 125.98 | 118.60 |
| 35 | E | 872 | A | N1-C6-N6 | 12.30 | 125.98 | 118.60 |
| 35 | E | 1794 | A | N1-C6-N6 | 12.29 | 125.98 | 118.60 |
| 35 | E | 788 | A | N1-C6-N6 | 12.29 | 125.97 | 118.60 |
| 35 | E | 1704 | A | N1-C6-N6 | 12.29 | 125.97 | 118.60 |
| 35 | E | 1768 | A | N1-C6-N6 | 12.28 | 125.97 | 118.60 |
| 35 | E | 1781 | A | N1-C6-N6 | 12.28 | 125.97 | 118.60 |
| 35 | E | 241 | A | N1-C6-N6 | 12.27 | 125.96 | 118.60 |
| 35 | E | 647 | A | N1-C6-N6 | 12.27 | 125.96 | 118.60 |
| 35 | E | 599 | A | N1-C6-N6 | 12.27 | 125.96 | 118.60 |
| 35 | E | 764 | A | N1-C6-N6 | 12.26 | 125.95 | 118.60 |
| 35 | E | 522 | A | N1-C6-N6 | 12.26 | 125.95 | 118.60 |
| 35 | E | 1797 | A | N1-C6-N6 | 12.25 | 125.95 | 118.60 |
| 35 | E | 2046 | A | N1-C6-N6 | 12.25 | 125.95 | 118.60 |
| 35 | E | 2262 | A | N1-C6-N6 | 12.25 | 125.95 | 118.60 |
| 35 | E | 257 | A | N1-C6-N6 | 12.25 | 125.95 | 118.60 |
| 35 | E | 569 | A | N1-C6-N6 | 12.25 | 125.95 | 118.60 |
| 35 | E | 653 | A | N1-C6-N6 | 12.25 | 125.95 | 118.60 |
| 35 | E | 432 | A | N1-C6-N6 | 12.24 | 125.95 | 118.60 |
| 35 | E | 703 | A | N1-C6-N6 | 12.24 | 125.95 | 118.60 |
| 35 | E | 1259 | A | N1-C6-N6 | 12.24 | 125.95 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 2111 | A | N1-C6-N6 | 12.24 | 125.95 | 118.60 |
| 35 | E | 1265 | A | N1-C6-N6 | 12.23 | 125.94 | 118.60 |
| 35 | E | 314 | A | N1-C6-N6 | 12.22 | 125.94 | 118.60 |
| 35 | E | 1217 | A | N1-C6-N6 | 12.22 | 125.93 | 118.60 |
| 35 | E | 438 | A | N1-C6-N6 | 12.22 | 125.93 | 118.60 |
| 35 | E | 1192 | A | N1-C6-N6 | 12.22 | 125.93 | 118.60 |
| 35 | E | 304 | A | N1-C6-N6 | 12.22 | 125.93 | 118.60 |
| 35 | E | 1561 | A | N1-C6-N6 | 12.21 | 125.93 | 118.60 |
| 35 | E | 256 | A | N1-C6-N6 | 12.21 | 125.93 | 118.60 |
| 35 | E | 1292 | A | N1-C6-N6 | 12.21 | 125.93 | 118.60 |
| 35 | E | 778 | A | N1-C6-N6 | 12.21 | 125.92 | 118.60 |
| 35 | E | 348 | A | N1-C6-N6 | 12.20 | 125.92 | 118.60 |
| 35 | E | 655 | A | N1-C6-N6 | 12.20 | 125.92 | 118.60 |
| 35 | E | 1832 | A | N1-C6-N6 | 12.20 | 125.92 | 118.60 |
| 35 | E | 2048 | A | N1-C6-N6 | 12.20 | 125.92 | 118.60 |
| 35 | E | 1822 | A | N1-C6-N6 | 12.20 | 125.92 | 118.60 |
| 35 | E | 576 | A | N1-C6-N6 | 12.19 | 125.91 | 118.60 |
| 35 | E | 10 | G | N1-C6-O6 | 12.19 | 127.21 | 119.90 |
| 35 | E | 1661 | A | N1-C6-N6 | 12.19 | 125.91 | 118.60 |
| 35 | E | 161 | A | N1-C6-N6 | 12.18 | 125.91 | 118.60 |
| 35 | E | 454 | A | N1-C6-N6 | 12.18 | 125.91 | 118.60 |
| 35 | E | 1205 | A | N1-C6-N6 | 12.18 | 125.91 | 118.60 |
| 35 | E | 742 | A | N1-C6-N6 | 12.18 | 125.91 | 118.60 |
| 35 | E | 1215 | A | N1-C6-N6 | 12.18 | 125.91 | 118.60 |
| 35 | E | 11 | A | N1-C6-N6 | 12.17 | 125.90 | 118.60 |
| 35 | E | 710 | A | N1-C6-N6 | 12.17 | 125.90 | 118.60 |
| 35 | E | 1913 | U | P-O3'-C3' | 12.17 | 134.30 | 119.70 |
| 35 | E | 1676 | A | N1-C6-N6 | 12.16 | 125.90 | 118.60 |
| 35 | E | 894 | A | N1-C6-N6 | 12.16 | 125.89 | 118.60 |
| 35 | E | 2167 | A | N1-C6-N6 | 12.16 | 125.89 | 118.60 |
| 35 | E | 1258 | A | N1-C6-N6 | 12.15 | 125.89 | 118.60 |
| 35 | E | 1176 | A | N1-C6-N6 | 12.15 | 125.89 | 118.60 |
| 35 | E | 1619 | A | N1-C6-N6 | 12.15 | 125.89 | 118.60 |
| 35 | E | 417 | A | N1-C6-N6 | 12.14 | 125.89 | 118.60 |
| 35 | E | 2031 | A | N1-C6-N6 | 12.14 | 125.89 | 118.60 |
| 35 | E | 1764 | A | N1-C6-N6 | 12.14 | 125.88 | 118.60 |
| 35 | E | 168 | A | N1-C6-N6 | 12.12 | 125.88 | 118.60 |
| 35 | E | 845 | A | N1-C6-N6 | 12.12 | 125.88 | 118.60 |
| 35 | E | 728 | A | N1-C6-N6 | 12.12 | 125.87 | 118.60 |
| 35 | E | 884 | A | N1-C6-N6 | 12.12 | 125.87 | 118.60 |
| 35 | E | 371 | A | N1-C6-N6 | 12.12 | 125.87 | 118.60 |
| 35 | E | 1385 | A | N1-C6-N6 | 12.11 | 125.87 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1592 | A | N1-C6-N6 | 12.11 | 125.87 | 118.60 |
| 35 | E | 28 | A | N1-C6-N6 | 12.11 | 125.87 | 118.60 |
| 35 | E | 2036 | A | N1-C6-N6 | 12.11 | 125.87 | 118.60 |
| 35 | E | 2083 | A | N1-C6-N6 | 12.11 | 125.86 | 118.60 |
| 35 | E | 142 | A | N1-C6-N6 | 12.11 | 125.86 | 118.60 |
| 35 | E | 592 | A | N1-C6-N6 | 12.10 | 125.86 | 118.60 |
| 35 | E | 826 | A | N1-C6-N6 | 12.10 | 125.86 | 118.60 |
| 35 | E | 1362 | A | N1-C6-N6 | 12.10 | 125.86 | 118.60 |
| 35 | E | 1611 | A | N1-C6-N6 | 12.10 | 125.86 | 118.60 |
| 35 | E | 2299 | A | N1-C6-N6 | 12.10 | 125.86 | 118.60 |
| 35 | E | 65 | A | N1-C6-N6 | 12.10 | 125.86 | 118.60 |
| 35 | E | 1825 | A | N1-C6-N6 | 12.10 | 125.86 | 118.60 |
| 35 | E | 1526 | A | N1-C6-N6 | 12.09 | 125.86 | 118.60 |
| 35 | E | 783 | A | N1-C6-N6 | 12.09 | 125.85 | 118.60 |
| 35 | E | 1865 | A | N1-C6-N6 | 12.09 | 125.85 | 118.60 |
| 35 | E | 586 | A | N1-C6-N6 | 12.09 | 125.85 | 118.60 |
| 35 | E | 659 | A | N1-C6-N6 | 12.08 | 125.85 | 118.60 |
| 35 | E | 1270 | A | N1-C6-N6 | 12.08 | 125.85 | 118.60 |
| 35 | E | 875 | A | N1-C6-N6 | 12.08 | 125.85 | 118.60 |
| 35 | E | 245 | A | N1-C6-N6 | 12.07 | 125.84 | 118.60 |
| 35 | E | 916 | A | N1-C6-N6 | 12.07 | 125.84 | 118.60 |
| 35 | E | 2294 | A | N1-C6-N6 | 12.07 | 125.84 | 118.60 |
| 35 | E | 577 | A | N1-C6-N6 | 12.07 | 125.84 | 118.60 |
| 35 | E | 503 | A | N1-C6-N6 | 12.06 | 125.84 | 118.60 |
| 35 | E | 2089 | A | N1-C6-N6 | 12.06 | 125.83 | 118.60 |
| 35 | E | 809 | A | N1-C6-N6 | 12.05 | 125.83 | 118.60 |
| 35 | E | 2076 | A | N1-C6-N6 | 12.05 | 125.83 | 118.60 |
| 35 | E | 26 | A | N1-C6-N6 | 12.05 | 125.83 | 118.60 |
| 35 | E | 935 | A | N1-C6-N6 | 12.04 | 125.83 | 118.60 |
| 35 | E | 974 | A | N1-C6-N6 | 12.04 | 125.83 | 118.60 |
| 35 | E | 124 | A | N1-C6-N6 | 12.04 | 125.82 | 118.60 |
| 35 | E | 507 | A | N1-C6-N6 | 12.04 | 125.82 | 118.60 |
| 35 | E | 977 | A | N1-C6-N6 | 12.04 | 125.82 | 118.60 |
| 35 | E | 2026 | A | N1-C6-N6 | 12.04 | 125.82 | 118.60 |
| 35 | E | 863 | A | N1-C6-N6 | 12.04 | 125.82 | 118.60 |
| 35 | E | 1175 | A | N1-C6-N6 | 12.04 | 125.82 | 118.60 |
| 35 | E | 2283 | A | N1-C6-N6 | 12.03 | 125.82 | 118.60 |
| 35 | E | 990 | A | N1-C6-N6 | 12.03 | 125.82 | 118.60 |
| 35 | E | 506 | A | N1-C6-N6 | 12.02 | 125.81 | 118.60 |
| 35 | E | 2189 | A | N1-C6-N6 | 12.02 | 125.81 | 118.60 |
| 35 | E | 610 | A | N1-C6-N6 | 12.02 | 125.81 | 118.60 |
| 35 | E | 246 | A | N1-C6-N6 | 12.02 | 125.81 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 295 | A | N1-C6-N6 | 12.02 | 125.81 | 118.60 |
| 35 | E | 891 | U | P-O3'-C3' | 12.02 | 134.12 | 119.70 |
| 35 | E | 386 | A | N1-C6-N6 | 12.01 | 125.81 | 118.60 |
| 35 | E | 833 | A | N1-C6-N6 | 12.01 | 125.81 | 118.60 |
| 35 | E | 2216 | A | N1-C6-N6 | 12.01 | 125.81 | 118.60 |
| 35 | E | 2 | A | N1-C6-N6 | 12.01 | 125.81 | 118.60 |
| 35 | E | 595 | A | N1-C6-N6 | 12.01 | 125.80 | 118.60 |
| 35 | E | 675 | A | N1-C6-N6 | 12.01 | 125.80 | 118.60 |
| 35 | E | 2126 | A | N1-C6-N6 | 12.01 | 125.80 | 118.60 |
| 35 | E | 905 | A | N1-C6-N6 | 12.00 | 125.80 | 118.60 |
| 35 | E | 1255 | A | N1-C6-N6 | 12.00 | 125.80 | 118.60 |
| 35 | E | 2272 | A | N1-C6-N6 | 12.00 | 125.80 | 118.60 |
| 35 | E | 504 | A | N1-C6-N6 | 12.00 | 125.80 | 118.60 |
| 35 | E | 499 | A | N1-C6-N6 | 11.99 | 125.80 | 118.60 |
| 35 | E | 2267 | A | N1-C6-N6 | 11.99 | 125.80 | 118.60 |
| 35 | E | 587 | A | N1-C6-N6 | 11.99 | 125.79 | 118.60 |
| 35 | E | 698 | C | P-O3'-C3' | 11.99 | 134.08 | 119.70 |
| 35 | E | 444 | A | N1-C6-N6 | 11.98 | 125.79 | 118.60 |
| 35 | E | 915 | A | N1-C6-N6 | 11.98 | 125.79 | 118.60 |
| 35 | E | 1984 | A | N1-C6-N6 | 11.98 | 125.79 | 118.60 |
| 35 | E | 1180 | A | N1-C6-N6 | 11.98 | 125.79 | 118.60 |
| 35 | E | 2011 | A | N1-C6-N6 | 11.98 | 125.79 | 118.60 |
| 35 | E | 2135 | A | N1-C6-N6 | 11.98 | 125.79 | 118.60 |
| 35 | E | 1903 | A | N1-C6-N6 | 11.97 | 125.78 | 118.60 |
| 35 | E | 858 | A | N1-C6-N6 | 11.97 | 125.78 | 118.60 |
| 35 | E | 300 | A | N1-C6-N6 | 11.97 | 125.78 | 118.60 |
| 35 | E | 1368 | A | N1-C6-N6 | 11.97 | 125.78 | 118.60 |
| 35 | E | 1633 | A | N1-C6-N6 | 11.97 | 125.78 | 118.60 |
| 35 | E | 1529 | A | N1-C6-N6 | 11.96 | 125.78 | 118.60 |
| 35 | E | 1902 | G | P-O3'-C3' | 11.96 | 134.06 | 119.70 |
| 35 | E | 2260 | A | N1-C6-N6 | 11.96 | 125.78 | 118.60 |
| 35 | E | 2037 | A | N1-C6-N6 | 11.96 | 125.78 | 118.60 |
| 35 | E | 979 | G | N1-C6-O6 | 11.96 | 127.08 | 119.90 |
| 35 | E | 1353 | A | N1-C6-N6 | 11.96 | 125.77 | 118.60 |
| 35 | E | 765 | A | N1-C6-N6 | 11.95 | 125.77 | 118.60 |
| 35 | E | 1960 | A | N1-C6-N6 | 11.95 | 125.77 | 118.60 |
| 35 | E | 1327 | A | N1-C6-N6 | 11.95 | 125.77 | 118.60 |
| 35 | E | 141 | A | N1-C6-N6 | 11.95 | 125.77 | 118.60 |
| 35 | E | 516 | A | N1-C6-N6 | 11.95 | 125.77 | 118.60 |
| 35 | E | 1087 | A | N1-C6-N6 | 11.94 | 125.77 | 118.60 |
| 35 | E | 68 | A | N1-C6-N6 | 11.94 | 125.77 | 118.60 |
| 35 | E | 531 | A | N1-C6-N6 | 11.94 | 125.77 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 781 | A | N1-C6-N6 | 11.94 | 125.76 | 118.60 |
| 35 | E | 598 | A | N1-C6-N6 | 11.94 | 125.76 | 118.60 |
| 35 | E | 1539 | A | N1-C6-N6 | 11.94 | 125.76 | 118.60 |
| 35 | E | 1568 | A | N1-C6-N6 | 11.93 | 125.76 | 118.60 |
| 35 | E | 40 | A | N1-C6-N6 | 11.93 | 125.76 | 118.60 |
| 35 | E | 242 | A | N1-C6-N6 | 11.93 | 125.76 | 118.60 |
| 35 | E | 498 | A | N1-C6-N6 | 11.93 | 125.76 | 118.60 |
| 35 | E | 467 | A | N1-C6-N6 | 11.92 | 125.75 | 118.60 |
| 35 | E | 2259 | A | N1-C6-N6 | 11.92 | 125.75 | 118.60 |
| 35 | E | 596 | A | N1-C6-N6 | 11.92 | 125.75 | 118.60 |
| 35 | E | 2065 | A | N1-C6-N6 | 11.92 | 125.75 | 118.60 |
| 35 | E | 107 | A | N1-C6-N6 | 11.92 | 125.75 | 118.60 |
| 35 | E | 782 | A | N1-C6-N6 | 11.92 | 125.75 | 118.60 |
| 35 | E | 793 | A | N1-C6-N6 | 11.91 | 125.75 | 118.60 |
| 35 | E | 960 | A | N1-C6-N6 | 11.91 | 125.75 | 118.60 |
| 35 | E | 912 | A | N1-C6-N6 | 11.91 | 125.75 | 118.60 |
| 35 | E | 562 | A | N1-C6-N6 | 11.91 | 125.74 | 118.60 |
| 35 | E | 1370 | A | N1-C6-N6 | 11.90 | 125.74 | 118.60 |
| 35 | E | 1333 | A | N1-C6-N6 | 11.90 | 125.74 | 118.60 |
| 35 | E | 525 | A | N1-C6-N6 | 11.90 | 125.74 | 118.60 |
| 35 | E | 2005 | A | N1-C6-N6 | 11.90 | 125.74 | 118.60 |
| 35 | E | 1343 | A | N1-C6-N6 | 11.89 | 125.74 | 118.60 |
| 35 | E | 529 | A | N1-C6-N6 | 11.89 | 125.73 | 118.60 |
| 35 | E | 2199 | A | N1-C6-N6 | 11.89 | 125.73 | 118.60 |
| 35 | E | 81 | A | N1-C6-N6 | 11.89 | 125.73 | 118.60 |
| 35 | E | 1264 | A | N1-C6-N6 | 11.89 | 125.73 | 118.60 |
| 35 | E | 1189 | A | N1-C6-N6 | 11.89 | 125.73 | 118.60 |
| 35 | E | 1888 | A | N1-C6-N6 | 11.89 | 125.73 | 118.60 |
| 35 | E | 1996 | A | N1-C6-N6 | 11.88 | 125.73 | 118.60 |
| 35 | E | 47 | A | N1-C6-N6 | 11.88 | 125.73 | 118.60 |
| 35 | E | 352 | A | N1-C6-N6 | 11.88 | 125.73 | 118.60 |
| 35 | E | 634 | A | N1-C6-N6 | 11.88 | 125.73 | 118.60 |
| 35 | E | 1743 | A | N1-C6-N6 | 11.88 | 125.73 | 118.60 |
| 35 | E | 1631 | A | N1-C6-N6 | 11.87 | 125.72 | 118.60 |
| 35 | E | 1733 | A | N1-C6-N6 | 11.87 | 125.72 | 118.60 |
| 35 | E | 2238 | A | N1-C6-N6 | 11.87 | 125.72 | 118.60 |
| 35 | E | 792 | G | N1-C6-O6 | 11.87 | 127.02 | 119.90 |
| 35 | E | 1662 | A | N1-C6-N6 | 11.87 | 125.72 | 118.60 |
| 35 | E | 1920 | A | N1-C6-N6 | 11.87 | 125.72 | 118.60 |
| 35 | E | 1999 | A | N1-C6-N6 | 11.87 | 125.72 | 118.60 |
| 35 | E | 64 | A | N1-C6-N6 | 11.86 | 125.72 | 118.60 |
| 35 | E | 501 | A | N1-C6-N6 | 11.87 | 125.72 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 607 | A | N1-C6-N6 | 11.87 | 125.72 | 118.60 |
| 35 | E | 769 | A | N1-C6-N6 | 11.86 | 125.72 | 118.60 |
| 35 | E | 571 | A | N1-C6-N6 | 11.86 | 125.72 | 118.60 |
| 35 | E | 2192 | A | N1-C6-N6 | 11.86 | 125.72 | 118.60 |
| 35 | E | 82 | A | N1-C6-N6 | 11.86 | 125.72 | 118.60 |
| 35 | E | 184 | A | N1-C6-N6 | 11.86 | 125.71 | 118.60 |
| 35 | E | 181 | A | N1-C6-N6 | 11.86 | 125.71 | 118.60 |
| 35 | E | 775 | A | N1-C6-N6 | 11.86 | 125.71 | 118.60 |
| 35 | E | 898 | A | N1-C6-N6 | 11.86 | 125.71 | 118.60 |
| 35 | E | 97 | A | N1-C6-N6 | 11.85 | 125.71 | 118.60 |
| 35 | E | 2103 | A | N1-C6-N6 | 11.85 | 125.71 | 118.60 |
| 35 | E | 1610 | A | N1-C6-N6 | 11.85 | 125.71 | 118.60 |
| 35 | E | 527 | A | N1-C6-N6 | 11.84 | 125.71 | 118.60 |
| 35 | E | 425 | A | N1-C6-N6 | 11.83 | 125.70 | 118.60 |
| 35 | E | 861 | A | N1-C6-N6 | 11.83 | 125.70 | 118.60 |
| 35 | E | 180 | A | N1-C6-N6 | 11.83 | 125.70 | 118.60 |
| 35 | E | 624 | A | N1-C6-N6 | 11.83 | 125.70 | 118.60 |
| 35 | E | 690 | A | N1-C6-N6 | 11.83 | 125.70 | 118.60 |
| 35 | E | 1651 | A | N1-C6-N6 | 11.83 | 125.70 | 118.60 |
| 35 | E | 1689 | A | N1-C6-N6 | 11.83 | 125.70 | 118.60 |
| 35 | E | 2273 | A | N1-C6-N6 | 11.83 | 125.70 | 118.60 |
| 35 | E | 992 | A | N1-C6-N6 | 11.83 | 125.70 | 118.60 |
| 35 | E | 1987 | A | N1-C6-N6 | 11.83 | 125.69 | 118.60 |
| 35 | E | 19 | A | N1-C6-N6 | 11.82 | 125.69 | 118.60 |
| 35 | E | 648 | A | N1-C6-N6 | 11.82 | 125.69 | 118.60 |
| 35 | E | 1975 | A | N1-C6-N6 | 11.82 | 125.69 | 118.60 |
| 35 | E | 917 | A | N1-C6-N6 | 11.82 | 125.69 | 118.60 |
| 35 | E | 177 | A | N1-C6-N6 | 11.82 | 125.69 | 118.60 |
| 35 | E | 1312 | A | N1-C6-N6 | 11.81 | 125.69 | 118.60 |
| 35 | E | 959 | A | N1-C6-N6 | 11.81 | 125.69 | 118.60 |
| 35 | E | 447 | A | N1-C6-N6 | 11.80 | 125.68 | 118.60 |
| 35 | E | 585 | A | N1-C6-N6 | 11.80 | 125.68 | 118.60 |
| 35 | E | 249 | A | N1-C6-N6 | 11.80 | 125.68 | 118.60 |
| 35 | E | 2035 | A | N1-C6-N6 | 11.80 | 125.68 | 118.60 |
| 35 | E | 112 | A | N1-C6-N6 | 11.80 | 125.68 | 118.60 |
| 35 | E | 902 | A | N1-C6-N6 | 11.80 | 125.68 | 118.60 |
| 35 | E | 1878 | A | N1-C6-N6 | 11.80 | 125.68 | 118.60 |
| 35 | E | 865 | A | N1-C6-N6 | 11.79 | 125.67 | 118.60 |
| 35 | E | 1248 | A | N1-C6-N6 | 11.79 | 125.67 | 118.60 |
| 35 | E | 1313 | A | N1-C6-N6 | 11.79 | 125.67 | 118.60 |
| 35 | E | 250 | A | N1-C6-N6 | 11.79 | 125.67 | 118.60 |
| 35 | E | 502 | A | N1-C6-N6 | 11.79 | 125.67 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 500 | A | N1-C6-N6 | 11.78 | 125.67 | 118.60 |
| 35 | E | 167 | A | N1-C6-N6 | 11.78 | 125.67 | 118.60 |
| 35 | E | 1724 | A | N1-C6-N6 | 11.78 | 125.67 | 118.60 |
| 35 | E | 1992 | A | N1-C6-N6 | 11.78 | 125.67 | 118.60 |
| 35 | E | 2008 | A | N1-C6-N6 | 11.78 | 125.67 | 118.60 |
| 35 | E | 493 | A | N1-C6-N6 | 11.78 | 125.67 | 118.60 |
| 35 | E | 2055 | A | N1-C6-N6 | 11.77 | 125.66 | 118.60 |
| 35 | E | 254 | A | N1-C6-N6 | 11.77 | 125.66 | 118.60 |
| 35 | E | 694 | A | N1-C6-N6 | 11.77 | 125.66 | 118.60 |
| 35 | E | 2274 | A | N1-C6-N6 | 11.77 | 125.66 | 118.60 |
| 35 | E | 1919 | A | N1-C6-N6 | 11.77 | 125.66 | 118.60 |
| 35 | E | 735 | A | N1-C6-N6 | 11.76 | 125.66 | 118.60 |
| 35 | E | 673 | A | N1-C6-N6 | 11.76 | 125.66 | 118.60 |
| 35 | E | 718 | A | N1-C6-N6 | 11.76 | 125.66 | 118.60 |
| 35 | E | 231 | A | N1-C6-N6 | 11.76 | 125.65 | 118.60 |
| 35 | E | 2069 | A | N1-C6-N6 | 11.76 | 125.65 | 118.60 |
| 35 | E | 1323 | A | N1-C6-N6 | 11.75 | 125.65 | 118.60 |
| 35 | E | 330 | A | N1-C6-N6 | 11.75 | 125.65 | 118.60 |
| 35 | E | 523 | A | N1-C6-N6 | 11.74 | 125.65 | 118.60 |
| 35 | E | 779 | A | N1-C6-N6 | 11.74 | 125.65 | 118.60 |
| 35 | E | 913 | A | N1-C6-N6 | 11.74 | 125.65 | 118.60 |
| 35 | E | 961 | A | N1-C6-N6 | 11.74 | 125.64 | 118.60 |
| 35 | E | 51 | A | N1-C6-N6 | 11.74 | 125.64 | 118.60 |
| 35 | E | 269 | A | N1-C6-N6 | 11.74 | 125.64 | 118.60 |
| 35 | E | 345 | A | N1-C6-N6 | 11.73 | 125.64 | 118.60 |
| 35 | E | 829 | C | P-O3'-C3' | 11.73 | 133.78 | 119.70 |
| 35 | E | 185 | A | N1-C6-N6 | 11.73 | 125.64 | 118.60 |
| 35 | E | 1197 | A | N1-C6-N6 | 11.73 | 125.64 | 118.60 |
| 35 | E | 43 | A | N1-C6-N6 | 11.72 | 125.63 | 118.60 |
| 35 | E | 786 | A | N1-C6-N6 | 11.72 | 125.63 | 118.60 |
| 35 | E | 812 | A | N1-C6-N6 | 11.72 | 125.63 | 118.60 |
| 35 | E | 2039 | A | N1-C6-N6 | 11.72 | 125.63 | 118.60 |
| 35 | E | 1942 | A | N1-C6-N6 | 11.72 | 125.63 | 118.60 |
| 35 | E | 149 | A | N1-C6-N6 | 11.72 | 125.63 | 118.60 |
| 35 | E | 771 | A | N1-C6-N6 | 11.71 | 125.63 | 118.60 |
| 35 | E | 932 | G | N1-C6-O6 | 11.71 | 126.93 | 119.90 |
| 35 | E | 972 | A | N1-C6-N6 | 11.71 | 125.63 | 118.60 |
| 35 | E | 1620 | A | N1-C6-N6 | 11.71 | 125.63 | 118.60 |
| 35 | E | 2315 | A | N1-C6-N6 | 11.71 | 125.62 | 118.60 |
| 35 | E | 55 | A | N1-C6-N6 | 11.70 | 125.62 | 118.60 |
| 35 | E | 2134 | A | N1-C6-N6 | 11.70 | 125.62 | 118.60 |
| 35 | E | 2169 | A | N1-C6-N6 | 11.70 | 125.62 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 866 | A | N1-C6-N6 | 11.70 | 125.62 | 118.60 |
| 35 | E | 2104 | A | N1-C6-N6 | 11.70 | 125.62 | 118.60 |
| 35 | E | 1803 | A | N1-C6-N6 | 11.69 | 125.61 | 118.60 |
| 35 | E | 1961 | A | N1-C6-N6 | 11.69 | 125.61 | 118.60 |
| 35 | E | 122 | A | N1-C6-N6 | 11.68 | 125.61 | 118.60 |
| 35 | E | 1601 | A | N1-C6-N6 | 11.68 | 125.61 | 118.60 |
| 35 | E | 729 | C | P-O3'-C3' | 11.68 | 133.71 | 119.70 |
| 35 | E | 1698 | A | N1-C6-N6 | 11.68 | 125.61 | 118.60 |
| 35 | E | 2284 | A | N1-C6-N6 | 11.68 | 125.61 | 118.60 |
| 35 | E | 520 | A | N1-C6-N6 | 11.67 | 125.60 | 118.60 |
| 35 | E | 689 | A | N1-C6-N6 | 11.67 | 125.60 | 118.60 |
| 35 | E | 784 | A | N1-C6-N6 | 11.66 | 125.60 | 118.60 |
| 35 | E | 102 | A | N1-C6-N6 | 11.66 | 125.59 | 118.60 |
| 35 | E | 1937 | A | N1-C6-N6 | 11.65 | 125.59 | 118.60 |
| 35 | E | 1348 | A | N1-C6-N6 | 11.65 | 125.59 | 118.60 |
| 35 | E | 901 | A | N1-C6-N6 | 11.64 | 125.59 | 118.60 |
| 35 | E | 2113 | G | N1-C6-O6 | 11.64 | 126.89 | 119.90 |
| 35 | E | 125 | A | N1-C6-N6 | 11.64 | 125.58 | 118.60 |
| 35 | E | 1695 | A | N1-C6-N6 | 11.64 | 125.58 | 118.60 |
| 35 | E | 817 | A | N1-C6-N6 | 11.63 | 125.58 | 118.60 |
| 35 | E | 1378 | A | N1-C6-N6 | 11.63 | 125.58 | 118.60 |
| 35 | E | 993 | A | N1-C6-N6 | 11.63 | 125.58 | 118.60 |
| 35 | E | 1599 | A | N1-C6-N6 | 11.63 | 125.58 | 118.60 |
| 35 | E | 1939 | A | N1-C6-N6 | 11.62 | 125.58 | 118.60 |
| 35 | E | 1566 | A | N1-C6-N6 | 11.62 | 125.57 | 118.60 |
| 35 | E | 39 | A | N1-C6-N6 | 11.61 | 125.57 | 118.60 |
| 35 | E | 900 | A | N1-C6-N6 | 11.61 | 125.56 | 118.60 |
| 35 | E | 2271 | A | N1-C6-N6 | 11.61 | 125.56 | 118.60 |
| 35 | E | 2300 | A | N1-C6-N6 | 11.60 | 125.56 | 118.60 |
| 35 | E | 2312 | A | N1-C6-N6 | 11.59 | 125.55 | 118.60 |
| 35 | E | 1812 | A | N1-C6-N6 | 11.58 | 125.55 | 118.60 |
| 35 | E | 885 | U | P-O3'-C3' | 11.56 | 133.57 | 119.70 |
| 35 | E | 1552 | A | N1-C6-N6 | 11.55 | 125.53 | 118.60 |
| 35 | E | 1671 | A | N1-C6-N6 | 11.55 | 125.53 | 118.60 |
| 35 | E | 2159 | A | N1-C6-N6 | 11.55 | 125.53 | 118.60 |
| 35 | E | 216 | A | N1-C6-N6 | 11.54 | 125.52 | 118.60 |
| 35 | E | 1076 | C | P-O3'-C3' | 11.54 | 133.54 | 119.70 |
| 35 | E | 1340 | A | N1-C6-N6 | 11.53 | 125.52 | 118.60 |
| 35 | E | 2227 | U | P-O3'-C3' | 11.53 | 133.53 | 119.70 |
| 35 | E | 532 | G | P-O3'-C3' | 11.52 | 133.52 | 119.70 |
| 35 | E | 674 | A | N1-C6-N6 | 11.51 | 125.51 | 118.60 |
| 35 | E | 351 | A | N1-C6-N6 | 11.50 | 125.50 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 367 | A | N1-C6-N6 | 11.50 | 125.50 | 118.60 |
| 35 | E | 162 | A | N1-C6-N6 | 11.49 | 125.50 | 118.60 |
| 35 | E | 1630 | A | N1-C6-N6 | 11.49 | 125.50 | 118.60 |
| 35 | E | 1328 | A | N1-C6-N6 | 11.48 | 125.49 | 118.60 |
| 35 | E | 1081 | G | P-O3'-C3' | 11.48 | 133.48 | 119.70 |
| 35 | E | 148 | G | N1-C6-O6 | 11.48 | 126.79 | 119.90 |
| 35 | E | 463 | A | N1-C6-N6 | 11.48 | 125.49 | 118.60 |
| 35 | E | 2239 | A | N1-C6-N6 | 11.48 | 125.49 | 118.60 |
| 35 | E | 446 | A | N1-C6-N6 | 11.47 | 125.48 | 118.60 |
| 35 | E | 90 | A | N1-C6-N6 | 11.46 | 125.48 | 118.60 |
| 35 | E | 360 | A | N1-C6-N6 | 11.46 | 125.47 | 118.60 |
| 35 | E | 2063 | A | N1-C6-N6 | 11.44 | 125.47 | 118.60 |
| 35 | E | 2056 | A | N1-C6-N6 | 11.44 | 125.47 | 118.60 |
| 35 | E | 719 | G | P-O3'-C3' | 11.44 | 133.42 | 119.70 |
| 35 | E | 967 | A | N1-C6-N6 | 11.43 | 125.46 | 118.60 |
| 35 | E | 1868 | G | N1-C6-O6 | 11.43 | 126.76 | 119.90 |
| 35 | E | 968 | U | P-O3'-C3' | 11.42 | 133.40 | 119.70 |
| 35 | E | 1085 | G | N1-C6-O6 | 11.42 | 126.75 | 119.90 |
| 35 | E | 1377 | A | N1-C6-N6 | 11.42 | 125.45 | 118.60 |
| 35 | E | 2034 | A | N1-C6-N6 | 11.41 | 125.45 | 118.60 |
| 35 | E | 288 | A | N1-C6-N6 | 11.41 | 125.44 | 118.60 |
| 35 | E | 835 | G | N1-C6-O6 | 11.40 | 126.74 | 119.90 |
| 35 | E | 1365 | A | N1-C6-N6 | 11.39 | 125.43 | 118.60 |
| 35 | E | 950 | G | N1-C6-O6 | 11.38 | 126.73 | 119.90 |
| 35 | E | 944 | G | N1-C6-O6 | 11.38 | 126.72 | 119.90 |
| 35 | E | 621 | A | N1-C6-N6 | 11.36 | 125.42 | 118.60 |
| 35 | E | 2038 | G | N1-C6-O6 | 11.36 | 126.72 | 119.90 |
| 35 | E | 980 | G | N1-C6-O6 | 11.32 | 126.69 | 119.90 |
| 35 | E | 485 | A | N1-C6-N6 | 11.32 | 125.39 | 118.60 |
| 35 | E | 706 | G | P-O5'-C5' | 11.32 | 139.00 | 120.90 |
| 35 | E | 2007 | A | N1-C6-N6 | 11.31 | 125.39 | 118.60 |
| 35 | E | 2213 | G | P-O3'-C3' | 11.31 | 133.27 | 119.70 |
| 35 | E | 777 | A | N1-C6-N6 | 11.30 | 125.38 | 118.60 |
| 35 | E | 1305 | A | N1-C6-N6 | 11.30 | 125.38 | 118.60 |
| 35 | E | 877 | A | N1-C6-N6 | 11.29 | 125.38 | 118.60 |
| 35 | E | 316 | A | N1-C6-N6 | 11.29 | 125.37 | 118.60 |
| 35 | E | 2107 | A | N1-C6-N6 | 11.27 | 125.36 | 118.60 |
| 35 | E | 2204 | A | N1-C6-N6 | 11.26 | 125.36 | 118.60 |
| 35 | E | 709 | C | P-O3'-C3' | 11.25 | 133.20 | 119.70 |
| 35 | E | 2148 | A | N1-C6-N6 | 11.25 | 125.35 | 118.60 |
| 35 | E | 2110 | A | N1-C6-N6 | 11.21 | 125.33 | 118.60 |
| 35 | E | 1338 | A | N1-C6-N6 | 11.20 | 125.32 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1746 | G | N1-C6-O6 | 11.20 | 126.62 | 119.90 |
| 35 | E | 940 | U | P-O3'-C3' | 11.20 | 133.14 | 119.70 |
| 35 | E | 1242 | A | N1-C6-N6 | 11.19 | 125.31 | 118.60 |
| 35 | E | 1250 | A | N1-C6-N6 | 11.18 | 125.31 | 118.60 |
| 35 | E | 237 | A | N1-C6-N6 | 11.17 | 125.30 | 118.60 |
| 35 | E | 172 | A | N1-C6-N6 | 11.17 | 125.30 | 118.60 |
| 35 | E | 1789 | A | N1-C6-N6 | 11.16 | 125.30 | 118.60 |
| 35 | E | 1664 | A | N1-C6-N6 | 11.16 | 125.30 | 118.60 |
| 35 | E | 575 | A | N1-C6-N6 | 11.13 | 125.28 | 118.60 |
| 35 | E | 684 | A | N1-C6-N6 | 11.13 | 125.28 | 118.60 |
| 35 | E | 1584 | A | N1-C6-N6 | 11.12 | 125.27 | 118.60 |
| 35 | E | 484 | A | N1-C6-N6 | 11.12 | 125.27 | 118.60 |
| 35 | E | 609 | A | N1-C6-N6 | 11.12 | 125.27 | 118.60 |
| 35 | E | 953 | G | N1-C6-O6 | 11.12 | 126.57 | 119.90 |
| 35 | E | 1808 | G | N1-C6-O6 | 11.09 | 126.55 | 119.90 |
| 35 | E | 633 | A | N1-C6-N6 | 11.06 | 125.24 | 118.60 |
| 35 | E | 979 | G | C5-C6-O6 | -11.05 | 121.97 | 128.60 |
| 35 | E | 2113 | G | C5-C6-O6 | -11.05 | 121.97 | 128.60 |
| 35 | E | 535 | G | N1-C6-O6 | 10.98 | 126.49 | 119.90 |
| 35 | E | 2224 | G | N1-C6-O6 | 10.98 | 126.49 | 119.90 |
| 35 | E | 63 | G | N1-C6-O6 | 10.98 | 126.49 | 119.90 |
| 35 | E | 285 | A | N1-C6-N6 | 10.97 | 125.18 | 118.60 |
| 35 | E | 1670 | A | N1-C6-N6 | 10.89 | 125.14 | 118.60 |
| 35 | E | 2240 | A | N1-C6-N6 | 10.89 | 125.13 | 118.60 |
| 35 | E | 862 | A | N1-C6-N6 | 10.88 | 125.12 | 118.60 |
| 35 | E | 975 | U | OP2-P-O3' | -10.86 | 81.31 | 105.20 |
| 35 | E | 788 | A | P-O3'-C3' | 10.83 | 132.70 | 119.70 |
| 35 | E | 335 | G | N1-C6-O6 | 10.83 | 126.40 | 119.90 |
| 35 | E | 23 | G | N1-C6-O6 | 10.80 | 126.38 | 119.90 |
| 35 | E | 822 | A | N1-C6-N6 | 10.79 | 125.08 | 118.60 |
| 35 | E | 71 | G | N1-C6-O6 | 10.79 | 126.37 | 119.90 |
| 35 | E | 931 | G | N1-C6-O6 | 10.77 | 126.36 | 119.90 |
| 35 | E | 2131 | A | N1-C6-N6 | 10.76 | 125.06 | 118.60 |
| 35 | E | 169 | G | N1-C6-O6 | 10.75 | 126.35 | 119.90 |
| 35 | E | 1953 | G | N1-C6-O6 | 10.75 | 126.35 | 119.90 |
| 35 | E | 1854 | G | N1-C6-O6 | 10.74 | 126.35 | 119.90 |
| 35 | E | 1361 | A | N1-C6-N6 | 10.74 | 125.05 | 118.60 |
| 35 | E | 2006 | A | N1-C6-N6 | 10.74 | 125.05 | 118.60 |
| 35 | E | 276 | G | N1-C6-O6 | 10.73 | 126.34 | 119.90 |
| 35 | E | 2051 | C | P-O3'-C3' | 10.73 | 132.58 | 119.70 |
| 35 | E | 263 | G | N1-C6-O6 | 10.73 | 126.34 | 119.90 |
| 35 | E | 1384 | G | N1-C6-O6 | 10.73 | 126.34 | 119.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 530 | G | N1-C6-O6 | 10.72 | 126.33 | 119.90 |
| 35 | E | 567 | G | N1-C6-O6 | 10.72 | 126.33 | 119.90 |
| 35 | E | 255 | A | N1-C6-N6 | 10.71 | 125.03 | 118.60 |
| 35 | E | 1605 | A | N1-C6-N6 | 10.71 | 125.03 | 118.60 |
| 35 | E | 1749 | G | N1-C6-O6 | 10.69 | 126.31 | 119.90 |
| 35 | E | 1886 | G | P-O3'-C3' | 10.68 | 132.51 | 119.70 |
| 35 | E | 1606 | A | N1-C6-N6 | 10.63 | 124.98 | 118.60 |
| 35 | E | 521 | A | N1-C6-N6 | 10.62 | 124.97 | 118.60 |
| 35 | E | 100 | A | N1-C6-N6 | 10.62 | 124.97 | 118.60 |
| 35 | E | 10 | G | C5-C6-O6 | -10.61 | 122.24 | 128.60 |
| 35 | E | 724 | A | C5-C6-N1 | -10.61 | 112.40 | 117.70 |
| 35 | E | 1644 | G | N1-C6-O6 | 10.60 | 126.26 | 119.90 |
| 35 | E | 1625 | A | N1-C6-N6 | 10.60 | 124.96 | 118.60 |
| 35 | E | 394 | G | N1-C6-O6 | 10.59 | 126.26 | 119.90 |
| 35 | E | 291 | G | N1-C6-O6 | 10.59 | 126.25 | 119.90 |
| 35 | E | 315 | A | N1-C6-N6 | 10.57 | 124.94 | 118.60 |
| 35 | E | 2122 | G | N1-C6-O6 | 10.55 | 126.23 | 119.90 |
| 35 | E | 1186 | U | P-O3'-C3' | 10.55 | 132.36 | 119.70 |
| 35 | E | 2165 | A | N1-C6-N6 | 10.54 | 124.92 | 118.60 |
| 35 | E | 1898 | G | N1-C6-O6 | 10.53 | 126.22 | 119.90 |
| 35 | E | 1306 | A | N1-C6-N6 | 10.53 | 124.92 | 118.60 |
| 35 | E | 1547 | A | N1-C6-N6 | 10.52 | 124.91 | 118.60 |
| 35 | E | 1873 | G | N1-C6-O6 | 10.50 | 126.20 | 119.90 |
| 35 | E | 133 | G | N1-C6-O6 | 10.47 | 126.19 | 119.90 |
| 35 | E | 1861 | A | N1-C6-N6 | 10.47 | 124.88 | 118.60 |
| 35 | E | 983 | C | O4'-C1'-N1 | 10.46 | 116.57 | 108.20 |
| 35 | E | 488 | G | N1-C6-O6 | 10.45 | 126.17 | 119.90 |
| 35 | E | 1598 | G | N1-C6-O6 | 10.45 | 126.17 | 119.90 |
| 35 | E | 53 | G | N1-C6-O6 | 10.45 | 126.17 | 119.90 |
| 35 | E | 712 | U | P-O3'-C3' | 10.45 | 132.24 | 119.70 |
| 35 | E | 79 | G | N1-C6-O6 | 10.44 | 126.16 | 119.90 |
| 35 | E | 2017 | G | P-O3'-C3' | 10.44 | 132.22 | 119.70 |
| 35 | E | 1824 | A | N1-C6-N6 | 10.43 | 124.86 | 118.60 |
| 35 | E | 1555 | G | N1-C6-O6 | 10.43 | 126.16 | 119.90 |
| 35 | E | 1277 | G | N1-C6-O6 | 10.41 | 126.15 | 119.90 |
| 35 | E | 2296 | G | N1-C6-O6 | 10.41 | 126.14 | 119.90 |
| 35 | E | 524 | G | N1-C6-O6 | 10.40 | 126.14 | 119.90 |
| 35 | E | 2289 | G | N1-C6-O6 | 10.39 | 126.13 | 119.90 |
| 35 | E | 895 | A | N1-C6-N6 | 10.38 | 124.83 | 118.60 |
| 35 | E | 2120 | A | N1-C6-N6 | 10.37 | 124.82 | 118.60 |
| 35 | E | 1871 | G | N1-C6-O6 | 10.36 | 126.12 | 119.90 |
| 35 | E | 420 | G | N1-C6-O6 | 10.36 | 126.11 | 119.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 555 | G | N1-C6-O6 | 10.35 | 126.11 | 119.90 |
| 35 | E | 766 | C | O4'-C1'-N1 | 10.34 | 116.47 | 108.20 |
| 35 | E | 106 | G | N1-C6-O6 | 10.34 | 126.10 | 119.90 |
| 35 | E | 2043 | G | N1-C6-O6 | 10.34 | 126.10 | 119.90 |
| 35 | E | 299 | A | N1-C6-N6 | 10.33 | 124.80 | 118.60 |
| 35 | E | 1210 | G | N1-C6-O6 | 10.33 | 126.10 | 119.90 |
| 35 | E | 855 | G | N1-C6-O6 | 10.32 | 126.09 | 119.90 |
| 35 | E | 2249 | A | N1-C6-N6 | 10.32 | 124.79 | 118.60 |
| 35 | E | 1233 | A | N1-C6-N6 | 10.31 | 124.79 | 118.60 |
| 35 | E | 857 | G | N1-C6-O6 | 10.29 | 126.08 | 119.90 |
| 35 | E | 2045 | A | N1-C6-N6 | 10.29 | 124.78 | 118.60 |
| 35 | E | 661 | G | N1-C6-O6 | 10.29 | 126.07 | 119.90 |
| 35 | E | 2214 | A | N1-C6-N6 | 10.29 | 124.77 | 118.60 |
| 35 | E | 1808 | G | C5-C6-O6 | -10.28 | 122.43 | 128.60 |
| 35 | E | 2195 | G | N1-C6-O6 | 10.27 | 126.06 | 119.90 |
| 35 | E | 188 | G | N1-C6-O6 | 10.27 | 126.06 | 119.90 |
| 35 | E | 2237 | G | N1-C6-O6 | 10.27 | 126.06 | 119.90 |
| 35 | E | 1869 | G | N1-C6-O6 | 10.26 | 126.05 | 119.90 |
| 35 | E | 702 | U | O4'-C1'-N1 | 10.25 | 116.40 | 108.20 |
| 35 | E | 907 | G | N1-C6-O6 | 10.25 | 126.05 | 119.90 |
| 35 | E | 711 | A | C5-C6-N1 | -10.25 | 112.58 | 117.70 |
| 35 | E | 1943 | G | N1-C6-O6 | 10.25 | 126.05 | 119.90 |
| 35 | E | 1182 | G | N1-C6-O6 | 10.23 | 126.04 | 119.90 |
| 35 | E | 975 | U | OP1-P-O3' | -10.22 | 82.72 | 105.20 |
| 35 | E | 1731 | G | N1-C6-O6 | 10.22 | 126.03 | 119.90 |
| 35 | E | 1900 | G | N1-C6-O6 | 10.21 | 126.02 | 119.90 |
| 35 | E | 970 | G | N1-C6-O6 | 10.20 | 126.02 | 119.90 |
| 35 | E | 943 | G | N1-C6-O6 | 10.19 | 126.02 | 119.90 |
| 35 | E | 706 | G | N1-C6-O6 | 10.19 | 126.01 | 119.90 |
| 35 | E | 552 | G | N1-C6-O6 | 10.18 | 126.01 | 119.90 |
| 35 | E | 541 | G | N1-C6-O6 | 10.18 | 126.01 | 119.90 |
| 35 | E | 86 | G | N1-C6-O6 | 10.17 | 126.00 | 119.90 |
| 35 | E | 1237 | G | N1-C6-O6 | 10.17 | 126.00 | 119.90 |
| 35 | E | 1545 | U | P-O3'-C3' | 10.17 | 131.90 | 119.70 |
| 35 | E | 1367 | G | N1-C6-O6 | 10.15 | 125.99 | 119.90 |
| 35 | E | 220 | G | N1-C6-O6 | 10.15 | 125.99 | 119.90 |
| 35 | E | 1763 | G | N1-C6-O6 | 10.15 | 125.99 | 119.90 |
| 35 | E | 223 | G | N1-C6-O6 | 10.14 | 125.98 | 119.90 |
| 35 | E | 1855 | G | N1-C6-O6 | 10.14 | 125.98 | 119.90 |
| 35 | E | 2139 | G | N1-C6-O6 | 10.13 | 125.98 | 119.90 |
| 35 | E | 2233 | G | N1-C6-O6 | 10.13 | 125.98 | 119.90 |
| 35 | E | 1927 | A | N1-C6-N6 | 10.12 | 124.67 | 118.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 508 | G | N1-C6-O6 | 10.12 | 125.97 | 119.90 |
| 35 | E | 347 | G | N1-C6-O6 | 10.11 | 125.96 | 119.90 |
| 35 | E | 2121 | G | N1-C6-O6 | 10.10 | 125.96 | 119.90 |
| 35 | E | 836 | G | N1-C6-O6 | 10.10 | 125.96 | 119.90 |
| 35 | E | 403 | G | N1-C6-O6 | 10.09 | 125.95 | 119.90 |
| 35 | E | 734 | G | C5-C6-O6 | -10.08 | 122.55 | 128.60 |
| 35 | E | 211 | G | N1-C6-O6 | 10.08 | 125.95 | 119.90 |
| 35 | E | 6 | G | N1-C6-O6 | 10.07 | 125.94 | 119.90 |
| 35 | E | 1817 | G | N1-C6-O6 | 10.07 | 125.94 | 119.90 |
| 35 | E | 1577 | G | N1-C6-O6 | 10.06 | 125.94 | 119.90 |
| 35 | E | 2152 | C | P-O3'-C3' | 10.05 | 131.76 | 119.70 |
| 35 | E | 943 | G | C5-C6-O6 | -10.04 | 122.58 | 128.60 |
| 35 | E | 713 | G | P-O3'-C3' | 10.04 | 131.75 | 119.70 |
| 35 | E | 204 | G | N1-C6-O6 | 10.04 | 125.92 | 119.90 |
| 35 | E | 1735 | G | N1-C6-O6 | 10.03 | 125.92 | 119.90 |
| 35 | E | 363 | A | N1-C6-N6 | 10.03 | 124.62 | 118.60 |
| 35 | E | 517 | G | N1-C6-O6 | 10.03 | 125.92 | 119.90 |
| 35 | E | 888 | G | N1-C6-O6 | 10.02 | 125.91 | 119.90 |
| 35 | E | 410 | G | N1-C6-O6 | 10.02 | 125.91 | 119.90 |
| 35 | E | 1274 | A | N1-C6-N6 | 10.01 | 124.61 | 118.60 |
| 35 | E | 954 | G | N1-C6-O6 | 10.00 | 125.90 | 119.90 |
| 35 | E | 564 | G | N1-C6-O6 | 10.00 | 125.90 | 119.90 |
| 35 | E | 42 | G | N1-C6-O6 | 9.99 | 125.90 | 119.90 |
| 35 | E | 651 | G | N1-C6-O6 | 9.98 | 125.89 | 119.90 |
| 35 | E | 470 | G | N1-C6-O6 | 9.97 | 125.88 | 119.90 |
| 35 | E | 431 | G | N1-C6-O6 | 9.97 | 125.88 | 119.90 |
| 35 | E | 1549 | G | N1-C6-O6 | 9.97 | 125.88 | 119.90 |
| 35 | E | 1776 | G | N1-C6-O6 | 9.96 | 125.88 | 119.90 |
| 35 | E | 230 | G | N1-C6-O6 | 9.96 | 125.87 | 119.90 |
| 35 | E | 7 | G | N1-C6-O6 | 9.95 | 125.87 | 119.90 |
| 35 | E | 717 | U | P-O3'-C3' | 9.95 | 131.64 | 119.70 |
| 35 | E | 996 | G | N1-C6-O6 | 9.95 | 125.87 | 119.90 |
| 35 | E | 2217 | G | N1-C6-O6 | 9.94 | 125.86 | 119.90 |
| 35 | E | 944 | G | C5-C6-O6 | -9.93 | 122.64 | 128.60 |
| 35 | E | 1687 | A | N1-C6-N6 | 9.93 | 124.56 | 118.60 |
| 35 | E | 532 | G | N1-C6-O6 | 9.93 | 125.86 | 119.90 |
| 35 | E | 2265 | G | N1-C6-O6 | 9.93 | 125.86 | 119.90 |
| 35 | E | 2304 | G | N1-C6-O6 | 9.93 | 125.86 | 119.90 |
| 35 | E | 1852 | G | N1-C6-O6 | 9.92 | 125.85 | 119.90 |
| 35 | E | 1870 | G | N1-C6-O6 | 9.92 | 125.85 | 119.90 |
| 35 | E | 785 | A | P-O3'-C3' | 9.92 | 131.60 | 119.70 |
| 35 | E | 1608 | G | N1-C6-O6 | 9.92 | 125.85 | 119.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 57 | G | N1-C6-O6 | 9.91 | 125.85 | 119.90 |
| 35 | E | 132 | G | N1-C6-O6 | 9.90 | 125.84 | 119.90 |
| 35 | E | 1213 | G | N1-C6-O6 | 9.90 | 125.84 | 119.90 |
| 35 | E | 2220 | G | N1-C6-O6 | 9.89 | 125.84 | 119.90 |
| 35 | E | 205 | G | N1-C6-O6 | 9.89 | 125.83 | 119.90 |
| 35 | E | 1880 | U | O4'-C1'-N1 | 9.88 | 116.10 | 108.20 |
| 35 | E | 982 | G | N1-C6-O6 | 9.87 | 125.82 | 119.90 |
| 35 | E | 2197 | G | N1-C6-O6 | 9.87 | 125.82 | 119.90 |
| 35 | E | 473 | G | N1-C6-O6 | 9.87 | 125.82 | 119.90 |
| 35 | E | 2176 | G | N1-C6-O6 | 9.87 | 125.82 | 119.90 |
| 35 | E | 208 | G | N1-C6-O6 | 9.87 | 125.82 | 119.90 |
| 35 | E | 835 | G | C5-C6-O6 | -9.87 | 122.68 | 128.60 |
| 35 | E | 409 | G | N1-C6-O6 | 9.86 | 125.82 | 119.90 |
| 35 | E | 756 | G | N1-C6-O6 | 9.86 | 125.81 | 119.90 |
| 35 | E | 2275 | G | N1-C6-O6 | 9.86 | 125.82 | 119.90 |
| 35 | E | 1220 | G | N1-C6-O6 | 9.86 | 125.81 | 119.90 |
| 35 | E | 1307 | G | N1-C6-O6 | 9.86 | 125.81 | 119.90 |
| 35 | E | 311 | G | N1-C6-O6 | 9.85 | 125.81 | 119.90 |
| 35 | E | 772 | U | P-O3'-C3' | 9.85 | 131.51 | 119.70 |
| 35 | E | 30 | G | N1-C6-O6 | 9.84 | 125.81 | 119.90 |
| 35 | E | 34 | G | N1-C6-O6 | 9.84 | 125.80 | 119.90 |
| 35 | E | 1381 | G | N1-C6-O6 | 9.83 | 125.80 | 119.90 |
| 35 | E | 466 | G | N1-C6-O6 | 9.83 | 125.80 | 119.90 |
| 35 | E | 189 | G | N1-C6-O6 | 9.82 | 125.80 | 119.90 |
| 35 | E | 233 | G | N1-C6-O6 | 9.82 | 125.79 | 119.90 |
| 35 | E | 963 | G | N1-C6-O6 | 9.82 | 125.79 | 119.90 |
| 35 | E | 971 | G | N1-C6-O6 | 9.82 | 125.79 | 119.90 |
| 35 | E | 1886 | G | N1-C6-O6 | 9.82 | 125.79 | 119.90 |
| 35 | E | 109 | G | N1-C6-O6 | 9.81 | 125.78 | 119.90 |
| 35 | E | 606 | G | N1-C6-O6 | 9.81 | 125.78 | 119.90 |
| 35 | E | 1635 | G | N1-C6-O6 | 9.80 | 125.78 | 119.90 |
| 35 | E | 1206 | G | N1-C6-O6 | 9.79 | 125.78 | 119.90 |
| 35 | E | 1997 | G | N1-C6-O6 | 9.79 | 125.78 | 119.90 |
| 35 | E | 413 | G | N1-C6-O6 | 9.79 | 125.78 | 119.90 |
| 35 | E | 229 | G | N1-C6-O6 | 9.79 | 125.77 | 119.90 |
| 35 | E | 430 | G | N1-C6-O6 | 9.79 | 125.77 | 119.90 |
| 35 | E | 2127 | G | N1-C6-O6 | 9.79 | 125.77 | 119.90 |
| 35 | E | 1666 | G | N1-C6-O6 | 9.79 | 125.77 | 119.90 |
| 35 | E | 156 | G | N1-C6-O6 | 9.78 | 125.77 | 119.90 |
| 35 | E | 1382 | G | N1-C6-O6 | 9.78 | 125.77 | 119.90 |
| 35 | E | 2163 | G | N1-C6-O6 | 9.78 | 125.77 | 119.90 |
| 35 | E | 514 | G | N1-C6-O6 | 9.76 | 125.76 | 119.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 611 | G | N1-C6-O6 | 9.76 | 125.76 | 119.90 |
| 35 | E | 1876 | G | C5-C6-O6 | -9.75 | 122.75 | 128.60 |
| 35 | E | 334 | G | N1-C6-O6 | 9.74 | 125.75 | 119.90 |
| 35 | E | 395 | G | N1-C6-O6 | 9.74 | 125.75 | 119.90 |
| 35 | E | 1777 | G | N1-C6-O6 | 9.74 | 125.75 | 119.90 |
| 35 | E | 93 | G | N1-C6-O6 | 9.74 | 125.74 | 119.90 |
| 35 | E | 1339 | G | N1-C6-O6 | 9.74 | 125.74 | 119.90 |
| 35 | E | 842 | G | N1-C6-O6 | 9.73 | 125.74 | 119.90 |
| 35 | E | 2278 | G | N1-C6-O6 | 9.73 | 125.74 | 119.90 |
| 35 | E | 1979 | G | N1-C6-O6 | 9.73 | 125.74 | 119.90 |
| 35 | E | 1594 | G | N1-C6-O6 | 9.73 | 125.74 | 119.90 |
| 35 | E | 2266 | G | N1-C6-O6 | 9.73 | 125.74 | 119.90 |
| 35 | E | 192 | G | N1-C6-O6 | 9.72 | 125.73 | 119.90 |
| 35 | E | 451 | G | N1-C6-O6 | 9.71 | 125.72 | 119.90 |
| 35 | E | 495 | G | N1-C6-O6 | 9.69 | 125.72 | 119.90 |
| 35 | E | 173 | A | N1-C6-N6 | 9.69 | 124.41 | 118.60 |
| 35 | E | 2222 | G | N1-C6-O6 | 9.69 | 125.71 | 119.90 |
| 35 | E | 1230 | G | N1-C6-O6 | 9.68 | 125.71 | 119.90 |
| 35 | E | 320 | G | N1-C6-O6 | 9.67 | 125.70 | 119.90 |
| 35 | E | 2194 | G | N1-C6-O6 | 9.67 | 125.70 | 119.90 |
| 35 | E | 2073 | G | N1-C6-O6 | 9.66 | 125.70 | 119.90 |
| 35 | E | 2206 | G | N1-C6-O6 | 9.65 | 125.69 | 119.90 |
| 35 | E | 207 | G | N1-C6-O6 | 9.65 | 125.69 | 119.90 |
| 35 | E | 401 | A | N1-C6-N6 | 9.65 | 124.39 | 118.60 |
| 35 | E | 1579 | G | N1-C6-O6 | 9.64 | 125.69 | 119.90 |
| 35 | E | 791 | G | N1-C6-O6 | 9.64 | 125.69 | 119.90 |
| 35 | E | 272 | G | N1-C6-O6 | 9.64 | 125.68 | 119.90 |
| 35 | E | 1289 | G | N1-C6-O6 | 9.64 | 125.68 | 119.90 |
| 35 | E | 566 | G | N1-C6-O6 | 9.63 | 125.68 | 119.90 |
| 35 | E | 1329 | G | N1-C6-O6 | 9.63 | 125.68 | 119.90 |
| 35 | E | 48 | G | N1-C6-O6 | 9.63 | 125.68 | 119.90 |
| 35 | E | 1867 | G | N1-C6-O6 | 9.63 | 125.68 | 119.90 |
| 35 | E | 2205 | G | N1-C6-O6 | 9.63 | 125.68 | 119.90 |
| 35 | E | 513 | G | N1-C6-O6 | 9.62 | 125.67 | 119.90 |
| 35 | E | 1793 | G | N1-C6-O6 | 9.62 | 125.67 | 119.90 |
| 35 | E | 389 | G | N1-C6-O6 | 9.62 | 125.67 | 119.90 |
| 35 | E | 987 | G | N1-C6-O6 | 9.62 | 125.67 | 119.90 |
| 35 | E | 1085 | G | C5-C6-O6 | -9.61 | 122.83 | 128.60 |
| 35 | E | 775 | A | P-O5'-C5' | 9.61 | 136.28 | 120.90 |
| 35 | E | 1563 | G | N1-C6-O6 | 9.61 | 125.67 | 119.90 |
| 35 | E | 2003 | G | N1-C6-O6 | 9.61 | 125.67 | 119.90 |
| 35 | E | 1786 | G | N1-C6-O6 | 9.61 | 125.66 | 119.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 2295 | G | N1-C6-O6 | 9.60 | 125.66 | 119.90 |
| 35 | E | 151 | A | N1-C6-N6 | 9.60 | 124.36 | 118.60 |
| 35 | E | 678 | G | N1-C6-O6 | 9.60 | 125.66 | 119.90 |
| 35 | E | 317 | G | N1-C6-O6 | 9.60 | 125.66 | 119.90 |
| 35 | E | 1697 | G | N1-C6-O6 | 9.60 | 125.66 | 119.90 |
| 35 | E | 477 | G | N1-C6-O6 | 9.59 | 125.65 | 119.90 |
| 35 | E | 1216 | G | N1-C6-O6 | 9.59 | 125.65 | 119.90 |
| 35 | E | 615 | G | N1-C6-O6 | 9.57 | 125.64 | 119.90 |
| 35 | E | 1746 | G | C5-C6-O6 | -9.57 | 122.86 | 128.60 |
| 35 | E | 1762 | G | N1-C6-O6 | 9.57 | 125.64 | 119.90 |
| 35 | E | 405 | G | N1-C6-O6 | 9.56 | 125.64 | 119.90 |
| 35 | E | 1165 | G | N1-C6-O6 | 9.55 | 125.63 | 119.90 |
| 35 | E | 2150 | G | N1-C6-O6 | 9.54 | 125.63 | 119.90 |
| 35 | E | 199 | G | N1-C6-O6 | 9.54 | 125.62 | 119.90 |
| 35 | E | 2292 | G | N1-C6-O6 | 9.53 | 125.62 | 119.90 |
| 35 | E | 412 | G | N1-C6-O6 | 9.53 | 125.62 | 119.90 |
| 35 | E | 633 | A | P-O3'-C3' | 9.53 | 131.13 | 119.70 |
| 35 | E | 404 | G | N1-C6-O6 | 9.52 | 125.61 | 119.90 |
| 35 | E | 1349 | G | N1-C6-O6 | 9.52 | 125.61 | 119.90 |
| 35 | E | 1600 | A | N1-C6-N6 | 9.52 | 124.31 | 118.60 |
| 35 | E | 1749 | G | C5-C6-O6 | -9.52 | 122.89 | 128.60 |
| 35 | E | 1578 | G | N1-C6-O6 | 9.51 | 125.61 | 119.90 |
| 35 | E | 616 | G | N1-C6-O6 | 9.51 | 125.61 | 119.90 |
| 35 | E | 2156 | G | N1-C6-O6 | 9.51 | 125.61 | 119.90 |
| 35 | E | 130 | G | N1-C6-O6 | 9.51 | 125.60 | 119.90 |
| 35 | E | 157 | G | N1-C6-O6 | 9.50 | 125.60 | 119.90 |
| 35 | E | 2147 | U | O4'-C1'-N1 | 9.50 | 115.80 | 108.20 |
| 35 | E | 148 | G | C5-C6-O6 | -9.49 | 122.90 | 128.60 |
| 35 | E | 1922 | G | N1-C6-O6 | 9.49 | 125.59 | 119.90 |
| 35 | E | 640 | G | N1-C6-O6 | 9.49 | 125.59 | 119.90 |
| 35 | E | 670 | G | N1-C6-O6 | 9.49 | 125.59 | 119.90 |
| 35 | E | 1332 | G | N1-C6-O6 | 9.48 | 125.59 | 119.90 |
| 35 | E | 1263 | G | N1-C6-O6 | 9.48 | 125.59 | 119.90 |
| 35 | E | 2208 | G | N1-C6-O6 | 9.47 | 125.58 | 119.90 |
| 35 | E | 738 | G | C5-C6-O6 | -9.47 | 122.92 | 128.60 |
| 35 | E | 1326 | G | N1-C6-O6 | 9.46 | 125.58 | 119.90 |
| 35 | E | 2141 | G | N1-C6-O6 | 9.46 | 125.58 | 119.90 |
| 35 | E | 919 | G | P-O3'-C3' | 9.46 | 131.05 | 119.70 |
| 35 | E | 2044 | G | N1-C6-O6 | 9.46 | 125.58 | 119.90 |
| 35 | E | 1319 | G | N1-C6-O6 | 9.46 | 125.57 | 119.90 |
| 35 | E | 1562 | G | N1-C6-O6 | 9.46 | 125.58 | 119.90 |
| 35 | E | 1705 | G | N1-C6-O6 | 9.46 | 125.58 | 119.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1970 | G | N1-C6-O6 | 9.46 | 125.57 | 119.90 |
| 35 | E | 708 | G | N1-C6-O6 | 9.45 | 125.57 | 119.90 |
| 35 | E | 370 | G | N1-C6-O6 | 9.45 | 125.57 | 119.90 |
| 35 | E | 878 | G | N1-C6-O6 | 9.45 | 125.57 | 119.90 |
| 35 | E | 812 | A | P-O3'-C3' | 9.45 | 131.03 | 119.70 |
| 35 | E | 71 | G | C5-C6-O6 | -9.44 | 122.94 | 128.60 |
| 35 | E | 364 | G | N1-C6-O6 | 9.44 | 125.56 | 119.90 |
| 35 | E | 568 | G | N1-C6-O6 | 9.44 | 125.56 | 119.90 |
| 35 | E | 1260 | G | N1-C6-O6 | 9.44 | 125.56 | 119.90 |
| 35 | E | 344 | G | N1-C6-O6 | 9.43 | 125.56 | 119.90 |
| 35 | E | 76 | G | N1-C6-O6 | 9.43 | 125.56 | 119.90 |
| 35 | E | 628 | G | N1-C6-O6 | 9.42 | 125.55 | 119.90 |
| 35 | E | 869 | G | N1-C6-O6 | 9.42 | 125.55 | 119.90 |
| 35 | E | 535 | G | C5-C6-O6 | -9.41 | 122.95 | 128.60 |
| 35 | E | 1944 | G | N1-C6-O6 | 9.41 | 125.55 | 119.90 |
| 35 | E | 322 | G | N1-C6-O6 | 9.41 | 125.55 | 119.90 |
| 35 | E | 664 | G | N1-C6-O6 | 9.40 | 125.54 | 119.90 |
| 35 | E | 980 | G | C5-C6-O6 | -9.40 | 122.96 | 128.60 |
| 35 | E | 1856 | G | N1-C6-O6 | 9.40 | 125.54 | 119.90 |
| 35 | E | 792 | G | P-O3'-C3' | 9.39 | 130.97 | 119.70 |
| 35 | E | 355 | G | N1-C6-O6 | 9.39 | 125.53 | 119.90 |
| 35 | E | 733 | G | N1-C6-O6 | 9.38 | 125.53 | 119.90 |
| 35 | E | 238 | G | N1-C6-O6 | 9.38 | 125.53 | 119.90 |
| 35 | E | 880 | A | N1-C6-N6 | 9.38 | 124.23 | 118.60 |
| 35 | E | 2241 | G | N1-C6-O6 | 9.38 | 125.53 | 119.90 |
| 35 | E | 1910 | G | N1-C6-O6 | 9.37 | 125.52 | 119.90 |
| 35 | E | 139 | G | N1-C6-O6 | 9.37 | 125.52 | 119.90 |
| 35 | E | 705 | G | N1-C6-O6 | 9.36 | 125.51 | 119.90 |
| 35 | E | 2118 | G | N1-C6-O6 | 9.36 | 125.51 | 119.90 |
| 35 | E | 908 | G | N1-C6-O6 | 9.35 | 125.51 | 119.90 |
| 35 | E | 1315 | G | N1-C6-O6 | 9.34 | 125.51 | 119.90 |
| 35 | E | 1203 | G | N1-C6-O6 | 9.34 | 125.50 | 119.90 |
| 35 | E | 605 | G | N1-C6-O6 | 9.34 | 125.50 | 119.90 |
| 35 | E | 481 | G | N1-C6-O6 | 9.33 | 125.50 | 119.90 |
| 35 | E | 276 | G | C5-C6-O6 | -9.33 | 123.00 | 128.60 |
| 35 | E | 1656 | G | N1-C6-O6 | 9.33 | 125.50 | 119.90 |
| 35 | E | 240 | G | N1-C6-O6 | 9.32 | 125.50 | 119.90 |
| 35 | E | 622 | G | N1-C6-O6 | 9.32 | 125.49 | 119.90 |
| 35 | E | 994 | G | N1-C6-O6 | 9.32 | 125.49 | 119.90 |
| 35 | E | 1950 | G | N1-C6-O6 | 9.32 | 125.49 | 119.90 |
| 35 | E | 1968 | G | N1-C6-O6 | 9.32 | 125.49 | 119.90 |
| 35 | E | 41 | G | N1-C6-O6 | 9.31 | 125.49 | 119.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 794 | G | N1-C6-O6 | 9.31 | 125.49 | 119.90 |
| 35 | E | 1569 | G | N1-C6-O6 | 9.31 | 125.49 | 119.90 |
| 35 | E | 435 | G | N1-C6-O6 | 9.31 | 125.48 | 119.90 |
| 35 | E | 1756 | G | N1-C6-O6 | 9.30 | 125.48 | 119.90 |
| 35 | E | 1868 | G | C5-C6-O6 | -9.30 | 123.02 | 128.60 |
| 35 | E | 244 | G | N1-C6-O6 | 9.30 | 125.48 | 119.90 |
| 35 | E | 1932 | G | N1-C6-O6 | 9.29 | 125.48 | 119.90 |
| 35 | E | 2310 | G | N1-C6-O6 | 9.29 | 125.47 | 119.90 |
| 35 | E | 1816 | G | N1-C6-O6 | 9.28 | 125.47 | 119.90 |
| 35 | E | 147 | G | N1-C6-O6 | 9.27 | 125.46 | 119.90 |
| 35 | E | 1876 | G | N1-C6-O6 | 9.27 | 125.46 | 119.90 |
| 35 | E | 1320 | G | N1-C6-O6 | 9.27 | 125.46 | 119.90 |
| 35 | E | 2172 | G | N1-C6-O6 | 9.27 | 125.46 | 119.90 |
| 35 | E | 712 | U | O4'-C1'-N1 | 9.27 | 115.61 | 108.20 |
| 35 | E | 1759 | G | N1-C6-O6 | 9.26 | 125.45 | 119.90 |
| 35 | E | 133 | G | C5-C6-O6 | -9.26 | 123.05 | 128.60 |
| 35 | E | 291 | G | C5-C6-O6 | -9.25 | 123.05 | 128.60 |
| 35 | E | 439 | G | N1-C6-O6 | 9.25 | 125.45 | 119.90 |
| 35 | E | 448 | A | N1-C6-N6 | 9.23 | 124.14 | 118.60 |
| 35 | E | 1214 | G | N1-C6-O6 | 9.23 | 125.44 | 119.90 |
| 35 | E | 1854 | G | C5-C6-O6 | -9.23 | 123.06 | 128.60 |
| 35 | E | 847 | U | P-O3'-C3' | 9.22 | 130.77 | 119.70 |
| 35 | E | 313 | G | N1-C6-O6 | 9.20 | 125.42 | 119.90 |
| 35 | E | 1972 | G | N1-C6-O6 | 9.20 | 125.42 | 119.90 |
| 35 | E | 106 | G | C5-C6-O6 | -9.20 | 123.08 | 128.60 |
| 35 | E | 1075 | G | N1-C6-O6 | 9.20 | 125.42 | 119.90 |
| 35 | E | 1623 | G | N1-C6-O6 | 9.20 | 125.42 | 119.90 |
| 35 | E | 2182 | G | N1-C6-O6 | 9.19 | 125.41 | 119.90 |
| 35 | E | 179 | G | N1-C6-O6 | 9.19 | 125.41 | 119.90 |
| 35 | E | 547 | G | N1-C6-O6 | 9.18 | 125.41 | 119.90 |
| 35 | E | 2086 | G | N1-C6-O6 | 9.17 | 125.40 | 119.90 |
| 35 | E | 2269 | G | N1-C6-O6 | 9.17 | 125.40 | 119.90 |
| 35 | E | 2038 | G | C5-C6-O6 | -9.17 | 123.10 | 128.60 |
| 35 | E | 1083 | G | N1-C6-O6 | 9.16 | 125.40 | 119.90 |
| 35 | E | 1898 | G | C5-C6-O6 | -9.15 | 123.11 | 128.60 |
| 35 | E | 1776 | G | C5-C6-O6 | -9.13 | 123.12 | 128.60 |
| 35 | E | 790 | G | N1-C6-O6 | 9.13 | 125.38 | 119.90 |
| 35 | E | 377 | G | N1-C6-O6 | 9.12 | 125.37 | 119.90 |
| 35 | E | 757 | G | N1-C6-O6 | 9.12 | 125.37 | 119.90 |
| 35 | E | 1212 | G | N1-C6-O6 | 9.12 | 125.37 | 119.90 |
| 35 | E | 469 | G | N1-C6-O6 | 9.11 | 125.37 | 119.90 |
| 35 | E | 468 | G | N1-C6-O6 | 9.11 | 125.36 | 119.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 699 | C | O4'-C1'-N1 | 9.11 | 115.48 | 108.20 |
| 35 | E | 1228 | G | N1-C6-O6 | 9.11 | 125.36 | 119.90 |
| 35 | E | 1940 | G | N1-C6-O6 | 9.10 | 125.36 | 119.90 |
| 35 | E | 1694 | G | N1-C6-O6 | 9.10 | 125.36 | 119.90 |
| 35 | E | 1555 | G | C5-C6-O6 | -9.10 | 123.14 | 128.60 |
| 35 | E | 567 | G | C5-C6-O6 | -9.09 | 123.14 | 128.60 |
| 35 | E | 1692 | G | N1-C6-O6 | 9.09 | 125.35 | 119.90 |
| 35 | E | 1337 | G | N1-C6-O6 | 9.08 | 125.35 | 119.90 |
| 35 | E | 2064 | G | N1-C6-O6 | 9.08 | 125.35 | 119.90 |
| 35 | E | 1538 | G | N1-C6-O6 | 9.08 | 125.35 | 119.90 |
| 35 | E | 2285 | G | N1-C6-O6 | 9.08 | 125.35 | 119.90 |
| 35 | E | 748 | G | N1-C6-O6 | 9.08 | 125.35 | 119.90 |
| 35 | E | 263 | G | C5-C6-O6 | -9.07 | 123.16 | 128.60 |
| 35 | E | 321 | G | N1-C6-O6 | 9.07 | 125.34 | 119.90 |
| 35 | E | 433 | G | N1-C6-O6 | 9.07 | 125.34 | 119.90 |
| 35 | E | 79 | G | C5-C6-O6 | -9.07 | 123.16 | 128.60 |
| 35 | E | 1234 | G | N1-C6-O6 | 9.06 | 125.34 | 119.90 |
| 35 | E | 228 | G | N1-C6-O6 | 9.06 | 125.34 | 119.90 |
| 35 | E | 1796 | G | N1-C6-O6 | 9.06 | 125.34 | 119.90 |
| 35 | E | 1798 | G | N1-C6-O6 | 9.06 | 125.34 | 119.90 |
| 35 | E | 931 | G | C5-C6-O6 | -9.05 | 123.17 | 128.60 |
| 35 | E | 119 | G | N1-C6-O6 | 9.05 | 125.33 | 119.90 |
| 35 | E | 1953 | G | C5-C6-O6 | -9.05 | 123.17 | 128.60 |
| 35 | E | 1317 | G | N1-C6-O6 | 9.05 | 125.33 | 119.90 |
| 35 | E | 1969 | G | N1-C6-O6 | 9.05 | 125.33 | 119.90 |
| 35 | E | 1288 | G | N1-C6-O6 | 9.05 | 125.33 | 119.90 |
| 35 | E | 530 | G | C5-C6-O6 | -9.04 | 123.18 | 128.60 |
| 35 | E | 792 | G | C5-C6-O6 | -9.04 | 123.18 | 128.60 |
| 35 | E | 824 | G | N1-C6-O6 | 9.04 | 125.32 | 119.90 |
| 35 | E | 918 | G | N1-C6-O6 | 9.04 | 125.32 | 119.90 |
| 35 | E | 1736 | G | N1-C6-O6 | 9.04 | 125.32 | 119.90 |
| 35 | E | 436 | G | N1-C6-O6 | 9.03 | 125.32 | 119.90 |
| 35 | E | 555 | G | C5-C6-O6 | -9.03 | 123.18 | 128.60 |
| 35 | E | 2224 | G | C5-C6-O6 | -9.03 | 123.18 | 128.60 |
| 35 | E | 539 | G | N1-C6-O6 | 9.03 | 125.32 | 119.90 |
| 35 | E | 1921 | G | N1-C6-O6 | 9.03 | 125.32 | 119.90 |
| 35 | E | 63 | G | C5-C6-O6 | -9.02 | 123.19 | 128.60 |
| 35 | E | 188 | G | C5-C6-O6 | -9.02 | 123.19 | 128.60 |
| 35 | E | 1277 | G | C5-C6-O6 | -9.02 | 123.19 | 128.60 |
| 35 | E | 273 | G | N1-C6-O6 | 9.02 | 125.31 | 119.90 |
| 35 | E | 2050 | C | P-O3'-C3' | 9.02 | 130.52 | 119.70 |
| 35 | E | 1614 | G | N1-C6-O6 | 9.01 | 125.31 | 119.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1253 | G | N1-C6-O6 | 9.01 | 125.31 | 119.90 |
| 35 | E | 1575 | G | N1-C6-O6 | 9.01 | 125.31 | 119.90 |
| 35 | E | 733 | G | C5-C6-O6 | -9.01 | 123.20 | 128.60 |
| 35 | E | 2144 | G | N1-C6-O6 | 9.00 | 125.30 | 119.90 |
| 35 | E | 1739 | G | N1-C6-O6 | 9.00 | 125.30 | 119.90 |
| 35 | E | 86 | G | C5-C6-O6 | -9.00 | 123.20 | 128.60 |
| 35 | E | 1644 | G | C5-C6-O6 | -9.00 | 123.20 | 128.60 |
| 35 | E | 1817 | G | C5-C6-O6 | -9.00 | 123.20 | 128.60 |
| 35 | E | 443 | G | N1-C6-O6 | 8.99 | 125.30 | 119.90 |
| 35 | E | 2020 | G | N1-C6-O6 | 8.99 | 125.30 | 119.90 |
| 35 | E | 1933 | G | N1-C6-O6 | 8.99 | 125.29 | 119.90 |
| 35 | E | 1914 | U | O4'-C1'-N1 | 8.99 | 115.39 | 108.20 |
| 35 | E | 2124 | G | N1-C6-O6 | 8.99 | 125.29 | 119.90 |
| 35 | E | 289 | G | N1-C6-O6 | 8.98 | 125.29 | 119.90 |
| 35 | E | 23 | G | C5-C6-O6 | -8.98 | 123.21 | 128.60 |
| 35 | E | 465 | G | N1-C6-O6 | 8.97 | 125.28 | 119.90 |
| 35 | E | 2061 | G | N1-C6-O6 | 8.97 | 125.28 | 119.90 |
| 35 | E | 1873 | G | C5-C6-O6 | -8.97 | 123.22 | 128.60 |
| 35 | E | 1701 | G | N1-C6-O6 | 8.96 | 125.28 | 119.90 |
| 35 | E | 2012 | C | P-O5'-C5' | 8.96 | 135.23 | 120.90 |
| 35 | E | 1617 | G | N1-C6-O6 | 8.95 | 125.27 | 119.90 |
| 35 | E | 921 | G | N1-C6-O6 | 8.95 | 125.27 | 119.90 |
| 35 | E | 1225 | G | N1-C6-O6 | 8.94 | 125.27 | 119.90 |
| 35 | E | 1995 | G | N1-C6-O6 | 8.94 | 125.27 | 119.90 |
| 35 | E | 479 | G | N1-C6-O6 | 8.94 | 125.26 | 119.90 |
| 35 | E | 888 | G | C5-C6-O6 | -8.94 | 123.24 | 128.60 |
| 35 | E | 164 | G | N1-C6-O6 | 8.93 | 125.26 | 119.90 |
| 35 | E | 249 | A | O4'-C1'-N9 | 8.93 | 115.35 | 108.20 |
| 35 | E | 512 | A | N1-C6-N6 | 8.93 | 123.96 | 118.60 |
| 35 | E | 682 | G | N1-C6-O6 | 8.93 | 125.26 | 119.90 |
| 35 | E | 1367 | G | C5-C6-O6 | -8.93 | 123.24 | 128.60 |
| 35 | E | 2023 | C | O4'-C1'-N1 | 8.93 | 115.35 | 108.20 |
| 35 | E | 2108 | G | N1-C6-O6 | 8.93 | 125.26 | 119.90 |
| 35 | E | 814 | C | C2-N1-C1' | 8.93 | 128.62 | 118.80 |
| 35 | E | 833 | A | P-O3'-C3' | 8.93 | 130.41 | 119.70 |
| 35 | E | 1713 | G | N1-C6-O6 | 8.93 | 125.26 | 119.90 |
| 35 | E | 1640 | G | N1-C6-O6 | 8.92 | 125.25 | 119.90 |
| 35 | E | 1823 | G | N1-C6-O6 | 8.92 | 125.25 | 119.90 |
| 35 | E | 400 | G | N1-C6-O6 | 8.91 | 125.25 | 119.90 |
| 35 | E | 838 | G | N1-C6-O6 | 8.91 | 125.25 | 119.90 |
| 35 | E | 1691 | G | N1-C6-O6 | 8.91 | 125.25 | 119.90 |
| 35 | E | 893 | G | N1-C6-O6 | 8.91 | 125.25 | 119.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 2212 | G | N1-C6-O6 | 8.91 | 125.25 | 119.90 |
| 35 | E | 1190 | G | N1-C6-O6 | 8.90 | 125.24 | 119.90 |
| 35 | E | 335 | G | C5-C6-O6 | -8.90 | 123.26 | 128.60 |
| 35 | E | 385 | G | N1-C6-O6 | 8.90 | 125.24 | 119.90 |
| 35 | E | 1199 | G | N1-C6-O6 | 8.90 | 125.24 | 119.90 |
| 35 | E | 685 | G | N1-C6-O6 | 8.90 | 125.24 | 119.90 |
| 35 | E | 761 | G | N1-C6-O6 | 8.90 | 125.24 | 119.90 |
| 35 | E | 796 | G | N1-C6-O6 | 8.90 | 125.24 | 119.90 |
| 35 | E | 1081 | G | N1-C6-O6 | 8.90 | 125.24 | 119.90 |
| 35 | E | 1560 | G | N1-C6-O6 | 8.90 | 125.24 | 119.90 |
| 35 | E | 213 | G | N1-C6-O6 | 8.89 | 125.24 | 119.90 |
| 35 | E | 985 | G | N1-C6-O6 | 8.89 | 125.24 | 119.90 |
| 35 | E | 1249 | G | N1-C6-O6 | 8.89 | 125.24 | 119.90 |
| 35 | E | 1875 | G | N1-C6-O6 | 8.89 | 125.23 | 119.90 |
| 35 | E | 1901 | G | N1-C6-O6 | 8.89 | 125.23 | 119.90 |
| 35 | E | 2123 | C | O4'-C1'-N1 | 8.89 | 115.31 | 108.20 |
| 35 | E | 745 | C | O4'-C1'-N1 | 8.88 | 115.31 | 108.20 |
| 35 | E | 1993 | G | N1-C6-O6 | 8.89 | 125.23 | 119.90 |
| 35 | E | 1183 | G | N1-C6-O6 | 8.88 | 125.23 | 119.90 |
| 35 | E | 693 | G | N1-C6-O6 | 8.88 | 125.23 | 119.90 |
| 35 | E | 511 | G | N1-C6-O6 | 8.88 | 125.22 | 119.90 |
| 35 | E | 1792 | G | N1-C6-O6 | 8.87 | 125.22 | 119.90 |
| 35 | E | 2049 | C | O4'-C1'-N1 | 8.87 | 115.30 | 108.20 |
| 35 | E | 2079 | G | N1-C6-O6 | 8.87 | 125.22 | 119.90 |
| 35 | E | 248 | G | N1-C6-O6 | 8.87 | 125.22 | 119.90 |
| 35 | E | 602 | G | N1-C6-O6 | 8.87 | 125.22 | 119.90 |
| 35 | E | 2151 | U | O4'-C1'-N1 | 8.86 | 115.29 | 108.20 |
| 35 | E | 661 | G | C5-C6-O6 | -8.86 | 123.28 | 128.60 |
| 35 | E | 53 | G | C5-C6-O6 | -8.86 | 123.28 | 128.60 |
| 35 | E | 419 | G | N1-C6-O6 | 8.86 | 125.22 | 119.90 |
| 35 | E | 1765 | G | N1-C6-O6 | 8.86 | 125.22 | 119.90 |
| 35 | E | 2043 | G | C5-C6-O6 | -8.86 | 123.28 | 128.60 |
| 35 | E | 1618 | G | N1-C6-O6 | 8.85 | 125.21 | 119.90 |
| 35 | E | 1198 | G | N1-C6-O6 | 8.84 | 125.20 | 119.90 |
| 35 | E | 2286 | G | N1-C6-O6 | 8.84 | 125.20 | 119.90 |
| 35 | E | 1072 | G | N1-C6-O6 | 8.84 | 125.20 | 119.90 |
| 35 | E | 1917 | G | N1-C6-O6 | 8.84 | 125.20 | 119.90 |
| 35 | E | 424 | G | N1-C6-O6 | 8.83 | 125.20 | 119.90 |
| 35 | E | 476 | G | N1-C6-O6 | 8.83 | 125.20 | 119.90 |
| 35 | E | 1364 | G | N1-C6-O6 | 8.83 | 125.20 | 119.90 |
| 35 | E | 1376 | G | N1-C6-O6 | 8.83 | 125.20 | 119.90 |
| 35 | E | 2179 | G | N1-C6-O6 | 8.83 | 125.20 | 119.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1738 | G | N1-C6-O6 | 8.83 | 125.20 | 119.90 |
| 35 | E | 1226 | G | N1-C6-O6 | 8.82 | 125.19 | 119.90 |
| 35 | E | 2109 | G | N1-C6-O6 | 8.82 | 125.19 | 119.90 |
| 35 | E | 1276 | G | N1-C6-O6 | 8.82 | 125.19 | 119.90 |
| 35 | E | 2074 | G | N1-C6-O6 | 8.82 | 125.19 | 119.90 |
| 35 | E | 815 | G | N1-C6-O6 | 8.82 | 125.19 | 119.90 |
| 35 | E | 1813 | G | N1-C6-O6 | 8.82 | 125.19 | 119.90 |
| 35 | E | 989 | G | N1-C6-O6 | 8.81 | 125.19 | 119.90 |
| 35 | E | 2030 | G | N1-C6-O6 | 8.81 | 125.19 | 119.90 |
| 35 | E | 631 | G | N1-C6-O6 | 8.80 | 125.18 | 119.90 |
| 35 | E | 411 | G | N1-C6-O6 | 8.80 | 125.18 | 119.90 |
| 35 | E | 1236 | G | N1-C6-O6 | 8.80 | 125.18 | 119.90 |
| 35 | E | 1322 | G | N1-C6-O6 | 8.80 | 125.18 | 119.90 |
| 35 | E | 1551 | G | N1-C6-O6 | 8.80 | 125.18 | 119.90 |
| 35 | E | 1924 | G | N1-C6-O6 | 8.80 | 125.18 | 119.90 |
| 35 | E | 137 | C | O4'-C1'-N1 | 8.79 | 115.24 | 108.20 |
| 35 | E | 212 | G | N1-C6-O6 | 8.80 | 125.18 | 119.90 |
| 35 | E | 2040 | G | N1-C6-O6 | 8.79 | 125.18 | 119.90 |
| 35 | E | 46 | U | O4'-C1'-N1 | 8.79 | 115.23 | 108.20 |
| 35 | E | 938 | G | N1-C6-O6 | 8.79 | 125.17 | 119.90 |
| 35 | E | 2011 | A | P-O3'-C3' | 8.79 | 130.25 | 119.70 |
| 35 | E | 1632 | G | N1-C6-O6 | 8.79 | 125.17 | 119.90 |
| 35 | E | 649 | G | N1-C6-O6 | 8.78 | 125.17 | 119.90 |
| 35 | E | 2101 | G | N1-C6-O6 | 8.78 | 125.17 | 119.90 |
| 35 | E | 379 | G | N1-C6-O6 | 8.78 | 125.17 | 119.90 |
| 35 | E | 1963 | G | N1-C6-O6 | 8.78 | 125.17 | 119.90 |
| 35 | E | 407 | G | N1-C6-O6 | 8.78 | 125.17 | 119.90 |
| 35 | E | 1590 | G | N1-C6-O6 | 8.77 | 125.17 | 119.90 |
| 35 | E | 309 | G | N1-C6-O6 | 8.77 | 125.16 | 119.90 |
| 35 | E | 930 | G | N1-C6-O6 | 8.77 | 125.16 | 119.90 |
| 35 | E | 1596 | G | N1-C6-O6 | 8.77 | 125.16 | 119.90 |
| 35 | E | 1084 | G | N1-C6-O6 | 8.77 | 125.16 | 119.90 |
| 35 | E | 1165 | G | C5-C6-O6 | -8.77 | 123.34 | 128.60 |
| 35 | E | 1890 | C | O4'-C1'-N1 | 8.76 | 115.21 | 108.20 |
| 35 | E | 20 | G | N1-C6-O6 | 8.76 | 125.16 | 119.90 |
| 35 | E | 754 | G | N1-C6-O6 | 8.76 | 125.16 | 119.90 |
| 35 | E | 909 | G | N1-C6-O6 | 8.76 | 125.16 | 119.90 |
| 35 | E | 1915 | G | N1-C6-O6 | 8.76 | 125.15 | 119.90 |
| 35 | E | 903 | G | N1-C6-O6 | 8.75 | 125.15 | 119.90 |
| 35 | E | 1383 | G | N1-C6-O6 | 8.75 | 125.15 | 119.90 |
| 35 | E | 919 | G | N1-C6-O6 | 8.75 | 125.15 | 119.90 |
| 35 | E | 30 | G | C5-C6-O6 | -8.74 | 123.35 | 128.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 828 | G | N1-C6-O6 | 8.74 | 125.15 | 119.90 |
| 35 | E | 1696 | G | N1-C6-O6 | 8.74 | 125.14 | 119.90 |
| 35 | E | 688 | G | N1-C6-O6 | 8.74 | 125.14 | 119.90 |
| 35 | E | 1622 | G | N1-C6-O6 | 8.74 | 125.14 | 119.90 |
| 35 | E | 2106 | G | N1-C6-O6 | 8.74 | 125.14 | 119.90 |
| 35 | E | 591 | G | N1-C6-O6 | 8.73 | 125.14 | 119.90 |
| 35 | E | 618 | G | N1-C6-O6 | 8.73 | 125.14 | 119.90 |
| 35 | E | 2081 | G | N1-C6-O6 | 8.73 | 125.14 | 119.90 |
| 35 | E | 667 | G | N1-C6-O6 | 8.73 | 125.14 | 119.90 |
| 35 | E | 1906 | C | O4'-C1'-N1 | 8.72 | 115.18 | 108.20 |
| 35 | E | 92 | G | N1-C6-O6 | 8.72 | 125.13 | 119.90 |
| 35 | E | 2152 | C | O4'-C1'-N1 | 8.72 | 115.17 | 108.20 |
| 35 | E | 1637 | G | N1-C6-O6 | 8.72 | 125.13 | 119.90 |
| 35 | E | 1358 | G | N1-C6-O6 | 8.71 | 125.13 | 119.90 |
| 35 | E | 1926 | G | N1-C6-O6 | 8.71 | 125.13 | 119.90 |
| 35 | E | 1772 | G | N1-C6-O6 | 8.71 | 125.13 | 119.90 |
| 35 | E | 2213 | G | N1-C6-O6 | 8.71 | 125.13 | 119.90 |
| 35 | E | 80 | G | N1-C6-O6 | 8.71 | 125.12 | 119.90 |
| 35 | E | 1549 | G | C5-C6-O6 | -8.71 | 123.38 | 128.60 |
| 35 | E | 1902 | G | N1-C6-O6 | 8.71 | 125.13 | 119.90 |
| 35 | E | 981 | G | N1-C6-O6 | 8.70 | 125.12 | 119.90 |
| 35 | E | 466 | G | C5-C6-O6 | -8.70 | 123.38 | 128.60 |
| 35 | E | 532 | G | C5-C6-O6 | -8.70 | 123.38 | 128.60 |
| 35 | E | 2296 | G | C5-C6-O6 | -8.70 | 123.38 | 128.60 |
| 35 | E | 1531 | G | N1-C6-O6 | 8.69 | 125.12 | 119.90 |
| 35 | E | 1853 | C | O4'-C1'-N1 | 8.69 | 115.16 | 108.20 |
| 35 | E | 2096 | G | N1-C6-O6 | 8.69 | 125.11 | 119.90 |
| 35 | E | 876 | A | N1-C6-N6 | 8.69 | 123.81 | 118.60 |
| 35 | E | 1384 | G | C5-C6-O6 | -8.68 | 123.39 | 128.60 |
| 35 | E | 412 | G | C5-C6-O6 | -8.68 | 123.39 | 128.60 |
| 35 | E | 1535 | U | O4'-C1'-N1 | 8.68 | 115.14 | 108.20 |
| 35 | E | 973 | G | N1-C6-O6 | 8.67 | 125.10 | 119.90 |
| 35 | E | 1201 | G | N1-C6-O6 | 8.67 | 125.10 | 119.90 |
| 35 | E | 397 | G | N1-C6-O6 | 8.67 | 125.10 | 119.90 |
| 35 | E | 1182 | G | C5-C6-O6 | -8.66 | 123.40 | 128.60 |
| 35 | E | 881 | G | N1-C6-O6 | 8.65 | 125.09 | 119.90 |
| 35 | E | 924 | G | N1-C6-O6 | 8.65 | 125.09 | 119.90 |
| 35 | E | 1580 | G | N1-C6-O6 | 8.65 | 125.09 | 119.90 |
| 35 | E | 2237 | G | C5-C6-O6 | -8.65 | 123.41 | 128.60 |
| 35 | E | 286 | G | N1-C6-O6 | 8.65 | 125.09 | 119.90 |
| 35 | E | 797 | G | N1-C6-O6 | 8.65 | 125.09 | 119.90 |
| 35 | E | 1187 | C | O4'-C1'-N1 | 8.65 | 115.12 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 16 | G | N1-C6-O6 | 8.65 | 125.09 | 119.90 |
| 35 | E | 1210 | G | C5-C6-O6 | -8.65 | 123.41 | 128.60 |
| 35 | E | 1943 | G | C5-C6-O6 | -8.65 | 123.41 | 128.60 |
| 35 | E | 2010 | G | N1-C6-O6 | 8.65 | 125.09 | 119.90 |
| 35 | E | 1321 | G | N1-C6-O6 | 8.65 | 125.09 | 119.90 |
| 35 | E | 867 | G | N1-C6-O6 | 8.64 | 125.08 | 119.90 |
| 35 | E | 819 | G | N1-C6-O6 | 8.64 | 125.08 | 119.90 |
| 35 | E | 899 | G | N1-C6-O6 | 8.63 | 125.08 | 119.90 |
| 35 | E | 132 | G | C5-C6-O6 | -8.63 | 123.42 | 128.60 |
| 35 | E | 440 | C | O4'-C1'-N1 | 8.63 | 115.10 | 108.20 |
| 35 | E | 6 | G | C5-C6-O6 | -8.63 | 123.42 | 128.60 |
| 35 | E | 418 | G | N1-C6-O6 | 8.63 | 125.08 | 119.90 |
| 35 | E | 2233 | G | C5-C6-O6 | -8.63 | 123.42 | 128.60 |
| 35 | E | 1977 | G | N1-C6-O6 | 8.63 | 125.08 | 119.90 |
| 35 | E | 1767 | G | N1-C6-O6 | 8.62 | 125.07 | 119.90 |
| 35 | E | 763 | G | N1-C6-O6 | 8.62 | 125.07 | 119.90 |
| 35 | E | 1723 | G | N1-C6-O6 | 8.61 | 125.07 | 119.90 |
| 35 | E | 2217 | G | C5-C6-O6 | -8.61 | 123.43 | 128.60 |
| 35 | E | 2248 | G | N1-C6-O6 | 8.61 | 125.06 | 119.90 |
| 35 | E | 223 | G | C5-C6-O6 | -8.61 | 123.44 | 128.60 |
| 35 | E | 337 | G | N1-C6-O6 | 8.60 | 125.06 | 119.90 |
| 35 | E | 519 | G | N1-C6-O6 | 8.60 | 125.06 | 119.90 |
| 35 | E | 1755 | G | N1-C6-O6 | 8.60 | 125.06 | 119.90 |
| 35 | E | 1646 | G | N1-C6-O6 | 8.59 | 125.06 | 119.90 |
| 35 | E | 768 | G | N1-C6-O6 | 8.59 | 125.05 | 119.90 |
| 35 | E | 677 | G | N1-C6-O6 | 8.59 | 125.05 | 119.90 |
| 35 | E | 696 | G | N1-C6-O6 | 8.59 | 125.05 | 119.90 |
| 35 | E | 1668 | G | N1-C6-O6 | 8.59 | 125.05 | 119.90 |
| 35 | E | 1731 | G | C5-C6-O6 | -8.59 | 123.45 | 128.60 |
| 35 | E | 108 | C | O4'-C1'-N1 | 8.58 | 115.06 | 108.20 |
| 35 | E | 159 | G | N1-C6-O6 | 8.58 | 125.05 | 119.90 |
| 35 | E | 676 | G | N1-C6-O6 | 8.58 | 125.05 | 119.90 |
| 35 | E | 697 | G | N1-C6-O6 | 8.58 | 125.05 | 119.90 |
| 35 | E | 368 | G | N1-C6-O6 | 8.57 | 125.05 | 119.90 |
| 35 | E | 252 | G | N1-C6-O6 | 8.57 | 125.04 | 119.90 |
| 35 | E | 1586 | G | N1-C6-O6 | 8.57 | 125.04 | 119.90 |
| 35 | E | 69 | C | O4'-C1'-N1 | 8.56 | 115.05 | 108.20 |
| 35 | E | 739 | G | N1-C6-O6 | 8.56 | 125.04 | 119.90 |
| 35 | E | 1709 | G | N1-C6-O6 | 8.56 | 125.04 | 119.90 |
| 35 | E | 116 | G | N1-C6-O6 | 8.56 | 125.03 | 119.90 |
| 35 | E | 970 | G | C5-C6-O6 | -8.56 | 123.47 | 128.60 |
| 35 | E | 169 | G | C5-C6-O6 | -8.55 | 123.47 | 128.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 2188 | G | N1-C6-O6 | 8.56 | 125.03 | 119.90 |
| 35 | E | 1780 | G | N1-C6-O6 | 8.55 | 125.03 | 119.90 |
| 35 | E | 1882 | G | N1-C6-O6 | 8.55 | 125.03 | 119.90 |
| 35 | E | 2021 | G | N1-C6-O6 | 8.55 | 125.03 | 119.90 |
| 35 | E | 695 | G | N1-C6-O6 | 8.54 | 125.03 | 119.90 |
| 35 | E | 871 | G | N1-C6-O6 | 8.55 | 125.03 | 119.90 |
| 35 | E | 2298 | G | N1-C6-O6 | 8.54 | 125.03 | 119.90 |
| 35 | E | 1256 | C | O4'-C1'-N1 | 8.54 | 115.03 | 108.20 |
| 35 | E | 808 | G | N1-C6-O6 | 8.54 | 125.02 | 119.90 |
| 35 | E | 2053 | G | N1-C6-O6 | 8.54 | 125.02 | 119.90 |
| 35 | E | 603 | G | N1-C6-O6 | 8.53 | 125.02 | 119.90 |
| 35 | E | 816 | C | O4'-C1'-N1 | 8.53 | 115.03 | 108.20 |
| 35 | E | 1934 | G | N1-C6-O6 | 8.53 | 125.02 | 119.90 |
| 35 | E | 714 | G | N1-C6-O6 | 8.52 | 125.01 | 119.90 |
| 35 | E | 311 | G | C5-C6-O6 | -8.52 | 123.49 | 128.60 |
| 35 | E | 724 | A | C2-N3-C4 | -8.52 | 106.34 | 110.60 |
| 35 | E | 1548 | C | C2-N1-C1' | 8.52 | 128.17 | 118.80 |
| 35 | E | 2191 | G | N1-C6-O6 | 8.51 | 125.01 | 119.90 |
| 35 | E | 997 | G | N1-C6-O6 | 8.51 | 125.01 | 119.90 |
| 35 | E | 2112 | U | O4'-C1'-N1 | 8.51 | 115.01 | 108.20 |
| 35 | E | 431 | G | C5-C6-O6 | -8.50 | 123.50 | 128.60 |
| 35 | E | 923 | A | P-O3'-C3' | 8.50 | 129.90 | 119.70 |
| 35 | E | 2054 | G | N1-C6-O6 | 8.50 | 125.00 | 119.90 |
| 35 | E | 2042 | G | N1-C6-O6 | 8.50 | 125.00 | 119.90 |
| 35 | E | 1805 | G | N1-C6-O6 | 8.49 | 125.00 | 119.90 |
| 35 | E | 1869 | G | C5-C6-O6 | -8.49 | 123.51 | 128.60 |
| 35 | E | 1989 | G | N1-C6-O6 | 8.49 | 124.99 | 119.90 |
| 35 | E | 2032 | U | O4'-C1'-N1 | 8.49 | 114.99 | 108.20 |
| 35 | E | 88 | G | N1-C6-O6 | 8.49 | 124.99 | 119.90 |
| 35 | E | 1891 | C | O4'-C1'-N1 | 8.49 | 114.99 | 108.20 |
| 35 | E | 2075 | G | N1-C6-O6 | 8.49 | 124.99 | 119.90 |
| 35 | E | 541 | G | C5-C6-O6 | -8.48 | 123.51 | 128.60 |
| 35 | E | 1582 | G | N1-C6-O6 | 8.48 | 124.99 | 119.90 |
| 35 | E | 220 | G | C5-C6-O6 | -8.47 | 123.52 | 128.60 |
| 35 | E | 564 | G | C5-C6-O6 | -8.47 | 123.52 | 128.60 |
| 35 | E | 2311 | G | N1-C6-O6 | 8.47 | 124.98 | 119.90 |
| 35 | E | 1075 | G | O4'-C1'-N9 | 8.46 | 114.97 | 108.20 |
| 35 | E | 2095 | G | N1-C6-O6 | 8.46 | 124.98 | 119.90 |
| 35 | E | 275 | A | C5-C6-N6 | -8.46 | 116.93 | 123.70 |
| 35 | E | 1527 | G | N1-C6-O6 | 8.46 | 124.98 | 119.90 |
| 35 | E | 698 | C | O4'-C1'-N1 | 8.46 | 114.97 | 108.20 |
| 35 | E | 1239 | G | N1-C6-O6 | 8.45 | 124.97 | 119.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 2017 | G | N1-C6-O6 | 8.45 | 124.97 | 119.90 |
| 35 | E | 857 | G | C5-C6-O6 | -8.45 | 123.53 | 128.60 |
| 35 | E | 1647 | G | N1-C6-O6 | 8.45 | 124.97 | 119.90 |
| 35 | E | 1202 | G | N1-C6-O6 | 8.45 | 124.97 | 119.90 |
| 35 | E | 2289 | G | C5-C6-O6 | -8.45 | 123.53 | 128.60 |
| 35 | E | 2263 | G | N1-C6-O6 | 8.45 | 124.97 | 119.90 |
| 35 | E | 834 | G | N1-C6-O6 | 8.44 | 124.96 | 119.90 |
| 35 | E | 713 | G | N1-C6-O6 | 8.43 | 124.96 | 119.90 |
| 35 | E | 950 | G | C5-C6-O6 | -8.42 | 123.55 | 128.60 |
| 35 | E | 445 | G | N1-C6-O6 | 8.42 | 124.95 | 119.90 |
| 35 | E | 1346 | G | N1-C6-O6 | 8.41 | 124.95 | 119.90 |
| 35 | E | 1910 | G | C5-C6-O6 | -8.41 | 123.55 | 128.60 |
| 35 | E | 1257 | C | O4'-C1'-N1 | 8.41 | 114.93 | 108.20 |
| 35 | E | 211 | G | C5-C6-O6 | -8.41 | 123.56 | 128.60 |
| 35 | E | 2122 | G | C5-C6-O6 | -8.41 | 123.56 | 128.60 |
| 35 | E | 1642 | G | N1-C6-O6 | 8.41 | 124.94 | 119.90 |
| 35 | E | 2023 | C | C2-N1-C1' | 8.41 | 128.05 | 118.80 |
| 35 | E | 1598 | G | C5-C6-O6 | -8.39 | 123.56 | 128.60 |
| 35 | E | 2139 | G | C5-C6-O6 | -8.39 | 123.56 | 128.60 |
| 35 | E | 963 | G | C5-C6-O6 | -8.39 | 123.57 | 128.60 |
| 35 | E | 832 | G | N1-C6-O6 | 8.39 | 124.93 | 119.90 |
| 35 | E | 749 | C | P-O3'-C3' | 8.39 | 129.76 | 119.70 |
| 35 | E | 753 | U | O4'-C1'-N1 | 8.38 | 114.91 | 108.20 |
| 35 | E | 719 | G | N1-C6-O6 | 8.38 | 124.93 | 119.90 |
| 35 | E | 1548 | C | O4'-C1'-N1 | 8.38 | 114.91 | 108.20 |
| 35 | E | 48 | G | C5-C6-O6 | -8.38 | 123.57 | 128.60 |
| 35 | E | 189 | G | C5-C6-O6 | -8.38 | 123.57 | 128.60 |
| 35 | E | 230 | G | C5-C6-O6 | -8.37 | 123.58 | 128.60 |
| 35 | E | 1076 | C | O4'-C1'-N1 | 8.38 | 114.90 | 108.20 |
| 35 | E | 996 | G | C5-C6-O6 | -8.37 | 123.58 | 128.60 |
| 35 | E | 1220 | G | C5-C6-O6 | -8.37 | 123.58 | 128.60 |
| 35 | E | 1 | G | N1-C6-O6 | 8.37 | 124.92 | 119.90 |
| 35 | E | 394 | G | C5-C6-O6 | -8.37 | 123.58 | 128.60 |
| 35 | E | 741 | G | N1-C6-O6 | 8.36 | 124.92 | 119.90 |
| 35 | E | 844 | G | N1-C6-O6 | 8.35 | 124.91 | 119.90 |
| 35 | E | 31 | C | O4'-C1'-N1 | 8.35 | 114.88 | 108.20 |
| 35 | E | 922 | C | P-O3'-C3' | 8.35 | 129.72 | 119.70 |
| 35 | E | 1195 | G | N1-C6-O6 | 8.35 | 124.91 | 119.90 |
| 35 | E | 1262 | C | O4'-C1'-N1 | 8.34 | 114.87 | 108.20 |
| 35 | E | 593 | G | N1-C6-O6 | 8.34 | 124.90 | 119.90 |
| 35 | E | 57 | G | C5-C6-O6 | -8.34 | 123.60 | 128.60 |
| 35 | E | 1864 | C | O4'-C1'-N1 | 8.33 | 114.87 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 262 | U | O4'-C1'-N1 | 8.33 | 114.86 | 108.20 |
| 35 | E | 932 | G | C5-C6-O6 | -8.33 | 123.60 | 128.60 |
| 35 | E | 1188 | C | O4'-C1'-N1 | 8.32 | 114.86 | 108.20 |
| 35 | E | 395 | G | C5-C6-O6 | -8.31 | 123.61 | 128.60 |
| 35 | E | 334 | G | C5-C6-O6 | -8.31 | 123.61 | 128.60 |
| 35 | E | 437 | G | N1-C6-O6 | 8.31 | 124.89 | 119.90 |
| 35 | E | 524 | G | C5-C6-O6 | -8.31 | 123.61 | 128.60 |
| 35 | E | 1850 | C | O4'-C1'-N1 | 8.31 | 114.85 | 108.20 |
| 35 | E | 272 | G | C5-C6-O6 | -8.30 | 123.62 | 128.60 |
| 35 | E | 1581 | A | N1-C6-N6 | 8.30 | 123.58 | 118.60 |
| 35 | E | 2222 | G | C5-C6-O6 | -8.30 | 123.62 | 128.60 |
| 35 | E | 641 | C | O4'-C1'-N1 | 8.30 | 114.84 | 108.20 |
| 35 | E | 2275 | G | C5-C6-O6 | -8.30 | 123.62 | 128.60 |
| 35 | E | 7 | G | C5-C6-O6 | -8.30 | 123.62 | 128.60 |
| 35 | E | 2307 | G | N1-C6-O6 | 8.30 | 124.88 | 119.90 |
| 35 | E | 514 | G | C5-C6-O6 | -8.29 | 123.63 | 128.60 |
| 35 | E | 1680 | G | N1-C6-O6 | 8.29 | 124.87 | 119.90 |
| 35 | E | 630 | G | N1-C6-O6 | 8.29 | 124.87 | 119.90 |
| 35 | E | 2121 | G | C5-C6-O6 | -8.29 | 123.63 | 128.60 |
| 35 | E | 320 | G | C5-C6-O6 | -8.28 | 123.64 | 128.60 |
| 35 | E | 2176 | G | C5-C6-O6 | -8.27 | 123.64 | 128.60 |
| 35 | E | 640 | G | C5-C6-O6 | -8.27 | 123.64 | 128.60 |
| 35 | E | 430 | G | C5-C6-O6 | -8.27 | 123.64 | 128.60 |
| 35 | E | 771 | A | P-O3'-C3' | 8.27 | 129.62 | 119.70 |
| 35 | E | 1074 | C | O4'-C1'-N1 | 8.27 | 114.81 | 108.20 |
| 35 | E | 1985 | C | O4'-C1'-N1 | 8.26 | 114.81 | 108.20 |
| 35 | E | 157 | G | C5-C6-O6 | -8.25 | 123.65 | 128.60 |
| 35 | E | 165 | C | O4'-C1'-N1 | 8.25 | 114.80 | 108.20 |
| 35 | E | 1741 | G | N1-C6-O6 | 8.25 | 124.85 | 119.90 |
| 35 | E | 2206 | G | C5-C6-O6 | -8.25 | 123.65 | 128.60 |
| 35 | E | 1685 | G | N1-C6-O6 | 8.25 | 124.85 | 119.90 |
| 35 | E | 1935 | C | O4'-C1'-N1 | 8.25 | 114.80 | 108.20 |
| 35 | E | 552 | G | C5-C6-O6 | -8.24 | 123.66 | 128.60 |
| 35 | E | 2174 | C | O4'-C1'-N1 | 8.24 | 114.79 | 108.20 |
| 35 | E | 373 | G | N1-C6-O6 | 8.24 | 124.84 | 119.90 |
| 35 | E | 238 | G | C5-C6-O6 | -8.23 | 123.66 | 128.60 |
| 35 | E | 294 | G | N1-C6-O6 | 8.23 | 124.84 | 119.90 |
| 35 | E | 420 | G | C5-C6-O6 | -8.23 | 123.66 | 128.60 |
| 35 | E | 488 | G | C5-C6-O6 | -8.23 | 123.66 | 128.60 |
| 35 | E | 776 | G | N1-C6-O6 | 8.23 | 124.84 | 119.90 |
| 35 | E | 1982 | C | O4'-C1'-N1 | 8.23 | 114.78 | 108.20 |
| 35 | E | 1594 | G | C5-C6-O6 | -8.22 | 123.67 | 128.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 428 | C | O4'-C1'-N1 | 8.22 | 114.78 | 108.20 |
| 35 | E | 478 | C | O4'-C1'-N1 | 8.22 | 114.78 | 108.20 |
| 35 | E | 1307 | G | C5-C6-O6 | -8.22 | 123.67 | 128.60 |
| 35 | E | 2235 | C | O4'-C1'-N1 | 8.21 | 114.77 | 108.20 |
| 35 | E | 606 | G | C5-C6-O6 | -8.21 | 123.68 | 128.60 |
| 35 | E | 2265 | G | C5-C6-O6 | -8.21 | 123.68 | 128.60 |
| 35 | E | 2290 | C | O4'-C1'-N1 | 8.20 | 114.76 | 108.20 |
| 35 | E | 1870 | G | C5-C6-O6 | -8.20 | 123.68 | 128.60 |
| 35 | E | 887 | C | O4'-C1'-N1 | 8.20 | 114.76 | 108.20 |
| 35 | E | 2302 | C | O4'-C1'-N1 | 8.20 | 114.76 | 108.20 |
| 35 | E | 700 | U | O4'-C1'-N1 | 8.19 | 114.76 | 108.20 |
| 35 | E | 1735 | G | C5-C6-O6 | -8.19 | 123.69 | 128.60 |
| 35 | E | 1339 | G | C5-C6-O6 | -8.19 | 123.69 | 128.60 |
| 35 | E | 1906 | C | C2-N1-C1' | 8.19 | 127.81 | 118.80 |
| 35 | E | 2278 | G | C5-C6-O6 | -8.19 | 123.69 | 128.60 |
| 35 | E | 34 | G | C5-C6-O6 | -8.19 | 123.69 | 128.60 |
| 35 | E | 389 | G | C5-C6-O6 | -8.19 | 123.69 | 128.60 |
| 35 | E | 2246 | C | O4'-C1'-N1 | 8.19 | 114.75 | 108.20 |
| 35 | E | 1750 | C | O4'-C1'-N1 | 8.18 | 114.75 | 108.20 |
| 35 | E | 1711 | G | N1-C6-O6 | 8.18 | 124.81 | 119.90 |
| 35 | E | 385 | G | C5-C6-O6 | -8.18 | 123.69 | 128.60 |
| 35 | E | 746 | A | C6-C5-N7 | -8.17 | 126.58 | 132.30 |
| 35 | E | 2198 | C | O4'-C1'-N1 | 8.17 | 114.74 | 108.20 |
| 35 | E | 2197 | G | C5-C6-O6 | -8.17 | 123.70 | 128.60 |
| 35 | E | 2220 | G | C5-C6-O6 | -8.17 | 123.70 | 128.60 |
| 35 | E | 1203 | G | C5-C6-O6 | -8.16 | 123.70 | 128.60 |
| 35 | E | 1540 | C | O4'-C1'-N1 | 8.16 | 114.73 | 108.20 |
| 35 | E | 718 | A | C5-C6-N1 | -8.16 | 113.62 | 117.70 |
| 35 | E | 192 | G | C5-C6-O6 | -8.15 | 123.71 | 128.60 |
| 35 | E | 204 | G | C5-C6-O6 | -8.15 | 123.71 | 128.60 |
| 35 | E | 1875 | G | P-O3'-C3' | 8.15 | 129.49 | 119.70 |
| 35 | E | 205 | G | C5-C6-O6 | -8.14 | 123.71 | 128.60 |
| 35 | E | 404 | G | C5-C6-O6 | -8.14 | 123.72 | 128.60 |
| 35 | E | 1793 | G | C5-C6-O6 | -8.14 | 123.72 | 128.60 |
| 35 | E | 2266 | G | C5-C6-O6 | -8.13 | 123.72 | 128.60 |
| 35 | E | 1219 | C | O4'-C1'-N1 | 8.13 | 114.70 | 108.20 |
| 35 | E | 1907 | C | O4'-C1'-N1 | 8.13 | 114.70 | 108.20 |
| 35 | E | 113 | U | O4'-C1'-N1 | 8.12 | 114.70 | 108.20 |
| 35 | E | 1579 | G | C5-C6-O6 | -8.12 | 123.73 | 128.60 |
| 35 | E | 1082 | U | O4'-C1'-N1 | 8.12 | 114.70 | 108.20 |
| 35 | E | 1230 | G | C5-C6-O6 | -8.12 | 123.73 | 128.60 |
| 35 | E | 1938 | C | O4'-C1'-N1 | 8.12 | 114.70 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1979 | G | C5-C6-O6 | -8.12 | 123.73 | 128.60 |
| 35 | E | 319 | C | O4'-C1'-N1 | 8.12 | 114.69 | 108.20 |
| 35 | E | 837 | C | O4'-C1'-N1 | 8.11 | 114.69 | 108.20 |
| 35 | E | 1983 | U | O4'-C1'-N1 | 8.11 | 114.69 | 108.20 |
| 35 | E | 2067 | C | O4'-C1'-N1 | 8.11 | 114.69 | 108.20 |
| 35 | E | 135 | C | O4'-C1'-N1 | 8.10 | 114.68 | 108.20 |
| 35 | E | 834 | G | P-O3'-C3' | 8.10 | 129.42 | 119.70 |
| 35 | E | 2194 | G | C5-C6-O6 | -8.10 | 123.74 | 128.60 |
| 35 | E | 391 | C | O4'-C1'-N1 | 8.10 | 114.68 | 108.20 |
| 35 | E | 84 | C | O4'-C1'-N1 | 8.10 | 114.68 | 108.20 |
| 35 | E | 318 | C | O4'-C1'-N1 | 8.10 | 114.68 | 108.20 |
| 35 | E | 186 | C | O4'-C1'-N1 | 8.09 | 114.67 | 108.20 |
| 35 | E | 405 | G | C5-C6-O6 | -8.09 | 123.74 | 128.60 |
| 35 | E | 232 | C | O4'-C1'-N1 | 8.09 | 114.67 | 108.20 |
| 35 | E | 559 | U | P-O3'-C3' | 8.09 | 129.41 | 119.70 |
| 35 | E | 942 | C | C2-N1-C1' | 8.09 | 127.70 | 118.80 |
| 35 | E | 982 | G | P-O3'-C3' | 8.09 | 129.41 | 119.70 |
| 35 | E | 331 | U | O4'-C1'-N1 | 8.09 | 114.67 | 108.20 |
| 35 | E | 508 | G | C5-C6-O6 | -8.09 | 123.75 | 128.60 |
| 35 | E | 423 | C | O4'-C1'-N1 | 8.08 | 114.66 | 108.20 |
| 35 | E | 1237 | G | C5-C6-O6 | -8.08 | 123.75 | 128.60 |
| 35 | E | 1900 | G | C5-C6-O6 | -8.08 | 123.75 | 128.60 |
| 35 | E | 1211 | G | N1-C6-O6 | 8.08 | 124.75 | 119.90 |
| 35 | E | 548 | C | O4'-C1'-N1 | 8.07 | 114.66 | 108.20 |
| 35 | E | 104 | C | O4'-C1'-N1 | 8.07 | 114.66 | 108.20 |
| 35 | E | 156 | G | C5-C6-O6 | -8.07 | 123.76 | 128.60 |
| 35 | E | 807 | U | O4'-C1'-N1 | 8.07 | 114.66 | 108.20 |
| 35 | E | 374 | G | N1-C6-O6 | 8.06 | 124.74 | 119.90 |
| 35 | E | 1273 | G | N1-C6-O6 | 8.05 | 124.73 | 119.90 |
| 35 | E | 722 | C | O4'-C1'-N1 | 8.05 | 114.64 | 108.20 |
| 35 | E | 720 | U | O4'-C1'-N1 | 8.05 | 114.64 | 108.20 |
| 35 | E | 1577 | G | C5-C6-O6 | -8.05 | 123.77 | 128.60 |
| 35 | E | 2114 | U | C2-N1-C1' | 8.05 | 127.36 | 117.70 |
| 35 | E | 517 | G | C5-C6-O6 | -8.04 | 123.77 | 128.60 |
| 35 | E | 2295 | G | C5-C6-O6 | -8.04 | 123.78 | 128.60 |
| 35 | E | 971 | G | C5-C6-O6 | -8.03 | 123.78 | 128.60 |
| 35 | E | 1957 | C | O4'-C1'-N1 | 8.03 | 114.62 | 108.20 |
| 35 | E | 668 | C | O4'-C1'-N1 | 8.02 | 114.62 | 108.20 |
| 35 | E | 470 | G | C5-C6-O6 | -8.02 | 123.79 | 128.60 |
| 35 | E | 579 | C | O4'-C1'-N1 | 8.02 | 114.61 | 108.20 |
| 35 | E | 409 | G | C5-C6-O6 | -8.01 | 123.79 | 128.60 |
| 35 | E | 1236 | G | O4'-C1'-N9 | 8.01 | 114.61 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1325 | C | O4'-C1'-N1 | 8.01 | 114.61 | 108.20 |
| 35 | E | 2157 | C | O4'-C1'-N1 | 8.01 | 114.61 | 108.20 |
| 35 | E | 1777 | G | C5-C6-O6 | -8.01 | 123.80 | 128.60 |
| 35 | E | 2125 | C | O4'-C1'-N1 | 8.01 | 114.61 | 108.20 |
| 35 | E | 2208 | G | C5-C6-O6 | -8.01 | 123.80 | 128.60 |
| 35 | E | 1851 | C | O4'-C1'-N1 | 8.01 | 114.60 | 108.20 |
| 35 | E | 208 | G | C5-C6-O6 | -8.00 | 123.80 | 128.60 |
| 35 | E | 376 | C | O4'-C1'-N1 | 8.00 | 114.60 | 108.20 |
| 35 | E | 217 | C | O4'-C1'-N1 | 8.00 | 114.60 | 108.20 |
| 35 | E | 2236 | C | O4'-C1'-N1 | 7.99 | 114.59 | 108.20 |
| 35 | E | 332 | C | O4'-C1'-N1 | 7.99 | 114.59 | 108.20 |
| 35 | E | 907 | G | C5-C6-O6 | -7.99 | 123.81 | 128.60 |
| 35 | E | 240 | G | C5-C6-O6 | -7.98 | 123.81 | 128.60 |
| 35 | E | 2158 | C | O4'-C1'-N1 | 7.97 | 114.58 | 108.20 |
| 35 | E | 1263 | G | C5-C6-O6 | -7.96 | 123.82 | 128.60 |
| 35 | E | 1289 | G | C5-C6-O6 | -7.96 | 123.82 | 128.60 |
| 35 | E | 1828 | G | N1-C6-O6 | 7.96 | 124.68 | 119.90 |
| 35 | E | 1911 | U | O4'-C1'-N1 | 7.96 | 114.57 | 108.20 |
| 35 | E | 477 | G | C5-C6-O6 | -7.96 | 123.82 | 128.60 |
| 35 | E | 746 | A | C5-C6-N1 | -7.96 | 113.72 | 117.70 |
| 35 | E | 162 | A | C4-C5-C6 | 7.96 | 120.98 | 117.00 |
| 35 | E | 2244 | C | O4'-C1'-N1 | 7.96 | 114.56 | 108.20 |
| 35 | E | 1809 | C | O4'-C1'-N1 | 7.95 | 114.56 | 108.20 |
| 35 | E | 619 | C | O4'-C1'-N1 | 7.95 | 114.56 | 108.20 |
| 35 | E | 563 | U | O4'-C1'-N1 | 7.94 | 114.55 | 108.20 |
| 35 | E | 1216 | G | C5-C6-O6 | -7.94 | 123.83 | 128.60 |
| 35 | E | 2149 | C | O4'-C1'-N1 | 7.94 | 114.55 | 108.20 |
| 35 | E | 370 | G | C5-C6-O6 | -7.94 | 123.84 | 128.60 |
| 35 | E | 364 | G | C5-C6-O6 | -7.93 | 123.84 | 128.60 |
| 35 | E | 473 | G | C5-C6-O6 | -7.93 | 123.84 | 128.60 |
| 35 | E | 2205 | G | C5-C6-O6 | -7.93 | 123.84 | 128.60 |
| 35 | E | 1282 | C | O4'-C1'-N1 | 7.93 | 114.54 | 108.20 |
| 35 | E | 167 | A | O4'-C1'-N9 | 7.92 | 114.54 | 108.20 |
| 35 | E | 410 | G | C5-C6-O6 | -7.92 | 123.85 | 128.60 |
| 35 | E | 1373 | C | O4'-C1'-N1 | 7.92 | 114.54 | 108.20 |
| 35 | E | 723 | C | O4'-C1'-N1 | 7.92 | 114.54 | 108.20 |
| 35 | E | 42 | G | C5-C6-O6 | -7.92 | 123.85 | 128.60 |
| 35 | E | 678 | G | C5-C6-O6 | -7.92 | 123.85 | 128.60 |
| 35 | E | 387 | C | O4'-C1'-N1 | 7.91 | 114.53 | 108.20 |
| 35 | E | 199 | G | C5-C6-O6 | -7.91 | 123.85 | 128.60 |
| 35 | E | 1638 | G | N1-C6-O6 | 7.91 | 124.65 | 119.90 |
| 35 | E | 1846 | C | O4'-C1'-N1 | 7.91 | 114.53 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 921 | G | P-O3'-C3' | 7.91 | 129.19 | 119.70 |
| 35 | E | 756 | G | C5-C6-O6 | -7.90 | 123.86 | 128.60 |
| 35 | E | 1872 | G | N1-C6-O6 | 7.90 | 124.64 | 119.90 |
| 35 | E | 1727 | C | O4'-C1'-N1 | 7.90 | 114.52 | 108.20 |
| 35 | E | 1786 | G | C5-C6-O6 | -7.90 | 123.86 | 128.60 |
| 35 | E | 542 | C | O4'-C1'-N1 | 7.89 | 114.52 | 108.20 |
| 35 | E | 347 | G | C5-C6-O6 | -7.89 | 123.86 | 128.60 |
| 35 | E | 2184 | U | O4'-C1'-N1 | 7.89 | 114.51 | 108.20 |
| 35 | E | 322 | G | C5-C6-O6 | -7.89 | 123.86 | 128.60 |
| 35 | E | 855 | G | C5-C6-O6 | -7.89 | 123.87 | 128.60 |
| 35 | E | 2060 | C | O4'-C1'-N1 | 7.89 | 114.51 | 108.20 |
| 35 | E | 131 | C | O4'-C1'-N1 | 7.88 | 114.51 | 108.20 |
| 35 | E | 566 | G | C5-C6-O6 | -7.88 | 123.87 | 128.60 |
| 35 | E | 1775 | U | O4'-C1'-N1 | 7.88 | 114.50 | 108.20 |
| 35 | E | 403 | G | C5-C6-O6 | -7.88 | 123.87 | 128.60 |
| 35 | E | 489 | C | O4'-C1'-N1 | 7.88 | 114.50 | 108.20 |
| 35 | E | 1634 | C | N3-C4-N4 | 7.88 | 123.51 | 118.00 |
| 35 | E | 260 | A | C5-C6-N1 | -7.87 | 113.77 | 117.70 |
| 35 | E | 2241 | G | C5-C6-O6 | -7.87 | 123.88 | 128.60 |
| 35 | E | 988 | U | O4'-C1'-N1 | 7.87 | 114.49 | 108.20 |
| 35 | E | 2141 | G | C5-C6-O6 | -7.87 | 123.88 | 128.60 |
| 35 | E | 384 | G | N1-C6-O6 | 7.86 | 124.62 | 119.90 |
| 35 | E | 382 | G | N1-C6-O6 | 7.86 | 124.61 | 119.90 |
| 35 | E | 355 | G | C5-C6-O6 | -7.86 | 123.89 | 128.60 |
| 35 | E | 757 | G | C5-C6-O6 | -7.86 | 123.89 | 128.60 |
| 35 | E | 1082 | U | P-O5'-C5' | 7.86 | 133.47 | 120.90 |
| 35 | E | 568 | G | C5-C6-O6 | -7.85 | 123.89 | 128.60 |
| 35 | E | 2270 | C | O4'-C1'-N1 | 7.85 | 114.48 | 108.20 |
| 32 | o | 70 | TYR | CB-CG-CD1 | -7.85 | 116.29 | 121.00 |
| 35 | E | 623 | C | O4'-C1'-N1 | 7.85 | 114.48 | 108.20 |
| 35 | E | 217 | C | C5'-C4'-C3' | 7.85 | 128.56 | 116.00 |
| 35 | E | 236 | C | O4'-C1'-N1 | 7.85 | 114.48 | 108.20 |
| 35 | E | 1251 | C | O4'-C1'-N1 | 7.85 | 114.48 | 108.20 |
| 35 | E | 1980 | C | O4'-C1'-N1 | 7.84 | 114.48 | 108.20 |
| 35 | E | 233 | G | C5-C6-O6 | -7.84 | 123.89 | 128.60 |
| 35 | E | 1683 | C | O4'-C1'-N1 | 7.84 | 114.47 | 108.20 |
| 35 | E | 1272 | C | O4'-C1'-N1 | 7.83 | 114.47 | 108.20 |
| 35 | E | 1645 | C | O4'-C1'-N1 | 7.83 | 114.47 | 108.20 |
| 35 | E | 2211 | C | O4'-C1'-N1 | 7.83 | 114.47 | 108.20 |
| 35 | E | 77 | C | O4'-C1'-N1 | 7.83 | 114.46 | 108.20 |
| 35 | E | 203 | C | O4'-C1'-N1 | 7.83 | 114.46 | 108.20 |
| 35 | E | 2137 | C | O4'-C1'-N1 | 7.83 | 114.46 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 2225 | C | O4'-C1'-N1 | 7.83 | 114.46 | 108.20 |
| 35 | E | 207 | G | C5-C6-O6 | -7.83 | 123.91 | 128.60 |
| 35 | E | 1335 | U | O4'-C1'-N1 | 7.83 | 114.46 | 108.20 |
| 35 | E | 1899 | C | O4'-C1'-N1 | 7.83 | 114.46 | 108.20 |
| 35 | E | 1971 | C | O4'-C1'-N1 | 7.82 | 114.46 | 108.20 |
| 35 | E | 158 | C | O4'-C1'-N1 | 7.82 | 114.46 | 108.20 |
| 35 | E | 1332 | G | C5-C6-O6 | -7.81 | 123.91 | 128.60 |
| 35 | E | 1569 | G | C5-C6-O6 | -7.81 | 123.91 | 128.60 |
| 35 | E | 2044 | G | C5-C6-O6 | -7.81 | 123.91 | 128.60 |
| 35 | E | 615 | G | C5-C6-O6 | -7.81 | 123.91 | 128.60 |
| 35 | E | 38 | C | O4'-C1'-N1 | 7.81 | 114.44 | 108.20 |
| 35 | E | 321 | G | C5-C6-O6 | -7.81 | 123.92 | 128.60 |
| 35 | E | 110 | U | O4'-C1'-N1 | 7.80 | 114.44 | 108.20 |
| 35 | E | 1181 | C | O4'-C1'-N1 | 7.80 | 114.44 | 108.20 |
| 35 | E | 1880 | U | C4'-C3'-C2' | -7.80 | 94.80 | 102.60 |
| 35 | E | 1855 | G | C5-C6-O6 | -7.80 | 123.92 | 128.60 |
| 35 | E | 358 | C | O4'-C1'-N1 | 7.80 | 114.44 | 108.20 |
| 35 | E | 221 | C | O4'-C1'-N1 | 7.79 | 114.44 | 108.20 |
| 35 | E | 282 | C | O4'-C1'-N1 | 7.79 | 114.43 | 108.20 |
| 35 | E | 955 | U | O4'-C1'-N1 | 7.79 | 114.43 | 108.20 |
| 35 | E | 72 | C | O4'-C1'-N1 | 7.79 | 114.43 | 108.20 |
| 35 | E | 560 | C | O4'-C1'-N1 | 7.79 | 114.43 | 108.20 |
| 35 | E | 885 | U | O4'-C1'-N1 | 7.79 | 114.43 | 108.20 |
| 35 | E | 725 | U | O4'-C1'-N1 | 7.78 | 114.42 | 108.20 |
| 35 | E | 2313 | U | O4'-C1'-N1 | 7.78 | 114.42 | 108.20 |
| 35 | E | 1291 | U | O4'-C1'-N1 | 7.78 | 114.42 | 108.20 |
| 35 | E | 2066 | C | O4'-C1'-N1 | 7.78 | 114.42 | 108.20 |
| 35 | E | 2189 | A | C4-C5-C6 | 7.78 | 120.89 | 117.00 |
| 35 | E | 2304 | G | C5-C6-O6 | -7.77 | 123.94 | 128.60 |
| 35 | E | 235 | C | O4'-C1'-N1 | 7.77 | 114.42 | 108.20 |
| 35 | E | 953 | G | C5-C6-O6 | -7.77 | 123.94 | 128.60 |
| 35 | E | 1320 | G | C5-C6-O6 | -7.77 | 123.94 | 128.60 |
| 35 | E | 482 | C | O4'-C1'-N1 | 7.76 | 114.41 | 108.20 |
| 35 | E | 1763 | G | C5-C6-O6 | -7.76 | 123.94 | 128.60 |
| 35 | E | 495 | G | C5-C6-O6 | -7.76 | 123.95 | 128.60 |
| 35 | E | 840 | C | O4'-C1'-N1 | 7.76 | 114.41 | 108.20 |
| 35 | E | 152 | A | N1-C6-N6 | 7.75 | 123.25 | 118.60 |
| 35 | E | 578 | C | O4'-C1'-N1 | 7.75 | 114.40 | 108.20 |
| 35 | E | 1889 | U | O4'-C1'-N1 | 7.75 | 114.40 | 108.20 |
| 35 | E | 1191 | G | N1-C6-O6 | 7.75 | 124.55 | 119.90 |
| 35 | E | 103 | U | O4'-C1'-N1 | 7.75 | 114.40 | 108.20 |
| 35 | E | 651 | G | C5-C6-O6 | -7.75 | 123.95 | 128.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 828 | G | P-O3'-C3' | 7.75 | 129.00 | 119.70 |
| 35 | E | 2156 | G | C5-C6-O6 | -7.75 | 123.95 | 128.60 |
| 35 | E | 2255 | C | O4'-C1'-N1 | 7.75 | 114.40 | 108.20 |
| 35 | E | 546 | U | O4'-C1'-N1 | 7.74 | 114.39 | 108.20 |
| 35 | E | 1166 | C | O4'-C1'-N1 | 7.74 | 114.39 | 108.20 |
| 35 | E | 1832 | A | P-O3'-C3' | 7.74 | 128.99 | 119.70 |
| 35 | E | 2247 | C | O4'-C1'-N1 | 7.74 | 114.39 | 108.20 |
| 35 | E | 147 | G | C5-C6-O6 | -7.74 | 123.96 | 128.60 |
| 35 | E | 452 | C | O4'-C1'-N1 | 7.74 | 114.39 | 108.20 |
| 35 | E | 683 | U | O4'-C1'-N1 | 7.74 | 114.39 | 108.20 |
| 35 | E | 825 | C | O4'-C1'-N1 | 7.74 | 114.39 | 108.20 |
| 35 | E | 1852 | G | C5-C6-O6 | -7.73 | 123.96 | 128.60 |
| 35 | E | 344 | G | C5-C6-O6 | -7.73 | 123.96 | 128.60 |
| 34 | h | 181 | TYR | CB-CG-CD2 | -7.73 | 116.36 | 121.00 |
| 35 | E | 2258 | C | O4'-C1'-N1 | 7.73 | 114.38 | 108.20 |
| 35 | E | 139 | G | C5-C6-O6 | -7.72 | 123.97 | 128.60 |
| 35 | E | 1563 | G | C5-C6-O6 | -7.72 | 123.97 | 128.60 |
| 35 | E | 2052 | C | O4'-C1'-N1 | 7.72 | 114.38 | 108.20 |
| 35 | E | 120 | C | O4'-C1'-N1 | 7.72 | 114.38 | 108.20 |
| 35 | E | 1686 | G | N1-C6-O6 | 7.72 | 124.53 | 119.90 |
| 35 | E | 2277 | C | O4'-C1'-N1 | 7.72 | 114.37 | 108.20 |
| 35 | E | 2102 | C | O4'-C1'-N1 | 7.71 | 114.37 | 108.20 |
| 35 | E | 650 | C | O4'-C1'-N1 | 7.71 | 114.37 | 108.20 |
| 35 | E | 547 | G | C5-C6-O6 | -7.71 | 123.97 | 128.60 |
| 35 | E | 1905 | U | O4'-C1'-N1 | 7.71 | 114.37 | 108.20 |
| 35 | E | 744 | C | O4'-C1'-N1 | 7.71 | 114.36 | 108.20 |
| 35 | E | 1886 | G | C5-C6-O6 | -7.71 | 123.98 | 128.60 |
| 35 | E | 365 | C | O4'-C1'-N1 | 7.71 | 114.36 | 108.20 |
| 35 | E | 87 | C | O4'-C1'-N1 | 7.70 | 114.36 | 108.20 |
| 35 | E | 176 | C | O4'-C1'-N1 | 7.70 | 114.36 | 108.20 |
| 35 | E | 153 | C | O4'-C1'-N1 | 7.70 | 114.36 | 108.20 |
| 35 | E | 218 | C | O4'-C1'-N1 | 7.70 | 114.36 | 108.20 |
| 35 | E | 333 | C | O4'-C1'-N1 | 7.69 | 114.35 | 108.20 |
| 35 | E | 2078 | C | O4'-C1'-N1 | 7.69 | 114.35 | 108.20 |
| 35 | E | 2310 | G | C5-C6-O6 | -7.69 | 123.99 | 128.60 |
| 35 | E | 513 | G | C5-C6-O6 | -7.69 | 123.99 | 128.60 |
| 35 | E | 681 | C | O4'-C1'-N1 | 7.69 | 114.35 | 108.20 |
| 35 | E | 413 | G | C5-C6-O6 | -7.68 | 123.99 | 128.60 |
| 35 | E | 853 | C | O4'-C1'-N1 | 7.68 | 114.35 | 108.20 |
| 35 | E | 1315 | G | C5-C6-O6 | -7.68 | 123.99 | 128.60 |
| 35 | E | 997 | G | O4'-C1'-N9 | 7.68 | 114.34 | 108.20 |
| 35 | E | 1974 | C | O4'-C1'-N1 | 7.68 | 114.35 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 197 | C | O4'-C1'-N1 | 7.68 | 114.34 | 108.20 |
| 35 | E | 1863 | C | O4'-C1'-N1 | 7.68 | 114.34 | 108.20 |
| 35 | E | 49 | C | O4'-C1'-N1 | 7.68 | 114.34 | 108.20 |
| 35 | E | 1073 | U | O4'-C1'-N1 | 7.67 | 114.34 | 108.20 |
| 35 | E | 1956 | C | O4'-C1'-N1 | 7.67 | 114.34 | 108.20 |
| 35 | E | 1327 | A | C4-C5-C6 | 7.67 | 120.84 | 117.00 |
| 35 | E | 1616 | C | O4'-C1'-N1 | 7.67 | 114.34 | 108.20 |
| 35 | E | 41 | G | C5-C6-O6 | -7.67 | 124.00 | 128.60 |
| 35 | E | 59 | C | O4'-C1'-N1 | 7.67 | 114.33 | 108.20 |
| 35 | E | 2292 | G | C5-C6-O6 | -7.67 | 124.00 | 128.60 |
| 35 | E | 1871 | G | C5-C6-O6 | -7.67 | 124.00 | 128.60 |
| 35 | E | 76 | G | C5-C6-O6 | -7.66 | 124.00 | 128.60 |
| 35 | E | 580 | C | O4'-C1'-N1 | 7.66 | 114.33 | 108.20 |
| 35 | E | 1228 | G | C5-C6-O6 | -7.66 | 124.00 | 128.60 |
| 35 | E | 1271 | G | N1-C6-O6 | 7.66 | 124.49 | 119.90 |
| 35 | E | 2173 | C | O4'-C1'-N1 | 7.65 | 114.32 | 108.20 |
| 35 | E | 1369 | C | O4'-C1'-N1 | 7.65 | 114.32 | 108.20 |
| 35 | E | 1862 | C | O4'-C1'-N1 | 7.65 | 114.32 | 108.20 |
| 35 | E | 2000 | C | O4'-C1'-N1 | 7.64 | 114.31 | 108.20 |
| 35 | E | 925 | C | O4'-C1'-N1 | 7.64 | 114.31 | 108.20 |
| 35 | E | 605 | G | C5-C6-O6 | -7.64 | 124.02 | 128.60 |
| 35 | E | 1916 | C | O4'-C1'-N1 | 7.64 | 114.31 | 108.20 |
| 35 | E | 2127 | G | C5-C6-O6 | -7.64 | 124.02 | 128.60 |
| 35 | E | 2195 | G | C5-C6-O6 | -7.64 | 124.02 | 128.60 |
| 35 | E | 1319 | G | C5-C6-O6 | -7.64 | 124.02 | 128.60 |
| 35 | E | 1897 | U | O4'-C1'-N1 | 7.64 | 114.31 | 108.20 |
| 35 | E | 2228 | C | O4'-C1'-N1 | 7.64 | 114.31 | 108.20 |
| 35 | E | 94 | C | O4'-C1'-N1 | 7.63 | 114.31 | 108.20 |
| 35 | E | 279 | A | C5-C6-N6 | -7.63 | 117.59 | 123.70 |
| 35 | E | 1354 | C | O4'-C1'-N1 | 7.63 | 114.31 | 108.20 |
| 35 | E | 244 | G | C5-C6-O6 | -7.63 | 124.02 | 128.60 |
| 35 | E | 357 | C | O4'-C1'-N1 | 7.63 | 114.30 | 108.20 |
| 35 | E | 986 | U | O4'-C1'-N1 | 7.63 | 114.30 | 108.20 |
| 35 | E | 1748 | C | O4'-C1'-N1 | 7.62 | 114.30 | 108.20 |
| 35 | E | 611 | G | C5-C6-O6 | -7.62 | 124.03 | 128.60 |
| 35 | E | 12 | U | O4'-C1'-N1 | 7.62 | 114.30 | 108.20 |
| 35 | E | 390 | C | O4'-C1'-N1 | 7.62 | 114.30 | 108.20 |
| 35 | E | 292 | U | O4'-C1'-N1 | 7.62 | 114.30 | 108.20 |
| 35 | E | 408 | C | O4'-C1'-N1 | 7.62 | 114.30 | 108.20 |
| 35 | E | 481 | G | C5-C6-O6 | -7.62 | 124.03 | 128.60 |
| 35 | E | 1288 | G | C5-C6-O6 | -7.62 | 124.03 | 128.60 |
| 35 | E | 1948 | G | N1-C6-O6 | 7.62 | 124.47 | 119.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 2172 | G | C5-C6-O6 | -7.62 | 124.03 | 128.60 |
| 35 | E | 441 | C | O4'-C1'-N1 | 7.62 | 114.29 | 108.20 |
| 35 | E | 303 | C | O4'-C1'-N1 | 7.61 | 114.29 | 108.20 |
| 35 | E | 228 | G | C5-C6-O6 | -7.61 | 124.04 | 128.60 |
| 35 | E | 1712 | U | O4'-C1'-N1 | 7.61 | 114.28 | 108.20 |
| 35 | E | 317 | G | C5-C6-O6 | -7.60 | 124.04 | 128.60 |
| 35 | E | 995 | C | O4'-C1'-N1 | 7.60 | 114.28 | 108.20 |
| 35 | E | 1324 | U | O4'-C1'-N1 | 7.60 | 114.28 | 108.20 |
| 35 | E | 1976 | C | O4'-C1'-N1 | 7.60 | 114.28 | 108.20 |
| 35 | E | 1940 | G | C5-C6-O6 | -7.60 | 124.04 | 128.60 |
| 35 | E | 933 | C | O4'-C1'-N1 | 7.60 | 114.28 | 108.20 |
| 35 | E | 1349 | G | C5-C6-O6 | -7.60 | 124.04 | 128.60 |
| 35 | E | 18 | C | O4'-C1'-N1 | 7.60 | 114.28 | 108.20 |
| 35 | E | 1543 | C | N3-C4-N4 | 7.60 | 123.32 | 118.00 |
| 35 | E | 2013 | U | O4'-C1'-N1 | 7.59 | 114.28 | 108.20 |
| 35 | E | 213 | G | N3-C2-N2 | 7.59 | 125.21 | 119.90 |
| 35 | E | 1918 | C | O4'-C1'-N1 | 7.59 | 114.27 | 108.20 |
| 35 | E | 89 | C | O4'-C1'-N1 | 7.59 | 114.27 | 108.20 |
| 35 | E | 490 | C | O4'-C1'-N1 | 7.59 | 114.27 | 108.20 |
| 35 | E | 1634 | C | O4'-C1'-N1 | 7.59 | 114.27 | 108.20 |
| 35 | E | 1666 | G | C5-C6-O6 | -7.59 | 124.05 | 128.60 |
| 35 | E | 313 | G | C5-C6-O6 | -7.58 | 124.05 | 128.60 |
| 35 | E | 1705 | G | C5-C6-O6 | -7.58 | 124.05 | 128.60 |
| 35 | E | 1703 | C | O4'-C1'-N1 | 7.58 | 114.27 | 108.20 |
| 35 | E | 455 | C | O4'-C1'-N1 | 7.58 | 114.26 | 108.20 |
| 35 | E | 869 | G | C5-C6-O6 | -7.58 | 124.06 | 128.60 |
| 35 | E | 1562 | G | C5-C6-O6 | -7.58 | 124.06 | 128.60 |
| 35 | E | 1310 | C | O4'-C1'-N1 | 7.57 | 114.26 | 108.20 |
| 35 | E | 1944 | G | C5-C6-O6 | -7.57 | 124.06 | 128.60 |
| 35 | E | 2187 | C | O4'-C1'-N1 | 7.57 | 114.26 | 108.20 |
| 35 | E | 537 | C | O4'-C1'-N1 | 7.57 | 114.26 | 108.20 |
| 35 | E | 2140 | U | O4'-C1'-N1 | 7.57 | 114.26 | 108.20 |
| 35 | E | 182 | C | O4'-C1'-N1 | 7.57 | 114.25 | 108.20 |
| 35 | E | 1756 | G | C5-C6-O6 | -7.56 | 124.06 | 128.60 |
| 35 | E | 1188 | C | N3-C4-N4 | 7.55 | 123.29 | 118.00 |
| 35 | E | 1530 | C | O4'-C1'-N1 | 7.55 | 114.24 | 108.20 |
| 35 | E | 2190 | U | O4'-C1'-N1 | 7.55 | 114.24 | 108.20 |
| 35 | E | 1254 | C | O4'-C1'-N1 | 7.55 | 114.24 | 108.20 |
| 35 | E | 1648 | U | O4'-C1'-N1 | 7.55 | 114.24 | 108.20 |
| 35 | E | 166 | C | O4'-C1'-N1 | 7.55 | 114.24 | 108.20 |
| 35 | E | 206 | C | O4'-C1'-N1 | 7.55 | 114.24 | 108.20 |
| 35 | E | 664 | G | C5-C6-O6 | -7.55 | 124.07 | 128.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 841 | C | O4'-C1'-N1 | 7.55 | 114.24 | 108.20 |
| 35 | E | 1283 | U | O4'-C1'-N1 | 7.55 | 114.24 | 108.20 |
| 35 | E | 2108 | G | C5-C6-O6 | -7.55 | 124.07 | 128.60 |
| 35 | E | 2058 | C | O4'-C1'-N1 | 7.54 | 114.24 | 108.20 |
| 35 | E | 274 | C | O4'-C1'-N1 | 7.54 | 114.23 | 108.20 |
| 35 | E | 2285 | G | C5-C6-O6 | -7.54 | 124.07 | 128.60 |
| 35 | E | 836 | G | C5-C6-O6 | -7.54 | 124.08 | 128.60 |
| 35 | E | 1974 | C | C2-N1-C1' | 7.54 | 127.10 | 118.80 |
| 35 | E | 842 | G | C5-C6-O6 | -7.54 | 124.08 | 128.60 |
| 35 | E | 117 | C | O4'-C1'-N1 | 7.54 | 114.23 | 108.20 |
| 35 | E | 1880 | U | P-O3'-C3' | 7.54 | 128.74 | 119.70 |
| 35 | E | 130 | G | C5-C6-O6 | -7.53 | 124.08 | 128.60 |
| 35 | E | 415 | U | O4'-C1'-N1 | 7.53 | 114.22 | 108.20 |
| 35 | E | 1623 | G | C5-C6-O6 | -7.53 | 124.08 | 128.60 |
| 35 | E | 239 | C | O4'-C1'-N1 | 7.53 | 114.22 | 108.20 |
| 35 | E | 1747 | C | O4'-C1'-N1 | 7.53 | 114.22 | 108.20 |
| 35 | E | 1223 | C | O4'-C1'-N1 | 7.52 | 114.22 | 108.20 |
| 35 | E | 1269 | C | O4'-C1'-N1 | 7.52 | 114.22 | 108.20 |
| 35 | E | 1571 | C | O4'-C1'-N1 | 7.52 | 114.22 | 108.20 |
| 35 | E | 2154 | C | O4'-C1'-N1 | 7.52 | 114.22 | 108.20 |
| 35 | E | 759 | C | C6-N1-C2 | -7.51 | 117.30 | 120.30 |
| 35 | E | 1908 | U | O4'-C1'-N1 | 7.51 | 114.21 | 108.20 |
| 35 | E | 1950 | G | C5-C6-O6 | -7.51 | 124.09 | 128.60 |
| 34 | h | 181 | TYR | CB-CG-CD1 | 7.51 | 125.51 | 121.00 |
| 35 | E | 662 | C | O4'-C1'-N1 | 7.51 | 114.21 | 108.20 |
| 35 | E | 1639 | A | C5-C6-N6 | -7.51 | 117.69 | 123.70 |
| 35 | E | 54 | C | O4'-C1'-N1 | 7.51 | 114.21 | 108.20 |
| 35 | E | 109 | G | C5-C6-O6 | -7.51 | 124.09 | 128.60 |
| 35 | E | 751 | C | O4'-C1'-N1 | 7.51 | 114.21 | 108.20 |
| 35 | E | 1867 | G | O4'-C1'-N9 | 7.51 | 114.21 | 108.20 |
| 35 | E | 5 | U | O4'-C1'-N1 | 7.50 | 114.20 | 108.20 |
| 35 | E | 1739 | G | C5-C6-O6 | -7.50 | 124.10 | 128.60 |
| 35 | E | 58 | C | O4'-C1'-N1 | 7.50 | 114.20 | 108.20 |
| 35 | E | 439 | G | C5-C6-O6 | -7.50 | 124.10 | 128.60 |
| 35 | E | 1758 | C | O4'-C1'-N1 | 7.50 | 114.20 | 108.20 |
| 35 | E | 1213 | G | C5-C6-O6 | -7.50 | 124.10 | 128.60 |
| 35 | E | 956 | U | O4'-C1'-N1 | 7.50 | 114.20 | 108.20 |
| 35 | E | 656 | U | O4'-C1'-N1 | 7.50 | 114.20 | 108.20 |
| 35 | E | 2100 | C | O4'-C1'-N1 | 7.50 | 114.20 | 108.20 |
| 35 | E | 435 | G | C5-C6-O6 | -7.49 | 124.10 | 128.60 |
| 35 | E | 458 | C | O4'-C1'-N1 | 7.49 | 114.19 | 108.20 |
| 35 | E | 265 | C | O4'-C1'-N1 | 7.49 | 114.19 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1932 | G | C5-C6-O6 | -7.49 | 124.11 | 128.60 |
| 35 | E | 2133 | C | O4'-C1'-N1 | 7.49 | 114.19 | 108.20 |
| 35 | E | 670 | G | C5-C6-O6 | -7.49 | 124.11 | 128.60 |
| 35 | E | 1593 | A | C4-C5-C6 | 7.49 | 120.74 | 117.00 |
| 35 | E | 1697 | G | C5-C6-O6 | -7.49 | 124.11 | 128.60 |
| 35 | E | 396 | C | O4'-C1'-N1 | 7.48 | 114.19 | 108.20 |
| 35 | E | 2182 | G | C5-C6-O6 | -7.48 | 124.11 | 128.60 |
| 35 | E | 818 | U | O4'-C1'-N1 | 7.48 | 114.18 | 108.20 |
| 35 | E | 787 | C | O4'-C1'-N1 | 7.48 | 114.18 | 108.20 |
| 35 | E | 2150 | G | C5-C6-O6 | -7.47 | 124.11 | 128.60 |
| 35 | E | 259 | C | N3-C4-C5 | -7.47 | 118.91 | 121.90 |
| 35 | E | 451 | G | C5-C6-O6 | -7.47 | 124.12 | 128.60 |
| 35 | E | 1557 | U | O4'-C1'-N1 | 7.47 | 114.18 | 108.20 |
| 35 | E | 1867 | G | C5-C6-O6 | -7.47 | 124.12 | 128.60 |
| 32 | o | 70 | TYR | CB-CG-CD2 | 7.47 | 125.48 | 121.00 |
| 35 | E | 1602 | C | O4'-C1'-N1 | 7.47 | 114.17 | 108.20 |
| 35 | E | 1744 | U | O4'-C1'-N1 | 7.46 | 114.17 | 108.20 |
| 35 | E | 628 | G | C5-C6-O6 | -7.46 | 124.12 | 128.60 |
| 35 | E | 2087 | C | O4'-C1'-N1 | 7.46 | 114.17 | 108.20 |
| 35 | E | 928 | C | O4'-C1'-N1 | 7.46 | 114.17 | 108.20 |
| 35 | E | 175 | A | C5-C6-N6 | -7.46 | 117.73 | 123.70 |
| 35 | E | 1188 | C | P-O3'-C3' | 7.46 | 128.65 | 119.70 |
| 35 | E | 1922 | G | C5-C6-O6 | -7.46 | 124.13 | 128.60 |
| 35 | E | 1329 | G | C5-C6-O6 | -7.46 | 124.13 | 128.60 |
| 35 | E | 627 | C | O4'-C1'-N1 | 7.45 | 114.16 | 108.20 |
| 35 | E | 2131 | A | O4'-C1'-N9 | 7.45 | 114.16 | 108.20 |
| 35 | E | 2242 | U | O4'-C1'-N1 | 7.45 | 114.16 | 108.20 |
| 35 | E | 1179 | C | O4'-C1'-N1 | 7.45 | 114.16 | 108.20 |
| 35 | E | 66 | U | O4'-C1'-N1 | 7.45 | 114.16 | 108.20 |
| 35 | E | 890 | C | O4'-C1'-N1 | 7.44 | 114.15 | 108.20 |
| 35 | E | 1656 | G | C5-C6-O6 | -7.44 | 124.14 | 128.60 |
| 35 | E | 1372 | C | O4'-C1'-N1 | 7.44 | 114.15 | 108.20 |
| 35 | E | 1382 | G | C5-C6-O6 | -7.43 | 124.14 | 128.60 |
| 35 | E | 118 | C | O4'-C1'-N1 | 7.43 | 114.15 | 108.20 |
| 35 | E | 209 | C | O4'-C1'-N1 | 7.43 | 114.14 | 108.20 |
| 35 | E | 212 | G | C5-C6-O6 | -7.43 | 124.14 | 128.60 |
| 35 | E | 375 | C | O4'-C1'-N1 | 7.43 | 114.14 | 108.20 |
| 35 | E | 706 | G | C5-C6-O6 | -7.43 | 124.14 | 128.60 |
| 35 | E | 726 | C | P-O3'-C3' | 7.43 | 128.61 | 119.70 |
| 35 | E | 722 | C | N3-C4-C5 | -7.42 | 118.93 | 121.90 |
| 35 | E | 802 | U | O4'-C1'-N1 | 7.42 | 114.14 | 108.20 |
| 35 | E | 1655 | U | O4'-C1'-N1 | 7.42 | 114.14 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 2183 | U | O4'-C1'-N1 | 7.42 | 114.14 | 108.20 |
| 35 | E | 93 | G | C5-C6-O6 | -7.42 | 124.15 | 128.60 |
| 35 | E | 749 | C | O4'-C1'-N1 | 7.42 | 114.13 | 108.20 |
| 35 | E | 1317 | G | C5-C6-O6 | -7.42 | 124.15 | 128.60 |
| 35 | E | 1823 | G | C5-C6-O6 | -7.42 | 124.15 | 128.60 |
| 35 | E | 969 | U | O4'-C1'-N1 | 7.41 | 114.13 | 108.20 |
| 35 | E | 149 | A | O4'-C1'-N9 | 7.41 | 114.13 | 108.20 |
| 35 | E | 622 | G | C5-C6-O6 | -7.41 | 124.15 | 128.60 |
| 35 | E | 1978 | C | O4'-C1'-N1 | 7.41 | 114.13 | 108.20 |
| 35 | E | 679 | U | O4'-C1'-N1 | 7.41 | 114.13 | 108.20 |
| 35 | E | 366 | C | O4'-C1'-N1 | 7.40 | 114.12 | 108.20 |
| 35 | E | 710 | A | O4'-C1'-N9 | 7.40 | 114.12 | 108.20 |
| 35 | E | 515 | C | O4'-C1'-N1 | 7.40 | 114.12 | 108.20 |
| 35 | E | 1081 | G | O4'-C1'-N9 | 7.40 | 114.12 | 108.20 |
| 35 | E | 1371 | C | O4'-C1'-N1 | 7.40 | 114.12 | 108.20 |
| 35 | E | 1893 | U | O4'-C1'-N1 | 7.40 | 114.12 | 108.20 |
| 35 | E | 2142 | C | O4'-C1'-N1 | 7.40 | 114.12 | 108.20 |
| 35 | E | 1663 | C | O4'-C1'-N1 | 7.39 | 114.11 | 108.20 |
| 35 | E | 2178 | C | O4'-C1'-N1 | 7.39 | 114.12 | 108.20 |
| 35 | E | 2163 | G | C5-C6-O6 | -7.39 | 124.16 | 128.60 |
| 35 | E | 1305 | A | C4-C5-C6 | 7.39 | 120.69 | 117.00 |
| 35 | E | 797 | G | P-O3'-C3' | 7.39 | 128.57 | 119.70 |
| 35 | E | 312 | C | O4'-C1'-N1 | 7.38 | 114.10 | 108.20 |
| 35 | E | 402 | C | O4'-C1'-N1 | 7.38 | 114.10 | 108.20 |
| 35 | E | 433 | G | C5-C6-O6 | -7.38 | 124.17 | 128.60 |
| 35 | E | 1260 | G | C5-C6-O6 | -7.38 | 124.17 | 128.60 |
| 35 | E | 1687 | A | O4'-C1'-N9 | 7.38 | 114.10 | 108.20 |
| 35 | E | 1736 | G | C5-C6-O6 | -7.38 | 124.17 | 128.60 |
| 35 | E | 2256 | U | O4'-C1'-N1 | 7.37 | 114.10 | 108.20 |
| 35 | E | 469 | G | C5-C6-O6 | -7.37 | 124.18 | 128.60 |
| 35 | E | 1352 | C | O4'-C1'-N1 | 7.37 | 114.10 | 108.20 |
| 35 | E | 378 | U | O4'-C1'-N1 | 7.37 | 114.09 | 108.20 |
| 35 | E | 1785 | C | O4'-C1'-N1 | 7.37 | 114.09 | 108.20 |
| 35 | E | 2020 | G | O4'-C1'-N9 | 7.37 | 114.10 | 108.20 |
| 35 | E | 15 | U | O4'-C1'-N1 | 7.37 | 114.09 | 108.20 |
| 35 | E | 1088 | A | C5-C6-N6 | -7.37 | 117.81 | 123.70 |
| 35 | E | 1300 | C | C6-N1-C1' | -7.36 | 111.96 | 120.80 |
| 35 | E | 1884 | U | C2-N1-C1' | 7.36 | 126.53 | 117.70 |
| 35 | E | 271 | C | O4'-C1'-N1 | 7.36 | 114.09 | 108.20 |
| 35 | E | 1608 | G | C5-C6-O6 | -7.36 | 124.18 | 128.60 |
| 35 | E | 109 | G | O4'-C1'-N9 | 7.36 | 114.09 | 108.20 |
| 35 | E | 616 | G | C5-C6-O6 | -7.36 | 124.19 | 128.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 2254 | U | O4'-C1'-N1 | 7.36 | 114.09 | 108.20 |
| 35 | E | 2186 | C | O4'-C1'-N1 | 7.36 | 114.08 | 108.20 |
| 35 | E | 626 | C | O4'-C1'-N1 | 7.35 | 114.08 | 108.20 |
| 35 | E | 1690 | G | N1-C6-O6 | 7.35 | 124.31 | 119.90 |
| 35 | E | 758 | U | O4'-C1'-N1 | 7.35 | 114.08 | 108.20 |
| 35 | E | 949 | U | O4'-C1'-N1 | 7.35 | 114.08 | 108.20 |
| 35 | E | 256 | A | C4-C5-C6 | 7.35 | 120.67 | 117.00 |
| 35 | E | 710 | A | C4-C5-C6 | 7.35 | 120.67 | 117.00 |
| 35 | E | 1208 | U | O4'-C1'-N1 | 7.35 | 114.08 | 108.20 |
| 35 | E | 1234 | G | C5-C6-O6 | -7.35 | 124.19 | 128.60 |
| 35 | E | 873 | C | C2-N1-C1' | 7.35 | 126.88 | 118.80 |
| 35 | E | 1084 | G | O4'-C1'-N9 | 7.35 | 114.08 | 108.20 |
| 35 | E | 572 | U | O4'-C1'-N1 | 7.34 | 114.08 | 108.20 |
| 35 | E | 2064 | G | C5-C6-O6 | -7.34 | 124.19 | 128.60 |
| 35 | E | 2203 | C | O4'-C1'-N1 | 7.34 | 114.08 | 108.20 |
| 35 | E | 2230 | C | O4'-C1'-N1 | 7.34 | 114.08 | 108.20 |
| 35 | E | 1997 | G | C5-C6-O6 | -7.34 | 124.19 | 128.60 |
| 35 | E | 2215 | C | O4'-C1'-N1 | 7.34 | 114.07 | 108.20 |
| 35 | E | 1573 | C | O4'-C1'-N1 | 7.34 | 114.07 | 108.20 |
| 35 | E | 709 | C | O4'-C1'-N1 | 7.33 | 114.06 | 108.20 |
| 35 | E | 1762 | G | C5-C6-O6 | -7.33 | 124.20 | 128.60 |
| 35 | E | 669 | U | O4'-C1'-N1 | 7.33 | 114.06 | 108.20 |
| 35 | E | 436 | G | C5-C6-O6 | -7.33 | 124.20 | 128.60 |
| 35 | E | 533 | C | O4'-C1'-N1 | 7.33 | 114.06 | 108.20 |
| 35 | E | 892 | U | O4'-C1'-N1 | 7.33 | 114.06 | 108.20 |
| 35 | E | 1895 | U | O4'-C1'-N1 | 7.33 | 114.06 | 108.20 |
| 35 | E | 2061 | G | C5-C6-O6 | -7.33 | 124.20 | 128.60 |
| 35 | E | 339 | C | O4'-C1'-N1 | 7.32 | 114.06 | 108.20 |
| 35 | E | 1356 | C | O4'-C1'-N1 | 7.32 | 114.06 | 108.20 |
| 35 | E | 146 | U | O4'-C1'-N1 | 7.32 | 114.06 | 108.20 |
| 35 | E | 353 | C | N3-C4-N4 | 7.32 | 123.12 | 118.00 |
| 35 | E | 796 | G | C5-C6-O6 | -7.32 | 124.21 | 128.60 |
| 35 | E | 2196 | U | O4'-C1'-N1 | 7.32 | 114.06 | 108.20 |
| 35 | E | 1845 | C | O4'-C1'-N1 | 7.32 | 114.05 | 108.20 |
| 35 | E | 2261 | U | O4'-C1'-N1 | 7.32 | 114.05 | 108.20 |
| 35 | E | 350 | C | O4'-C1'-N1 | 7.32 | 114.05 | 108.20 |
| 35 | E | 1578 | G | C5-C6-O6 | -7.32 | 124.21 | 128.60 |
| 35 | E | 1816 | G | C5-C6-O6 | -7.32 | 124.21 | 128.60 |
| 35 | E | 1917 | G | C5-C6-O6 | -7.32 | 124.21 | 128.60 |
| 35 | E | 1856 | G | C5-C6-O6 | -7.31 | 124.21 | 128.60 |
| 35 | E | 2104 | A | C4-C5-C6 | 7.31 | 120.66 | 117.00 |
| 35 | E | 2216 | A | O4'-C1'-N9 | 7.31 | 114.05 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 2019 | C | N3-C4-N4 | 7.31 | 123.11 | 118.00 |
| 35 | E | 536 | A | C5-C6-N6 | -7.30 | 117.86 | 123.70 |
| 35 | E | 2023 | C | C6-N1-C1' | -7.30 | 112.04 | 120.80 |
| 35 | E | 2118 | G | C5-C6-O6 | -7.30 | 124.22 | 128.60 |
| 35 | E | 2210 | U | O4'-C1'-N1 | 7.30 | 114.04 | 108.20 |
| 35 | E | 1226 | G | C5-C6-O6 | -7.30 | 124.22 | 128.60 |
| 35 | E | 904 | C | O4'-C1'-N1 | 7.30 | 114.04 | 108.20 |
| 35 | E | 1903 | A | P-O5'-C5' | 7.30 | 132.58 | 120.90 |
| 35 | E | 518 | C | O4'-C1'-N1 | 7.29 | 114.04 | 108.20 |
| 35 | E | 1872 | G | O4'-C1'-N9 | 7.29 | 114.03 | 108.20 |
| 35 | E | 1169 | U | O4'-C1'-N1 | 7.29 | 114.03 | 108.20 |
| 35 | E | 1523 | C | O4'-C1'-N1 | 7.29 | 114.03 | 108.20 |
| 35 | E | 748 | G | C5-C6-O6 | -7.28 | 124.23 | 128.60 |
| 35 | E | 1344 | U | O4'-C1'-N1 | 7.28 | 114.02 | 108.20 |
| 35 | E | 680 | U | O4'-C1'-N1 | 7.28 | 114.02 | 108.20 |
| 35 | E | 1677 | C | O4'-C1'-N1 | 7.28 | 114.02 | 108.20 |
| 35 | E | 1209 | C | O4'-C1'-N1 | 7.28 | 114.02 | 108.20 |
| 35 | E | 1694 | G | C5-C6-O6 | -7.27 | 124.24 | 128.60 |
| 35 | E | 814 | C | C6-N1-C1' | -7.27 | 112.08 | 120.80 |
| 35 | E | 1206 | G | C5-C6-O6 | -7.27 | 124.24 | 128.60 |
| 35 | E | 1341 | C | O4'-C1'-N1 | 7.26 | 114.01 | 108.20 |
| 35 | E | 2257 | U | O4'-C1'-N1 | 7.26 | 114.01 | 108.20 |
| 35 | E | 1723 | G | C5-C6-O6 | -7.26 | 124.24 | 128.60 |
| 35 | E | 1654 | U | O4'-C1'-N1 | 7.26 | 114.01 | 108.20 |
| 35 | E | 878 | G | C5-C6-O6 | -7.26 | 124.25 | 128.60 |
| 35 | E | 2082 | U | O4'-C1'-N1 | 7.26 | 114.01 | 108.20 |
| 35 | E | 1303 | U | O4'-C1'-N1 | 7.25 | 114.00 | 108.20 |
| 35 | E | 421 | U | O4'-C1'-N1 | 7.25 | 114.00 | 108.20 |
| 35 | E | 456 | C | O4'-C1'-N1 | 7.25 | 114.00 | 108.20 |
| 35 | E | 1665 | C | O4'-C1'-N1 | 7.25 | 114.00 | 108.20 |
| 35 | E | 2062 | U | O4'-C1'-N1 | 7.25 | 114.00 | 108.20 |
| 35 | E | 2175 | C | O4'-C1'-N1 | 7.25 | 114.00 | 108.20 |
| 35 | E | 479 | G | C5-C6-O6 | -7.25 | 124.25 | 128.60 |
| 35 | E | 1719 | U | O4'-C1'-N1 | 7.25 | 114.00 | 108.20 |
| 35 | E | 2075 | G | C5-C6-O6 | -7.25 | 124.25 | 128.60 |
| 35 | E | 270 | C | O4'-C1'-N1 | 7.24 | 113.99 | 108.20 |
| 35 | E | 590 | C | O4'-C1'-N1 | 7.24 | 113.99 | 108.20 |
| 35 | E | 1575 | G | C5-C6-O6 | -7.24 | 124.26 | 128.60 |
| 35 | E | 1607 | A | C5-C6-N6 | -7.24 | 117.91 | 123.70 |
| 35 | E | 480 | C | O4'-C1'-N1 | 7.23 | 113.98 | 108.20 |
| 35 | E | 554 | C | N3-C4-N4 | 7.23 | 123.06 | 118.00 |
| 35 | E | 755 | U | O4'-C1'-N1 | 7.23 | 113.99 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 13 | U | O4'-C1'-N1 | 7.23 | 113.98 | 108.20 |
| 35 | E | 850 | U | O4'-C1'-N1 | 7.23 | 113.98 | 108.20 |
| 35 | E | 1083 | G | C5-C6-O6 | -7.23 | 124.26 | 128.60 |
| 35 | E | 2138 | U | O4'-C1'-N1 | 7.23 | 113.98 | 108.20 |
| 35 | E | 1339 | G | O4'-C1'-N9 | 7.22 | 113.98 | 108.20 |
| 35 | E | 1554 | A | C4-C5-C6 | 7.22 | 120.61 | 117.00 |
| 35 | E | 1635 | G | C5-C6-O6 | -7.22 | 124.27 | 128.60 |
| 35 | E | 1768 | A | C4-C5-C6 | 7.22 | 120.61 | 117.00 |
| 35 | E | 1278 | C | O4'-C1'-N1 | 7.22 | 113.98 | 108.20 |
| 35 | E | 1629 | C | O4'-C1'-N1 | 7.22 | 113.97 | 108.20 |
| 35 | E | 649 | G | C5-C6-O6 | -7.21 | 124.27 | 128.60 |
| 35 | E | 734 | G | N1-C2-N3 | -7.21 | 119.57 | 123.90 |
| 35 | E | 1668 | G | C5-C6-O6 | -7.21 | 124.27 | 128.60 |
| 35 | E | 422 | U | O4'-C1'-N1 | 7.21 | 113.97 | 108.20 |
| 35 | E | 654 | U | O4'-C1'-N1 | 7.21 | 113.97 | 108.20 |
| 35 | E | 1381 | G | C5-C6-O6 | -7.21 | 124.28 | 128.60 |
| 35 | E | 2143 | C | O4'-C1'-N1 | 7.21 | 113.97 | 108.20 |
| 35 | E | 346 | C | O4'-C1'-N1 | 7.21 | 113.96 | 108.20 |
| 35 | E | 620 | C | O4'-C1'-N1 | 7.21 | 113.96 | 108.20 |
| 35 | E | 926 | C | O4'-C1'-N1 | 7.20 | 113.96 | 108.20 |
| 35 | E | 1970 | G | O4'-C1'-N9 | 7.20 | 113.96 | 108.20 |
| 35 | E | 2193 | U | O4'-C1'-N1 | 7.20 | 113.96 | 108.20 |
| 35 | E | 1170 | C | O4'-C1'-N1 | 7.20 | 113.96 | 108.20 |
| 35 | E | 1193 | A | C5-C6-N6 | -7.20 | 117.94 | 123.70 |
| 35 | E | 1229 | C | O4'-C1'-N1 | 7.20 | 113.96 | 108.20 |
| 35 | E | 377 | G | C5-C6-O6 | -7.20 | 124.28 | 128.60 |
| 35 | E | 1926 | G | C5-C6-O6 | -7.20 | 124.28 | 128.60 |
| 35 | E | 1284 | U | O4'-C1'-N1 | 7.20 | 113.96 | 108.20 |
| 35 | E | 1072 | G | C5-C6-O6 | -7.20 | 124.28 | 128.60 |
| 35 | E | 1295 | U | O4'-C1'-N1 | 7.19 | 113.95 | 108.20 |
| 35 | E | 1721 | U | O4'-C1'-N1 | 7.19 | 113.95 | 108.20 |
| 35 | E | 202 | C | N3-C4-N4 | 7.19 | 123.03 | 118.00 |
| 35 | E | 1225 | G | C5-C6-O6 | -7.19 | 124.28 | 128.60 |
| 35 | E | 1692 | G | C5-C6-O6 | -7.19 | 124.28 | 128.60 |
| 35 | E | 310 | U | O4'-C1'-N1 | 7.19 | 113.95 | 108.20 |
| 35 | E | 1970 | G | C5-C6-O6 | -7.19 | 124.29 | 128.60 |
| 35 | E | 584 | C | N3-C4-N4 | 7.19 | 123.03 | 118.00 |
| 35 | E | 97 | A | C4-C5-C6 | 7.19 | 120.59 | 117.00 |
| 35 | E | 2306 | A | C5-C6-N6 | -7.19 | 117.95 | 123.70 |
| 35 | E | 67 | C | O4'-C1'-N1 | 7.18 | 113.95 | 108.20 |
| 35 | E | 921 | G | C5-C6-O6 | -7.18 | 124.29 | 128.60 |
| 35 | E | 229 | G | C5-C6-O6 | -7.18 | 124.29 | 128.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1899 | C | N3-C4-N4 | 7.18 | 123.03 | 118.00 |
| 35 | E | 429 | C | O4'-C1'-N1 | 7.18 | 113.94 | 108.20 |
| 35 | E | 1968 | G | C5-C6-O6 | -7.18 | 124.29 | 128.60 |
| 35 | E | 874 | C | O4'-C1'-N1 | 7.18 | 113.94 | 108.20 |
| 35 | E | 994 | G | C5-C6-O6 | -7.18 | 124.29 | 128.60 |
| 35 | E | 1293 | C | O4'-C1'-N1 | 7.17 | 113.94 | 108.20 |
| 35 | E | 497 | C | O4'-C1'-N1 | 7.17 | 113.94 | 108.20 |
| 35 | E | 1729 | C | O4'-C1'-N1 | 7.17 | 113.94 | 108.20 |
| 35 | E | 1811 | C | O4'-C1'-N1 | 7.17 | 113.93 | 108.20 |
| 35 | E | 224 | C | O4'-C1'-N1 | 7.17 | 113.93 | 108.20 |
| 35 | E | 1678 | C | O4'-C1'-N1 | 7.17 | 113.93 | 108.20 |
| 35 | E | 1243 | U | O4'-C1'-N1 | 7.16 | 113.93 | 108.20 |
| 35 | E | 1796 | G | C5-C6-O6 | -7.16 | 124.31 | 128.60 |
| 35 | E | 2253 | U | O4'-C1'-N1 | 7.16 | 113.92 | 108.20 |
| 35 | E | 633 | A | O4'-C1'-N9 | 7.15 | 113.92 | 108.20 |
| 35 | E | 1894 | C | O4'-C1'-N1 | 7.15 | 113.92 | 108.20 |
| 35 | E | 884 | A | O4'-C1'-N9 | 7.15 | 113.92 | 108.20 |
| 35 | E | 1546 | C | O4'-C1'-N1 | 7.15 | 113.92 | 108.20 |
| 35 | E | 138 | C | O4'-C1'-N1 | 7.15 | 113.92 | 108.20 |
| 35 | E | 794 | G | C5-C6-O6 | -7.15 | 124.31 | 128.60 |
| 35 | E | 830 | C | O4'-C1'-N1 | 7.15 | 113.92 | 108.20 |
| 35 | E | 1847 | C | O4'-C1'-N1 | 7.15 | 113.92 | 108.20 |
| 35 | E | 1879 | U | O4'-C1'-N1 | 7.14 | 113.91 | 108.20 |
| 35 | E | 1311 | C | O4'-C1'-N1 | 7.14 | 113.91 | 108.20 |
| 35 | E | 1990 | U | O4'-C1'-N1 | 7.14 | 113.91 | 108.20 |
| 35 | E | 2084 | U | O4'-C1'-N1 | 7.14 | 113.91 | 108.20 |
| 35 | E | 2264 | A | C4-C5-C6 | 7.13 | 120.57 | 117.00 |
| 35 | E | 1791 | C | O4'-C1'-N1 | 7.13 | 113.90 | 108.20 |
| 35 | E | 815 | G | O4'-C1'-N9 | 7.13 | 113.90 | 108.20 |
| 35 | E | 2029 | U | O4'-C1'-N1 | 7.13 | 113.90 | 108.20 |
| 35 | E | 539 | G | C5-C6-O6 | -7.13 | 124.32 | 128.60 |
| 35 | E | 1830 | C | O4'-C1'-N1 | 7.12 | 113.90 | 108.20 |
| 35 | E | 1266 | C | O4'-C1'-N1 | 7.12 | 113.89 | 108.20 |
| 35 | E | 790 | G | C5-C6-O6 | -7.12 | 124.33 | 128.60 |
| 35 | E | 2061 | G | C4-N9-C1' | 7.12 | 135.75 | 126.50 |
| 35 | E | 1585 | C | O4'-C1'-N1 | 7.12 | 113.89 | 108.20 |
| 35 | E | 2308 | C | O4'-C1'-N1 | 7.12 | 113.89 | 108.20 |
| 35 | E | 1185 | A | C5-C6-N1 | -7.11 | 114.14 | 117.70 |
| 35 | E | 388 | U | O4'-C1'-N1 | 7.11 | 113.89 | 108.20 |
| 35 | E | 2057 | U | O4'-C1'-N1 | 7.11 | 113.89 | 108.20 |
| 35 | E | 801 | C | O4'-C1'-N1 | 7.10 | 113.88 | 108.20 |
| 35 | E | 686 | U | O4'-C1'-N1 | 7.10 | 113.88 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 134 | U | O4'-C1'-N1 | 7.10 | 113.88 | 108.20 |
| 35 | E | 962 | A | C5-C6-N6 | -7.10 | 118.02 | 123.70 |
| 35 | E | 1548 | C | C6-N1-C1' | -7.10 | 112.28 | 120.80 |
| 35 | E | 827 | U | O4'-C1'-N1 | 7.10 | 113.88 | 108.20 |
| 35 | E | 2105 | C | O4'-C1'-N1 | 7.10 | 113.88 | 108.20 |
| 35 | E | 2181 | U | O4'-C1'-N1 | 7.10 | 113.88 | 108.20 |
| 35 | E | 187 | C | O4'-C1'-N1 | 7.10 | 113.88 | 108.20 |
| 35 | E | 1224 | U | O4'-C1'-N1 | 7.09 | 113.87 | 108.20 |
| 35 | E | 1245 | C | O4'-C1'-N1 | 7.09 | 113.87 | 108.20 |
| 35 | E | 671 | U | O4'-C1'-N1 | 7.09 | 113.87 | 108.20 |
| 35 | E | 1348 | A | C4-C5-C6 | 7.09 | 120.54 | 117.00 |
| 35 | E | 2146 | U | O4'-C1'-N1 | 7.09 | 113.87 | 108.20 |
| 35 | E | 908 | G | C5-C6-O6 | -7.08 | 124.35 | 128.60 |
| 35 | E | 1347 | U | O4'-C1'-N1 | 7.08 | 113.87 | 108.20 |
| 35 | E | 1667 | G | N1-C6-O6 | 7.08 | 124.15 | 119.90 |
| 35 | E | 900 | A | O4'-C1'-N9 | 7.08 | 113.86 | 108.20 |
| 35 | E | 1685 | G | C5-C6-O6 | -7.08 | 124.35 | 128.60 |
| 35 | E | 1714 | U | O4'-C1'-N1 | 7.08 | 113.86 | 108.20 |
| 35 | E | 1947 | U | O4'-C1'-N1 | 7.08 | 113.86 | 108.20 |
| 35 | E | 1377 | A | O4'-C1'-N9 | 7.07 | 113.86 | 108.20 |
| 35 | E | 1326 | G | C5-C6-O6 | -7.07 | 124.36 | 128.60 |
| 35 | E | 1376 | G | O4'-C1'-N9 | 7.07 | 113.86 | 108.20 |
| 35 | E | 17 | C | O4'-C1'-N1 | 7.07 | 113.86 | 108.20 |
| 35 | E | 2301 | C | O4'-C1'-N1 | 7.07 | 113.86 | 108.20 |
| 35 | E | 1183 | G | C5-C6-O6 | -7.07 | 124.36 | 128.60 |
| 35 | E | 1185 | A | O4'-C1'-N9 | 7.07 | 113.85 | 108.20 |
| 35 | E | 1331 | U | O4'-C1'-N1 | 7.07 | 113.85 | 108.20 |
| 35 | E | 1379 | U | O4'-C1'-N1 | 7.07 | 113.85 | 108.20 |
| 35 | E | 1622 | G | C5-C6-O6 | -7.07 | 124.36 | 128.60 |
| 35 | E | 85 | U | O4'-C1'-N1 | 7.07 | 113.85 | 108.20 |
| 35 | E | 1694 | G | O4'-C1'-N9 | 7.07 | 113.85 | 108.20 |
| 35 | E | 368 | G | O4'-C1'-N9 | 7.06 | 113.85 | 108.20 |
| 35 | E | 1909 | U | O4'-C1'-N1 | 7.06 | 113.85 | 108.20 |
| 35 | E | 225 | C | O4'-C1'-N1 | 7.06 | 113.85 | 108.20 |
| 35 | E | 534 | C | O4'-C1'-N1 | 7.06 | 113.85 | 108.20 |
| 35 | E | 1075 | G | C5-C6-O6 | -7.06 | 124.37 | 128.60 |
| 35 | E | 2318 | U | O4'-C1'-N1 | 7.05 | 113.84 | 108.20 |
| 35 | E | 465 | G | C5-C6-O6 | -7.05 | 124.37 | 128.60 |
| 35 | E | 2201 | U | O4'-C1'-N1 | 7.05 | 113.84 | 108.20 |
| 35 | E | 573 | U | O4'-C1'-N1 | 7.05 | 113.84 | 108.20 |
| 35 | E | 32 | U | O4'-C1'-N1 | 7.05 | 113.84 | 108.20 |
| 35 | E | 1716 | C | O4'-C1'-N1 | 7.05 | 113.84 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1901 | G | C5-C6-O6 | -7.05 | 124.37 | 128.60 |
| 35 | E | 2161 | U | O4'-C1'-N1 | 7.05 | 113.84 | 108.20 |
| 35 | E | 2219 | C | O4'-C1'-N1 | 7.05 | 113.84 | 108.20 |
| 35 | E | 92 | G | C5-C6-O6 | -7.04 | 124.37 | 128.60 |
| 35 | E | 1640 | G | C5-C6-O6 | -7.04 | 124.37 | 128.60 |
| 35 | E | 384 | G | C5-C6-O6 | -7.04 | 124.38 | 128.60 |
| 35 | E | 407 | G | C5-C6-O6 | -7.04 | 124.38 | 128.60 |
| 35 | E | 1337 | G | C5-C6-O6 | -7.04 | 124.38 | 128.60 |
| 35 | E | 27 | U | O4'-C1'-N1 | 7.04 | 113.83 | 108.20 |
| 35 | E | 1871 | G | O4'-C1'-N9 | 7.04 | 113.83 | 108.20 |
| 35 | E | 115 | U | O4'-C1'-N1 | 7.04 | 113.83 | 108.20 |
| 35 | E | 1285 | C | O4'-C1'-N1 | 7.04 | 113.83 | 108.20 |
| 35 | E | 534 | C | N3-C4-N4 | 7.04 | 122.92 | 118.00 |
| 35 | E | 1538 | G | C5-C6-O6 | -7.04 | 124.38 | 128.60 |
| 35 | E | 2012 | C | O4'-C1'-N1 | 7.04 | 113.83 | 108.20 |
| 35 | E | 745 | C | N3-C4-N4 | 7.03 | 122.92 | 118.00 |
| 35 | E | 779 | A | C4-C5-C6 | 7.03 | 120.52 | 117.00 |
| 35 | E | 1624 | C | O4'-C1'-N1 | 7.03 | 113.82 | 108.20 |
| 35 | E | 178 | U | O4'-C1'-N1 | 7.03 | 113.82 | 108.20 |
| 35 | E | 1252 | C | O4'-C1'-N1 | 7.03 | 113.82 | 108.20 |
| 35 | E | 155 | U | O4'-C1'-N1 | 7.03 | 113.82 | 108.20 |
| 35 | E | 719 | G | O4'-C1'-N9 | 7.03 | 113.82 | 108.20 |
| 35 | E | 883 | C | N3-C4-N4 | 7.03 | 122.92 | 118.00 |
| 35 | E | 1184 | C | O4'-C1'-N1 | 7.03 | 113.82 | 108.20 |
| 35 | E | 1600 | A | C4-C5-C6 | 7.02 | 120.51 | 117.00 |
| 35 | E | 1536 | C | O4'-C1'-N1 | 7.02 | 113.82 | 108.20 |
| 35 | E | 1618 | G | C5-C6-O6 | -7.02 | 124.39 | 128.60 |
| 35 | E | 441 | C | N3-C4-N4 | 7.02 | 122.92 | 118.00 |
| 35 | E | 1798 | G | C5-C6-O6 | -7.02 | 124.39 | 128.60 |
| 35 | E | 50 | C | O4'-C1'-N1 | 7.02 | 113.81 | 108.20 |
| 35 | E | 964 | U | O4'-C1'-N1 | 7.02 | 113.81 | 108.20 |
| 35 | E | 1081 | G | C5-C6-O6 | -7.02 | 124.39 | 128.60 |
| 35 | E | 280 | C | O4'-C1'-N1 | 7.02 | 113.81 | 108.20 |
| 35 | E | 724 | A | N1-C2-N3 | 7.02 | 132.81 | 129.30 |
| 35 | E | 1556 | C | O4'-C1'-N1 | 7.02 | 113.81 | 108.20 |
| 35 | E | 643 | C | O4'-C1'-N1 | 7.01 | 113.81 | 108.20 |
| 35 | E | 266 | U | O4'-C1'-N1 | 7.01 | 113.81 | 108.20 |
| 35 | E | 772 | U | O4'-C1'-C2' | -7.01 | 98.79 | 105.80 |
| 35 | E | 1760 | G | N1-C6-O6 | 7.01 | 124.11 | 119.90 |
| 35 | E | 298 | C | N3-C4-N4 | 7.01 | 122.91 | 118.00 |
| 35 | E | 1342 | C | O4'-C1'-N1 | 7.01 | 113.81 | 108.20 |
| 35 | E | 286 | G | C5-C6-O6 | -7.01 | 124.39 | 128.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 708 | G | O4'-C1'-N9 | 7.01 | 113.81 | 108.20 |
| 35 | E | 1171 | C | O4'-C1'-N1 | 7.01 | 113.81 | 108.20 |
| 35 | E | 2160 | U | O4'-C1'-N1 | 7.01 | 113.81 | 108.20 |
| 35 | E | 1820 | U | O4'-C1'-N1 | 7.00 | 113.80 | 108.20 |
| 35 | E | 918 | G | C5-C6-O6 | -7.00 | 124.40 | 128.60 |
| 35 | E | 1364 | G | C5-C6-O6 | -7.00 | 124.40 | 128.60 |
| 35 | E | 2034 | A | O4'-C1'-N9 | 7.00 | 113.80 | 108.20 |
| 35 | E | 612 | U | O4'-C1'-N1 | 7.00 | 113.80 | 108.20 |
| 35 | E | 971 | G | O4'-C1'-N9 | 7.00 | 113.80 | 108.20 |
| 35 | E | 1928 | U | O4'-C1'-N1 | 7.00 | 113.80 | 108.20 |
| 35 | E | 14 | C | O4'-C1'-N1 | 6.99 | 113.79 | 108.20 |
| 35 | E | 289 | G | C5-C6-O6 | -6.99 | 124.40 | 128.60 |
| 35 | E | 642 | U | O4'-C1'-N1 | 6.99 | 113.79 | 108.20 |
| 35 | E | 897 | U | O4'-C1'-N1 | 6.99 | 113.79 | 108.20 |
| 35 | E | 1921 | G | C5-C6-O6 | -6.99 | 124.41 | 128.60 |
| 35 | E | 1550 | C | O4'-C1'-N1 | 6.99 | 113.79 | 108.20 |
| 35 | E | 234 | U | O4'-C1'-N1 | 6.99 | 113.79 | 108.20 |
| 35 | E | 1949 | U | O4'-C1'-N1 | 6.98 | 113.79 | 108.20 |
| 35 | E | 2086 | G | C5-C6-O6 | -6.98 | 124.41 | 128.60 |
| 35 | E | 459 | U | O4'-C1'-N1 | 6.98 | 113.78 | 108.20 |
| 35 | E | 471 | C | O4'-C1'-N1 | 6.98 | 113.78 | 108.20 |
| 35 | E | 638 | C | O4'-C1'-N1 | 6.98 | 113.78 | 108.20 |
| 35 | E | 667 | G | C5-C6-O6 | -6.98 | 124.41 | 128.60 |
| 35 | E | 914 | C | O4'-C1'-N1 | 6.98 | 113.78 | 108.20 |
| 35 | E | 1636 | U | O4'-C1'-N1 | 6.98 | 113.78 | 108.20 |
| 35 | E | 652 | U | O4'-C1'-N1 | 6.98 | 113.78 | 108.20 |
| 35 | E | 705 | G | C5-C6-O6 | -6.98 | 124.41 | 128.60 |
| 35 | E | 1872 | G | C5-C6-O6 | -6.98 | 124.41 | 128.60 |
| 35 | E | 1961 | A | C4-C5-C6 | 6.98 | 120.49 | 117.00 |
| 35 | E | 613 | C | O4'-C1'-N1 | 6.97 | 113.78 | 108.20 |
| 35 | E | 264 | C | O4'-C1'-N1 | 6.97 | 113.78 | 108.20 |
| 35 | E | 554 | C | O4'-C1'-N1 | 6.97 | 113.78 | 108.20 |
| 35 | E | 1718 | U | O4'-C1'-N1 | 6.97 | 113.78 | 108.20 |
| 35 | E | 1589 | C | O4'-C1'-N1 | 6.97 | 113.77 | 108.20 |
| 35 | E | 637 | C | O4'-C1'-N1 | 6.96 | 113.77 | 108.20 |
| 35 | E | 859 | C | O4'-C1'-N1 | 6.96 | 113.77 | 108.20 |
| 35 | E | 1198 | G | C5-C6-O6 | -6.96 | 124.42 | 128.60 |
| 35 | E | 2019 | C | O4'-C1'-N1 | 6.96 | 113.77 | 108.20 |
| 35 | E | 731 | U | O4'-C1'-N1 | 6.96 | 113.77 | 108.20 |
| 26 | j | 100 | TYR | CB-CG-CD1 | 6.96 | 125.17 | 121.00 |
| 35 | E | 1806 | C | O4'-C1'-N1 | 6.96 | 113.76 | 108.20 |
| 35 | E | 546 | U | C2-N1-C1' | 6.95 | 126.04 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1576 | G | N1-C6-O6 | 6.95 | 124.07 | 119.90 |
| 35 | E | 1198 | G | P-O3'-C3' | 6.95 | 128.04 | 119.70 |
| 35 | E | 617 | U | O4'-C1'-N1 | 6.95 | 113.76 | 108.20 |
| 35 | E | 1351 | C | O4'-C1'-N1 | 6.95 | 113.76 | 108.20 |
| 35 | E | 1903 | A | O4'-C1'-N9 | 6.95 | 113.76 | 108.20 |
| 35 | E | 210 | A | C5-C6-N6 | -6.95 | 118.14 | 123.70 |
| 35 | E | 1755 | G | C5-C6-O6 | -6.95 | 124.43 | 128.60 |
| 35 | E | 150 | U | O4'-C1'-N1 | 6.94 | 113.75 | 108.20 |
| 35 | E | 2228 | C | N3-C4-N4 | 6.94 | 122.86 | 118.00 |
| 35 | E | 657 | U | O4'-C1'-N1 | 6.94 | 113.75 | 108.20 |
| 35 | E | 726 | C | O4'-C1'-N1 | 6.94 | 113.75 | 108.20 |
| 35 | E | 910 | A | C5-C6-N6 | -6.94 | 118.15 | 123.70 |
| 35 | E | 1931 | U | O4'-C1'-N1 | 6.94 | 113.75 | 108.20 |
| 35 | E | 2162 | U | O4'-C1'-N1 | 6.94 | 113.75 | 108.20 |
| 35 | E | 528 | U | O4'-C1'-N1 | 6.93 | 113.75 | 108.20 |
| 35 | E | 824 | G | C5-C6-O6 | -6.93 | 124.44 | 128.60 |
| 35 | E | 987 | G | O4'-C1'-N9 | 6.93 | 113.75 | 108.20 |
| 35 | E | 353 | C | O4'-C1'-N1 | 6.93 | 113.75 | 108.20 |
| 35 | E | 2021 | G | C5-C6-O6 | -6.93 | 124.44 | 128.60 |
| 35 | E | 2128 | C | O4'-C1'-N1 | 6.93 | 113.75 | 108.20 |
| 35 | E | 305 | U | O4'-C1'-N1 | 6.93 | 113.75 | 108.20 |
| 35 | E | 1544 | U | O4'-C1'-N1 | 6.93 | 113.75 | 108.20 |
| 35 | E | 346 | C | N3-C4-N4 | 6.93 | 122.85 | 118.00 |
| 35 | E | 789 | C | O4'-C1'-N1 | 6.93 | 113.74 | 108.20 |
| 35 | E | 1322 | G | C5-C6-O6 | -6.93 | 124.44 | 128.60 |
| 35 | E | 752 | U | O4'-C1'-N1 | 6.93 | 113.74 | 108.20 |
| 35 | E | 2252 | U | O4'-C1'-N1 | 6.93 | 113.74 | 108.20 |
| 35 | E | 91 | U | O4'-C1'-N1 | 6.92 | 113.74 | 108.20 |
| 35 | E | 719 | G | C5-C6-O6 | -6.92 | 124.45 | 128.60 |
| 35 | E | 938 | G | C5-C6-O6 | -6.92 | 124.45 | 128.60 |
| 35 | E | 1614 | G | C5-C6-O6 | -6.92 | 124.45 | 128.60 |
| 35 | E | 323 | U | O4'-C1'-N1 | 6.92 | 113.74 | 108.20 |
| 35 | E | 618 | G | C5-C6-O6 | -6.92 | 124.45 | 128.60 |
| 35 | E | 1772 | G | C5-C6-O6 | -6.92 | 124.45 | 128.60 |
| 35 | E | 1896 | C | O4'-C1'-N1 | 6.92 | 113.74 | 108.20 |
| 35 | E | 416 | U | O4'-C1'-N1 | 6.92 | 113.74 | 108.20 |
| 35 | E | 424 | G | C5-C6-O6 | -6.92 | 124.45 | 128.60 |
| 35 | E | 970 | G | O4'-C1'-N9 | 6.92 | 113.73 | 108.20 |
| 35 | E | 2250 | U | O4'-C1'-N1 | 6.92 | 113.73 | 108.20 |
| 35 | E | 2282 | C | O4'-C1'-N1 | 6.91 | 113.73 | 108.20 |
| 35 | E | 565 | G | N1-C6-O6 | 6.91 | 124.05 | 119.90 |
| 35 | E | 37 | U | O4'-C1'-N1 | 6.91 | 113.72 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 336 | C | O4'-C1'-N1 | 6.91 | 113.72 | 108.20 |
| 35 | E | 492 | A | C5-C6-N6 | -6.91 | 118.18 | 123.70 |
| 35 | E | 833 | A | O4'-C1'-N9 | 6.91 | 113.72 | 108.20 |
| 35 | E | 1810 | C | O4'-C1'-N1 | 6.91 | 113.72 | 108.20 |
| 35 | E | 2074 | G | C5-C6-O6 | -6.91 | 124.46 | 128.60 |
| 35 | E | 550 | U | O4'-C1'-N1 | 6.90 | 113.72 | 108.20 |
| 35 | E | 614 | U | O4'-C1'-N1 | 6.90 | 113.72 | 108.20 |
| 35 | E | 750 | C | O4'-C1'-N1 | 6.90 | 113.72 | 108.20 |
| 35 | E | 780 | C | O4'-C1'-N1 | 6.90 | 113.72 | 108.20 |
| 35 | E | 77 | C | N3-C4-N4 | 6.90 | 122.83 | 118.00 |
| 35 | E | 179 | G | C5-C6-O6 | -6.90 | 124.46 | 128.60 |
| 35 | E | 2180 | U | O4'-C1'-N1 | 6.89 | 113.72 | 108.20 |
| 35 | E | 2053 | G | C5-C6-O6 | -6.89 | 124.47 | 128.60 |
| 35 | E | 1713 | G | C5-C6-O6 | -6.89 | 124.47 | 128.60 |
| 35 | E | 114 | C | O4'-C1'-N1 | 6.89 | 113.71 | 108.20 |
| 35 | E | 164 | G | C5-C6-O6 | -6.89 | 124.47 | 128.60 |
| 35 | E | 2207 | U | O4'-C1'-N1 | 6.89 | 113.71 | 108.20 |
| 26 | j | 100 | TYR | CB-CG-CD2 | -6.88 | 116.87 | 121.00 |
| 35 | E | 51 | A | C4-C5-C6 | 6.88 | 120.44 | 117.00 |
| 35 | E | 1864 | C | N3-C4-N4 | 6.88 | 122.82 | 118.00 |
| 35 | E | 1873 | G | C4-N9-C1' | -6.88 | 117.55 | 126.50 |
| 35 | E | 309 | G | C5-C6-O6 | -6.88 | 124.47 | 128.60 |
| 35 | E | 99 | U | O4'-C1'-N1 | 6.88 | 113.71 | 108.20 |
| 35 | E | 137 | C | N3-C4-N4 | 6.88 | 122.82 | 118.00 |
| 35 | E | 1706 | A | C4-C5-C6 | 6.88 | 120.44 | 117.00 |
| 35 | E | 1906 | C | C6-N1-C1' | -6.88 | 112.54 | 120.80 |
| 35 | E | 1873 | G | C8-N9-C1' | 6.88 | 135.94 | 127.00 |
| 35 | E | 2136 | A | C5-C6-N6 | -6.88 | 118.20 | 123.70 |
| 35 | E | 2280 | A | C4-C5-C6 | 6.88 | 120.44 | 117.00 |
| 35 | E | 267 | U | O4'-C1'-N1 | 6.88 | 113.70 | 108.20 |
| 35 | E | 327 | U | O4'-C1'-N1 | 6.88 | 113.70 | 108.20 |
| 35 | E | 570 | U | O4'-C1'-N1 | 6.88 | 113.70 | 108.20 |
| 35 | E | 729 | C | O4'-C1'-N1 | 6.88 | 113.70 | 108.20 |
| 35 | E | 948 | U | O4'-C1'-N1 | 6.88 | 113.70 | 108.20 |
| 35 | E | 1757 | U | O4'-C1'-N1 | 6.88 | 113.70 | 108.20 |
| 35 | E | 301 | U | O4'-C1'-N1 | 6.87 | 113.70 | 108.20 |
| 35 | E | 446 | A | C4-C5-C6 | 6.87 | 120.44 | 117.00 |
| 35 | E | 511 | G | C5-C6-O6 | -6.87 | 124.48 | 128.60 |
| 35 | E | 2212 | G | C5-C6-O6 | -6.87 | 124.48 | 128.60 |
| 35 | E | 362 | C | O4'-C1'-N1 | 6.87 | 113.69 | 108.20 |
| 35 | E | 2303 | U | O4'-C1'-N1 | 6.86 | 113.69 | 108.20 |
| 35 | E | 592 | A | C4-C5-C6 | 6.86 | 120.43 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 797 | G | C5-C6-O6 | -6.86 | 124.48 | 128.60 |
| 35 | E | 1321 | G | C5-C6-O6 | -6.86 | 124.48 | 128.60 |
| 35 | E | 160 | A | C5-C6-N6 | -6.86 | 118.21 | 123.70 |
| 35 | E | 247 | U | O4'-C1'-N1 | 6.85 | 113.68 | 108.20 |
| 35 | E | 2025 | U | O4'-C1'-N1 | 6.85 | 113.68 | 108.20 |
| 35 | E | 2276 | U | O4'-C1'-N1 | 6.85 | 113.68 | 108.20 |
| 35 | E | 2010 | G | C5-C6-O6 | -6.85 | 124.49 | 128.60 |
| 35 | E | 1172 | C | O4'-C1'-N1 | 6.85 | 113.68 | 108.20 |
| 35 | E | 52 | U | O4'-C1'-N1 | 6.85 | 113.68 | 108.20 |
| 35 | E | 163 | C | O4'-C1'-N1 | 6.85 | 113.68 | 108.20 |
| 35 | E | 714 | G | C5-C6-O6 | -6.85 | 124.49 | 128.60 |
| 35 | E | 1770 | U | O4'-C1'-N1 | 6.85 | 113.68 | 108.20 |
| 35 | E | 1780 | G | C5-C6-O6 | -6.85 | 124.49 | 128.60 |
| 35 | E | 1969 | G | C5-C6-O6 | -6.85 | 124.49 | 128.60 |
| 35 | E | 1819 | U | O4'-C1'-N1 | 6.85 | 113.68 | 108.20 |
| 35 | E | 1556 | C | N3-C4-N4 | 6.84 | 122.79 | 118.00 |
| 35 | E | 1672 | C | O4'-C1'-N1 | 6.84 | 113.67 | 108.20 |
| 35 | E | 342 | U | O4'-C1'-N1 | 6.84 | 113.67 | 108.20 |
| 35 | E | 1632 | G | C5-C6-O6 | -6.84 | 124.49 | 128.60 |
| 35 | E | 1813 | G | C5-C6-O6 | -6.84 | 124.49 | 128.60 |
| 35 | E | 2177 | U | O4'-C1'-N1 | 6.84 | 113.67 | 108.20 |
| 35 | E | 20 | G | C5-C6-O6 | -6.84 | 124.50 | 128.60 |
| 35 | E | 1253 | G | C5-C6-O6 | -6.84 | 124.50 | 128.60 |
| 35 | E | 1915 | G | C5-C6-O6 | -6.84 | 124.50 | 128.60 |
| 35 | E | 154 | U | O4'-C1'-N1 | 6.84 | 113.67 | 108.20 |
| 35 | E | 1856 | G | O4'-C1'-N9 | 6.84 | 113.67 | 108.20 |
| 35 | E | 40 | A | C4-C5-C6 | 6.84 | 120.42 | 117.00 |
| 35 | E | 1754 | U | O4'-C1'-N1 | 6.84 | 113.67 | 108.20 |
| 35 | E | 2091 | U | O4'-C1'-N1 | 6.84 | 113.67 | 108.20 |
| 35 | E | 171 | U | O4'-C1'-N1 | 6.83 | 113.67 | 108.20 |
| 35 | E | 947 | U | O4'-C1'-N1 | 6.83 | 113.67 | 108.20 |
| 35 | E | 1617 | G | C5-C6-O6 | -6.83 | 124.50 | 128.60 |
| 35 | E | 1621 | U | O4'-C1'-N1 | 6.83 | 113.67 | 108.20 |
| 35 | E | 2012 | C | N3-C4-N4 | 6.83 | 122.78 | 118.00 |
| 35 | E | 2185 | U | O4'-C1'-N1 | 6.83 | 113.67 | 108.20 |
| 35 | E | 937 | C | N3-C4-N4 | 6.83 | 122.78 | 118.00 |
| 35 | E | 775 | A | P-O3'-C3' | 6.82 | 127.89 | 119.70 |
| 35 | E | 1297 | C | O4'-C1'-N1 | 6.82 | 113.66 | 108.20 |
| 35 | E | 1631 | A | O4'-C1'-N9 | 6.82 | 113.66 | 108.20 |
| 35 | E | 88 | G | C5-C6-O6 | -6.82 | 124.51 | 128.60 |
| 35 | E | 895 | A | C4-C5-C6 | 6.82 | 120.41 | 117.00 |
| 35 | E | 973 | G | C5-C6-O6 | -6.82 | 124.51 | 128.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1204 | U | O4'-C1'-N1 | 6.82 | 113.66 | 108.20 |
| 35 | E | 551 | U | O4'-C1'-N1 | 6.82 | 113.66 | 108.20 |
| 35 | E | 924 | G | C5-C6-O6 | -6.82 | 124.51 | 128.60 |
| 35 | E | 934 | C | O4'-C1'-N1 | 6.82 | 113.65 | 108.20 |
| 35 | E | 2030 | G | C5-C6-O6 | -6.82 | 124.51 | 128.60 |
| 35 | E | 631 | G | C5-C6-O6 | -6.82 | 124.51 | 128.60 |
| 35 | E | 806 | C | O4'-C1'-N1 | 6.82 | 113.65 | 108.20 |
| 35 | E | 965 | C | O4'-C1'-N1 | 6.82 | 113.65 | 108.20 |
| 35 | E | 2027 | C | C2-N1-C1' | 6.81 | 126.29 | 118.80 |
| 35 | E | 128 | U | O4'-C1'-N1 | 6.81 | 113.65 | 108.20 |
| 35 | E | 308 | C | O4'-C1'-N1 | 6.81 | 113.65 | 108.20 |
| 35 | E | 574 | U | O4'-C1'-N1 | 6.81 | 113.65 | 108.20 |
| 35 | E | 630 | G | C5-C6-O6 | -6.81 | 124.52 | 128.60 |
| 35 | E | 1696 | G | C5-C6-O6 | -6.81 | 124.51 | 128.60 |
| 35 | E | 1221 | U | O4'-C1'-N1 | 6.81 | 113.65 | 108.20 |
| 35 | E | 1720 | C | O4'-C1'-N1 | 6.81 | 113.65 | 108.20 |
| 35 | E | 1972 | G | C5-C6-O6 | -6.81 | 124.52 | 128.60 |
| 35 | E | 1998 | A | C5-C6-N6 | -6.81 | 118.25 | 123.70 |
| 35 | E | 899 | G | C5-C6-O6 | -6.80 | 124.52 | 128.60 |
| 35 | E | 1993 | G | C5-C6-O6 | -6.80 | 124.52 | 128.60 |
| 35 | E | 998 | C | O4'-C1'-N1 | 6.80 | 113.64 | 108.20 |
| 35 | E | 896 | U | O4'-C1'-N1 | 6.80 | 113.64 | 108.20 |
| 35 | E | 1187 | C | N3-C4-C5 | -6.80 | 119.18 | 121.90 |
| 35 | E | 2076 | A | O4'-C1'-N9 | 6.80 | 113.64 | 108.20 |
| 35 | E | 2213 | G | C5-C6-O6 | -6.80 | 124.52 | 128.60 |
| 35 | E | 29 | U | O4'-C1'-N1 | 6.80 | 113.64 | 108.20 |
| 35 | E | 372 | U | O4'-C1'-N1 | 6.80 | 113.64 | 108.20 |
| 35 | E | 727 | C | O4'-C1'-N1 | 6.80 | 113.64 | 108.20 |
| 35 | E | 1281 | U | O4'-C1'-N1 | 6.80 | 113.64 | 108.20 |
| 35 | E | 116 | G | C5-C6-O6 | -6.80 | 124.52 | 128.60 |
| 35 | E | 252 | G | C5-C6-O6 | -6.80 | 124.52 | 128.60 |
| 35 | E | 1691 | G | C5-C6-O6 | -6.80 | 124.52 | 128.60 |
| 35 | E | 1883 | C | O4'-C1'-N1 | 6.80 | 113.64 | 108.20 |
| 35 | E | 1913 | U | O4'-C1'-N1 | 6.80 | 113.64 | 108.20 |
| 35 | E | 1933 | G | C5-C6-O6 | -6.80 | 124.52 | 128.60 |
| 35 | E | 2099 | G | N1-C6-O6 | 6.80 | 123.98 | 119.90 |
| 35 | E | 397 | G | C5-C6-O6 | -6.79 | 124.52 | 128.60 |
| 35 | E | 688 | G | C5-C6-O6 | -6.79 | 124.52 | 128.60 |
| 35 | E | 437 | G | O4'-C1'-N9 | 6.79 | 113.64 | 108.20 |
| 35 | E | 500 | A | C4-C5-C6 | 6.79 | 120.40 | 117.00 |
| 35 | E | 893 | G | C5-C6-O6 | -6.79 | 124.52 | 128.60 |
| 35 | E | 1963 | G | C5-C6-O6 | -6.79 | 124.53 | 128.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 2145 | A | C4-C5-C6 | 6.79 | 120.39 | 117.00 |
| 35 | E | 1825 | A | C4-C5-C6 | 6.79 | 120.39 | 117.00 |
| 35 | E | 759 | C | O4'-C1'-N1 | 6.79 | 113.63 | 108.20 |
| 35 | E | 819 | G | C5-C6-O6 | -6.79 | 124.53 | 128.60 |
| 35 | E | 909 | G | C5-C6-O6 | -6.79 | 124.53 | 128.60 |
| 35 | E | 90 | A | C4-C5-C6 | 6.78 | 120.39 | 117.00 |
| 35 | E | 693 | G | C5-C6-O6 | -6.78 | 124.53 | 128.60 |
| 35 | E | 2243 | U | O4'-C1'-N1 | 6.78 | 113.62 | 108.20 |
| 35 | E | 379 | G | C5-C6-O6 | -6.78 | 124.53 | 128.60 |
| 3 | r | 135 | TRP | C-N-CA | 6.78 | 136.53 | 122.30 |
| 35 | E | 144 | A | C5-C6-N6 | -6.78 | 118.28 | 123.70 |
| 35 | E | 966 | C | O4'-C1'-N1 | 6.78 | 113.62 | 108.20 |
| 35 | E | 2017 | G | C5-C6-O6 | -6.78 | 124.53 | 128.60 |
| 35 | E | 2022 | A | O4'-C1'-N9 | 6.78 | 113.62 | 108.20 |
| 35 | E | 426 | U | O4'-C1'-N1 | 6.78 | 113.62 | 108.20 |
| 35 | E | 1688 | C | N3-C4-N4 | 6.78 | 122.74 | 118.00 |
| 35 | E | 1717 | U | O4'-C1'-N1 | 6.78 | 113.62 | 108.20 |
| 35 | E | 2235 | C | N3-C4-N4 | 6.77 | 122.74 | 118.00 |
| 35 | E | 981 | G | C5-C6-O6 | -6.77 | 124.54 | 128.60 |
| 35 | E | 2298 | G | C5-C6-O6 | -6.77 | 124.54 | 128.60 |
| 35 | E | 1942 | A | O4'-C1'-N9 | 6.77 | 113.62 | 108.20 |
| 35 | E | 252 | G | O4'-C1'-N9 | 6.77 | 113.61 | 108.20 |
| 35 | E | 772 | U | C4'-C3'-C2' | -6.77 | 95.83 | 102.60 |
| 35 | E | 1304 | C | O4'-C1'-N1 | 6.77 | 113.61 | 108.20 |
| 35 | E | 1531 | G | C5-C6-O6 | -6.77 | 124.54 | 128.60 |
| 35 | E | 2101 | G | C5-C6-O6 | -6.77 | 124.54 | 128.60 |
| 35 | E | 1722 | C | O4'-C1'-N1 | 6.77 | 113.61 | 108.20 |
| 35 | E | 2229 | A | C5-C6-N6 | -6.77 | 118.29 | 123.70 |
| 35 | E | 302 | U | O4'-C1'-N1 | 6.77 | 113.61 | 108.20 |
| 35 | E | 1941 | C | N3-C4-N4 | 6.77 | 122.74 | 118.00 |
| 35 | E | 2073 | G | C5-C6-O6 | -6.77 | 124.54 | 128.60 |
| 5 | u | 43 | TYR | CB-CG-CD2 | -6.76 | 116.94 | 121.00 |
| 35 | E | 172 | A | C4-C5-C6 | 6.76 | 120.38 | 117.00 |
| 35 | E | 2291 | U | O4'-C1'-N1 | 6.76 | 113.61 | 108.20 |
| 35 | E | 170 | C | O4'-C1'-N1 | 6.76 | 113.61 | 108.20 |
| 35 | E | 1550 | C | N3-C4-N4 | 6.76 | 122.73 | 118.00 |
| 35 | E | 1698 | A | C4-C5-C6 | 6.76 | 120.38 | 117.00 |
| 35 | E | 2155 | U | O4'-C1'-N1 | 6.76 | 113.61 | 108.20 |
| 35 | E | 1227 | U | O4'-C1'-N1 | 6.76 | 113.61 | 108.20 |
| 35 | E | 2280 | A | C5-C6-N6 | -6.76 | 118.30 | 123.70 |
| 35 | E | 1954 | C | O4'-C1'-N1 | 6.75 | 113.60 | 108.20 |
| 35 | E | 621 | A | C4-C5-C6 | 6.75 | 120.38 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1765 | G | C5-C6-O6 | -6.75 | 124.55 | 128.60 |
| 35 | E | 819 | G | P-O3'-C3' | 6.75 | 127.80 | 119.70 |
| 35 | E | 687 | U | O4'-C1'-N1 | 6.75 | 113.60 | 108.20 |
| 35 | E | 1902 | G | C5-C6-O6 | -6.75 | 124.55 | 128.60 |
| 35 | E | 419 | G | C5-C6-O6 | -6.75 | 124.55 | 128.60 |
| 35 | E | 919 | G | C5-C6-O6 | -6.75 | 124.55 | 128.60 |
| 35 | E | 461 | C | O4'-C1'-N1 | 6.75 | 113.60 | 108.20 |
| 35 | E | 16 | G | C5-C6-O6 | -6.74 | 124.55 | 128.60 |
| 35 | E | 557 | U | O4'-C1'-N1 | 6.74 | 113.59 | 108.20 |
| 35 | E | 629 | C | O4'-C1'-N1 | 6.74 | 113.59 | 108.20 |
| 35 | E | 1191 | G | C2'-C3'-O3' | 6.74 | 124.49 | 113.70 |
| 35 | E | 839 | C | O4'-C1'-N1 | 6.74 | 113.59 | 108.20 |
| 35 | E | 1977 | G | C5-C6-O6 | -6.74 | 124.56 | 128.60 |
| 35 | E | 494 | U | O4'-C1'-N1 | 6.74 | 113.59 | 108.20 |
| 35 | E | 776 | G | C5-C6-O6 | -6.74 | 124.56 | 128.60 |
| 35 | E | 1287 | A | C5-C6-N6 | -6.74 | 118.31 | 123.70 |
| 35 | E | 1580 | G | C5-C6-O6 | -6.74 | 124.56 | 128.60 |
| 35 | E | 1875 | G | C5-C6-O6 | -6.74 | 124.56 | 128.60 |
| 35 | E | 400 | G | C5-C6-O6 | -6.74 | 124.56 | 128.60 |
| 35 | E | 834 | G | C5-C6-O6 | -6.74 | 124.56 | 128.60 |
| 35 | E | 274 | C | N3-C4-N4 | 6.74 | 122.72 | 118.00 |
| 35 | E | 697 | G | C5-C6-O6 | -6.73 | 124.56 | 128.60 |
| 35 | E | 1167 | C | N3-C4-N4 | 6.73 | 122.71 | 118.00 |
| 35 | E | 1588 | U | O4'-C1'-N1 | 6.73 | 113.59 | 108.20 |
| 35 | E | 84 | C | N3-C4-N4 | 6.73 | 122.71 | 118.00 |
| 35 | E | 984 | A | C5-C6-N6 | -6.73 | 118.31 | 123.70 |
| 35 | E | 985 | G | O4'-C1'-N9 | 6.73 | 113.59 | 108.20 |
| 35 | E | 261 | A | C5-C6-N6 | -6.73 | 118.32 | 123.70 |
| 35 | E | 2031 | A | C4-C5-C6 | 6.73 | 120.36 | 117.00 |
| 35 | E | 2109 | G | C5-C6-O6 | -6.73 | 124.56 | 128.60 |
| 35 | E | 1829 | C | O4'-C1'-N1 | 6.73 | 113.58 | 108.20 |
| 35 | E | 298 | C | O4'-C1'-N1 | 6.73 | 113.58 | 108.20 |
| 35 | E | 1358 | G | C5-C6-O6 | -6.72 | 124.56 | 128.60 |
| 35 | E | 2308 | C | N3-C4-N4 | 6.72 | 122.71 | 118.00 |
| 25 | i | 116 | PHE | CB-CG-CD1 | 6.72 | 125.51 | 120.80 |
| 35 | E | 194 | U | O4'-C1'-N1 | 6.72 | 113.58 | 108.20 |
| 35 | E | 354 | U | O4'-C1'-N1 | 6.72 | 113.58 | 108.20 |
| 35 | E | 923 | A | C4-C5-C6 | 6.72 | 120.36 | 117.00 |
| 35 | E | 1849 | U | O4'-C1'-N1 | 6.72 | 113.58 | 108.20 |
| 35 | E | 2191 | G | O4'-C1'-N9 | 6.72 | 113.58 | 108.20 |
| 35 | E | 561 | A | C5-C6-N6 | -6.72 | 118.33 | 123.70 |
| 35 | E | 987 | G | C5-C6-O6 | -6.72 | 124.57 | 128.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1987 | A | C4-C5-C6 | 6.72 | 120.36 | 117.00 |
| 35 | E | 259 | C | N3-C4-N4 | 6.71 | 122.70 | 118.00 |
| 35 | E | 871 | G | C5-C6-O6 | -6.71 | 124.57 | 128.60 |
| 35 | E | 1599 | A | C4-C5-C6 | 6.71 | 120.36 | 117.00 |
| 35 | E | 2230 | C | N3-C4-N4 | 6.71 | 122.70 | 118.00 |
| 35 | E | 474 | C | O4'-C1'-N1 | 6.71 | 113.57 | 108.20 |
| 35 | E | 801 | C | N3-C4-N4 | 6.71 | 122.70 | 118.00 |
| 35 | E | 997 | G | C5-C6-O6 | -6.71 | 124.57 | 128.60 |
| 35 | E | 1641 | C | O4'-C1'-N1 | 6.71 | 113.57 | 108.20 |
| 35 | E | 2144 | G | C5-C6-O6 | -6.71 | 124.57 | 128.60 |
| 35 | E | 443 | G | C5-C6-O6 | -6.71 | 124.57 | 128.60 |
| 35 | E | 1383 | G | C5-C6-O6 | -6.71 | 124.58 | 128.60 |
| 35 | E | 1542 | U | O4'-C1'-N1 | 6.71 | 113.57 | 108.20 |
| 35 | E | 1912 | U | O4'-C1'-N1 | 6.71 | 113.57 | 108.20 |
| 35 | E | 737 | U | O4'-C1'-N1 | 6.71 | 113.56 | 108.20 |
| 35 | E | 1084 | G | C5-C6-O6 | -6.71 | 124.58 | 128.60 |
| 35 | E | 341 | U | O4'-C1'-N1 | 6.71 | 113.56 | 108.20 |
| 35 | E | 559 | U | O4'-C1'-N1 | 6.71 | 113.56 | 108.20 |
| 35 | E | 175 | A | C4-C5-C6 | 6.70 | 120.35 | 117.00 |
| 35 | E | 248 | G | C5-C6-O6 | -6.70 | 124.58 | 128.60 |
| 35 | E | 522 | A | C5-C6-N1 | -6.70 | 114.35 | 117.70 |
| 35 | E | 1528 | C | O4'-C1'-N1 | 6.70 | 113.56 | 108.20 |
| 35 | E | 903 | G | C5-C6-O6 | -6.70 | 124.58 | 128.60 |
| 35 | E | 930 | G | C5-C6-O6 | -6.70 | 124.58 | 128.60 |
| 35 | E | 1236 | G | C5-C6-O6 | -6.70 | 124.58 | 128.60 |
| 35 | E | 58 | C | N3-C4-N4 | 6.70 | 122.69 | 118.00 |
| 35 | E | 95 | U | O4'-C1'-N1 | 6.70 | 113.56 | 108.20 |
| 35 | E | 460 | U | O4'-C1'-N1 | 6.70 | 113.56 | 108.20 |
| 35 | E | 129 | U | O4'-C1'-N1 | 6.69 | 113.56 | 108.20 |
| 35 | E | 1296 | U | O4'-C1'-N1 | 6.69 | 113.55 | 108.20 |
| 35 | E | 33 | U | O4'-C1'-N1 | 6.69 | 113.55 | 108.20 |
| 35 | E | 172 | A | C5-C6-N1 | -6.69 | 114.36 | 117.70 |
| 35 | E | 505 | A | C4-C5-C6 | 6.69 | 120.34 | 117.00 |
| 35 | E | 613 | C | N3-C4-N4 | 6.69 | 122.68 | 118.00 |
| 35 | E | 791 | G | C5-C6-O6 | -6.69 | 124.59 | 128.60 |
| 35 | E | 1615 | A | C4-C5-C6 | 6.69 | 120.34 | 117.00 |
| 35 | E | 1768 | A | C5-C6-N1 | -6.68 | 114.36 | 117.70 |
| 35 | E | 1924 | G | C5-C6-O6 | -6.68 | 124.59 | 128.60 |
| 35 | E | 461 | C | N3-C4-N4 | 6.68 | 122.68 | 118.00 |
| 35 | E | 1741 | G | C5-C6-O6 | -6.68 | 124.59 | 128.60 |
| 35 | E | 2020 | G | C5-C6-O6 | -6.68 | 124.59 | 128.60 |
| 35 | E | 591 | G | O4'-C1'-N9 | 6.68 | 113.54 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1805 | G | C5-C6-O6 | -6.68 | 124.59 | 128.60 |
| 35 | E | 1930 | U | O4'-C1'-N1 | 6.68 | 113.54 | 108.20 |
| 35 | E | 1995 | G | C5-C6-O6 | -6.68 | 124.59 | 128.60 |
| 35 | E | 2106 | G | C5-C6-O6 | -6.68 | 124.59 | 128.60 |
| 35 | E | 2311 | G | C5-C6-O6 | -6.67 | 124.60 | 128.60 |
| 35 | E | 69 | C | N3-C4-N4 | 6.67 | 122.67 | 118.00 |
| 35 | E | 70 | U | O4'-C1'-N1 | 6.67 | 113.54 | 108.20 |
| 35 | E | 359 | U | O4'-C1'-N1 | 6.67 | 113.54 | 108.20 |
| 35 | E | 768 | G | C5-C6-O6 | -6.67 | 124.60 | 128.60 |
| 35 | E | 991 | C | O4'-C1'-N1 | 6.67 | 113.53 | 108.20 |
| 35 | E | 2307 | G | C5-C6-O6 | -6.67 | 124.60 | 128.60 |
| 35 | E | 759 | C | N3-C4-C5 | -6.67 | 119.23 | 121.90 |
| 35 | E | 849 | U | O4'-C1'-N1 | 6.67 | 113.53 | 108.20 |
| 35 | E | 982 | G | C5-C6-O6 | -6.67 | 124.60 | 128.60 |
| 35 | E | 224 | C | N3-C4-N4 | 6.67 | 122.67 | 118.00 |
| 35 | E | 236 | C | N3-C4-N4 | 6.66 | 122.67 | 118.00 |
| 35 | E | 1328 | A | C4-C5-C6 | 6.66 | 120.33 | 117.00 |
| 35 | E | 496 | U | O4'-C1'-N1 | 6.66 | 113.53 | 108.20 |
| 35 | E | 1967 | U | O4'-C1'-N1 | 6.66 | 113.53 | 108.20 |
| 35 | E | 213 | G | C5-C6-O6 | -6.66 | 124.61 | 128.60 |
| 35 | E | 1334 | U | O4'-C1'-N1 | 6.66 | 113.53 | 108.20 |
| 35 | E | 1612 | U | O4'-C1'-N1 | 6.66 | 113.53 | 108.20 |
| 35 | E | 1759 | G | C5-C6-O6 | -6.66 | 124.60 | 128.60 |
| 35 | E | 593 | G | C5-C6-O6 | -6.66 | 124.61 | 128.60 |
| 35 | E | 602 | G | C5-C6-O6 | -6.66 | 124.61 | 128.60 |
| 35 | E | 808 | G | C5-C6-O6 | -6.66 | 124.61 | 128.60 |
| 35 | E | 1276 | G | C5-C6-O6 | -6.66 | 124.61 | 128.60 |
| 35 | E | 2269 | G | C5-C6-O6 | -6.66 | 124.61 | 128.60 |
| 35 | E | 2293 | U | O4'-C1'-N1 | 6.66 | 113.52 | 108.20 |
| 35 | E | 1 | G | O4'-C1'-N9 | 6.65 | 113.52 | 108.20 |
| 35 | E | 591 | G | C5-C6-O6 | -6.65 | 124.61 | 128.60 |
| 35 | E | 920 | A | C5-C6-N6 | -6.65 | 118.38 | 123.70 |
| 35 | E | 1174 | C | O4'-C1'-N1 | 6.65 | 113.52 | 108.20 |
| 35 | E | 1214 | G | C5-C6-O6 | -6.65 | 124.61 | 128.60 |
| 35 | E | 1923 | U | O4'-C1'-N1 | 6.65 | 113.52 | 108.20 |
| 35 | E | 1980 | C | N3-C4-N4 | 6.65 | 122.66 | 118.00 |
| 35 | E | 634 | A | C5-C6-N6 | -6.65 | 118.38 | 123.70 |
| 35 | E | 857 | G | O4'-C1'-N9 | 6.65 | 113.52 | 108.20 |
| 35 | E | 181 | A | C4-C5-C6 | 6.65 | 120.32 | 117.00 |
| 35 | E | 1603 | U | O4'-C1'-N1 | 6.64 | 113.51 | 108.20 |
| 35 | E | 609 | A | C4-C5-C6 | 6.64 | 120.32 | 117.00 |
| 35 | E | 634 | A | C4-C5-C6 | 6.64 | 120.32 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 140 | C | O4'-C1'-N1 | 6.64 | 113.51 | 108.20 |
| 35 | E | 2134 | A | C4-C5-C6 | 6.64 | 120.32 | 117.00 |
| 35 | E | 1278 | C | N3-C4-N4 | 6.63 | 122.64 | 118.00 |
| 35 | E | 216 | A | O4'-C1'-N9 | 6.63 | 113.51 | 108.20 |
| 35 | E | 583 | C | O4'-C1'-N1 | 6.63 | 113.51 | 108.20 |
| 35 | E | 726 | C | N3-C4-C5 | -6.63 | 119.25 | 121.90 |
| 35 | E | 701 | C | O4'-C1'-N1 | 6.63 | 113.50 | 108.20 |
| 35 | E | 368 | G | C5-C6-O6 | -6.63 | 124.62 | 128.60 |
| 35 | E | 805 | C | O4'-C1'-N1 | 6.63 | 113.50 | 108.20 |
| 35 | E | 1198 | G | O4'-C1'-N9 | 6.63 | 113.50 | 108.20 |
| 35 | E | 1567 | C | N3-C4-N4 | 6.63 | 122.64 | 118.00 |
| 35 | E | 834 | G | O4'-C1'-N9 | 6.63 | 113.50 | 108.20 |
| 35 | E | 868 | U | O4'-C1'-N1 | 6.63 | 113.50 | 108.20 |
| 35 | E | 1534 | A | C5-C6-N1 | -6.63 | 114.39 | 117.70 |
| 35 | E | 1582 | G | C5-C6-O6 | -6.63 | 124.62 | 128.60 |
| 35 | E | 1590 | G | C5-C6-O6 | -6.63 | 124.62 | 128.60 |
| 35 | E | 2305 | C | O4'-C1'-N1 | 6.63 | 113.50 | 108.20 |
| 35 | E | 375 | C | N3-C4-N4 | 6.62 | 122.64 | 118.00 |
| 35 | E | 1682 | U | O4'-C1'-N1 | 6.62 | 113.50 | 108.20 |
| 35 | E | 2179 | G | C5-C6-O6 | -6.62 | 124.63 | 128.60 |
| 35 | E | 1272 | C | N3-C4-N4 | 6.62 | 122.63 | 118.00 |
| 35 | E | 25 | C | O4'-C1'-N1 | 6.62 | 113.50 | 108.20 |
| 35 | E | 1583 | U | O4'-C1'-N1 | 6.62 | 113.50 | 108.20 |
| 35 | E | 1767 | G | C5-C6-O6 | -6.62 | 124.63 | 128.60 |
| 35 | E | 901 | A | O4'-C1'-N9 | 6.62 | 113.49 | 108.20 |
| 35 | E | 1200 | A | C5-C6-N6 | -6.62 | 118.41 | 123.70 |
| 35 | E | 1551 | G | C5-C6-O6 | -6.62 | 124.63 | 128.60 |
| 35 | E | 1738 | G | C5-C6-O6 | -6.62 | 124.63 | 128.60 |
| 35 | E | 937 | C | O4'-C1'-N1 | 6.61 | 113.49 | 108.20 |
| 35 | E | 965 | C | N3-C4-N4 | 6.61 | 122.63 | 118.00 |
| 35 | E | 1989 | G | C5-C6-O6 | -6.61 | 124.63 | 128.60 |
| 35 | E | 2188 | G | C5-C6-O6 | -6.61 | 124.63 | 128.60 |
| 35 | E | 237 | A | O4'-C1'-N9 | 6.61 | 113.49 | 108.20 |
| 35 | E | 691 | U | O4'-C1'-N1 | 6.61 | 113.49 | 108.20 |
| 35 | E | 1799 | A | C4-C5-C6 | 6.61 | 120.30 | 117.00 |
| 35 | E | 1868 | G | O4'-C1'-N9 | 6.61 | 113.48 | 108.20 |
| 35 | E | 2316 | U | O4'-C1'-N1 | 6.61 | 113.48 | 108.20 |
| 35 | E | 2204 | A | C4-C5-C6 | 6.60 | 120.30 | 117.00 |
| 35 | E | 411 | G | C5-C6-O6 | -6.60 | 124.64 | 128.60 |
| 35 | E | 1545 | U | O4'-C1'-N1 | 6.60 | 113.48 | 108.20 |
| 35 | E | 1643 | U | O4'-C1'-N1 | 6.60 | 113.48 | 108.20 |
| 35 | E | 2054 | G | C5-C6-O6 | -6.60 | 124.64 | 128.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 418 | G | C5-C6-O6 | -6.60 | 124.64 | 128.60 |
| 35 | E | 1318 | U | O4'-C1'-N1 | 6.60 | 113.48 | 108.20 |
| 35 | E | 2092 | A | C5-C6-N6 | -6.60 | 118.42 | 123.70 |
| 35 | E | 524 | G | O4'-C1'-N9 | 6.60 | 113.48 | 108.20 |
| 35 | E | 749 | C | N3-C4-C5 | -6.60 | 119.26 | 121.90 |
| 35 | E | 1276 | G | O4'-C1'-N9 | 6.60 | 113.48 | 108.20 |
| 35 | E | 1659 | U | O4'-C1'-N1 | 6.60 | 113.48 | 108.20 |
| 35 | E | 1688 | C | O4'-C1'-N1 | 6.60 | 113.48 | 108.20 |
| 35 | E | 2147 | U | C2-N1-C1' | 6.60 | 125.62 | 117.70 |
| 35 | E | 843 | U | O4'-C1'-N1 | 6.60 | 113.48 | 108.20 |
| 35 | E | 24 | U | O4'-C1'-N1 | 6.59 | 113.47 | 108.20 |
| 35 | E | 1858 | U | O4'-C1'-N1 | 6.59 | 113.47 | 108.20 |
| 35 | E | 80 | G | C5-C6-O6 | -6.59 | 124.64 | 128.60 |
| 35 | E | 734 | G | C6-C5-N7 | -6.59 | 126.44 | 130.40 |
| 35 | E | 2249 | A | C4-C5-C6 | 6.59 | 120.30 | 117.00 |
| 35 | E | 218 | C | N3-C4-N4 | 6.59 | 122.61 | 118.00 |
| 35 | E | 462 | U | O4'-C1'-N1 | 6.59 | 113.47 | 108.20 |
| 35 | E | 2014 | C | O4'-C1'-N1 | 6.59 | 113.47 | 108.20 |
| 35 | E | 2166 | C | O4'-C1'-N1 | 6.59 | 113.47 | 108.20 |
| 35 | E | 1804 | A | C5-C6-N6 | -6.58 | 118.43 | 123.70 |
| 35 | E | 114 | C | N3-C4-N4 | 6.58 | 122.61 | 118.00 |
| 35 | E | 650 | C | N3-C4-N4 | 6.58 | 122.61 | 118.00 |
| 35 | E | 856 | U | O4'-C1'-N1 | 6.58 | 113.47 | 108.20 |
| 35 | E | 1831 | C | O4'-C1'-N1 | 6.58 | 113.47 | 108.20 |
| 35 | E | 685 | G | C5-C6-O6 | -6.58 | 124.65 | 128.60 |
| 35 | E | 1587 | U | O4'-C1'-N1 | 6.58 | 113.46 | 108.20 |
| 35 | E | 2022 | A | C5-C6-N6 | -6.58 | 118.44 | 123.70 |
| 35 | E | 119 | G | C5-C6-O6 | -6.58 | 124.65 | 128.60 |
| 35 | E | 1300 | C | N3-C4-C5 | -6.58 | 119.27 | 121.90 |
| 35 | E | 87 | C | N3-C4-N4 | 6.58 | 122.60 | 118.00 |
| 35 | E | 1647 | G | C5-C6-O6 | -6.58 | 124.65 | 128.60 |
| 35 | E | 1873 | G | C6-N1-C2 | -6.58 | 121.15 | 125.10 |
| 35 | E | 2079 | G | C5-C6-O6 | -6.58 | 124.65 | 128.60 |
| 35 | E | 743 | C | O4'-C1'-N1 | 6.57 | 113.46 | 108.20 |
| 35 | E | 1848 | U | O4'-C1'-N1 | 6.57 | 113.46 | 108.20 |
| 35 | E | 831 | A | C4-C5-C6 | 6.57 | 120.28 | 117.00 |
| 35 | E | 1669 | G | N1-C6-O6 | 6.57 | 123.84 | 119.90 |
| 35 | E | 832 | G | C5-C6-O6 | -6.57 | 124.66 | 128.60 |
| 35 | E | 1704 | A | C5-C6-N6 | -6.57 | 118.45 | 123.70 |
| 35 | E | 1709 | G | C5-C6-O6 | -6.57 | 124.66 | 128.60 |
| 35 | E | 1964 | U | O4'-C1'-N1 | 6.57 | 113.45 | 108.20 |
| 35 | E | 560 | C | N3-C4-N4 | 6.56 | 122.59 | 118.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 996 | G | O4'-C1'-N9 | 6.56 | 113.45 | 108.20 |
| 35 | E | 1166 | C | N3-C4-N4 | 6.56 | 122.59 | 118.00 |
| 35 | E | 1199 | G | C5-C6-O6 | -6.56 | 124.66 | 128.60 |
| 35 | E | 957 | U | O4'-C1'-N1 | 6.56 | 113.45 | 108.20 |
| 35 | E | 1885 | U | O4'-C1'-N1 | 6.56 | 113.45 | 108.20 |
| 35 | E | 1969 | G | O4'-C1'-N9 | 6.56 | 113.45 | 108.20 |
| 35 | E | 1986 | A | C5-C6-N6 | -6.56 | 118.45 | 123.70 |
| 35 | E | 884 | A | C4-C5-C6 | 6.55 | 120.28 | 117.00 |
| 35 | E | 2068 | C | O4'-C1'-N1 | 6.55 | 113.44 | 108.20 |
| 35 | E | 778 | A | C4-C5-C6 | 6.55 | 120.28 | 117.00 |
| 35 | E | 862 | A | O4'-C1'-N9 | 6.55 | 113.44 | 108.20 |
| 35 | E | 985 | G | C5-C6-O6 | -6.55 | 124.67 | 128.60 |
| 35 | E | 1646 | G | C5-C6-O6 | -6.55 | 124.67 | 128.60 |
| 35 | E | 226 | A | C5-C6-N6 | -6.55 | 118.46 | 123.70 |
| 35 | E | 338 | U | O4'-C1'-N1 | 6.55 | 113.44 | 108.20 |
| 35 | E | 18 | C | N3-C4-N4 | 6.55 | 122.58 | 118.00 |
| 35 | E | 483 | A | C5-C6-N6 | -6.55 | 118.46 | 123.70 |
| 35 | E | 2142 | C | N3-C4-N4 | 6.55 | 122.58 | 118.00 |
| 35 | E | 774 | C | N3-C4-N4 | 6.54 | 122.58 | 118.00 |
| 35 | E | 815 | G | C5-C6-O6 | -6.54 | 124.67 | 128.60 |
| 35 | E | 820 | U | O4'-C1'-N1 | 6.54 | 113.43 | 108.20 |
| 35 | E | 863 | A | C4-C5-C6 | 6.54 | 120.27 | 117.00 |
| 35 | E | 1860 | U | O4'-C1'-N1 | 6.54 | 113.43 | 108.20 |
| 35 | E | 47 | A | C4-C5-C6 | 6.54 | 120.27 | 117.00 |
| 35 | E | 603 | G | C5-C6-O6 | -6.54 | 124.68 | 128.60 |
| 35 | E | 1801 | C | O4'-C1'-N1 | 6.54 | 113.43 | 108.20 |
| 35 | E | 1802 | C | O4'-C1'-N1 | 6.54 | 113.43 | 108.20 |
| 35 | E | 828 | G | C5-C6-O6 | -6.53 | 124.68 | 128.60 |
| 35 | E | 847 | U | O4'-C1'-N1 | 6.53 | 113.42 | 108.20 |
| 35 | E | 596 | A | O4'-C1'-N9 | 6.53 | 113.42 | 108.20 |
| 35 | E | 708 | G | C5-C6-O6 | -6.53 | 124.68 | 128.60 |
| 35 | E | 1249 | G | C5-C6-O6 | -6.53 | 124.68 | 128.60 |
| 35 | E | 1790 | A | C4-C5-C6 | 6.53 | 120.27 | 117.00 |
| 35 | E | 2232 | U | O4'-C1'-N1 | 6.53 | 113.42 | 108.20 |
| 35 | E | 198 | U | O4'-C1'-N1 | 6.53 | 113.42 | 108.20 |
| 35 | E | 445 | G | C5-C6-O6 | -6.53 | 124.68 | 128.60 |
| 35 | E | 2248 | G | C5-C6-O6 | -6.53 | 124.68 | 128.60 |
| 35 | E | 2317 | U | O4'-C1'-N1 | 6.53 | 113.42 | 108.20 |
| 35 | E | 851 | U | O4'-C1'-N1 | 6.53 | 113.42 | 108.20 |
| 35 | E | 1570 | U | O4'-C1'-N1 | 6.52 | 113.42 | 108.20 |
| 35 | E | 2096 | G | C5-C6-O6 | -6.52 | 124.69 | 128.60 |
| 35 | E | 222 | U | O4'-C1'-N1 | 6.52 | 113.42 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 804 | U | O4'-C1'-N1 | 6.52 | 113.42 | 108.20 |
| 35 | E | 1593 | A | C5-C6-N1 | -6.52 | 114.44 | 117.70 |
| 35 | E | 2153 | C | O4'-C1'-N1 | 6.52 | 113.42 | 108.20 |
| 35 | E | 489 | C | N3-C4-N4 | 6.52 | 122.56 | 118.00 |
| 35 | E | 226 | A | C4-C5-C6 | 6.52 | 120.26 | 117.00 |
| 35 | E | 954 | G | C5-C6-O6 | -6.52 | 124.69 | 128.60 |
| 35 | E | 1239 | G | C5-C6-O6 | -6.52 | 124.69 | 128.60 |
| 35 | E | 1637 | G | C5-C6-O6 | -6.52 | 124.69 | 128.60 |
| 35 | E | 2036 | A | C4-C5-C6 | 6.52 | 120.26 | 117.00 |
| 35 | E | 2215 | C | N3-C4-N4 | 6.52 | 122.56 | 118.00 |
| 35 | E | 1192 | A | C4-C5-C6 | 6.52 | 120.26 | 117.00 |
| 35 | E | 1918 | C | N3-C4-N4 | 6.52 | 122.56 | 118.00 |
| 35 | E | 1925 | A | C5-C6-N6 | -6.51 | 118.49 | 123.70 |
| 35 | E | 677 | G | C5-C6-O6 | -6.51 | 124.69 | 128.60 |
| 35 | E | 219 | U | O4'-C1'-N1 | 6.51 | 113.41 | 108.20 |
| 35 | E | 1941 | C | O4'-C1'-N1 | 6.51 | 113.41 | 108.20 |
| 35 | E | 2095 | G | C5-C6-O6 | -6.51 | 124.69 | 128.60 |
| 35 | E | 761 | G | C5-C6-O6 | -6.51 | 124.70 | 128.60 |
| 35 | E | 1852 | G | O4'-C1'-N9 | 6.51 | 113.41 | 108.20 |
| 35 | E | 1882 | G | C5-C6-O6 | -6.51 | 124.70 | 128.60 |
| 35 | E | 1218 | A | C5-C6-N6 | -6.50 | 118.50 | 123.70 |
| 35 | E | 2051 | C | N3-C4-N4 | 6.50 | 122.55 | 118.00 |
| 35 | E | 665 | U | O4'-C1'-N1 | 6.50 | 113.40 | 108.20 |
| 35 | E | 1177 | C | P-O3'-C3' | 6.50 | 127.50 | 119.70 |
| 35 | E | 1212 | G | C5-C6-O6 | -6.50 | 124.70 | 128.60 |
| 35 | E | 2081 | G | C5-C6-O6 | -6.50 | 124.70 | 128.60 |
| 35 | E | 881 | G | C5-C6-O6 | -6.50 | 124.70 | 128.60 |
| 35 | E | 340 | U | O4'-C1'-N1 | 6.50 | 113.40 | 108.20 |
| 35 | E | 1822 | A | C4-C5-C6 | 6.50 | 120.25 | 117.00 |
| 35 | E | 558 | U | O4'-C1'-N1 | 6.50 | 113.40 | 108.20 |
| 35 | E | 1553 | A | C4-C5-C6 | 6.50 | 120.25 | 117.00 |
| 35 | E | 21 | U | O4'-C1'-N1 | 6.50 | 113.40 | 108.20 |
| 35 | E | 577 | A | C4-C5-C6 | 6.49 | 120.25 | 117.00 |
| 35 | E | 1364 | G | O4'-C1'-N9 | 6.49 | 113.39 | 108.20 |
| 35 | E | 696 | G | C5-C6-O6 | -6.49 | 124.71 | 128.60 |
| 35 | E | 2055 | A | C4-C5-C6 | 6.49 | 120.25 | 117.00 |
| 35 | E | 2144 | G | N3-C2-N2 | 6.49 | 124.44 | 119.90 |
| 35 | E | 209 | C | N3-C4-N4 | 6.49 | 122.54 | 118.00 |
| 35 | E | 1711 | G | C5-C6-O6 | -6.49 | 124.71 | 128.60 |
| 35 | E | 2024 | C | O4'-C1'-N1 | 6.49 | 113.39 | 108.20 |
| 35 | E | 17 | C | N3-C4-N4 | 6.49 | 122.54 | 118.00 |
| 35 | E | 660 | U | O4'-C1'-N1 | 6.49 | 113.39 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1525 | C | O4'-C1'-N1 | 6.49 | 113.39 | 108.20 |
| 35 | E | 1615 | A | C5-C6-N6 | -6.49 | 118.51 | 123.70 |
| 35 | E | 1270 | A | C4-C5-C6 | 6.48 | 120.24 | 117.00 |
| 35 | E | 1604 | U | O4'-C1'-N1 | 6.48 | 113.39 | 108.20 |
| 35 | E | 243 | U | O4'-C1'-N1 | 6.48 | 113.39 | 108.20 |
| 35 | E | 333 | C | N3-C4-N4 | 6.48 | 122.54 | 118.00 |
| 35 | E | 477 | G | O4'-C1'-N9 | 6.48 | 113.39 | 108.20 |
| 35 | E | 510 | U | O4'-C1'-N1 | 6.48 | 113.38 | 108.20 |
| 35 | E | 929 | U | O4'-C1'-N1 | 6.48 | 113.38 | 108.20 |
| 35 | E | 1323 | A | C4-C5-C6 | 6.48 | 120.24 | 117.00 |
| 35 | E | 1664 | A | C4-C5-C6 | 6.48 | 120.24 | 117.00 |
| 35 | E | 2043 | G | O4'-C1'-N9 | 6.48 | 113.38 | 108.20 |
| 35 | E | 2132 | U | O4'-C1'-N1 | 6.48 | 113.38 | 108.20 |
| 35 | E | 251 | A | O4'-C1'-N9 | 6.48 | 113.38 | 108.20 |
| 35 | E | 1350 | U | O4'-C1'-N1 | 6.48 | 113.38 | 108.20 |
| 35 | E | 1704 | A | C4-C5-C6 | 6.48 | 120.24 | 117.00 |
| 35 | E | 82 | A | O4'-C1'-N9 | 6.47 | 113.38 | 108.20 |
| 35 | E | 1625 | A | C4-C5-C6 | 6.47 | 120.24 | 117.00 |
| 35 | E | 1850 | C | N3-C4-N4 | 6.47 | 122.53 | 118.00 |
| 35 | E | 1934 | G | C5-C6-O6 | -6.47 | 124.72 | 128.60 |
| 35 | E | 748 | G | P-O3'-C3' | 6.47 | 127.47 | 119.70 |
| 35 | E | 1271 | G | C5-C6-O6 | -6.47 | 124.72 | 128.60 |
| 35 | E | 1865 | A | C4-C5-C6 | 6.47 | 120.24 | 117.00 |
| 35 | E | 2099 | G | O4'-C1'-N9 | 6.47 | 113.38 | 108.20 |
| 35 | E | 1945 | U | O4'-C1'-N1 | 6.47 | 113.38 | 108.20 |
| 35 | E | 2268 | A | C5-C6-N6 | -6.47 | 118.52 | 123.70 |
| 35 | E | 1327 | A | C5-C6-N1 | -6.47 | 114.47 | 117.70 |
| 35 | E | 499 | A | C4-C5-C6 | 6.47 | 120.23 | 117.00 |
| 35 | E | 2223 | U | O4'-C1'-N1 | 6.47 | 113.37 | 108.20 |
| 35 | E | 722 | C | N3-C4-N4 | 6.46 | 122.53 | 118.00 |
| 35 | E | 2076 | A | C4-C5-C6 | 6.46 | 120.23 | 117.00 |
| 35 | E | 83 | U | O4'-C1'-N1 | 6.46 | 113.37 | 108.20 |
| 35 | E | 278 | A | C5-C6-N6 | -6.46 | 118.53 | 123.70 |
| 35 | E | 540 | U | O4'-C1'-N1 | 6.46 | 113.37 | 108.20 |
| 35 | E | 1809 | C | N3-C4-N4 | 6.46 | 122.52 | 118.00 |
| 35 | E | 44 | C | O4'-C1'-N1 | 6.46 | 113.36 | 108.20 |
| 35 | E | 483 | A | C4-C5-C6 | 6.46 | 120.23 | 117.00 |
| 35 | E | 1642 | G | C5-C6-O6 | -6.46 | 124.73 | 128.60 |
| 35 | E | 611 | G | O4'-C1'-N9 | 6.45 | 113.36 | 108.20 |
| 35 | E | 715 | U | O4'-C1'-N1 | 6.45 | 113.36 | 108.20 |
| 35 | E | 1761 | U | O4'-C1'-N1 | 6.45 | 113.36 | 108.20 |
| 35 | E | 2231 | U | O4'-C1'-N1 | 6.45 | 113.36 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1259 | A | C5-C6-N1 | -6.45 | 114.47 | 117.70 |
| 35 | E | 294 | G | C5-C6-O6 | -6.45 | 124.73 | 128.60 |
| 35 | E | 1544 | U | P-O3'-C3' | 6.45 | 127.44 | 119.70 |
| 35 | E | 1866 | A | C5-C6-N1 | -6.45 | 114.47 | 117.70 |
| 35 | E | 1890 | C | N3-C4-N4 | 6.45 | 122.52 | 118.00 |
| 35 | E | 279 | A | C4-C5-C6 | 6.45 | 120.22 | 117.00 |
| 35 | E | 390 | C | N3-C4-N4 | 6.45 | 122.51 | 118.00 |
| 35 | E | 1363 | C | O4'-C1'-N1 | 6.45 | 113.36 | 108.20 |
| 35 | E | 1708 | U | O4'-C1'-N1 | 6.45 | 113.36 | 108.20 |
| 35 | E | 2126 | A | C4-C5-C6 | 6.45 | 120.22 | 117.00 |
| 35 | E | 695 | G | C5-C6-O6 | -6.45 | 124.73 | 128.60 |
| 35 | E | 1262 | C | N3-C4-N4 | 6.45 | 122.51 | 118.00 |
| 35 | E | 183 | C | O4'-C1'-N1 | 6.45 | 113.36 | 108.20 |
| 35 | E | 1541 | U | O4'-C1'-N1 | 6.45 | 113.36 | 108.20 |
| 35 | E | 2125 | C | N3-C4-N4 | 6.45 | 122.51 | 118.00 |
| 35 | E | 2288 | A | C5-C6-N6 | -6.45 | 118.54 | 123.70 |
| 5 | u | 84 | PHE | CB-CG-CD1 | 6.44 | 125.31 | 120.80 |
| 35 | E | 1732 | A | C4-C5-C6 | 6.44 | 120.22 | 117.00 |
| 35 | E | 264 | C | N3-C4-C5 | -6.44 | 119.32 | 121.90 |
| 35 | E | 2048 | A | C4-C5-C6 | 6.44 | 120.22 | 117.00 |
| 35 | E | 940 | U | O4'-C1'-N1 | 6.44 | 113.35 | 108.20 |
| 35 | E | 1343 | A | C4-C5-C6 | 6.44 | 120.22 | 117.00 |
| 35 | E | 682 | G | C5-C6-O6 | -6.44 | 124.74 | 128.60 |
| 35 | E | 769 | A | C4-C5-C6 | 6.44 | 120.22 | 117.00 |
| 35 | E | 1167 | C | O4'-C1'-N1 | 6.44 | 113.35 | 108.20 |
| 35 | E | 1537 | U | O4'-C1'-N1 | 6.44 | 113.35 | 108.20 |
| 35 | E | 206 | C | N3-C4-N4 | 6.44 | 122.50 | 118.00 |
| 35 | E | 1078 | U | P-O3'-C3' | 6.44 | 127.42 | 119.70 |
| 35 | E | 1168 | U | O4'-C1'-N1 | 6.44 | 113.35 | 108.20 |
| 35 | E | 1250 | A | C4-C5-C6 | 6.44 | 120.22 | 117.00 |
| 35 | E | 754 | G | C5-C6-O6 | -6.43 | 124.74 | 128.60 |
| 35 | E | 1988 | U | O4'-C1'-N1 | 6.43 | 113.34 | 108.20 |
| 35 | E | 2152 | C | N3-C4-N4 | 6.43 | 122.50 | 118.00 |
| 35 | E | 519 | G | C5-C6-O6 | -6.43 | 124.74 | 128.60 |
| 35 | E | 739 | G | C5-C6-O6 | -6.43 | 124.74 | 128.60 |
| 35 | E | 923 | A | C5-C6-N6 | -6.43 | 118.56 | 123.70 |
| 35 | E | 1197 | A | C4-C5-C6 | 6.43 | 120.22 | 117.00 |
| 35 | E | 453 | U | O4'-C1'-N1 | 6.43 | 113.34 | 108.20 |
| 35 | E | 756 | G | O4'-C1'-N9 | 6.43 | 113.34 | 108.20 |
| 35 | E | 257 | A | C4-C5-C6 | 6.42 | 120.21 | 117.00 |
| 35 | E | 1376 | G | C5-C6-O6 | -6.42 | 124.75 | 128.60 |
| 35 | E | 271 | C | N3-C4-N4 | 6.42 | 122.50 | 118.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 989 | G | C5-C6-O6 | -6.42 | 124.75 | 128.60 |
| 35 | E | 1921 | G | O4'-C1'-N9 | 6.42 | 113.34 | 108.20 |
| 35 | E | 9 | U | O4'-C1'-N1 | 6.42 | 113.34 | 108.20 |
| 35 | E | 96 | C | N3-C4-N4 | 6.42 | 122.50 | 118.00 |
| 35 | E | 1186 | U | O4'-C1'-N1 | 6.42 | 113.34 | 108.20 |
| 35 | E | 1965 | U | O4'-C1'-N1 | 6.42 | 113.34 | 108.20 |
| 35 | E | 2251 | A | C5-C6-N6 | -6.42 | 118.56 | 123.70 |
| 35 | E | 1351 | C | N3-C4-N4 | 6.42 | 122.49 | 118.00 |
| 35 | E | 1360 | A | C4-C5-C6 | 6.42 | 120.21 | 117.00 |
| 35 | E | 2277 | C | N3-C4-N4 | 6.42 | 122.49 | 118.00 |
| 35 | E | 1524 | U | O4'-C1'-N1 | 6.42 | 113.33 | 108.20 |
| 35 | E | 2052 | C | C1'-O4'-C4' | -6.42 | 104.77 | 109.90 |
| 35 | E | 328 | U | O4'-C1'-N1 | 6.42 | 113.33 | 108.20 |
| 35 | E | 1952 | U | O4'-C1'-N1 | 6.42 | 113.33 | 108.20 |
| 35 | E | 1748 | C | N3-C4-N4 | 6.41 | 122.49 | 118.00 |
| 35 | E | 1821 | C | O4'-C1'-N1 | 6.41 | 113.33 | 108.20 |
| 35 | E | 105 | A | C4-C5-C6 | 6.41 | 120.20 | 117.00 |
| 35 | E | 521 | A | C4-C5-C6 | 6.41 | 120.20 | 117.00 |
| 35 | E | 2218 | U | O4'-C1'-N1 | 6.41 | 113.33 | 108.20 |
| 35 | E | 2281 | A | C5-C6-N6 | -6.41 | 118.57 | 123.70 |
| 35 | E | 1074 | C | N3-C4-N4 | 6.41 | 122.49 | 118.00 |
| 35 | E | 1676 | A | C4-C5-C6 | 6.41 | 120.20 | 117.00 |
| 35 | E | 2306 | A | C4-C5-C6 | 6.41 | 120.20 | 117.00 |
| 35 | E | 1797 | A | C4-C5-C6 | 6.41 | 120.20 | 117.00 |
| 35 | E | 2003 | G | C5-C6-O6 | -6.41 | 124.76 | 128.60 |
| 35 | E | 73 | A | C5-C6-N6 | -6.40 | 118.58 | 123.70 |
| 35 | E | 81 | A | C4-C5-C6 | 6.40 | 120.20 | 117.00 |
| 35 | E | 284 | C | O4'-C1'-N1 | 6.40 | 113.32 | 108.20 |
| 35 | E | 689 | A | C4-C5-C6 | 6.40 | 120.20 | 117.00 |
| 35 | E | 699 | C | N3-C4-N4 | 6.40 | 122.48 | 118.00 |
| 35 | E | 337 | G | C5-C6-O6 | -6.40 | 124.76 | 128.60 |
| 35 | E | 1974 | C | C6-N1-C1' | -6.40 | 113.12 | 120.80 |
| 35 | E | 371 | A | C4-C5-C6 | 6.40 | 120.20 | 117.00 |
| 35 | E | 1927 | A | C4-C5-C6 | 6.40 | 120.20 | 117.00 |
| 35 | E | 1078 | U | O4'-C1'-N1 | 6.39 | 113.32 | 108.20 |
| 35 | E | 738 | G | N1-C2-N3 | -6.39 | 120.06 | 123.90 |
| 35 | E | 1649 | U | O4'-C1'-N1 | 6.39 | 113.31 | 108.20 |
| 35 | E | 2077 | C | O4'-C1'-N1 | 6.39 | 113.31 | 108.20 |
| 35 | E | 2114 | U | C6-N1-C1' | -6.39 | 112.25 | 121.20 |
| 35 | E | 568 | G | O4'-C1'-N9 | 6.39 | 113.31 | 108.20 |
| 35 | E | 1601 | A | C4-C5-C6 | 6.39 | 120.20 | 117.00 |
| 35 | E | 2035 | A | C4-C5-C6 | 6.39 | 120.20 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1171 | C | N3-C4-N4 | 6.39 | 122.47 | 118.00 |
| 35 | E | 1261 | A | C5-C6-N6 | -6.39 | 118.59 | 123.70 |
| 35 | E | 1374 | A | C5-C6-N6 | -6.39 | 118.59 | 123.70 |
| 35 | E | 2164 | U | O4'-C1'-N1 | 6.39 | 113.31 | 108.20 |
| 35 | E | 307 | C | O4'-C1'-N1 | 6.39 | 113.31 | 108.20 |
| 35 | E | 538 | A | C5-C6-N6 | -6.39 | 118.59 | 123.70 |
| 35 | E | 1962 | U | O4'-C1'-N1 | 6.39 | 113.31 | 108.20 |
| 35 | E | 875 | A | C4-C5-C6 | 6.39 | 120.19 | 117.00 |
| 35 | E | 1554 | A | C5-C6-N6 | -6.39 | 118.59 | 123.70 |
| 35 | E | 2150 | G | O4'-C1'-N9 | 6.39 | 113.31 | 108.20 |
| 35 | E | 2286 | G | C5-C6-O6 | -6.39 | 124.77 | 128.60 |
| 35 | E | 711 | A | O3'-P-O5' | -6.38 | 91.87 | 104.00 |
| 35 | E | 1790 | A | C5-C6-N6 | -6.38 | 118.59 | 123.70 |
| 35 | E | 776 | G | P-O5'-C5' | 6.38 | 131.11 | 120.90 |
| 35 | E | 713 | G | O4'-C1'-N9 | 6.38 | 113.31 | 108.20 |
| 35 | E | 1785 | C | N3-C4-N4 | 6.38 | 122.47 | 118.00 |
| 35 | E | 1374 | A | C4-C5-C6 | 6.38 | 120.19 | 117.00 |
| 35 | E | 1732 | A | C5-C6-N6 | -6.38 | 118.60 | 123.70 |
| 35 | E | 672 | U | O4'-C1'-N1 | 6.38 | 113.30 | 108.20 |
| 35 | E | 744 | C | C6-N1-C2 | -6.38 | 117.75 | 120.30 |
| 35 | E | 526 | A | C5-C6-N6 | -6.38 | 118.60 | 123.70 |
| 35 | E | 641 | C | N3-C4-N4 | 6.38 | 122.46 | 118.00 |
| 35 | E | 1870 | G | O4'-C1'-N9 | 6.38 | 113.30 | 108.20 |
| 35 | E | 476 | G | C5-C6-O6 | -6.37 | 124.78 | 128.60 |
| 35 | E | 589 | U | O4'-C1'-N1 | 6.37 | 113.30 | 108.20 |
| 35 | E | 1533 | U | O4'-C1'-N1 | 6.37 | 113.30 | 108.20 |
| 35 | E | 2279 | U | O4'-C1'-N1 | 6.37 | 113.30 | 108.20 |
| 25 | i | 116 | PHE | CB-CG-CD2 | -6.37 | 116.34 | 120.80 |
| 35 | E | 1527 | G | C5-C6-O6 | -6.37 | 124.78 | 128.60 |
| 35 | E | 100 | A | C4-C5-C6 | 6.37 | 120.18 | 117.00 |
| 35 | E | 468 | G | C5-C6-O6 | -6.37 | 124.78 | 128.60 |
| 35 | E | 484 | A | C4-C5-C6 | 6.37 | 120.18 | 117.00 |
| 35 | E | 2001 | A | C5-C6-N6 | -6.37 | 118.61 | 123.70 |
| 1 | p | 105 | PHE | CB-CG-CD2 | 6.36 | 125.25 | 120.80 |
| 35 | E | 2214 | A | C4-C5-C6 | 6.36 | 120.18 | 117.00 |
| 35 | E | 131 | C | N3-C4-N4 | 6.36 | 122.45 | 118.00 |
| 35 | E | 285 | A | O4'-C1'-N9 | 6.36 | 113.29 | 108.20 |
| 35 | E | 423 | C | N3-C4-N4 | 6.36 | 122.45 | 118.00 |
| 35 | E | 2083 | A | C4-C5-C6 | 6.36 | 120.18 | 117.00 |
| 35 | E | 502 | A | C4-C5-C6 | 6.36 | 120.18 | 117.00 |
| 35 | E | 1244 | U | O4'-C1'-N1 | 6.36 | 113.29 | 108.20 |
| 35 | E | 1734 | U | O4'-C1'-N1 | 6.36 | 113.29 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1775 | U | C2-N1-C1' | 6.36 | 125.33 | 117.70 |
| 35 | E | 1887 | U | C3'-C2'-C1' | 6.36 | 106.59 | 101.50 |
| 35 | E | 576 | A | C4-C5-C6 | 6.36 | 120.18 | 117.00 |
| 35 | E | 2022 | A | C4-C5-C6 | 6.36 | 120.18 | 117.00 |
| 35 | E | 2040 | G | C5-C6-O6 | -6.36 | 124.78 | 128.60 |
| 35 | E | 537 | C | N3-C4-N4 | 6.36 | 122.45 | 118.00 |
| 35 | E | 1201 | G | C5-C6-O6 | -6.36 | 124.79 | 128.60 |
| 35 | E | 1282 | C | N3-C4-N4 | 6.36 | 122.45 | 118.00 |
| 35 | E | 2004 | A | C5-C6-N6 | -6.36 | 118.61 | 123.70 |
| 35 | E | 525 | A | C4-C5-C6 | 6.35 | 120.18 | 117.00 |
| 35 | E | 2042 | G | C5-C6-O6 | -6.35 | 124.79 | 128.60 |
| 35 | E | 1179 | C | N3-C4-C5 | -6.35 | 119.36 | 121.90 |
| 35 | E | 1689 | A | C4-C5-C6 | 6.35 | 120.18 | 117.00 |
| 35 | E | 2246 | C | N3-C4-N4 | 6.35 | 122.45 | 118.00 |
| 35 | E | 447 | A | C4-C5-C6 | 6.35 | 120.17 | 117.00 |
| 35 | E | 105 | A | C5-C6-N6 | -6.35 | 118.62 | 123.70 |
| 35 | E | 225 | C | N3-C4-N4 | 6.35 | 122.44 | 118.00 |
| 35 | E | 153 | C | N3-C4-N4 | 6.34 | 122.44 | 118.00 |
| 35 | E | 515 | C | N3-C4-N4 | 6.34 | 122.44 | 118.00 |
| 35 | E | 151 | A | O4'-C1'-N9 | 6.34 | 113.27 | 108.20 |
| 35 | E | 1248 | A | C4-C5-C6 | 6.34 | 120.17 | 117.00 |
| 35 | E | 527 | A | C4-C5-C6 | 6.34 | 120.17 | 117.00 |
| 35 | E | 626 | C | N3-C4-N4 | 6.34 | 122.44 | 118.00 |
| 35 | E | 1815 | A | C4-C5-C6 | 6.34 | 120.17 | 117.00 |
| 35 | E | 721 | C | N3-C4-N4 | 6.34 | 122.44 | 118.00 |
| 35 | E | 1787 | U | O4'-C1'-N1 | 6.34 | 113.27 | 108.20 |
| 35 | E | 1940 | G | O4'-C1'-N9 | 6.34 | 113.27 | 108.20 |
| 35 | E | 920 | A | C4-C5-C6 | 6.34 | 120.17 | 117.00 |
| 35 | E | 191 | U | O4'-C1'-N1 | 6.34 | 113.27 | 108.20 |
| 35 | E | 278 | A | C4-C5-C6 | 6.34 | 120.17 | 117.00 |
| 35 | E | 774 | C | N3-C4-C5 | -6.34 | 119.37 | 121.90 |
| 35 | E | 1321 | G | O4'-C1'-N9 | 6.34 | 113.27 | 108.20 |
| 35 | E | 1611 | A | C4-C5-C6 | 6.33 | 120.17 | 117.00 |
| 35 | E | 19 | A | O4'-C1'-N9 | 6.33 | 113.27 | 108.20 |
| 35 | E | 1336 | A | C5-C6-N6 | -6.33 | 118.63 | 123.70 |
| 35 | E | 1751 | U | O4'-C1'-N1 | 6.33 | 113.27 | 108.20 |
| 35 | E | 2020 | G | P-O3'-C3' | 6.33 | 127.30 | 119.70 |
| 35 | E | 2294 | A | C4-C5-C6 | 6.33 | 120.17 | 117.00 |
| 35 | E | 867 | G | C5-C6-O6 | -6.33 | 124.80 | 128.60 |
| 35 | E | 1986 | A | C4-C5-C6 | 6.33 | 120.17 | 117.00 |
| 35 | E | 82 | A | C4-C5-C6 | 6.33 | 120.17 | 117.00 |
| 35 | E | 1242 | A | C4-C5-C6 | 6.33 | 120.17 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1792 | G | C5-C6-O6 | -6.33 | 124.80 | 128.60 |
| 35 | E | 732 | C | O4'-C1'-N1 | 6.33 | 113.26 | 108.20 |
| 35 | E | 1207 | U | O4'-C1'-N1 | 6.33 | 113.26 | 108.20 |
| 35 | E | 1791 | C | N3-C4-N4 | 6.33 | 122.43 | 118.00 |
| 35 | E | 2077 | C | N3-C4-N4 | 6.33 | 122.43 | 118.00 |
| 35 | E | 864 | A | C5-C6-N6 | -6.33 | 118.64 | 123.70 |
| 35 | E | 1359 | C | O4'-C1'-N1 | 6.33 | 113.26 | 108.20 |
| 35 | E | 2301 | C | N3-C4-N4 | 6.33 | 122.43 | 118.00 |
| 35 | E | 381 | A | C4-C5-C6 | 6.33 | 120.16 | 117.00 |
| 35 | E | 437 | G | C5-C6-O6 | -6.33 | 124.81 | 128.60 |
| 35 | E | 1319 | G | O4'-C1'-N9 | 6.33 | 113.26 | 108.20 |
| 35 | E | 2008 | A | C4-C5-C6 | 6.33 | 120.16 | 117.00 |
| 35 | E | 927 | U | O4'-C1'-N1 | 6.32 | 113.26 | 108.20 |
| 35 | E | 1293 | C | N3-C4-N4 | 6.32 | 122.42 | 118.00 |
| 35 | E | 935 | A | C4-C5-C6 | 6.32 | 120.16 | 117.00 |
| 35 | E | 1320 | G | O4'-C1'-N9 | 6.32 | 113.26 | 108.20 |
| 35 | E | 1903 | A | C5'-C4'-C3' | 6.32 | 126.11 | 116.00 |
| 35 | E | 2024 | C | N3-C4-N4 | 6.32 | 122.42 | 118.00 |
| 35 | E | 506 | A | C4-C5-C6 | 6.32 | 120.16 | 117.00 |
| 35 | E | 1638 | G | C5-C6-O6 | -6.32 | 124.81 | 128.60 |
| 35 | E | 2110 | A | C4-C5-C6 | 6.32 | 120.16 | 117.00 |
| 35 | E | 130 | G | O4'-C1'-N9 | 6.32 | 113.25 | 108.20 |
| 35 | E | 480 | C | N3-C4-N4 | 6.32 | 122.42 | 118.00 |
| 35 | E | 936 | C | N3-C4-N4 | 6.32 | 122.42 | 118.00 |
| 35 | E | 1330 | A | C4-C5-C6 | 6.32 | 120.16 | 117.00 |
| 35 | E | 221 | C | N3-C4-N4 | 6.32 | 122.42 | 118.00 |
| 35 | E | 586 | A | C4-C5-C6 | 6.32 | 120.16 | 117.00 |
| 35 | E | 1187 | C | O3'-P-O5' | 6.32 | 116.00 | 104.00 |
| 35 | E | 933 | C | N3-C4-N4 | 6.31 | 122.42 | 118.00 |
| 35 | E | 1202 | G | C5-C6-O6 | -6.31 | 124.81 | 128.60 |
| 35 | E | 1273 | G | C5-C6-O6 | -6.31 | 124.81 | 128.60 |
| 35 | E | 2255 | C | N3-C4-N4 | 6.31 | 122.42 | 118.00 |
| 35 | E | 1 | G | C5-C6-O6 | -6.31 | 124.81 | 128.60 |
| 35 | E | 1707 | U | O4'-C1'-N1 | 6.31 | 113.25 | 108.20 |
| 35 | E | 2148 | A | O4'-C1'-N9 | 6.31 | 113.25 | 108.20 |
| 35 | E | 2191 | G | C5-C6-O6 | -6.31 | 124.81 | 128.60 |
| 35 | E | 1686 | G | C5-C6-O6 | -6.31 | 124.81 | 128.60 |
| 35 | E | 1294 | C | N3-C4-N4 | 6.31 | 122.42 | 118.00 |
| 35 | E | 1560 | G | C5-C6-O6 | -6.31 | 124.81 | 128.60 |
| 35 | E | 1561 | A | C4-C5-C6 | 6.31 | 120.15 | 117.00 |
| 35 | E | 996 | G | P-O3'-C3' | -6.31 | 112.13 | 119.70 |
| 35 | E | 1269 | C | N3-C4-N4 | 6.30 | 122.41 | 118.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1828 | G | C5-C6-O6 | -6.30 | 124.82 | 128.60 |
| 35 | E | 2239 | A | C4-C5-C6 | 6.30 | 120.15 | 117.00 |
| 35 | E | 159 | G | C5-C6-O6 | -6.30 | 124.82 | 128.60 |
| 35 | E | 900 | A | C4-C5-C6 | 6.30 | 120.15 | 117.00 |
| 35 | E | 1534 | A | C5-C6-N6 | -6.30 | 118.66 | 123.70 |
| 35 | E | 2234 | A | O4'-C1'-N9 | 6.30 | 113.24 | 108.20 |
| 35 | E | 144 | A | C4-C5-C6 | 6.30 | 120.15 | 117.00 |
| 35 | E | 984 | A | O4'-C1'-N9 | 6.30 | 113.24 | 108.20 |
| 35 | E | 2258 | C | N3-C4-N4 | 6.30 | 122.41 | 118.00 |
| 35 | E | 2115 | C | N3-C4-N4 | 6.29 | 122.41 | 118.00 |
| 35 | E | 312 | C | N3-C4-N4 | 6.29 | 122.41 | 118.00 |
| 35 | E | 1225 | G | O4'-C1'-N9 | 6.29 | 113.23 | 108.20 |
| 35 | E | 2058 | C | N3-C4-N4 | 6.29 | 122.41 | 118.00 |
| 35 | E | 454 | A | C5-C6-N1 | -6.29 | 114.55 | 117.70 |
| 35 | E | 1706 | A | C5-C6-N1 | -6.29 | 114.56 | 117.70 |
| 35 | E | 1703 | C | N3-C4-N4 | 6.29 | 122.40 | 118.00 |
| 35 | E | 1958 | U | O4'-C1'-N1 | 6.29 | 113.23 | 108.20 |
| 35 | E | 509 | A | C4-C5-C6 | 6.29 | 120.14 | 117.00 |
| 35 | E | 1189 | A | C4-C5-C6 | 6.29 | 120.14 | 117.00 |
| 35 | E | 1568 | A | C4-C5-C6 | 6.29 | 120.14 | 117.00 |
| 35 | E | 1937 | A | C4-C5-C6 | 6.29 | 120.14 | 117.00 |
| 35 | E | 264 | C | N3-C4-N4 | 6.29 | 122.40 | 118.00 |
| 35 | E | 647 | A | C5-C6-N6 | -6.29 | 118.67 | 123.70 |
| 35 | E | 68 | A | C4-C5-C6 | 6.28 | 120.14 | 117.00 |
| 35 | E | 548 | C | N3-C4-N4 | 6.28 | 122.40 | 118.00 |
| 35 | E | 674 | A | C4-C5-C6 | 6.28 | 120.14 | 117.00 |
| 35 | E | 2129 | U | O4'-C1'-N1 | 6.28 | 113.23 | 108.20 |
| 35 | E | 954 | G | C5-C6-N1 | -6.28 | 108.36 | 111.50 |
| 35 | E | 1878 | A | C4-C5-C6 | 6.28 | 120.14 | 117.00 |
| 35 | E | 55 | A | C4-C5-C6 | 6.28 | 120.14 | 117.00 |
| 35 | E | 873 | C | C6-N1-C1' | -6.28 | 113.26 | 120.80 |
| 35 | E | 1190 | G | C5-C6-O6 | -6.28 | 124.83 | 128.60 |
| 35 | E | 2002 | A | C5-C6-N6 | -6.28 | 118.68 | 123.70 |
| 35 | E | 96 | C | O4'-C1'-N1 | 6.28 | 113.22 | 108.20 |
| 35 | E | 261 | A | O4'-C1'-N9 | 6.28 | 113.22 | 108.20 |
| 35 | E | 357 | C | N3-C4-N4 | 6.28 | 122.39 | 118.00 |
| 35 | E | 2131 | A | C4-C5-C6 | 6.28 | 120.14 | 117.00 |
| 35 | E | 2274 | A | C4-C5-C6 | 6.28 | 120.14 | 117.00 |
| 35 | E | 161 | A | C4-C5-C6 | 6.28 | 120.14 | 117.00 |
| 35 | E | 383 | U | O4'-C1'-N1 | 6.28 | 113.22 | 108.20 |
| 35 | E | 1265 | A | C4-C5-C6 | 6.28 | 120.14 | 117.00 |
| 35 | E | 2085 | U | O4'-C1'-N1 | 6.28 | 113.22 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 358 | C | N3-C4-N4 | 6.27 | 122.39 | 118.00 |
| 35 | E | 472 | A | C5-C6-N6 | -6.27 | 118.68 | 123.70 |
| 35 | E | 1960 | A | C4-C5-C6 | 6.27 | 120.14 | 117.00 |
| 35 | E | 1552 | A | C4-C5-C6 | 6.27 | 120.14 | 117.00 |
| 35 | E | 2124 | G | C5-C6-O6 | -6.27 | 124.84 | 128.60 |
| 35 | E | 1641 | C | N3-C4-N4 | 6.27 | 122.39 | 118.00 |
| 35 | E | 1832 | A | C4-C5-C6 | 6.27 | 120.14 | 117.00 |
| 35 | E | 43 | A | C4-C5-C6 | 6.27 | 120.13 | 117.00 |
| 35 | E | 297 | U | O4'-C1'-N1 | 6.27 | 113.21 | 108.20 |
| 35 | E | 784 | A | C4-C5-C6 | 6.27 | 120.13 | 117.00 |
| 35 | E | 111 | A | C5-C6-N6 | -6.27 | 118.69 | 123.70 |
| 35 | E | 2245 | A | C5-C6-N6 | -6.27 | 118.69 | 123.70 |
| 35 | E | 232 | C | N3-C4-N4 | 6.26 | 122.39 | 118.00 |
| 35 | E | 345 | A | C4-C5-C6 | 6.26 | 120.13 | 117.00 |
| 35 | E | 596 | A | C4-C5-C6 | 6.26 | 120.13 | 117.00 |
| 35 | E | 906 | U | O4'-C1'-N1 | 6.26 | 113.21 | 108.20 |
| 35 | E | 1589 | C | N3-C4-N4 | 6.26 | 122.39 | 118.00 |
| 35 | E | 2119 | U | O4'-C1'-N1 | 6.26 | 113.21 | 108.20 |
| 35 | E | 2120 | A | C4-C5-C6 | 6.26 | 120.13 | 117.00 |
| 35 | E | 62 | A | C4-C5-C6 | 6.26 | 120.13 | 117.00 |
| 35 | E | 587 | A | C4-C5-C6 | 6.26 | 120.13 | 117.00 |
| 35 | E | 49 | C | N3-C4-N4 | 6.26 | 122.38 | 118.00 |
| 35 | E | 54 | C | N3-C4-N4 | 6.26 | 122.38 | 118.00 |
| 35 | E | 239 | C | N3-C4-N4 | 6.26 | 122.38 | 118.00 |
| 35 | E | 1223 | C | N3-C4-N4 | 6.26 | 122.38 | 118.00 |
| 35 | E | 1596 | G | C5-C6-O6 | -6.26 | 124.84 | 128.60 |
| 5 | u | 84 | PHE | CB-CG-CD2 | -6.26 | 116.42 | 120.80 |
| 35 | E | 104 | C | N3-C4-N4 | 6.26 | 122.38 | 118.00 |
| 35 | E | 373 | G | C5-C6-O6 | -6.26 | 124.85 | 128.60 |
| 35 | E | 735 | A | C6-N1-C2 | -6.26 | 114.85 | 118.60 |
| 35 | E | 1246 | U | O4'-C1'-N1 | 6.26 | 113.21 | 108.20 |
| 35 | E | 1650 | U | O4'-C1'-N1 | 6.26 | 113.21 | 108.20 |
| 35 | E | 1884 | U | P-O3'-C3' | 6.26 | 127.21 | 119.70 |
| 35 | E | 78 | A | C4-C5-C6 | 6.25 | 120.13 | 117.00 |
| 35 | E | 251 | A | C5-C6-N6 | -6.25 | 118.70 | 123.70 |
| 35 | E | 1571 | C | N3-C4-N4 | 6.25 | 122.38 | 118.00 |
| 35 | E | 1673 | U | O4'-C1'-N1 | 6.25 | 113.20 | 108.20 |
| 35 | E | 1951 | A | C5-C6-N6 | -6.25 | 118.70 | 123.70 |
| 35 | E | 434 | A | C5-C6-N6 | -6.25 | 118.70 | 123.70 |
| 35 | E | 444 | A | C4-C5-C6 | 6.25 | 120.13 | 117.00 |
| 35 | E | 833 | A | C4-C5-C6 | 6.25 | 120.13 | 117.00 |
| 35 | E | 1611 | A | C5-C6-N1 | -6.25 | 114.58 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1939 | A | C4-C5-C6 | 6.25 | 120.12 | 117.00 |
| 35 | E | 2137 | C | N3-C4-N4 | 6.25 | 122.38 | 118.00 |
| 35 | E | 216 | A | C4-C5-C6 | 6.25 | 120.12 | 117.00 |
| 35 | E | 478 | C | N3-C4-N4 | 6.25 | 122.37 | 118.00 |
| 35 | E | 750 | C | N3-C4-N4 | 6.25 | 122.37 | 118.00 |
| 35 | E | 1532 | U | O4'-C1'-N1 | 6.25 | 113.20 | 108.20 |
| 35 | E | 1710 | A | C4-C5-C6 | 6.25 | 120.12 | 117.00 |
| 35 | E | 1859 | U | O4'-C1'-N1 | 6.25 | 113.20 | 108.20 |
| 35 | E | 2229 | A | C4-C5-C6 | 6.25 | 120.12 | 117.00 |
| 35 | E | 1252 | C | N3-C4-N4 | 6.24 | 122.37 | 118.00 |
| 35 | E | 1818 | A | C5-C6-N1 | -6.24 | 114.58 | 117.70 |
| 35 | E | 281 | A | C4-C5-C6 | 6.24 | 120.12 | 117.00 |
| 35 | E | 2216 | A | C5-C6-N1 | -6.24 | 114.58 | 117.70 |
| 35 | E | 1310 | C | N3-C4-N4 | 6.24 | 122.37 | 118.00 |
| 35 | E | 2186 | C | N3-C4-N4 | 6.24 | 122.37 | 118.00 |
| 35 | E | 2238 | A | C4-C5-C6 | 6.24 | 120.12 | 117.00 |
| 35 | E | 339 | C | N3-C4-N4 | 6.24 | 122.37 | 118.00 |
| 35 | E | 386 | A | C4-C5-C6 | 6.24 | 120.12 | 117.00 |
| 35 | E | 475 | A | C5-C6-N6 | -6.24 | 118.71 | 123.70 |
| 35 | E | 713 | G | C5-C6-O6 | -6.24 | 124.86 | 128.60 |
| 35 | E | 1360 | A | C5-C6-N6 | -6.23 | 118.71 | 123.70 |
| 35 | E | 2221 | A | C5-C6-N6 | -6.23 | 118.71 | 123.70 |
| 35 | E | 777 | A | C4-C5-C6 | 6.23 | 120.12 | 117.00 |
| 35 | E | 1313 | A | O4'-C1'-N9 | 6.23 | 113.19 | 108.20 |
| 35 | E | 1847 | C | N3-C4-N4 | 6.23 | 122.36 | 118.00 |
| 35 | E | 235 | C | N3-C4-N4 | 6.23 | 122.36 | 118.00 |
| 35 | E | 872 | A | C4-C5-C6 | 6.23 | 120.11 | 117.00 |
| 35 | E | 1586 | G | C5-C6-O6 | -6.23 | 124.86 | 128.60 |
| 35 | E | 1196 | A | C5-C6-N1 | -6.23 | 114.59 | 117.70 |
| 35 | E | 1336 | A | C4-C5-C6 | 6.22 | 120.11 | 117.00 |
| 35 | E | 2075 | G | O4'-C1'-N9 | 6.22 | 113.18 | 108.20 |
| 35 | E | 501 | A | C4-C5-C6 | 6.22 | 120.11 | 117.00 |
| 35 | E | 1585 | C | N3-C4-N4 | 6.22 | 122.36 | 118.00 |
| 35 | E | 491 | C | O4'-C1'-N1 | 6.22 | 113.18 | 108.20 |
| 35 | E | 166 | C | N3-C4-N4 | 6.22 | 122.35 | 118.00 |
| 35 | E | 250 | A | C4-C5-C6 | 6.22 | 120.11 | 117.00 |
| 35 | E | 1259 | A | C4-C5-C6 | 6.22 | 120.11 | 117.00 |
| 35 | E | 2189 | A | C5-C6-N1 | -6.22 | 114.59 | 117.70 |
| 35 | E | 503 | A | C4-C5-C6 | 6.22 | 120.11 | 117.00 |
| 35 | E | 808 | G | O4'-C1'-N9 | 6.22 | 113.17 | 108.20 |
| 35 | E | 911 | U | O4'-C1'-N1 | 6.22 | 113.17 | 108.20 |
| 35 | E | 1660 | C | O4'-C1'-N1 | 6.22 | 113.17 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1861 | A | C4-C5-C6 | 6.22 | 120.11 | 117.00 |
| 35 | E | 149 | A | C4-C5-C6 | 6.21 | 120.11 | 117.00 |
| 35 | E | 840 | C | N3-C4-N4 | 6.21 | 122.35 | 118.00 |
| 35 | E | 1549 | G | O4'-C1'-N9 | 6.21 | 113.17 | 108.20 |
| 35 | E | 2 | A | O4'-C1'-N9 | 6.21 | 113.17 | 108.20 |
| 35 | E | 1662 | A | C4-C5-C6 | 6.21 | 120.11 | 117.00 |
| 35 | E | 658 | A | C5-C6-N6 | -6.21 | 118.73 | 123.70 |
| 35 | E | 894 | A | C4-C5-C6 | 6.21 | 120.10 | 117.00 |
| 35 | E | 2199 | A | C4-C5-C6 | 6.21 | 120.11 | 117.00 |
| 4 | t | 60 | ALA | N-CA-CB | 6.21 | 118.79 | 110.10 |
| 35 | E | 1193 | A | C4-C5-C6 | 6.21 | 120.10 | 117.00 |
| 35 | E | 1305 | A | C5-C6-N1 | -6.21 | 114.60 | 117.70 |
| 35 | E | 64 | A | C4-C5-C6 | 6.20 | 120.10 | 117.00 |
| 35 | E | 162 | A | C5-C6-N1 | -6.20 | 114.60 | 117.70 |
| 35 | E | 785 | A | C4-C5-C6 | 6.20 | 120.10 | 117.00 |
| 35 | E | 1268 | A | C5-C6-N6 | -6.20 | 118.74 | 123.70 |
| 35 | E | 1865 | A | C5-C6-N6 | -6.20 | 118.74 | 123.70 |
| 35 | E | 504 | A | C4-C5-C6 | 6.20 | 120.10 | 117.00 |
| 35 | E | 561 | A | C4-C5-C6 | 6.20 | 120.10 | 117.00 |
| 35 | E | 457 | A | C5-C6-N6 | -6.20 | 118.74 | 123.70 |
| 35 | E | 705 | G | O4'-C1'-N9 | 6.20 | 113.16 | 108.20 |
| 35 | E | 936 | C | N3-C4-C5 | -6.20 | 119.42 | 121.90 |
| 35 | E | 1286 | A | C5-C6-N1 | -6.20 | 114.60 | 117.70 |
| 35 | E | 1342 | C | N3-C4-N4 | 6.20 | 122.34 | 118.00 |
| 35 | E | 1539 | A | C4-C5-C6 | 6.20 | 120.10 | 117.00 |
| 35 | E | 588 | A | C4-C5-C6 | 6.20 | 120.10 | 117.00 |
| 35 | E | 645 | A | C4-C5-C6 | 6.20 | 120.10 | 117.00 |
| 35 | E | 658 | A | C4-C5-C6 | 6.20 | 120.10 | 117.00 |
| 35 | E | 829 | C | O4'-C1'-N1 | 6.20 | 113.16 | 108.20 |
| 35 | E | 959 | A | C4-C5-C6 | 6.20 | 120.10 | 117.00 |
| 35 | E | 2182 | G | O4'-C1'-N9 | 6.20 | 113.16 | 108.20 |
| 35 | E | 1825 | A | C5-C6-N1 | -6.20 | 114.60 | 117.70 |
| 35 | E | 381 | A | C5-C6-N6 | -6.20 | 118.74 | 123.70 |
| 35 | E | 694 | A | C4-C5-C6 | 6.20 | 120.10 | 117.00 |
| 35 | E | 905 | A | C5-C6-N1 | -6.20 | 114.60 | 117.70 |
| 35 | E | 942 | C | C6-N1-C1' | -6.20 | 113.36 | 120.80 |
| 35 | E | 2026 | A | C4-C5-C6 | 6.20 | 120.10 | 117.00 |
| 35 | E | 759 | C | N3-C4-N4 | 6.19 | 122.34 | 118.00 |
| 35 | E | 584 | C | O4'-C1'-N1 | 6.19 | 113.15 | 108.20 |
| 35 | E | 932 | G | O4'-C1'-N9 | 6.19 | 113.15 | 108.20 |
| 35 | E | 22 | A | C4-C5-C6 | 6.19 | 120.10 | 117.00 |
| 35 | E | 125 | A | C4-C5-C6 | 6.19 | 120.09 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 356 | C | O4'-C1'-N1 | 6.19 | 113.15 | 108.20 |
| 35 | E | 562 | A | C4-C5-C6 | 6.19 | 120.09 | 117.00 |
| 35 | E | 1309 | A | C5-C6-N6 | -6.19 | 118.75 | 123.70 |
| 35 | E | 1218 | A | C4-C5-C6 | 6.19 | 120.09 | 117.00 |
| 35 | E | 295 | A | C4-C5-C6 | 6.19 | 120.09 | 117.00 |
| 35 | E | 961 | A | C4-C5-C6 | 6.19 | 120.09 | 117.00 |
| 35 | E | 2305 | C | N3-C4-N4 | 6.19 | 122.33 | 118.00 |
| 35 | E | 872 | A | C5-C6-N6 | -6.19 | 118.75 | 123.70 |
| 35 | E | 1966 | C | O4'-C1'-N1 | 6.19 | 113.15 | 108.20 |
| 35 | E | 972 | A | C4-C5-C6 | 6.18 | 120.09 | 117.00 |
| 35 | E | 1241 | A | C4-C5-C6 | 6.18 | 120.09 | 117.00 |
| 35 | E | 2178 | C | N3-C4-N4 | 6.18 | 122.33 | 118.00 |
| 35 | E | 2315 | A | C4-C5-C6 | 6.18 | 120.09 | 117.00 |
| 35 | E | 696 | G | O4'-C1'-N9 | 6.18 | 113.14 | 108.20 |
| 35 | E | 741 | G | C5-C6-O6 | -6.18 | 124.89 | 128.60 |
| 35 | E | 1170 | C | N3-C4-N4 | 6.18 | 122.33 | 118.00 |
| 35 | E | 210 | A | C4-C5-C6 | 6.18 | 120.09 | 117.00 |
| 35 | E | 1609 | A | C4-C5-C6 | 6.18 | 120.09 | 117.00 |
| 35 | E | 22 | A | C5-C6-N6 | -6.18 | 118.76 | 123.70 |
| 35 | E | 185 | A | C4-C5-C6 | 6.18 | 120.09 | 117.00 |
| 35 | E | 2069 | A | C4-C5-C6 | 6.18 | 120.09 | 117.00 |
| 35 | E | 14 | C | N3-C4-N4 | 6.18 | 122.32 | 118.00 |
| 35 | E | 265 | C | N3-C4-N4 | 6.18 | 122.32 | 118.00 |
| 35 | E | 425 | A | C4-C5-C6 | 6.18 | 120.09 | 117.00 |
| 35 | E | 538 | A | C4-C5-C6 | 6.18 | 120.09 | 117.00 |
| 35 | E | 863 | A | C5-C6-N1 | -6.18 | 114.61 | 117.70 |
| 35 | E | 1308 | A | C4-C5-C6 | 6.18 | 120.09 | 117.00 |
| 35 | E | 1652 | A | C5-C6-N6 | -6.18 | 118.76 | 123.70 |
| 35 | E | 1973 | A | C4-C5-C6 | 6.18 | 120.09 | 117.00 |
| 35 | E | 1258 | A | C4-C5-C6 | 6.17 | 120.09 | 117.00 |
| 35 | E | 1681 | A | C4-C5-C6 | 6.17 | 120.09 | 117.00 |
| 35 | E | 1795 | C | N3-C4-N4 | 6.17 | 122.32 | 118.00 |
| 35 | E | 1312 | A | C4-C5-C6 | 6.17 | 120.09 | 117.00 |
| 35 | E | 287 | A | C4-C5-C6 | 6.17 | 120.08 | 117.00 |
| 35 | E | 1639 | A | C4-C5-C6 | 6.17 | 120.09 | 117.00 |
| 35 | E | 2234 | A | C5-C6-N6 | -6.17 | 118.76 | 123.70 |
| 35 | E | 1702 | A | C4-C5-C6 | 6.17 | 120.08 | 117.00 |
| 35 | E | 78 | A | C5-C6-N6 | -6.17 | 118.77 | 123.70 |
| 35 | E | 299 | A | C4-C5-C6 | 6.17 | 120.08 | 117.00 |
| 35 | E | 450 | A | C4-C5-C6 | 6.17 | 120.08 | 117.00 |
| 35 | E | 2128 | C | N3-C4-C5 | -6.17 | 119.43 | 121.90 |
| 35 | E | 1795 | C | O4'-C1'-N1 | 6.17 | 113.13 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 595 | A | C4-C5-C6 | 6.16 | 120.08 | 117.00 |
| 35 | E | 744 | C | N3-C4-C5 | -6.16 | 119.44 | 121.90 |
| 35 | E | 1235 | A | C4-C5-C6 | 6.16 | 120.08 | 117.00 |
| 35 | E | 2289 | G | O4'-C1'-N9 | 6.16 | 113.13 | 108.20 |
| 35 | E | 140 | C | N3-C4-N4 | 6.16 | 122.31 | 118.00 |
| 35 | E | 251 | A | C4-C5-C6 | 6.16 | 120.08 | 117.00 |
| 35 | E | 316 | A | C4-C5-C6 | 6.16 | 120.08 | 117.00 |
| 4 | t | 122 | TYR | CB-CG-CD2 | -6.16 | 117.31 | 121.00 |
| 35 | E | 205 | G | O4'-C1'-N9 | 6.16 | 113.13 | 108.20 |
| 35 | E | 503 | A | O4'-C1'-N9 | 6.16 | 113.13 | 108.20 |
| 35 | E | 2290 | C | N3-C4-N4 | 6.16 | 122.31 | 118.00 |
| 35 | E | 1799 | A | C5-C6-N6 | -6.16 | 118.78 | 123.70 |
| 35 | E | 429 | C | N3-C4-N4 | 6.15 | 122.31 | 118.00 |
| 35 | E | 1779 | U | O4'-C1'-N1 | 6.15 | 113.12 | 108.20 |
| 35 | E | 2157 | C | N3-C4-N4 | 6.15 | 122.31 | 118.00 |
| 35 | E | 2266 | G | O4'-C1'-N9 | 6.15 | 113.12 | 108.20 |
| 35 | E | 1197 | A | O4'-C1'-N9 | 6.15 | 113.12 | 108.20 |
| 35 | E | 1314 | A | C4-C5-C6 | 6.15 | 120.08 | 117.00 |
| 35 | E | 2206 | G | O4'-C1'-N9 | 6.15 | 113.12 | 108.20 |
| 35 | E | 2282 | C | N3-C4-N4 | 6.15 | 122.31 | 118.00 |
| 35 | E | 1088 | A | C4-C5-C6 | 6.15 | 120.07 | 117.00 |
| 35 | E | 1302 | A | C5-C6-N6 | -6.15 | 118.78 | 123.70 |
| 35 | E | 2219 | C | N3-C4-N4 | 6.15 | 122.30 | 118.00 |
| 35 | E | 926 | C | N3-C4-N4 | 6.15 | 122.30 | 118.00 |
| 35 | E | 1722 | C | N3-C4-N4 | 6.15 | 122.30 | 118.00 |
| 35 | E | 168 | A | C4-C5-C6 | 6.14 | 120.07 | 117.00 |
| 35 | E | 1526 | A | C4-C5-C6 | 6.14 | 120.07 | 117.00 |
| 35 | E | 1613 | U | O4'-C1'-N1 | 6.14 | 113.12 | 108.20 |
| 35 | E | 1633 | A | C4-C5-C6 | 6.14 | 120.07 | 117.00 |
| 35 | E | 138 | C | N3-C4-N4 | 6.14 | 122.30 | 118.00 |
| 35 | E | 1602 | C | N3-C4-N4 | 6.14 | 122.30 | 118.00 |
| 35 | E | 1674 | U | O4'-C1'-N1 | 6.14 | 113.11 | 108.20 |
| 35 | E | 259 | C | C6-N1-C2 | -6.14 | 117.84 | 120.30 |
| 35 | E | 273 | G | C5-C6-O6 | -6.14 | 124.92 | 128.60 |
| 35 | E | 450 | A | C5-C6-N6 | -6.14 | 118.79 | 123.70 |
| 35 | E | 1326 | G | N3-C2-N2 | 6.14 | 124.20 | 119.90 |
| 35 | E | 1328 | A | O4'-C1'-N9 | 6.14 | 113.11 | 108.20 |
| 35 | E | 2209 | A | C4-C5-C6 | 6.14 | 120.07 | 117.00 |
| 35 | E | 45 | U | O4'-C1'-N1 | 6.14 | 113.11 | 108.20 |
| 35 | E | 102 | A | C4-C5-C6 | 6.14 | 120.07 | 117.00 |
| 35 | E | 281 | A | C5-C6-N6 | -6.14 | 118.79 | 123.70 |
| 35 | E | 527 | A | O4'-C1'-N9 | 6.14 | 113.11 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 664 | G | O4'-C1'-N9 | 6.14 | 113.11 | 108.20 |
| 35 | E | 753 | U | C4'-C3'-C2' | -6.14 | 96.46 | 102.60 |
| 35 | E | 853 | C | N3-C4-N4 | 6.14 | 122.30 | 118.00 |
| 35 | E | 915 | A | C4-C5-C6 | 6.14 | 120.07 | 117.00 |
| 35 | E | 1264 | A | C4-C5-C6 | 6.14 | 120.07 | 117.00 |
| 35 | E | 1285 | C | N3-C4-N4 | 6.14 | 122.30 | 118.00 |
| 35 | E | 2002 | A | C4-C5-C6 | 6.14 | 120.07 | 117.00 |
| 35 | E | 2302 | C | N3-C4-N4 | 6.14 | 122.30 | 118.00 |
| 35 | E | 2175 | C | N3-C4-N4 | 6.14 | 122.30 | 118.00 |
| 35 | E | 16 | G | O4'-C1'-N9 | 6.14 | 113.11 | 108.20 |
| 35 | E | 170 | C | N3-C4-N4 | 6.14 | 122.30 | 118.00 |
| 35 | E | 1226 | G | O4'-C1'-N9 | 6.14 | 113.11 | 108.20 |
| 35 | E | 2083 | A | C5-C6-N6 | -6.14 | 118.79 | 123.70 |
| 35 | E | 2088 | A | C5-C6-N6 | -6.14 | 118.79 | 123.70 |
| 35 | E | 230 | G | O4'-C1'-N9 | 6.13 | 113.11 | 108.20 |
| 35 | E | 242 | A | C4-C5-C6 | 6.13 | 120.07 | 117.00 |
| 35 | E | 406 | A | C4-C5-C6 | 6.13 | 120.07 | 117.00 |
| 35 | E | 844 | G | C5-C6-O6 | -6.13 | 124.92 | 128.60 |
| 35 | E | 1572 | U | O4'-C1'-N1 | 6.13 | 113.11 | 108.20 |
| 35 | E | 1724 | A | C4-C5-C6 | 6.13 | 120.07 | 117.00 |
| 35 | E | 2047 | A | O4'-C1'-N9 | 6.13 | 113.11 | 108.20 |
| 35 | E | 960 | A | C4-C5-C6 | 6.13 | 120.07 | 117.00 |
| 35 | E | 1195 | G | C5-C6-O6 | -6.13 | 124.92 | 128.60 |
| 35 | E | 1378 | A | C4-C5-C6 | 6.13 | 120.06 | 117.00 |
| 35 | E | 176 | C | N3-C4-N4 | 6.13 | 122.29 | 118.00 |
| 35 | E | 215 | A | C4-C5-C6 | 6.13 | 120.06 | 117.00 |
| 35 | E | 356 | C | N3-C4-N4 | 6.13 | 122.29 | 118.00 |
| 35 | E | 374 | G | C5-C6-O6 | -6.13 | 124.92 | 128.60 |
| 35 | E | 676 | G | C5-C6-O6 | -6.12 | 124.92 | 128.60 |
| 35 | E | 1981 | A | C4-C5-C6 | 6.12 | 120.06 | 117.00 |
| 35 | E | 2061 | G | C8-N9-C1' | -6.12 | 119.04 | 127.00 |
| 35 | E | 2263 | G | C5-C6-O6 | -6.12 | 124.92 | 128.60 |
| 35 | E | 768 | G | P-O3'-C3' | 6.12 | 127.05 | 119.70 |
| 35 | E | 1607 | A | C4-C5-C6 | 6.12 | 120.06 | 117.00 |
| 35 | E | 1759 | G | O4'-C1'-N9 | 6.12 | 113.10 | 108.20 |
| 35 | E | 2221 | A | C4-C5-C6 | 6.12 | 120.06 | 117.00 |
| 35 | E | 2264 | A | C5-C6-N6 | -6.12 | 118.80 | 123.70 |
| 35 | E | 1087 | A | C4-C5-C6 | 6.12 | 120.06 | 117.00 |
| 35 | E | 363 | A | C4-C5-C6 | 6.12 | 120.06 | 117.00 |
| 35 | E | 2047 | A | C4-C5-C6 | 6.12 | 120.06 | 117.00 |
| 35 | E | 2205 | G | O4'-C1'-N9 | 6.12 | 113.10 | 108.20 |
| 35 | E | 319 | C | N3-C4-N4 | 6.12 | 122.28 | 118.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 456 | C | N3-C4-N4 | 6.12 | 122.28 | 118.00 |
| 35 | E | 790 | G | O4'-C1'-N9 | 6.12 | 113.09 | 108.20 |
| 35 | E | 1219 | C | N3-C4-N4 | 6.12 | 122.28 | 118.00 |
| 35 | E | 1286 | A | O4'-C1'-N9 | 6.12 | 113.09 | 108.20 |
| 35 | E | 1920 | A | C4-C5-C6 | 6.12 | 120.06 | 117.00 |
| 35 | E | 2202 | A | C4-C5-C6 | 6.12 | 120.06 | 117.00 |
| 35 | E | 2234 | A | C4-C5-C6 | 6.12 | 120.06 | 117.00 |
| 35 | E | 1998 | A | O4'-C1'-N9 | 6.12 | 113.09 | 108.20 |
| 35 | E | 1200 | A | C4-C5-C6 | 6.11 | 120.06 | 117.00 |
| 35 | E | 1592 | A | C4-C5-C6 | 6.11 | 120.06 | 117.00 |
| 35 | E | 1597 | U | O4'-C1'-N1 | 6.11 | 113.09 | 108.20 |
| 35 | E | 2247 | C | N3-C4-N4 | 6.11 | 122.28 | 118.00 |
| 35 | E | 1371 | C | N3-C4-N4 | 6.11 | 122.28 | 118.00 |
| 35 | E | 2268 | A | C4-C5-C6 | 6.11 | 120.06 | 117.00 |
| 35 | E | 432 | A | C5-C6-N1 | -6.11 | 114.64 | 117.70 |
| 35 | E | 434 | A | C4-C5-C6 | 6.11 | 120.06 | 117.00 |
| 35 | E | 1177 | C | N3-C4-N4 | 6.11 | 122.28 | 118.00 |
| 35 | E | 392 | A | C5-C6-N1 | -6.11 | 114.65 | 117.70 |
| 35 | E | 783 | A | C4-C5-C6 | 6.11 | 120.05 | 117.00 |
| 35 | E | 1559 | U | O4'-C1'-N1 | 6.11 | 113.08 | 108.20 |
| 35 | E | 531 | A | C4-C5-C6 | 6.10 | 120.05 | 117.00 |
| 35 | E | 1974 | C | N3-C4-N4 | 6.10 | 122.27 | 118.00 |
| 35 | E | 349 | A | C5-C6-N6 | -6.10 | 118.82 | 123.70 |
| 35 | E | 646 | A | C5-C6-N6 | -6.10 | 118.82 | 123.70 |
| 35 | E | 1079 | U | O4'-C1'-N1 | 6.10 | 113.08 | 108.20 |
| 35 | E | 352 | A | C4-C5-C6 | 6.10 | 120.05 | 117.00 |
| 35 | E | 430 | G | O4'-C1'-N9 | 6.10 | 113.08 | 108.20 |
| 35 | E | 520 | A | C5-C6-N6 | -6.10 | 118.82 | 123.70 |
| 35 | E | 1076 | C | N3-C4-N4 | 6.10 | 122.27 | 118.00 |
| 35 | E | 1716 | C | N3-C4-N4 | 6.10 | 122.27 | 118.00 |
| 35 | E | 1920 | A | O4'-C1'-N9 | 6.10 | 113.08 | 108.20 |
| 35 | E | 865 | A | C4-C5-C6 | 6.10 | 120.05 | 117.00 |
| 35 | E | 1306 | A | C4-C5-C6 | 6.10 | 120.05 | 117.00 |
| 35 | E | 1619 | A | C5-C6-N1 | -6.10 | 114.65 | 117.70 |
| 35 | E | 1702 | A | C5-C6-N6 | -6.10 | 118.82 | 123.70 |
| 35 | E | 196 | U | O4'-C1'-N1 | 6.10 | 113.08 | 108.20 |
| 35 | E | 1222 | A | C4-C5-C6 | 6.10 | 120.05 | 117.00 |
| 35 | E | 314 | A | C4-C5-C6 | 6.09 | 120.05 | 117.00 |
| 35 | E | 1233 | A | C4-C5-C6 | 6.09 | 120.05 | 117.00 |
| 35 | E | 1369 | C | N3-C4-N4 | 6.09 | 122.27 | 118.00 |
| 35 | E | 1695 | A | C4-C5-C6 | 6.09 | 120.05 | 117.00 |
| 35 | E | 2009 | C | N3-C4-N4 | 6.09 | 122.27 | 118.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 442 | U | O4'-C1'-N1 | 6.09 | 113.07 | 108.20 |
| 35 | E | 637 | C | N3-C4-N4 | 6.09 | 122.27 | 118.00 |
| 35 | E | 1330 | A | C5-C6-N1 | -6.09 | 114.65 | 117.70 |
| 35 | E | 1743 | A | C5-C6-N6 | -6.09 | 118.83 | 123.70 |
| 35 | E | 745 | C | N3-C4-C5 | -6.09 | 119.46 | 121.90 |
| 35 | E | 1999 | A | C4-C5-C6 | 6.09 | 120.05 | 117.00 |
| 35 | E | 2133 | C | N3-C4-N4 | 6.09 | 122.27 | 118.00 |
| 35 | E | 2262 | A | C4-C5-C6 | 6.09 | 120.05 | 117.00 |
| 35 | E | 326 | U | O4'-C1'-N1 | 6.09 | 113.07 | 108.20 |
| 35 | E | 1215 | A | C4-C5-C6 | 6.09 | 120.05 | 117.00 |
| 35 | E | 1240 | A | C5-C6-N6 | -6.09 | 118.83 | 123.70 |
| 35 | E | 1595 | A | C5-C6-N6 | -6.09 | 118.83 | 123.70 |
| 35 | E | 1656 | G | O4'-C1'-N9 | 6.09 | 113.07 | 108.20 |
| 35 | E | 1745 | G | N1-C6-O6 | 6.09 | 123.55 | 119.90 |
| 35 | E | 1764 | A | C4-C5-C6 | 6.09 | 120.05 | 117.00 |
| 35 | E | 817 | A | C4-C5-C6 | 6.09 | 120.04 | 117.00 |
| 35 | E | 1268 | A | C4-C5-C6 | 6.09 | 120.04 | 117.00 |
| 35 | E | 1313 | A | C4-C5-C6 | 6.09 | 120.04 | 117.00 |
| 35 | E | 1710 | A | C5-C6-N1 | -6.09 | 114.66 | 117.70 |
| 35 | E | 1957 | C | N3-C4-N4 | 6.09 | 122.26 | 118.00 |
| 35 | E | 300 | A | C4-C5-C6 | 6.09 | 120.04 | 117.00 |
| 35 | E | 701 | C | C6-N1-C2 | -6.09 | 117.86 | 120.30 |
| 35 | E | 852 | A | C4-C5-C6 | 6.09 | 120.04 | 117.00 |
| 35 | E | 967 | A | C4-C5-C6 | 6.09 | 120.04 | 117.00 |
| 35 | E | 1340 | A | C4-C5-C6 | 6.09 | 120.04 | 117.00 |
| 35 | E | 1373 | C | N3-C4-N4 | 6.09 | 122.26 | 118.00 |
| 35 | E | 1630 | A | C4-C5-C6 | 6.09 | 120.04 | 117.00 |
| 35 | E | 2088 | A | C4-C5-C6 | 6.09 | 120.04 | 117.00 |
| 35 | E | 2192 | A | C4-C5-C6 | 6.09 | 120.04 | 117.00 |
| 35 | E | 1784 | C | N3-C4-N4 | 6.08 | 122.26 | 118.00 |
| 35 | E | 414 | A | C4-C5-C6 | 6.08 | 120.04 | 117.00 |
| 35 | E | 741 | G | O4'-C1'-N9 | 6.08 | 113.07 | 108.20 |
| 35 | E | 958 | U | O4'-C1'-N1 | 6.08 | 113.07 | 108.20 |
| 35 | E | 1810 | C | N3-C4-N4 | 6.08 | 122.26 | 118.00 |
| 35 | E | 2074 | G | N3-C2-N2 | 6.08 | 124.16 | 119.90 |
| 35 | E | 392 | A | C4-C5-C6 | 6.08 | 120.04 | 117.00 |
| 35 | E | 455 | C | N3-C4-N4 | 6.08 | 122.26 | 118.00 |
| 35 | E | 977 | A | C5-C6-N6 | -6.08 | 118.84 | 123.70 |
| 35 | E | 1175 | A | C4-C5-C6 | 6.08 | 120.04 | 117.00 |
| 35 | E | 1306 | A | O4'-C1'-N9 | 6.08 | 113.06 | 108.20 |
| 35 | E | 1996 | A | C4-C5-C6 | 6.08 | 120.04 | 117.00 |
| 35 | E | 365 | C | N3-C4-N4 | 6.08 | 122.25 | 118.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 505 | A | C5-C6-N6 | -6.08 | 118.84 | 123.70 |
| 35 | E | 1355 | A | C5-C6-N1 | -6.08 | 114.66 | 117.70 |
| 35 | E | 2011 | A | C4-C5-C6 | 6.08 | 120.04 | 117.00 |
| 35 | E | 161 | A | O4'-C1'-N9 | 6.08 | 113.06 | 108.20 |
| 35 | E | 1896 | C | N3-C4-N4 | 6.08 | 122.25 | 118.00 |
| 35 | E | 440 | C | N3-C4-N4 | 6.08 | 122.25 | 118.00 |
| 35 | E | 508 | G | O4'-C1'-N9 | 6.08 | 113.06 | 108.20 |
| 35 | E | 1624 | C | N3-C4-N4 | 6.08 | 122.25 | 118.00 |
| 35 | E | 556 | U | O4'-C1'-N1 | 6.07 | 113.06 | 108.20 |
| 35 | E | 1362 | A | C4-C5-C6 | 6.07 | 120.04 | 117.00 |
| 35 | E | 1661 | A | C4-C5-C6 | 6.07 | 120.04 | 117.00 |
| 35 | E | 1758 | C | N3-C4-N4 | 6.07 | 122.25 | 118.00 |
| 35 | E | 490 | C | N3-C4-N4 | 6.07 | 122.25 | 118.00 |
| 35 | E | 864 | A | C4-C5-C6 | 6.07 | 120.04 | 117.00 |
| 35 | E | 2103 | A | C4-C5-C6 | 6.07 | 120.04 | 117.00 |
| 35 | E | 124 | A | C4-C5-C6 | 6.07 | 120.03 | 117.00 |
| 35 | E | 402 | C | N3-C4-N4 | 6.07 | 122.25 | 118.00 |
| 35 | E | 536 | A | C4-C5-C6 | 6.07 | 120.03 | 117.00 |
| 35 | E | 1370 | A | O4'-C1'-N9 | 6.07 | 113.06 | 108.20 |
| 35 | E | 432 | A | C4-C5-C6 | 6.07 | 120.03 | 117.00 |
| 35 | E | 485 | A | C4-C5-C6 | 6.07 | 120.03 | 117.00 |
| 35 | E | 497 | C | N3-C4-N4 | 6.07 | 122.25 | 118.00 |
| 35 | E | 1981 | A | C5-C6-N6 | -6.07 | 118.84 | 123.70 |
| 35 | E | 255 | A | C4-C5-C6 | 6.07 | 120.03 | 117.00 |
| 35 | E | 549 | A | C5-C6-N6 | -6.07 | 118.85 | 123.70 |
| 35 | E | 624 | A | C4-C5-C6 | 6.07 | 120.03 | 117.00 |
| 35 | E | 1211 | G | C5-C6-O6 | -6.07 | 124.96 | 128.60 |
| 35 | E | 2115 | C | N3-C4-C5 | -6.07 | 119.47 | 121.90 |
| 35 | E | 304 | A | C4-C5-C6 | 6.07 | 120.03 | 117.00 |
| 35 | E | 588 | A | C5-C6-N6 | -6.07 | 118.85 | 123.70 |
| 35 | E | 800 | C | N3-C4-C5 | -6.07 | 119.47 | 121.90 |
| 35 | E | 904 | C | N3-C4-N4 | 6.07 | 122.25 | 118.00 |
| 35 | E | 1984 | A | C4-C5-C6 | 6.07 | 120.03 | 117.00 |
| 35 | E | 599 | A | C4-C5-C6 | 6.06 | 120.03 | 117.00 |
| 35 | E | 681 | C | N3-C4-N4 | 6.06 | 122.25 | 118.00 |
| 35 | E | 604 | A | C5-C6-N6 | -6.06 | 118.85 | 123.70 |
| 35 | E | 655 | A | C4-C5-C6 | 6.06 | 120.03 | 117.00 |
| 35 | E | 763 | G | C5-C6-O6 | -6.06 | 124.96 | 128.60 |
| 35 | E | 917 | A | C4-C5-C6 | 6.06 | 120.03 | 117.00 |
| 35 | E | 1087 | A | C5-C6-N1 | -6.06 | 114.67 | 117.70 |
| 35 | E | 1180 | A | C4-C5-C6 | 6.06 | 120.03 | 117.00 |
| 35 | E | 1325 | C | N3-C4-N4 | 6.06 | 122.24 | 118.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1645 | C | N3-C4-N4 | 6.06 | 122.24 | 118.00 |
| 35 | E | 2300 | A | C4-C5-C6 | 6.06 | 120.03 | 117.00 |
| 35 | E | 764 | A | C5-C6-N6 | -6.06 | 118.85 | 123.70 |
| 35 | E | 1258 | A | C5-C6-N6 | -6.06 | 118.85 | 123.70 |
| 35 | E | 167 | A | C4-C5-C6 | 6.06 | 120.03 | 117.00 |
| 35 | E | 180 | A | O4'-C1'-N9 | 6.06 | 113.05 | 108.20 |
| 35 | E | 952 | U | O4'-C1'-N1 | 6.06 | 113.05 | 108.20 |
| 35 | E | 766 | C | N3-C4-N4 | 6.06 | 122.24 | 118.00 |
| 35 | E | 1628 | A | C5-C6-N6 | -6.06 | 118.86 | 123.70 |
| 35 | E | 742 | A | C5-C6-N1 | -6.06 | 114.67 | 117.70 |
| 35 | E | 1925 | A | C4-C5-C6 | 6.06 | 120.03 | 117.00 |
| 35 | E | 1998 | A | C4-C5-C6 | 6.06 | 120.03 | 117.00 |
| 35 | E | 2251 | A | C4-C5-C6 | 6.06 | 120.03 | 117.00 |
| 35 | E | 2299 | A | C4-C5-C6 | 6.06 | 120.03 | 117.00 |
| 35 | E | 916 | A | C4-C5-C6 | 6.05 | 120.03 | 117.00 |
| 35 | E | 1677 | C | N3-C4-N4 | 6.05 | 122.24 | 118.00 |
| 35 | E | 2008 | A | O4'-C1'-N9 | 6.05 | 113.04 | 108.20 |
| 35 | E | 306 | U | O4'-C1'-N1 | 6.05 | 113.04 | 108.20 |
| 35 | E | 757 | G | P-O3'-C3' | 6.05 | 126.96 | 119.70 |
| 35 | E | 1309 | A | C4-C5-C6 | 6.05 | 120.03 | 117.00 |
| 35 | E | 1657 | A | C4-C5-C6 | 6.05 | 120.03 | 117.00 |
| 35 | E | 1333 | A | C4-C5-C6 | 6.05 | 120.03 | 117.00 |
| 35 | E | 371 | A | C5-C6-N6 | -6.05 | 118.86 | 123.70 |
| 35 | E | 2059 | A | C5-C6-N1 | -6.05 | 114.68 | 117.70 |
| 35 | E | 882 | U | O4'-C1'-N1 | 6.05 | 113.04 | 108.20 |
| 35 | E | 2065 | A | O4'-C1'-N9 | 6.05 | 113.04 | 108.20 |
| 35 | E | 121 | A | C5-C6-N6 | -6.05 | 118.86 | 123.70 |
| 35 | E | 782 | A | C4-C5-C6 | 6.05 | 120.02 | 117.00 |
| 35 | E | 1938 | C | N3-C4-N4 | 6.05 | 122.23 | 118.00 |
| 35 | E | 147 | G | O4'-C1'-N9 | 6.04 | 113.03 | 108.20 |
| 35 | E | 877 | A | C4-C5-C6 | 6.04 | 120.02 | 117.00 |
| 35 | E | 913 | A | C4-C5-C6 | 6.04 | 120.02 | 117.00 |
| 35 | E | 1680 | G | C5-C6-O6 | -6.04 | 124.97 | 128.60 |
| 35 | E | 2039 | A | C4-C5-C6 | 6.04 | 120.02 | 117.00 |
| 35 | E | 2139 | G | O4'-C1'-N9 | 6.04 | 113.03 | 108.20 |
| 35 | E | 2159 | A | C4-C5-C6 | 6.04 | 120.02 | 117.00 |
| 35 | E | 180 | A | C4-C5-C6 | 6.04 | 120.02 | 117.00 |
| 35 | E | 348 | A | C4-C5-C6 | 6.04 | 120.02 | 117.00 |
| 35 | E | 406 | A | C5-C6-N6 | -6.04 | 118.87 | 123.70 |
| 35 | E | 417 | A | C4-C5-C6 | 6.04 | 120.02 | 117.00 |
| 35 | E | 743 | C | C6-N1-C2 | -6.04 | 117.88 | 120.30 |
| 35 | E | 777 | A | C5-C6-N1 | -6.04 | 114.68 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1216 | G | O4'-C1'-N9 | 6.04 | 113.03 | 108.20 |
| 35 | E | 1287 | A | C4-C5-C6 | 6.04 | 120.02 | 117.00 |
| 35 | E | 1679 | A | C5-C6-N1 | -6.04 | 114.68 | 117.70 |
| 35 | E | 2148 | A | C4-C5-C6 | 6.04 | 120.02 | 117.00 |
| 35 | E | 571 | A | C4-C5-C6 | 6.04 | 120.02 | 117.00 |
| 35 | E | 1536 | C | N3-C4-C5 | -6.04 | 119.48 | 121.90 |
| 35 | E | 36 | U | O4'-C1'-N1 | 6.04 | 113.03 | 108.20 |
| 35 | E | 82 | A | P-O3'-C3' | 6.04 | 126.95 | 119.70 |
| 35 | E | 1633 | A | C5-C6-N1 | -6.04 | 114.68 | 117.70 |
| 35 | E | 1781 | A | C4-C5-C6 | 6.04 | 120.02 | 117.00 |
| 35 | E | 2194 | G | O4'-C1'-N9 | 6.04 | 113.03 | 108.20 |
| 35 | E | 608 | C | O4'-C1'-N1 | 6.04 | 113.03 | 108.20 |
| 35 | E | 989 | G | C5'-C4'-C3' | -6.04 | 106.34 | 116.00 |
| 35 | E | 122 | A | C4-C5-C6 | 6.04 | 120.02 | 117.00 |
| 35 | E | 826 | A | C4-C5-C6 | 6.04 | 120.02 | 117.00 |
| 35 | E | 1804 | A | C4-C5-C6 | 6.04 | 120.02 | 117.00 |
| 35 | E | 701 | C | N3-C4-C5 | -6.03 | 119.49 | 121.90 |
| 35 | E | 1554 | A | C5-C6-N1 | -6.03 | 114.68 | 117.70 |
| 35 | E | 2284 | A | C4-C5-C6 | 6.03 | 120.02 | 117.00 |
| 35 | E | 410 | G | O4'-C1'-N9 | 6.03 | 113.02 | 108.20 |
| 35 | E | 889 | A | C5-C6-N1 | -6.03 | 114.68 | 117.70 |
| 35 | E | 2080 | A | C5-C6-N6 | -6.03 | 118.88 | 123.70 |
| 35 | E | 2143 | C | N3-C4-N4 | 6.03 | 122.22 | 118.00 |
| 35 | E | 2226 | U | O4'-C1'-N1 | 6.03 | 113.03 | 108.20 |
| 35 | E | 1723 | G | O4'-C1'-N9 | 6.03 | 113.02 | 108.20 |
| 35 | E | 1876 | G | O4'-C1'-N9 | 6.03 | 113.02 | 108.20 |
| 35 | E | 1979 | G | O4'-C1'-N9 | 6.03 | 113.02 | 108.20 |
| 35 | E | 111 | A | C4-C5-C6 | 6.03 | 120.01 | 117.00 |
| 35 | E | 569 | A | C4-C5-C6 | 6.03 | 120.01 | 117.00 |
| 35 | E | 1238 | U | O4'-C1'-N1 | 6.03 | 113.02 | 108.20 |
| 35 | E | 2070 | C | N3-C4-C5 | -6.03 | 119.49 | 121.90 |
| 35 | E | 2111 | A | C4-C5-C6 | 6.03 | 120.01 | 117.00 |
| 35 | E | 2015 | U | P-O3'-C3' | 6.03 | 126.93 | 119.70 |
| 35 | E | 2037 | A | C4-C5-C6 | 6.02 | 120.01 | 117.00 |
| 35 | E | 11 | A | C5-C6-N1 | -6.02 | 114.69 | 117.70 |
| 35 | E | 576 | A | C5-C6-N6 | -6.02 | 118.88 | 123.70 |
| 35 | E | 692 | U | O4'-C1'-N1 | 6.02 | 113.02 | 108.20 |
| 35 | E | 839 | C | N3-C4-C5 | -6.02 | 119.49 | 121.90 |
| 35 | E | 992 | A | C4-C5-C6 | 6.02 | 120.01 | 117.00 |
| 35 | E | 1200 | A | C5-C6-N1 | -6.02 | 114.69 | 117.70 |
| 35 | E | 190 | A | C4-C5-C6 | 6.02 | 120.01 | 117.00 |
| 35 | E | 1815 | A | C5-C6-N6 | -6.02 | 118.88 | 123.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 646 | A | C5-C6-N1 | -6.02 | 114.69 | 117.70 |
| 35 | E | 901 | A | C5-C6-N6 | -6.02 | 118.89 | 123.70 |
| 35 | E | 1174 | C | N3-C4-N4 | 6.02 | 122.21 | 118.00 |
| 35 | E | 1632 | G | O4'-C1'-N9 | 6.02 | 113.02 | 108.20 |
| 35 | E | 1701 | G | C5-C6-O6 | -6.02 | 124.99 | 128.60 |
| 35 | E | 690 | A | C4-C5-C6 | 6.02 | 120.01 | 117.00 |
| 35 | E | 845 | A | C4-C5-C6 | 6.02 | 120.01 | 117.00 |
| 35 | E | 1242 | A | O4'-C1'-N9 | 6.02 | 113.02 | 108.20 |
| 35 | E | 1275 | A | O4'-C1'-N9 | 6.02 | 113.01 | 108.20 |
| 35 | E | 1380 | U | O4'-C1'-N1 | 6.02 | 113.02 | 108.20 |
| 35 | E | 439 | G | O4'-C1'-N9 | 6.02 | 113.01 | 108.20 |
| 35 | E | 454 | A | C4-C5-C6 | 6.02 | 120.01 | 117.00 |
| 35 | E | 858 | A | C4-C5-C6 | 6.02 | 120.01 | 117.00 |
| 35 | E | 1176 | A | C4-C5-C6 | 6.02 | 120.01 | 117.00 |
| 35 | E | 1547 | A | C4-C5-C6 | 6.01 | 120.01 | 117.00 |
| 35 | E | 1591 | C | O4'-C1'-N1 | 6.01 | 113.01 | 108.20 |
| 35 | E | 118 | C | N3-C4-N4 | 6.01 | 122.21 | 118.00 |
| 35 | E | 121 | A | C4-C5-C6 | 6.01 | 120.01 | 117.00 |
| 35 | E | 653 | A | C4-C5-C6 | 6.01 | 120.01 | 117.00 |
| 35 | E | 728 | A | C4-C5-C6 | 6.01 | 120.01 | 117.00 |
| 35 | E | 743 | C | N3-C4-C5 | -6.01 | 119.50 | 121.90 |
| 35 | E | 889 | A | C5-C6-N6 | -6.01 | 118.89 | 123.70 |
| 35 | E | 1187 | C | N3-C4-N4 | 6.01 | 122.21 | 118.00 |
| 35 | E | 2006 | A | C4-C5-C6 | 6.01 | 120.01 | 117.00 |
| 30 | m | 143 | GLY | C-N-CA | 6.01 | 136.72 | 121.70 |
| 35 | E | 28 | A | C4-C5-C6 | 6.01 | 120.00 | 117.00 |
| 35 | E | 195 | C | N3-C4-N4 | 6.01 | 122.21 | 118.00 |
| 35 | E | 269 | A | C4-C5-C6 | 6.01 | 120.00 | 117.00 |
| 35 | E | 400 | G | N3-C2-N2 | 6.01 | 124.11 | 119.90 |
| 35 | E | 781 | A | C4-C5-C6 | 6.01 | 120.00 | 117.00 |
| 35 | E | 1769 | U | O4'-C1'-N1 | 6.01 | 113.01 | 108.20 |
| 35 | E | 241 | A | C4-C5-C6 | 6.01 | 120.00 | 117.00 |
| 35 | E | 608 | C | N3-C4-N4 | 6.01 | 122.21 | 118.00 |
| 35 | E | 993 | A | C4-C5-C6 | 6.01 | 120.00 | 117.00 |
| 35 | E | 1240 | A | C4-C5-C6 | 6.01 | 120.00 | 117.00 |
| 35 | E | 1764 | A | C5-C6-N6 | -6.01 | 118.89 | 123.70 |
| 35 | E | 2065 | A | C4-C5-C6 | 6.01 | 120.00 | 117.00 |
| 35 | E | 2080 | A | C4-C5-C6 | 6.01 | 120.00 | 117.00 |
| 35 | E | 751 | C | P-O3'-C3' | 6.01 | 126.91 | 119.70 |
| 35 | E | 1269 | C | N3-C4-C5 | -6.01 | 119.50 | 121.90 |
| 35 | E | 1802 | C | N3-C4-N4 | 6.01 | 122.20 | 118.00 |
| 35 | E | 414 | A | C5-C6-N6 | -6.00 | 118.90 | 123.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1891 | C | N3-C4-N4 | 6.00 | 122.20 | 118.00 |
| 35 | E | 72 | C | N3-C4-N4 | 6.00 | 122.20 | 118.00 |
| 35 | E | 402 | C | N3-C4-C5 | -6.00 | 119.50 | 121.90 |
| 35 | E | 774 | C | O3'-P-O5' | 6.00 | 115.41 | 104.00 |
| 35 | E | 1771 | U | O4'-C1'-N1 | 6.00 | 113.00 | 108.20 |
| 35 | E | 2118 | G | O4'-C1'-N9 | 6.00 | 113.00 | 108.20 |
| 35 | E | 2136 | A | C4-C5-C6 | 6.00 | 120.00 | 117.00 |
| 35 | E | 785 | A | C5-C6-N6 | -6.00 | 118.90 | 123.70 |
| 35 | E | 876 | A | C4-C5-C6 | 6.00 | 120.00 | 117.00 |
| 1 | p | 105 | PHE | CB-CG-CD1 | -6.00 | 116.60 | 120.80 |
| 35 | E | 734 | G | C8-N9-C4 | 6.00 | 108.80 | 106.40 |
| 35 | E | 789 | C | N3-C4-N4 | 6.00 | 122.20 | 118.00 |
| 35 | E | 794 | G | O4'-C1'-N9 | 6.00 | 113.00 | 108.20 |
| 35 | E | 2053 | G | O4'-C1'-N9 | 6.00 | 113.00 | 108.20 |
| 35 | E | 2063 | A | O4'-C1'-N9 | 6.00 | 113.00 | 108.20 |
| 35 | E | 349 | A | C4-C5-C6 | 6.00 | 120.00 | 117.00 |
| 35 | E | 2111 | A | O4'-C1'-N9 | 6.00 | 113.00 | 108.20 |
| 35 | E | 360 | A | C4-C5-C6 | 5.99 | 120.00 | 117.00 |
| 35 | E | 481 | G | O4'-C1'-N9 | 5.99 | 113.00 | 108.20 |
| 35 | E | 1201 | G | O4'-C1'-N9 | 5.99 | 112.99 | 108.20 |
| 35 | E | 2200 | A | C5-C6-N6 | -5.99 | 118.91 | 123.70 |
| 35 | E | 575 | A | C4-C5-C6 | 5.99 | 120.00 | 117.00 |
| 35 | E | 1301 | A | C4-C5-C6 | 5.99 | 120.00 | 117.00 |
| 35 | E | 1720 | C | N3-C4-C5 | -5.99 | 119.50 | 121.90 |
| 35 | E | 1794 | A | C4-C5-C6 | 5.99 | 120.00 | 117.00 |
| 35 | E | 2092 | A | C4-C5-C6 | 5.99 | 120.00 | 117.00 |
| 35 | E | 2135 | A | C4-C5-C6 | 5.99 | 120.00 | 117.00 |
| 35 | E | 498 | A | C4-C5-C6 | 5.99 | 120.00 | 117.00 |
| 35 | E | 1301 | A | C5-C6-N6 | -5.99 | 118.91 | 123.70 |
| 35 | E | 861 | A | C5-C6-N1 | -5.99 | 114.71 | 117.70 |
| 35 | E | 990 | A | C4-C5-C6 | 5.99 | 119.99 | 117.00 |
| 35 | E | 1205 | A | C4-C5-C6 | 5.99 | 119.99 | 117.00 |
| 35 | E | 1314 | A | C5-C6-N6 | -5.99 | 118.91 | 123.70 |
| 35 | E | 516 | A | C4-C5-C6 | 5.99 | 119.99 | 117.00 |
| 35 | E | 581 | A | C5-C6-N6 | -5.99 | 118.91 | 123.70 |
| 35 | E | 607 | A | C4-C5-C6 | 5.99 | 119.99 | 117.00 |
| 35 | E | 1854 | G | O4'-C1'-N9 | 5.99 | 112.99 | 108.20 |
| 35 | E | 1349 | G | O4'-C1'-N9 | 5.98 | 112.99 | 108.20 |
| 35 | E | 2015 | U | O4'-C1'-N1 | 5.98 | 112.99 | 108.20 |
| 35 | E | 350 | C | N3-C4-N4 | 5.98 | 122.19 | 118.00 |
| 35 | E | 549 | A | C4-C5-C6 | 5.98 | 119.99 | 117.00 |
| 35 | E | 1690 | G | C5-C6-O6 | -5.98 | 125.01 | 128.60 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1732 | A | O4'-C1'-N9 | 5.98 | 112.99 | 108.20 |
| 35 | E | 577 | A | O4'-C1'-N9 | 5.98 | 112.98 | 108.20 |
| 35 | E | 582 | U | O4'-C1'-N1 | 5.98 | 112.98 | 108.20 |
| 35 | E | 1354 | C | N3-C4-N4 | 5.98 | 122.19 | 118.00 |
| 35 | E | 1631 | A | C4-C5-C6 | 5.98 | 119.99 | 117.00 |
| 35 | E | 1919 | A | C4-C5-C6 | 5.98 | 119.99 | 117.00 |
| 14 | V | 57 | ALA | N-CA-CB | 5.98 | 118.47 | 110.10 |
| 35 | E | 231 | A | C5-C6-N1 | -5.98 | 114.71 | 117.70 |
| 35 | E | 1345 | U | O4'-C1'-N1 | 5.98 | 112.98 | 108.20 |
| 35 | E | 659 | A | C4-C5-C6 | 5.98 | 119.99 | 117.00 |
| 35 | E | 1657 | A | C5-C6-N6 | -5.98 | 118.92 | 123.70 |
| 35 | E | 2265 | G | O4'-C1'-N9 | 5.98 | 112.98 | 108.20 |
| 35 | E | 2034 | A | C4-C5-C6 | 5.98 | 119.99 | 117.00 |
| 35 | E | 655 | A | C5-C6-N6 | -5.97 | 118.92 | 123.70 |
| 35 | E | 1228 | G | O4'-C1'-N9 | 5.97 | 112.98 | 108.20 |
| 35 | E | 1353 | A | C4-C5-C6 | 5.97 | 119.99 | 117.00 |
| 35 | E | 1592 | A | C5-C6-N1 | -5.97 | 114.71 | 117.70 |
| 35 | E | 1679 | A | C4-C5-C6 | 5.97 | 119.99 | 117.00 |
| 35 | E | 1730 | U | O4'-C1'-N1 | 5.97 | 112.98 | 108.20 |
| 35 | E | 838 | G | C5-C6-O6 | -5.97 | 125.02 | 128.60 |
| 35 | E | 954 | G | C6-C5-N7 | -5.97 | 126.82 | 130.40 |
| 35 | E | 1377 | A | C4-C5-C6 | 5.97 | 119.99 | 117.00 |
| 35 | E | 1829 | C | N3-C4-N4 | 5.97 | 122.18 | 118.00 |
| 35 | E | 2005 | A | C4-C5-C6 | 5.97 | 119.99 | 117.00 |
| 35 | E | 2187 | C | N3-C4-N4 | 5.97 | 122.18 | 118.00 |
| 35 | E | 1311 | C | N3-C4-N4 | 5.97 | 122.18 | 118.00 |
| 35 | E | 2260 | A | C4-C5-C6 | 5.97 | 119.99 | 117.00 |
| 35 | E | 311 | G | O4'-C1'-N9 | 5.97 | 112.97 | 108.20 |
| 35 | E | 598 | A | C4-C5-C6 | 5.97 | 119.98 | 117.00 |
| 35 | E | 1302 | A | C4-C5-C6 | 5.97 | 119.98 | 117.00 |
| 35 | E | 2312 | A | C4-C5-C6 | 5.97 | 119.98 | 117.00 |
| 35 | E | 525 | A | C5-C6-N1 | -5.97 | 114.72 | 117.70 |
| 35 | E | 1185 | A | C4-C5-C6 | 5.97 | 119.98 | 117.00 |
| 35 | E | 2244 | C | N3-C4-N4 | 5.97 | 122.18 | 118.00 |
| 35 | E | 62 | A | C5-C6-N6 | -5.97 | 118.93 | 123.70 |
| 35 | E | 184 | A | C4-C5-C6 | 5.97 | 119.98 | 117.00 |
| 35 | E | 587 | A | O4'-C1'-N9 | 5.96 | 112.97 | 108.20 |
| 35 | E | 721 | C | O4'-C1'-N1 | 5.96 | 112.97 | 108.20 |
| 35 | E | 780 | C | N3-C4-C5 | -5.96 | 119.51 | 121.90 |
| 35 | E | 1209 | C | N3-C4-N4 | 5.96 | 122.17 | 118.00 |
| 35 | E | 2083 | A | O4'-C1'-N9 | 5.96 | 112.97 | 108.20 |
| 35 | E | 195 | C | O4'-C1'-N1 | 5.96 | 112.97 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1304 | C | N3-C4-N4 | 5.96 | 122.17 | 118.00 |
| 35 | E | 2166 | C | N3-C4-N4 | 5.96 | 122.17 | 118.00 |
| 35 | E | 809 | A | C4-C5-C6 | 5.96 | 119.98 | 117.00 |
| 35 | E | 165 | C | N3-C4-N4 | 5.96 | 122.17 | 118.00 |
| 35 | E | 562 | A | O4'-C1'-N9 | 5.96 | 112.97 | 108.20 |
| 35 | E | 638 | C | N3-C4-N4 | 5.96 | 122.17 | 118.00 |
| 35 | E | 812 | A | C4-C5-C6 | 5.96 | 119.98 | 117.00 |
| 35 | E | 866 | A | C5-C6-N1 | -5.96 | 114.72 | 117.70 |
| 35 | E | 2202 | A | C5-C6-N6 | -5.96 | 118.93 | 123.70 |
| 35 | E | 913 | A | C5-C6-N1 | -5.96 | 114.72 | 117.70 |
| 35 | E | 1705 | G | O4'-C1'-N9 | 5.96 | 112.97 | 108.20 |
| 35 | E | 1954 | C | N3-C4-N4 | 5.96 | 122.17 | 118.00 |
| 35 | E | 2288 | A | C4-C5-C6 | 5.96 | 119.98 | 117.00 |
| 21 | d | 81 | SER | N-CA-CB | 5.96 | 119.43 | 110.50 |
| 35 | E | 448 | A | C4-C5-C6 | 5.96 | 119.98 | 117.00 |
| 35 | E | 1981 | A | C5-C6-N1 | -5.96 | 114.72 | 117.70 |
| 20 | f | 172 | TYR | CB-CG-CD2 | -5.95 | 117.43 | 121.00 |
| 35 | E | 4 | C | N3-C4-N4 | 5.95 | 122.17 | 118.00 |
| 35 | E | 143 | C | N3-C4-N4 | 5.95 | 122.17 | 118.00 |
| 35 | E | 520 | A | C4-C5-C6 | 5.95 | 119.98 | 117.00 |
| 35 | E | 521 | A | O4'-C1'-N9 | 5.95 | 112.96 | 108.20 |
| 35 | E | 553 | U | O4'-C1'-N1 | 5.95 | 112.96 | 108.20 |
| 35 | E | 684 | A | C4-C5-C6 | 5.95 | 119.98 | 117.00 |
| 35 | E | 1229 | C | N3-C4-N4 | 5.95 | 122.17 | 118.00 |
| 35 | E | 1573 | C | N3-C4-N4 | 5.95 | 122.17 | 118.00 |
| 35 | E | 2027 | C | N3-C4-C5 | -5.95 | 119.52 | 121.90 |
| 35 | E | 2127 | G | O4'-C1'-N9 | 5.95 | 112.96 | 108.20 |
| 35 | E | 2171 | C | O4'-C1'-N1 | 5.95 | 112.96 | 108.20 |
| 35 | E | 789 | C | N3-C4-C5 | -5.95 | 119.52 | 121.90 |
| 35 | E | 1973 | A | C5-C6-N6 | -5.95 | 118.94 | 123.70 |
| 35 | E | 2004 | A | C4-C5-C6 | 5.95 | 119.98 | 117.00 |
| 35 | E | 2047 | A | C5-C6-N1 | -5.95 | 114.72 | 117.70 |
| 35 | E | 581 | A | C4-C5-C6 | 5.95 | 119.98 | 117.00 |
| 35 | E | 585 | A | C4-C5-C6 | 5.95 | 119.97 | 117.00 |
| 35 | E | 2046 | A | C5-C6-N6 | -5.95 | 118.94 | 123.70 |
| 35 | E | 332 | C | N3-C4-N4 | 5.95 | 122.16 | 118.00 |
| 35 | E | 989 | G | O4'-C1'-N9 | 5.95 | 112.96 | 108.20 |
| 35 | E | 1235 | A | C5-C6-N1 | -5.95 | 114.73 | 117.70 |
| 35 | E | 1275 | A | C5-C6-N6 | -5.95 | 118.94 | 123.70 |
| 35 | E | 1939 | A | O4'-C1'-N9 | 5.95 | 112.96 | 108.20 |
| 35 | E | 1984 | A | O4'-C1'-N9 | 5.95 | 112.96 | 108.20 |
| 35 | E | 2010 | G | O4'-C1'-N9 | 5.95 | 112.96 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 31 | C | N3-C4-N4 | 5.95 | 122.16 | 118.00 |
| 35 | E | 127 | C | O4'-C1'-N1 | 5.95 | 112.96 | 108.20 |
| 35 | E | 393 | U | O4'-C1'-N1 | 5.95 | 112.96 | 108.20 |
| 35 | E | 645 | A | C5-C6-N6 | -5.95 | 118.94 | 123.70 |
| 35 | E | 1566 | A | C4-C5-C6 | 5.95 | 119.97 | 117.00 |
| 35 | E | 2273 | A | C4-C5-C6 | 5.95 | 119.97 | 117.00 |
| 35 | E | 1385 | A | C5-C6-N6 | -5.94 | 118.94 | 123.70 |
| 35 | E | 1936 | A | C5-C6-N6 | -5.94 | 118.94 | 123.70 |
| 35 | E | 156 | G | O4'-C1'-N9 | 5.94 | 112.95 | 108.20 |
| 35 | E | 464 | C | O4'-C1'-N1 | 5.94 | 112.95 | 108.20 |
| 35 | E | 1254 | C | N3-C4-N4 | 5.94 | 122.16 | 118.00 |
| 35 | E | 2079 | G | O4'-C1'-N9 | 5.94 | 112.95 | 108.20 |
| 35 | E | 898 | A | C4-C5-C6 | 5.94 | 119.97 | 117.00 |
| 35 | E | 245 | A | C4-C5-C6 | 5.94 | 119.97 | 117.00 |
| 35 | E | 2004 | A | O4'-C1'-N9 | 5.94 | 112.95 | 108.20 |
| 35 | E | 1361 | A | C4-C5-C6 | 5.94 | 119.97 | 117.00 |
| 35 | E | 249 | A | C4-C5-C6 | 5.93 | 119.97 | 117.00 |
| 35 | E | 2262 | A | C5-C6-N1 | -5.93 | 114.73 | 117.70 |
| 35 | E | 1087 | A | O4'-C1'-N9 | 5.93 | 112.94 | 108.20 |
| 35 | E | 1593 | A | C5-C6-N6 | -5.93 | 118.95 | 123.70 |
| 35 | E | 2298 | G | O4'-C1'-N9 | 5.93 | 112.95 | 108.20 |
| 35 | E | 837 | C | N3-C4-C5 | -5.93 | 119.53 | 121.90 |
| 35 | E | 1332 | G | O4'-C1'-N9 | 5.93 | 112.94 | 108.20 |
| 35 | E | 709 | C | N3-C4-N4 | 5.93 | 122.15 | 118.00 |
| 35 | E | 912 | A | C4-C5-C6 | 5.93 | 119.96 | 117.00 |
| 35 | E | 1179 | C | N3-C4-N4 | 5.93 | 122.15 | 118.00 |
| 35 | E | 793 | A | C5-C6-N1 | -5.93 | 114.74 | 117.70 |
| 35 | E | 1561 | A | C5-C6-N1 | -5.93 | 114.74 | 117.70 |
| 35 | E | 703 | A | C5-C6-N1 | -5.93 | 114.74 | 117.70 |
| 35 | E | 744 | C | N3-C4-N4 | 5.93 | 122.15 | 118.00 |
| 35 | E | 1373 | C | N3-C4-C5 | -5.93 | 119.53 | 121.90 |
| 35 | E | 1574 | A | C4-C5-C6 | 5.93 | 119.96 | 117.00 |
| 35 | E | 2240 | A | C5-C6-N6 | -5.93 | 118.96 | 123.70 |
| 35 | E | 604 | A | C4-C5-C6 | 5.92 | 119.96 | 117.00 |
| 35 | E | 1256 | C | N3-C4-N4 | 5.92 | 122.15 | 118.00 |
| 35 | E | 507 | A | C5-C6-N6 | -5.92 | 118.96 | 123.70 |
| 35 | E | 523 | A | C5-C6-N1 | -5.92 | 114.74 | 117.70 |
| 35 | E | 799 | A | C5-C6-N6 | -5.92 | 118.96 | 123.70 |
| 35 | E | 1301 | A | C5-C6-N1 | -5.92 | 114.74 | 117.70 |
| 35 | E | 1874 | C | N3-C4-C5 | -5.92 | 119.53 | 121.90 |
| 35 | E | 287 | A | C5-C6-N6 | -5.92 | 118.96 | 123.70 |
| 35 | E | 598 | A | O4'-C1'-N9 | 5.92 | 112.94 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1888 | A | C4-C5-C6 | 5.92 | 119.96 | 117.00 |
| 35 | E | 1992 | A | C4-C5-C6 | 5.92 | 119.96 | 117.00 |
| 35 | E | 231 | A | C4-C5-C6 | 5.92 | 119.96 | 117.00 |
| 35 | E | 275 | A | C4-C5-C6 | 5.92 | 119.96 | 117.00 |
| 35 | E | 531 | A | C5-C6-N6 | -5.92 | 118.97 | 123.70 |
| 35 | E | 925 | C | N3-C4-N4 | 5.92 | 122.14 | 118.00 |
| 35 | E | 1316 | U | O4'-C1'-N1 | 5.92 | 112.93 | 108.20 |
| 35 | E | 1629 | C | N3-C4-N4 | 5.92 | 122.14 | 118.00 |
| 35 | E | 1917 | G | O4'-C1'-N9 | 5.92 | 112.93 | 108.20 |
| 35 | E | 2260 | A | O4'-C1'-N9 | 5.92 | 112.94 | 108.20 |
| 35 | E | 751 | C | N3-C4-C5 | -5.92 | 119.53 | 121.90 |
| 35 | E | 891 | U | O4'-C1'-N1 | 5.92 | 112.93 | 108.20 |
| 35 | E | 1382 | G | O4'-C1'-N9 | 5.92 | 112.93 | 108.20 |
| 35 | E | 1609 | A | C5-C6-N6 | -5.92 | 118.97 | 123.70 |
| 35 | E | 1818 | A | C4-C5-C6 | 5.92 | 119.96 | 117.00 |
| 35 | E | 2200 | A | C4-C5-C6 | 5.92 | 119.96 | 117.00 |
| 35 | E | 1297 | C | N3-C4-C5 | -5.92 | 119.53 | 121.90 |
| 35 | E | 2 | A | C4-C5-C6 | 5.91 | 119.96 | 117.00 |
| 35 | E | 245 | A | C5-C6-N1 | -5.91 | 114.74 | 117.70 |
| 35 | E | 526 | A | C4-C5-C6 | 5.91 | 119.96 | 117.00 |
| 35 | E | 639 | A | C4-C5-C6 | 5.91 | 119.96 | 117.00 |
| 35 | E | 734 | G | N3-C4-C5 | 5.91 | 131.56 | 128.60 |
| 35 | E | 1610 | A | C4-C5-C6 | 5.91 | 119.96 | 117.00 |
| 35 | E | 1740 | U | O4'-C1'-N1 | 5.91 | 112.93 | 108.20 |
| 35 | E | 1191 | G | C5-C6-O6 | -5.91 | 125.05 | 128.60 |
| 35 | E | 509 | A | C5-C6-N6 | -5.91 | 118.97 | 123.70 |
| 35 | E | 1368 | A | C4-C5-C6 | 5.91 | 119.95 | 117.00 |
| 35 | E | 2087 | C | N3-C4-N4 | 5.91 | 122.14 | 118.00 |
| 35 | E | 107 | A | C4-C5-C6 | 5.91 | 119.95 | 117.00 |
| 35 | E | 313 | G | C4-N9-C1' | 5.91 | 134.18 | 126.50 |
| 35 | E | 610 | A | C5-C6-N1 | -5.91 | 114.75 | 117.70 |
| 35 | E | 512 | A | C4-C5-C6 | 5.91 | 119.95 | 117.00 |
| 35 | E | 967 | A | C5-C6-N1 | -5.91 | 114.75 | 117.70 |
| 35 | E | 1733 | A | C4-C5-C6 | 5.91 | 119.95 | 117.00 |
| 35 | E | 703 | A | C4-C5-C6 | 5.91 | 119.95 | 117.00 |
| 35 | E | 999 | U | O4'-C1'-N1 | 5.91 | 112.92 | 108.20 |
| 35 | E | 1085 | G | O4'-C1'-N9 | 5.91 | 112.92 | 108.20 |
| 35 | E | 1355 | A | C4-C5-C6 | 5.91 | 119.95 | 117.00 |
| 35 | E | 1385 | A | C4-C5-C6 | 5.91 | 119.95 | 117.00 |
| 35 | E | 2039 | A | O4'-C1'-N9 | 5.91 | 112.92 | 108.20 |
| 35 | E | 2245 | A | C4-C5-C6 | 5.91 | 119.95 | 117.00 |
| 35 | E | 2259 | A | C4-C5-C6 | 5.90 | 119.95 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1180 | A | O4'-C1'-N9 | 5.90 | 112.92 | 108.20 |
| 35 | E | 2271 | A | C4-C5-C6 | 5.90 | 119.95 | 117.00 |
| 35 | E | 285 | A | C4-C5-C6 | 5.90 | 119.95 | 117.00 |
| 35 | E | 330 | A | C4-C5-C6 | 5.90 | 119.95 | 117.00 |
| 35 | E | 901 | A | C4-C5-C6 | 5.90 | 119.95 | 117.00 |
| 35 | E | 2046 | A | C4-C5-C6 | 5.90 | 119.95 | 117.00 |
| 35 | E | 26 | A | C4-C5-C6 | 5.90 | 119.95 | 117.00 |
| 35 | E | 64 | A | C5-C6-N1 | -5.90 | 114.75 | 117.70 |
| 35 | E | 192 | G | O4'-C1'-N9 | 5.90 | 112.92 | 108.20 |
| 35 | E | 1266 | C | N3-C4-N4 | 5.90 | 122.13 | 118.00 |
| 35 | E | 1308 | A | C5-C6-N6 | -5.90 | 118.98 | 123.70 |
| 35 | E | 141 | A | O4'-C1'-N9 | 5.89 | 112.92 | 108.20 |
| 35 | E | 1271 | G | O4'-C1'-N9 | 5.89 | 112.92 | 108.20 |
| 35 | E | 2089 | A | C4-C5-C6 | 5.89 | 119.95 | 117.00 |
| 35 | E | 2169 | A | C4-C5-C6 | 5.89 | 119.95 | 117.00 |
| 35 | E | 25 | C | N3-C4-N4 | 5.89 | 122.12 | 118.00 |
| 35 | E | 1794 | A | C5-C6-N6 | -5.89 | 118.99 | 123.70 |
| 35 | E | 1961 | A | O4'-C1'-N9 | 5.89 | 112.91 | 108.20 |
| 35 | E | 492 | A | O4'-C1'-N9 | 5.89 | 112.91 | 108.20 |
| 35 | E | 2272 | A | C4-C5-C6 | 5.89 | 119.94 | 117.00 |
| 35 | E | 1333 | A | O4'-C1'-N9 | 5.89 | 112.91 | 108.20 |
| 35 | E | 2267 | A | C4-C5-C6 | 5.89 | 119.94 | 117.00 |
| 35 | E | 962 | A | C4-C5-C6 | 5.89 | 119.94 | 117.00 |
| 35 | E | 2027 | C | O4'-C1'-N1 | 5.89 | 112.91 | 108.20 |
| 35 | E | 241 | A | C5-C6-N6 | -5.89 | 118.99 | 123.70 |
| 35 | E | 248 | G | N3-C2-N2 | 5.89 | 124.02 | 119.90 |
| 35 | E | 451 | G | O4'-C1'-N9 | 5.89 | 112.91 | 108.20 |
| 35 | E | 1951 | A | O4'-C1'-N9 | 5.89 | 112.91 | 108.20 |
| 35 | E | 2269 | G | O4'-C1'-N9 | 5.89 | 112.91 | 108.20 |
| 35 | E | 583 | C | N3-C4-N4 | 5.88 | 122.12 | 118.00 |
| 35 | E | 764 | A | C4-C5-C6 | 5.88 | 119.94 | 117.00 |
| 35 | E | 788 | A | C4-C5-C6 | 5.88 | 119.94 | 117.00 |
| 35 | E | 1370 | A | C4-C5-C6 | 5.88 | 119.94 | 117.00 |
| 35 | E | 1814 | U | O4'-C1'-N1 | 5.88 | 112.91 | 108.20 |
| 35 | E | 1888 | A | C5-C6-N1 | -5.88 | 114.76 | 117.70 |
| 35 | E | 1973 | A | C5-C6-N1 | -5.88 | 114.76 | 117.70 |
| 35 | E | 2063 | A | C4-C5-C6 | 5.88 | 119.94 | 117.00 |
| 35 | E | 2281 | A | C4-C5-C6 | 5.88 | 119.94 | 117.00 |
| 35 | E | 704 | A | C4-C5-C6 | 5.88 | 119.94 | 117.00 |
| 35 | E | 1667 | G | C5-C6-O6 | -5.88 | 125.07 | 128.60 |
| 35 | E | 653 | A | C5-C6-N6 | -5.88 | 118.99 | 123.70 |
| 35 | E | 1290 | A | C5-C6-N1 | -5.88 | 114.76 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 2089 | A | C5-C6-N1 | -5.88 | 114.76 | 117.70 |
| 35 | E | 2098 | C | N3-C4-C5 | -5.88 | 119.55 | 121.90 |
| 35 | E | 472 | A | C4-C5-C6 | 5.88 | 119.94 | 117.00 |
| 35 | E | 523 | A | C4-C5-C6 | 5.88 | 119.94 | 117.00 |
| 35 | E | 765 | A | C4-C5-C6 | 5.88 | 119.94 | 117.00 |
| 35 | E | 775 | A | C5-C6-N6 | -5.88 | 119.00 | 123.70 |
| 35 | E | 1217 | A | C4-C5-C6 | 5.88 | 119.94 | 117.00 |
| 35 | E | 463 | A | C4-C5-C6 | 5.88 | 119.94 | 117.00 |
| 35 | E | 491 | C | N3-C4-N4 | 5.88 | 122.11 | 118.00 |
| 35 | E | 866 | A | C4-C5-C6 | 5.88 | 119.94 | 117.00 |
| 35 | E | 912 | A | C5-C6-N1 | -5.88 | 114.76 | 117.70 |
| 35 | E | 1241 | A | C5-C6-N6 | -5.88 | 119.00 | 123.70 |
| 35 | E | 1245 | C | N3-C4-N4 | 5.88 | 122.11 | 118.00 |
| 35 | E | 1290 | A | C5-C6-N6 | -5.88 | 119.00 | 123.70 |
| 35 | E | 1352 | C | N3-C4-N4 | 5.88 | 122.11 | 118.00 |
| 35 | E | 1375 | U | O4'-C1'-N1 | 5.88 | 112.90 | 108.20 |
| 35 | E | 1971 | C | N3-C4-N4 | 5.88 | 122.11 | 118.00 |
| 35 | E | 2135 | A | C5-C6-N1 | -5.88 | 114.76 | 117.70 |
| 35 | E | 786 | A | C4-C5-C6 | 5.88 | 119.94 | 117.00 |
| 35 | E | 1646 | G | O4'-C1'-N9 | 5.88 | 112.90 | 108.20 |
| 35 | E | 464 | C | N3-C4-N4 | 5.87 | 122.11 | 118.00 |
| 35 | E | 467 | A | C4-C5-C6 | 5.87 | 119.94 | 117.00 |
| 35 | E | 645 | A | C5-C6-N1 | -5.87 | 114.76 | 117.70 |
| 35 | E | 1927 | A | O4'-C1'-N9 | 5.87 | 112.90 | 108.20 |
| 35 | E | 81 | A | O4'-C1'-N9 | 5.87 | 112.90 | 108.20 |
| 35 | E | 303 | C | N3-C4-N4 | 5.87 | 122.11 | 118.00 |
| 35 | E | 1285 | C | N3-C4-C5 | -5.87 | 119.55 | 121.90 |
| 35 | E | 1975 | A | C4-C5-C6 | 5.87 | 119.94 | 117.00 |
| 35 | E | 11 | A | C4-C5-C6 | 5.87 | 119.94 | 117.00 |
| 35 | E | 902 | A | C4-C5-C6 | 5.87 | 119.93 | 117.00 |
| 35 | E | 995 | C | N3-C4-N4 | 5.87 | 122.11 | 118.00 |
| 35 | E | 1615 | A | O4'-C1'-N9 | 5.87 | 112.89 | 108.20 |
| 35 | E | 1956 | C | N3-C4-N4 | 5.87 | 122.11 | 118.00 |
| 35 | E | 2128 | C | N3-C4-N4 | 5.87 | 122.11 | 118.00 |
| 35 | E | 646 | A | C4-C5-C6 | 5.87 | 119.93 | 117.00 |
| 35 | E | 1338 | A | C4-C5-C6 | 5.87 | 119.93 | 117.00 |
| 35 | E | 1584 | A | C4-C5-C6 | 5.87 | 119.93 | 117.00 |
| 35 | E | 1663 | C | N3-C4-N4 | 5.87 | 122.11 | 118.00 |
| 35 | E | 2100 | C | N3-C4-C5 | -5.86 | 119.55 | 121.90 |
| 35 | E | 647 | A | C4-C5-C6 | 5.86 | 119.93 | 117.00 |
| 35 | E | 578 | C | N3-C4-N4 | 5.86 | 122.10 | 118.00 |
| 35 | E | 889 | A | C4-C5-C6 | 5.86 | 119.93 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 2021 | G | O4'-C1'-N9 | 5.86 | 112.89 | 108.20 |
| 35 | E | 2059 | A | C5-C6-N6 | -5.86 | 119.01 | 123.70 |
| 35 | E | 19 | A | C4-C5-C6 | 5.86 | 119.93 | 117.00 |
| 35 | E | 649 | G | O4'-C1'-N9 | 5.86 | 112.89 | 108.20 |
| 35 | E | 732 | C | C2-N1-C1' | 5.86 | 125.24 | 118.80 |
| 35 | E | 734 | G | O4'-C1'-N9 | 5.86 | 112.89 | 108.20 |
| 35 | E | 1985 | C | N3-C4-N4 | 5.86 | 122.10 | 118.00 |
| 35 | E | 2009 | C | N3-C4-C5 | -5.86 | 119.56 | 121.90 |
| 35 | E | 2056 | A | C4-C5-C6 | 5.86 | 119.93 | 117.00 |
| 35 | E | 2209 | A | C5-C6-N1 | -5.86 | 114.77 | 117.70 |
| 35 | E | 1083 | G | O4'-C1'-N9 | 5.86 | 112.89 | 108.20 |
| 35 | E | 1362 | A | C5-C6-N6 | -5.86 | 119.02 | 123.70 |
| 35 | E | 2042 | G | O4'-C1'-N9 | 5.86 | 112.89 | 108.20 |
| 35 | E | 2103 | A | C5-C6-N1 | -5.86 | 114.77 | 117.70 |
| 35 | E | 2179 | G | O4'-C1'-N9 | 5.86 | 112.89 | 108.20 |
| 35 | E | 2209 | A | C5-C6-N6 | -5.86 | 119.02 | 123.70 |
| 35 | E | 593 | G | O4'-C1'-N9 | 5.85 | 112.88 | 108.20 |
| 35 | E | 800 | C | O4'-C1'-N1 | 5.85 | 112.88 | 108.20 |
| 1 | p | 301 | TYR | CB-CG-CD2 | -5.85 | 117.49 | 121.00 |
| 35 | E | 173 | A | C4-C5-C6 | 5.85 | 119.92 | 117.00 |
| 35 | E | 800 | C | N3-C4-N4 | 5.85 | 122.09 | 118.00 |
| 35 | E | 1634 | C | C5-C4-N4 | -5.85 | 116.11 | 120.20 |
| 35 | E | 2018 | U | O4'-C1'-N1 | 5.85 | 112.88 | 108.20 |
| 35 | E | 2259 | A | O4'-C1'-N9 | 5.85 | 112.88 | 108.20 |
| 35 | E | 401 | A | C4-C5-C6 | 5.85 | 119.92 | 117.00 |
| 35 | E | 592 | A | C5-C6-N1 | -5.85 | 114.78 | 117.70 |
| 35 | E | 1187 | C | C4'-C3'-C2' | -5.85 | 96.75 | 102.60 |
| 35 | E | 1333 | A | C5-C6-N6 | -5.85 | 119.02 | 123.70 |
| 35 | E | 1774 | U | O4'-C1'-N1 | 5.85 | 112.88 | 108.20 |
| 35 | E | 1942 | A | C4-C5-C6 | 5.85 | 119.92 | 117.00 |
| 35 | E | 2170 | C | N3-C4-N4 | 5.85 | 122.09 | 118.00 |
| 35 | E | 280 | C | N3-C4-N4 | 5.85 | 122.09 | 118.00 |
| 35 | E | 852 | A | C5-C6-N1 | -5.85 | 114.78 | 117.70 |
| 35 | E | 246 | A | C5-C6-N1 | -5.84 | 114.78 | 117.70 |
| 35 | E | 991 | C | N3-C4-N4 | 5.84 | 122.09 | 118.00 |
| 35 | E | 1290 | A | C4-C5-C6 | 5.84 | 119.92 | 117.00 |
| 35 | E | 1728 | C | O4'-C1'-N1 | 5.84 | 112.88 | 108.20 |
| 35 | E | 1747 | C | N3-C4-N4 | 5.84 | 122.09 | 118.00 |
| 35 | E | 123 | A | C5-C6-N6 | -5.84 | 119.03 | 123.70 |
| 35 | E | 905 | A | C4-C5-C6 | 5.84 | 119.92 | 117.00 |
| 35 | E | 1595 | A | C4-C5-C6 | 5.84 | 119.92 | 117.00 |
| 35 | E | 844 | G | O4'-C1'-N9 | 5.84 | 112.87 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1526 | A | C5-C6-N6 | -5.84 | 119.03 | 123.70 |
| 35 | E | 2059 | A | C4-C5-C6 | 5.84 | 119.92 | 117.00 |
| 35 | E | 190 | A | C5-C6-N6 | -5.84 | 119.03 | 123.70 |
| 35 | E | 1955 | U | O4'-C1'-N1 | 5.84 | 112.87 | 108.20 |
| 35 | E | 2271 | A | C5-C6-N1 | -5.84 | 114.78 | 117.70 |
| 35 | E | 2192 | A | O4'-C1'-N9 | 5.83 | 112.87 | 108.20 |
| 35 | E | 760 | C | N3-C4-N4 | 5.83 | 122.08 | 118.00 |
| 35 | E | 2068 | C | N3-C4-N4 | 5.83 | 122.08 | 118.00 |
| 35 | E | 810 | U | O4'-C1'-N1 | 5.83 | 112.86 | 108.20 |
| 35 | E | 2117 | C | N3-C4-N4 | 5.83 | 122.08 | 118.00 |
| 35 | E | 805 | C | N3-C4-N4 | 5.83 | 122.08 | 118.00 |
| 35 | E | 1853 | C | N3-C4-N4 | 5.83 | 122.08 | 118.00 |
| 35 | E | 39 | A | C4-C5-C6 | 5.83 | 119.91 | 117.00 |
| 35 | E | 1346 | G | C5-C6-O6 | -5.83 | 125.10 | 128.60 |
| 35 | E | 457 | A | C4-C5-C6 | 5.83 | 119.91 | 117.00 |
| 35 | E | 1742 | C | N3-C4-N4 | 5.83 | 122.08 | 118.00 |
| 35 | E | 1801 | C | N3-C4-N4 | 5.83 | 122.08 | 118.00 |
| 35 | E | 2263 | G | N3-C2-N2 | 5.83 | 123.98 | 119.90 |
| 35 | E | 1616 | C | N3-C4-N4 | 5.82 | 122.08 | 118.00 |
| 35 | E | 1177 | C | O4'-C1'-N1 | 5.82 | 112.86 | 108.20 |
| 35 | E | 2281 | A | C5-C6-N1 | -5.82 | 114.79 | 117.70 |
| 35 | E | 65 | A | C5-C6-N6 | -5.82 | 119.04 | 123.70 |
| 35 | E | 351 | A | C4-C5-C6 | 5.82 | 119.91 | 117.00 |
| 35 | E | 1298 | C | N3-C4-N4 | 5.82 | 122.07 | 118.00 |
| 35 | E | 1797 | A | C5-C6-N6 | -5.82 | 119.04 | 123.70 |
| 35 | E | 1939 | A | C5-C6-N1 | -5.82 | 114.79 | 117.70 |
| 35 | E | 2274 | A | O4'-C1'-N9 | 5.82 | 112.86 | 108.20 |
| 35 | E | 1803 | A | C4-C5-C6 | 5.82 | 119.91 | 117.00 |
| 35 | E | 2080 | A | C5-C6-N1 | -5.82 | 114.79 | 117.70 |
| 35 | E | 98 | U | O4'-C1'-N1 | 5.82 | 112.85 | 108.20 |
| 35 | E | 502 | A | O4'-C1'-N9 | 5.82 | 112.85 | 108.20 |
| 35 | E | 547 | G | C5'-C4'-C3' | 5.82 | 125.31 | 116.00 |
| 35 | E | 1591 | C | N3-C4-N4 | 5.82 | 122.07 | 118.00 |
| 35 | E | 1665 | C | N3-C4-N4 | 5.82 | 122.07 | 118.00 |
| 35 | E | 177 | A | C4-C5-C6 | 5.82 | 119.91 | 117.00 |
| 35 | E | 1529 | A | C4-C5-C6 | 5.82 | 119.91 | 117.00 |
| 35 | E | 1832 | A | C5-C6-N6 | -5.82 | 119.05 | 123.70 |
| 35 | E | 2070 | C | N3-C4-N4 | 5.82 | 122.07 | 118.00 |
| 35 | E | 884 | A | C5-C6-N6 | -5.81 | 119.05 | 123.70 |
| 35 | E | 1335 | U | C2-N1-C1' | 5.81 | 124.68 | 117.70 |
| 35 | E | 431 | G | O4'-C1'-N9 | 5.81 | 112.85 | 108.20 |
| 35 | E | 839 | C | N3-C4-N4 | 5.81 | 122.07 | 118.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 845 | A | C5-C6-N6 | -5.81 | 119.05 | 123.70 |
| 35 | E | 975 | U | O4'-C1'-N1 | 5.81 | 112.85 | 108.20 |
| 35 | E | 1086 | A | C5-C6-N1 | -5.81 | 114.79 | 117.70 |
| 35 | E | 1363 | C | N3-C4-N4 | 5.81 | 122.07 | 118.00 |
| 35 | E | 1936 | A | C4-C5-C6 | 5.81 | 119.91 | 117.00 |
| 35 | E | 648 | A | C5-C6-N1 | -5.81 | 114.80 | 117.70 |
| 35 | E | 507 | A | C4-C5-C6 | 5.81 | 119.90 | 117.00 |
| 35 | E | 1302 | A | O4'-C1'-N9 | 5.81 | 112.85 | 108.20 |
| 35 | E | 1750 | C | N3-C4-N4 | 5.81 | 122.07 | 118.00 |
| 35 | E | 4 | C | O4'-C1'-N1 | 5.81 | 112.84 | 108.20 |
| 35 | E | 2 | A | C5-C6-N6 | -5.80 | 119.06 | 123.70 |
| 35 | E | 273 | G | O4'-C1'-N9 | 5.80 | 112.84 | 108.20 |
| 35 | E | 321 | G | O4'-C1'-N9 | 5.80 | 112.84 | 108.20 |
| 35 | E | 609 | A | C5-C6-N1 | -5.80 | 114.80 | 117.70 |
| 35 | E | 47 | A | C5-C6-N1 | -5.80 | 114.80 | 117.70 |
| 35 | E | 382 | G | C5-C6-O6 | -5.80 | 125.12 | 128.60 |
| 35 | E | 543 | U | O4'-C1'-N1 | 5.80 | 112.84 | 108.20 |
| 35 | E | 1260 | G | O4'-C1'-N9 | 5.80 | 112.84 | 108.20 |
| 35 | E | 1652 | A | C5-C6-N1 | -5.80 | 114.80 | 117.70 |
| 35 | E | 1653 | U | O4'-C1'-N1 | 5.80 | 112.84 | 108.20 |
| 35 | E | 1222 | A | C5-C6-N6 | -5.80 | 119.06 | 123.70 |
| 35 | E | 1756 | G | O4'-C1'-N9 | 5.80 | 112.84 | 108.20 |
| 35 | E | 367 | A | O4'-C1'-N9 | 5.80 | 112.84 | 108.20 |
| 35 | E | 1205 | A | C5-C6-N6 | -5.80 | 119.06 | 123.70 |
| 35 | E | 1883 | C | N3-C4-N4 | 5.80 | 122.06 | 118.00 |
| 35 | E | 65 | A | C4-C5-C6 | 5.80 | 119.90 | 117.00 |
| 35 | E | 257 | A | C5-C6-N1 | -5.80 | 114.80 | 117.70 |
| 35 | E | 684 | A | O4'-C1'-N9 | 5.80 | 112.84 | 108.20 |
| 35 | E | 826 | A | C5-C6-N6 | -5.80 | 119.06 | 123.70 |
| 35 | E | 1985 | C | N3-C4-C5 | -5.80 | 119.58 | 121.90 |
| 35 | E | 2111 | A | C5-C6-N6 | -5.80 | 119.06 | 123.70 |
| 35 | E | 215 | A | C5-C6-N6 | -5.79 | 119.06 | 123.70 |
| 35 | E | 438 | A | C5-C6-N1 | -5.79 | 114.80 | 117.70 |
| 35 | E | 817 | A | C5-C6-N1 | -5.79 | 114.80 | 117.70 |
| 35 | E | 1181 | C | N3-C4-C5 | -5.79 | 119.58 | 121.90 |
| 35 | E | 1806 | C | N3-C4-C5 | -5.79 | 119.58 | 121.90 |
| 35 | E | 2014 | C | N3-C4-N4 | 5.79 | 122.06 | 118.00 |
| 35 | E | 831 | A | C5-C6-N6 | -5.79 | 119.06 | 123.70 |
| 35 | E | 840 | C | N3-C4-C5 | -5.79 | 119.58 | 121.90 |
| 35 | E | 1280 | U | O4'-C1'-N1 | 5.79 | 112.83 | 108.20 |
| 35 | E | 1346 | G | N3-C2-N2 | 5.79 | 123.95 | 119.90 |
| 35 | E | 458 | C | N3-C4-N4 | 5.79 | 122.05 | 118.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 706 | G | O4'-C1'-N9 | 5.79 | 112.83 | 108.20 |
| 35 | E | 830 | C | N3-C4-N4 | 5.79 | 122.05 | 118.00 |
| 35 | E | 939 | U | O4'-C1'-N1 | 5.79 | 112.83 | 108.20 |
| 35 | E | 1365 | A | C4-C5-C6 | 5.79 | 119.90 | 117.00 |
| 35 | E | 1574 | A | C5-C6-N6 | -5.79 | 119.07 | 123.70 |
| 35 | E | 1627 | C | N3-C4-N4 | 5.79 | 122.06 | 118.00 |
| 35 | E | 186 | C | N3-C4-N4 | 5.79 | 122.05 | 118.00 |
| 35 | E | 643 | C | N3-C4-N4 | 5.79 | 122.05 | 118.00 |
| 35 | E | 1652 | A | C4-C5-C6 | 5.79 | 119.89 | 117.00 |
| 35 | E | 1669 | G | O4'-C1'-N9 | 5.79 | 112.83 | 108.20 |
| 35 | E | 161 | A | C5-C6-N1 | -5.79 | 114.81 | 117.70 |
| 35 | E | 396 | C | N3-C4-N4 | 5.79 | 122.05 | 118.00 |
| 35 | E | 867 | G | N3-C2-N2 | 5.79 | 123.95 | 119.90 |
| 35 | E | 1681 | A | C5-C6-N6 | -5.79 | 119.07 | 123.70 |
| 35 | E | 1881 | C | N3-C4-C5 | -5.79 | 119.58 | 121.90 |
| 35 | E | 2058 | C | N3-C4-C5 | -5.79 | 119.58 | 121.90 |
| 35 | E | 898 | A | C5-C6-N1 | -5.79 | 114.81 | 117.70 |
| 35 | E | 1620 | A | C4-C5-C6 | 5.79 | 119.89 | 117.00 |
| 35 | E | 88 | G | O4'-C1'-N9 | 5.79 | 112.83 | 108.20 |
| 35 | E | 330 | A | O4'-C1'-N9 | 5.79 | 112.83 | 108.20 |
| 35 | E | 336 | C | N3-C4-N4 | 5.79 | 122.05 | 118.00 |
| 35 | E | 941 | U | O4'-C1'-N1 | 5.79 | 112.83 | 108.20 |
| 35 | E | 1292 | A | C5-C6-N6 | -5.79 | 119.07 | 123.70 |
| 35 | E | 1948 | G | C5-C6-O6 | -5.79 | 125.13 | 128.60 |
| 35 | E | 428 | C | N3-C4-N4 | 5.78 | 122.05 | 118.00 |
| 35 | E | 546 | U | C6-N1-C1' | -5.78 | 113.10 | 121.20 |
| 35 | E | 2295 | G | O4'-C1'-N9 | 5.78 | 112.83 | 108.20 |
| 35 | E | 63 | G | O4'-C1'-N9 | 5.78 | 112.83 | 108.20 |
| 35 | E | 242 | A | C5-C6-N6 | -5.78 | 119.08 | 123.70 |
| 35 | E | 1222 | A | C5-C6-N1 | -5.78 | 114.81 | 117.70 |
| 35 | E | 2292 | G | O4'-C1'-N9 | 5.78 | 112.82 | 108.20 |
| 35 | E | 1822 | A | C5-C6-N1 | -5.78 | 114.81 | 117.70 |
| 35 | E | 704 | A | C5-C6-N6 | -5.78 | 119.08 | 123.70 |
| 35 | E | 1847 | C | N3-C4-C5 | -5.78 | 119.59 | 121.90 |
| 35 | E | 164 | G | O4'-C1'-N9 | 5.78 | 112.82 | 108.20 |
| 35 | E | 260 | A | C5-C6-N6 | -5.78 | 119.08 | 123.70 |
| 35 | E | 307 | C | N3-C4-N4 | 5.78 | 122.04 | 118.00 |
| 35 | E | 348 | A | O4'-C1'-N9 | 5.78 | 112.82 | 108.20 |
| 35 | E | 1372 | C | N3-C4-N4 | 5.78 | 122.04 | 118.00 |
| 35 | E | 1903 | A | C5-C6-N6 | -5.78 | 119.08 | 123.70 |
| 35 | E | 495 | G | O4'-C1'-N9 | 5.77 | 112.82 | 108.20 |
| 35 | E | 499 | A | O4'-C1'-N9 | 5.77 | 112.82 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 529 | A | C4-C5-C6 | 5.77 | 119.89 | 117.00 |
| 35 | E | 646 | A | O4'-C1'-N9 | 5.77 | 112.82 | 108.20 |
| 35 | E | 1086 | A | O4'-C1'-N9 | 5.77 | 112.82 | 108.20 |
| 35 | E | 324 | U | O4'-C1'-N1 | 5.77 | 112.82 | 108.20 |
| 35 | E | 142 | A | C4-C5-C6 | 5.77 | 119.89 | 117.00 |
| 35 | E | 149 | A | C5-C6-N6 | -5.77 | 119.08 | 123.70 |
| 35 | E | 417 | A | C5-C6-N6 | -5.77 | 119.08 | 123.70 |
| 35 | E | 519 | G | N3-C2-N2 | 5.77 | 123.94 | 119.90 |
| 35 | E | 590 | C | N3-C4-N4 | 5.77 | 122.04 | 118.00 |
| 35 | E | 783 | A | O4'-C1'-N9 | 5.77 | 112.82 | 108.20 |
| 35 | E | 1800 | U | O4'-C1'-N1 | 5.77 | 112.82 | 108.20 |
| 35 | E | 1932 | G | O4'-C1'-N9 | 5.77 | 112.81 | 108.20 |
| 35 | E | 2078 | C | N3-C4-N4 | 5.77 | 122.04 | 118.00 |
| 35 | E | 39 | A | C5-C6-N1 | -5.77 | 114.82 | 117.70 |
| 35 | E | 1698 | A | O4'-C1'-N9 | 5.77 | 112.81 | 108.20 |
| 35 | E | 890 | C | N3-C4-C5 | -5.77 | 119.59 | 121.90 |
| 35 | E | 2045 | A | C4-C5-C6 | 5.77 | 119.88 | 117.00 |
| 35 | E | 288 | A | C4-C5-C6 | 5.76 | 119.88 | 117.00 |
| 35 | E | 304 | A | C5-C6-N6 | -5.76 | 119.09 | 123.70 |
| 35 | E | 471 | C | N3-C4-N4 | 5.76 | 122.03 | 118.00 |
| 35 | E | 2173 | C | N3-C4-C5 | -5.76 | 119.59 | 121.90 |
| 35 | E | 1356 | C | N3-C4-N4 | 5.76 | 122.03 | 118.00 |
| 35 | E | 2159 | A | O4'-C1'-N9 | 5.76 | 112.81 | 108.20 |
| 35 | E | 1600 | A | C5-C6-N1 | -5.76 | 114.82 | 117.70 |
| 35 | E | 2134 | A | C5-C6-N1 | -5.76 | 114.82 | 117.70 |
| 35 | E | 94 | C | N3-C4-N4 | 5.76 | 122.03 | 118.00 |
| 35 | E | 974 | A | C4-C5-C6 | 5.76 | 119.88 | 117.00 |
| 35 | E | 1184 | C | N3-C4-N4 | 5.76 | 122.03 | 118.00 |
| 35 | E | 254 | A | C4-C5-C6 | 5.76 | 119.88 | 117.00 |
| 35 | E | 386 | A | C5-C6-N1 | -5.76 | 114.82 | 117.70 |
| 35 | E | 387 | C | N3-C4-N4 | 5.76 | 122.03 | 118.00 |
| 35 | E | 710 | A | C5-C6-N6 | -5.76 | 119.10 | 123.70 |
| 35 | E | 1176 | A | C5-C6-N6 | -5.76 | 119.09 | 123.70 |
| 35 | E | 1231 | U | O4'-C1'-N1 | 5.76 | 112.80 | 108.20 |
| 35 | E | 1830 | C | N3-C4-N4 | 5.76 | 122.03 | 118.00 |
| 35 | E | 778 | A | C5-C6-N1 | -5.75 | 114.82 | 117.70 |
| 35 | E | 934 | C | N3-C4-C5 | -5.75 | 119.60 | 121.90 |
| 35 | E | 493 | A | C5-C6-N6 | -5.75 | 119.10 | 123.70 |
| 35 | E | 518 | C | N3-C4-N4 | 5.75 | 122.03 | 118.00 |
| 35 | E | 666 | U | O4'-C1'-N1 | 5.75 | 112.80 | 108.20 |
| 35 | E | 977 | A | C4-C5-C6 | 5.75 | 119.88 | 117.00 |
| 35 | E | 1261 | A | C4-C5-C6 | 5.75 | 119.88 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 26 | A | C5-C6-N6 | -5.75 | 119.10 | 123.70 |
| 35 | E | 427 | U | O4'-C1'-N1 | 5.75 | 112.80 | 108.20 |
| 35 | E | 531 | A | O4'-C1'-N9 | 5.75 | 112.80 | 108.20 |
| 35 | E | 788 | A | C5-C6-N6 | -5.75 | 119.10 | 123.70 |
| 35 | E | 1251 | C | N3-C4-N4 | 5.75 | 122.03 | 118.00 |
| 35 | E | 1661 | A | C5-C6-N6 | -5.75 | 119.10 | 123.70 |
| 35 | E | 2069 | A | C5-C6-N1 | -5.75 | 114.82 | 117.70 |
| 35 | E | 2130 | C | N3-C4-N4 | 5.75 | 122.03 | 118.00 |
| 35 | E | 781 | A | C5-C6-N6 | -5.75 | 119.10 | 123.70 |
| 35 | E | 894 | A | C5-C6-N6 | -5.75 | 119.10 | 123.70 |
| 35 | E | 1601 | A | C5-C6-N6 | -5.75 | 119.10 | 123.70 |
| 35 | E | 2102 | C | N3-C4-N4 | 5.75 | 122.03 | 118.00 |
| 35 | E | 2123 | C | N3-C4-N4 | 5.75 | 122.03 | 118.00 |
| 35 | E | 14 | C | N3-C4-C5 | -5.75 | 119.60 | 121.90 |
| 35 | E | 246 | A | C4-C5-C6 | 5.75 | 119.87 | 117.00 |
| 35 | E | 1279 | A | C5-C6-N1 | -5.75 | 114.83 | 117.70 |
| 35 | E | 1553 | A | C5-C6-N6 | -5.75 | 119.10 | 123.70 |
| 35 | E | 1581 | A | C4-C5-C6 | 5.75 | 119.87 | 117.00 |
| 35 | E | 1772 | G | N3-C2-N2 | 5.75 | 123.92 | 119.90 |
| 35 | E | 1830 | C | N3-C4-C5 | -5.75 | 119.60 | 121.90 |
| 35 | E | 2294 | A | C5-C6-N6 | -5.75 | 119.10 | 123.70 |
| 35 | E | 295 | A | C5-C6-N6 | -5.75 | 119.10 | 123.70 |
| 35 | E | 873 | C | N3-C4-C5 | -5.75 | 119.60 | 121.90 |
| 35 | E | 1817 | G | O4'-C1'-N9 | 5.75 | 112.80 | 108.20 |
| 35 | E | 214 | C | N3-C4-N4 | 5.74 | 122.02 | 118.00 |
| 35 | E | 675 | A | C5-C6-N1 | -5.74 | 114.83 | 117.70 |
| 35 | E | 1716 | C | N3-C4-C5 | -5.74 | 119.60 | 121.90 |
| 35 | E | 624 | A | C5-C6-N1 | -5.74 | 114.83 | 117.70 |
| 35 | E | 640 | G | O4'-C1'-N9 | 5.74 | 112.79 | 108.20 |
| 35 | E | 1171 | C | N3-C4-C5 | -5.74 | 119.60 | 121.90 |
| 35 | E | 1629 | C | N3-C4-C5 | -5.74 | 119.60 | 121.90 |
| 35 | E | 1651 | A | C5-C6-N6 | -5.74 | 119.11 | 123.70 |
| 35 | E | 2145 | A | C5-C6-N6 | -5.74 | 119.11 | 123.70 |
| 35 | E | 2283 | A | C4-C5-C6 | 5.74 | 119.87 | 117.00 |
| 35 | E | 599 | A | C5-C6-N1 | -5.74 | 114.83 | 117.70 |
| 35 | E | 1628 | A | C4-C5-C6 | 5.74 | 119.87 | 117.00 |
| 35 | E | 2174 | C | N3-C4-N4 | 5.74 | 122.02 | 118.00 |
| 35 | E | 438 | A | C4-C5-C6 | 5.74 | 119.87 | 117.00 |
| 35 | E | 529 | A | C5-C6-N1 | -5.74 | 114.83 | 117.70 |
| 35 | E | 619 | C | N3-C4-N4 | 5.74 | 122.02 | 118.00 |
| 35 | E | 1217 | A | C5-C6-N6 | -5.74 | 119.11 | 123.70 |
| 35 | E | 2228 | C | N3-C4-C5 | -5.74 | 119.61 | 121.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 504 | A | O4'-C1'-N9 | 5.74 | 112.79 | 108.20 |
| 35 | E | 659 | A | C5-C6-N6 | -5.74 | 119.11 | 123.70 |
| 35 | E | 1265 | A | C5-C6-N6 | -5.74 | 119.11 | 123.70 |
| 35 | E | 1279 | A | C5-C6-N6 | -5.74 | 119.11 | 123.70 |
| 35 | E | 1875 | G | O4'-C1'-N9 | 5.74 | 112.79 | 108.20 |
| 35 | E | 167 | A | C5-C6-N6 | -5.73 | 119.11 | 123.70 |
| 35 | E | 369 | C | O4'-C1'-N1 | 5.73 | 112.79 | 108.20 |
| 35 | E | 618 | G | O4'-C1'-N9 | 5.73 | 112.79 | 108.20 |
| 35 | E | 775 | A | C4-C5-C6 | 5.73 | 119.87 | 117.00 |
| 35 | E | 1235 | A | C5-C6-N6 | -5.73 | 119.11 | 123.70 |
| 35 | E | 1240 | A | C5-C6-N1 | -5.73 | 114.83 | 117.70 |
| 35 | E | 1812 | A | C4-C5-C6 | 5.73 | 119.87 | 117.00 |
| 35 | E | 28 | A | O4'-C1'-N9 | 5.73 | 112.79 | 108.20 |
| 35 | E | 552 | G | O4'-C1'-N9 | 5.73 | 112.79 | 108.20 |
| 35 | E | 773 | U | O4'-C1'-N1 | 5.73 | 112.78 | 108.20 |
| 35 | E | 787 | C | N3-C4-N4 | 5.73 | 122.01 | 118.00 |
| 35 | E | 791 | G | O4'-C1'-N9 | 5.73 | 112.78 | 108.20 |
| 35 | E | 1255 | A | C4-C5-C6 | 5.73 | 119.87 | 117.00 |
| 35 | E | 2031 | A | C5-C6-N1 | -5.73 | 114.83 | 117.70 |
| 35 | E | 28 | A | C5-C6-N6 | -5.73 | 119.12 | 123.70 |
| 35 | E | 516 | A | O4'-C1'-N9 | 5.73 | 112.78 | 108.20 |
| 35 | E | 694 | A | P-O3'-C3' | 5.73 | 126.58 | 119.70 |
| 35 | E | 701 | C | N3-C4-N4 | 5.73 | 122.01 | 118.00 |
| 35 | E | 783 | A | C5-C6-N6 | -5.73 | 119.12 | 123.70 |
| 35 | E | 142 | A | C5-C6-N6 | -5.73 | 119.12 | 123.70 |
| 35 | E | 1368 | A | C5-C6-N6 | -5.73 | 119.12 | 123.70 |
| 35 | E | 1616 | C | N3-C4-C5 | -5.73 | 119.61 | 121.90 |
| 35 | E | 114 | C | N3-C4-C5 | -5.72 | 119.61 | 121.90 |
| 35 | E | 978 | U | O4'-C1'-N1 | 5.72 | 112.78 | 108.20 |
| 35 | E | 1175 | A | C5-C6-N6 | -5.72 | 119.12 | 123.70 |
| 35 | E | 1671 | A | C5-C6-N6 | -5.72 | 119.12 | 123.70 |
| 35 | E | 1781 | A | C5-C6-N6 | -5.72 | 119.12 | 123.70 |
| 35 | E | 1984 | A | C5-C6-N1 | -5.72 | 114.84 | 117.70 |
| 35 | E | 2237 | G | O4'-C1'-N9 | 5.72 | 112.78 | 108.20 |
| 35 | E | 249 | A | C5-C6-N6 | -5.72 | 119.12 | 123.70 |
| 35 | E | 408 | C | N3-C4-N4 | 5.72 | 122.01 | 118.00 |
| 35 | E | 507 | A | O4'-C1'-N9 | 5.72 | 112.78 | 108.20 |
| 35 | E | 639 | A | C5-C6-N1 | -5.72 | 114.84 | 117.70 |
| 35 | E | 1289 | G | O4'-C1'-N9 | 5.72 | 112.78 | 108.20 |
| 35 | E | 1974 | C | N3-C4-C5 | -5.72 | 119.61 | 121.90 |
| 35 | E | 2122 | G | O4'-C1'-N9 | 5.72 | 112.78 | 108.20 |
| 35 | E | 916 | A | C5-C6-N6 | -5.72 | 119.12 | 123.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1553 | A | C5-C6-N1 | -5.72 | 114.84 | 117.70 |
| 35 | E | 875 | A | C5-C6-N6 | -5.72 | 119.12 | 123.70 |
| 35 | E | 942 | C | C2'-C3'-O3' | 5.72 | 122.85 | 113.70 |
| 35 | E | 974 | A | C5-C6-N6 | -5.72 | 119.12 | 123.70 |
| 35 | E | 1862 | C | N3-C4-N4 | 5.72 | 122.00 | 118.00 |
| 35 | E | 2238 | A | C5-C6-N1 | -5.72 | 114.84 | 117.70 |
| 35 | E | 20 | G | O4'-C1'-N9 | 5.72 | 112.77 | 108.20 |
| 35 | E | 809 | A | C5-C6-N6 | -5.72 | 119.13 | 123.70 |
| 35 | E | 822 | A | C4-C5-C6 | 5.72 | 119.86 | 117.00 |
| 35 | E | 1172 | C | N3-C4-N4 | 5.72 | 122.00 | 118.00 |
| 35 | E | 1248 | A | O4'-C1'-N9 | 5.72 | 112.77 | 108.20 |
| 35 | E | 1370 | A | C5-C6-N6 | -5.72 | 119.13 | 123.70 |
| 35 | E | 1681 | A | C5-C6-N1 | -5.72 | 114.84 | 117.70 |
| 35 | E | 1966 | C | C2-N1-C1' | 5.72 | 125.09 | 118.80 |
| 35 | E | 2167 | A | C5-C6-N6 | -5.72 | 119.13 | 123.70 |
| 35 | E | 288 | A | O4'-C1'-N9 | 5.71 | 112.77 | 108.20 |
| 35 | E | 984 | A | C4-C5-C6 | 5.71 | 119.86 | 117.00 |
| 35 | E | 2145 | A | C5-C6-N1 | -5.71 | 114.84 | 117.70 |
| 35 | E | 2165 | A | C4-C5-C6 | 5.71 | 119.86 | 117.00 |
| 35 | E | 466 | G | O4'-C1'-N9 | 5.71 | 112.77 | 108.20 |
| 35 | E | 873 | C | O4'-C1'-N1 | 5.71 | 112.77 | 108.20 |
| 35 | E | 1210 | G | O4'-C1'-N9 | 5.71 | 112.77 | 108.20 |
| 35 | E | 261 | A | C4-C5-C6 | 5.71 | 119.86 | 117.00 |
| 35 | E | 1167 | C | N3-C4-C5 | -5.71 | 119.61 | 121.90 |
| 35 | E | 2001 | A | C4-C5-C6 | 5.71 | 119.86 | 117.00 |
| 35 | E | 2273 | A | C5-C6-N1 | -5.71 | 114.84 | 117.70 |
| 35 | E | 73 | A | C4-C5-C6 | 5.71 | 119.86 | 117.00 |
| 35 | E | 148 | G | O4'-C1'-N9 | 5.71 | 112.77 | 108.20 |
| 35 | E | 182 | C | N3-C4-N4 | 5.71 | 122.00 | 118.00 |
| 35 | E | 1086 | A | C4-C5-C6 | 5.71 | 119.86 | 117.00 |
| 35 | E | 2216 | A | C4-C5-C6 | 5.71 | 119.86 | 117.00 |
| 35 | E | 711 | A | C4-C5-C6 | 5.71 | 119.85 | 117.00 |
| 35 | E | 2005 | A | C5-C6-N6 | -5.71 | 119.13 | 123.70 |
| 35 | E | 2167 | A | C4-C5-C6 | 5.71 | 119.85 | 117.00 |
| 35 | E | 1076 | C | N3-C4-C5 | -5.71 | 119.62 | 121.90 |
| 35 | E | 532 | G | O4'-C1'-N9 | 5.70 | 112.76 | 108.20 |
| 35 | E | 718 | A | O4'-C1'-N9 | 5.70 | 112.76 | 108.20 |
| 35 | E | 883 | C | O4'-C1'-N1 | 5.70 | 112.76 | 108.20 |
| 35 | E | 1672 | C | N3-C4-N4 | 5.70 | 121.99 | 118.00 |
| 35 | E | 596 | A | C5-C6-N6 | -5.70 | 119.14 | 123.70 |
| 35 | E | 1250 | A | C5-C6-N1 | -5.70 | 114.85 | 117.70 |
| 35 | E | 1292 | A | C4-C5-C6 | 5.70 | 119.85 | 117.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1534 | A | C4-C5-C6 | 5.70 | 119.85 | 117.00 |
| 35 | E | 610 | A | C4-C5-C6 | 5.70 | 119.85 | 117.00 |
| 35 | E | 861 | A | C4-C5-C6 | 5.70 | 119.85 | 117.00 |
| 35 | E | 915 | A | C5-C6-N6 | -5.70 | 119.14 | 123.70 |
| 35 | E | 1088 | A | C5-C6-N1 | -5.70 | 114.85 | 117.70 |
| 35 | E | 1192 | A | C5-C6-N6 | -5.70 | 119.14 | 123.70 |
| 35 | E | 469 | G | O4'-C1'-N9 | 5.70 | 112.76 | 108.20 |
| 35 | E | 1077 | C | O4'-C1'-N1 | 5.70 | 112.76 | 108.20 |
| 35 | E | 1263 | G | O4'-C1'-N9 | 5.70 | 112.76 | 108.20 |
| 35 | E | 1529 | A | O4'-C1'-N9 | 5.70 | 112.76 | 108.20 |
| 35 | E | 1676 | A | C5-C6-N1 | -5.70 | 114.85 | 117.70 |
| 35 | E | 1866 | A | C5-C6-N6 | -5.70 | 119.14 | 123.70 |
| 35 | E | 1966 | C | N3-C4-N4 | 5.70 | 121.99 | 118.00 |
| 35 | E | 2211 | C | N3-C4-N4 | 5.70 | 121.99 | 118.00 |
| 35 | E | 152 | A | C4-C5-C6 | 5.70 | 119.85 | 117.00 |
| 35 | E | 742 | A | C4-C5-C6 | 5.70 | 119.85 | 117.00 |
| 35 | E | 934 | C | N3-C4-N4 | 5.70 | 121.99 | 118.00 |
| 35 | E | 569 | A | C5-C6-N6 | -5.69 | 119.14 | 123.70 |
| 35 | E | 745 | C | C6-N1-C2 | -5.69 | 118.02 | 120.30 |
| 35 | E | 935 | A | C5-C6-N1 | -5.69 | 114.85 | 117.70 |
| 35 | E | 123 | A | C4-C5-C6 | 5.69 | 119.85 | 117.00 |
| 35 | E | 168 | A | C5-C6-N6 | -5.69 | 119.15 | 123.70 |
| 35 | E | 498 | A | C5-C6-N6 | -5.69 | 119.15 | 123.70 |
| 35 | E | 586 | A | C5-C6-N6 | -5.69 | 119.15 | 123.70 |
| 35 | E | 723 | C | N3-C4-N4 | 5.69 | 121.98 | 118.00 |
| 35 | E | 1568 | A | C5-C6-N6 | -5.69 | 119.15 | 123.70 |
| 35 | E | 1595 | A | C5-C6-N1 | -5.69 | 114.85 | 117.70 |
| 35 | E | 1799 | A | C5-C6-N1 | -5.69 | 114.85 | 117.70 |
| 35 | E | 1845 | C | N3-C4-N4 | 5.69 | 121.98 | 118.00 |
| 35 | E | 227 | U | O4'-C1'-N1 | 5.69 | 112.75 | 108.20 |
| 35 | E | 1627 | C | O4'-C1'-N1 | 5.69 | 112.75 | 108.20 |
| 35 | E | 1926 | G | O4'-C1'-N9 | 5.69 | 112.75 | 108.20 |
| 35 | E | 542 | C | N3-C4-N4 | 5.69 | 121.98 | 118.00 |
| 35 | E | 668 | C | N3-C4-N4 | 5.69 | 121.98 | 118.00 |
| 35 | E | 1896 | C | N3-C4-C5 | -5.69 | 119.62 | 121.90 |
| 35 | E | 2090 | U | O4'-C1'-N1 | 5.69 | 112.75 | 108.20 |
| 35 | E | 1275 | A | C4-C5-C6 | 5.69 | 119.84 | 117.00 |
| 35 | E | 639 | A | C5-C6-N6 | -5.68 | 119.15 | 123.70 |
| 35 | E | 1257 | C | N3-C4-N4 | 5.68 | 121.98 | 118.00 |
| 35 | E | 68 | A | C5-C6-N6 | -5.68 | 119.16 | 123.70 |
| 35 | E | 1205 | A | O4'-C1'-N9 | 5.68 | 112.75 | 108.20 |
| 35 | E | 1539 | A | C5-C6-N6 | -5.68 | 119.16 | 123.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 112 | A | C4-C5-C6 | 5.68 | 119.84 | 117.00 |
| 35 | E | 479 | G | O4'-C1'-N9 | 5.68 | 112.74 | 108.20 |
| 35 | E | 1807 | U | O4'-C1'-N1 | 5.68 | 112.74 | 108.20 |
| 35 | E | 1811 | C | N3-C4-N4 | 5.68 | 121.97 | 118.00 |
| 35 | E | 2032 | U | C2-N1-C1' | 5.68 | 124.52 | 117.70 |
| 35 | E | 2149 | C | N3-C4-N4 | 5.68 | 121.98 | 118.00 |
| 35 | E | 945 | C | N3-C4-N4 | 5.68 | 121.97 | 118.00 |
| 35 | E | 2245 | A | O4'-C1'-N9 | 5.68 | 112.74 | 108.20 |
| 35 | E | 256 | A | C5-C6-N6 | -5.68 | 119.16 | 123.70 |
| 35 | E | 522 | A | C4-C5-C6 | 5.68 | 119.84 | 117.00 |
| 35 | E | 735 | A | C5-C6-N6 | -5.68 | 119.16 | 123.70 |
| 35 | E | 2047 | A | C5-C6-N6 | -5.68 | 119.16 | 123.70 |
| 35 | E | 2245 | A | C5-C6-N1 | -5.68 | 114.86 | 117.70 |
| 35 | E | 417 | A | O4'-C1'-N9 | 5.67 | 112.74 | 108.20 |
| 35 | E | 467 | A | C5-C6-N1 | -5.67 | 114.86 | 117.70 |
| 35 | E | 2267 | A | O4'-C1'-N9 | 5.67 | 112.74 | 108.20 |
| 35 | E | 782 | A | C5-C6-N6 | -5.67 | 119.16 | 123.70 |
| 35 | E | 2048 | A | O4'-C1'-N9 | 5.67 | 112.74 | 108.20 |
| 35 | E | 44 | C | N3-C4-C5 | -5.67 | 119.63 | 121.90 |
| 35 | E | 314 | A | C5-C6-N6 | -5.67 | 119.16 | 123.70 |
| 35 | E | 598 | A | C5-C6-N6 | -5.67 | 119.16 | 123.70 |
| 35 | E | 698 | C | N3-C4-N4 | 5.67 | 121.97 | 118.00 |
| 35 | E | 732 | C | P-O3'-C3' | 5.67 | 126.51 | 119.70 |
| 35 | E | 1987 | A | O4'-C1'-N9 | 5.67 | 112.74 | 108.20 |
| 35 | E | 690 | A | C5-C6-N1 | -5.67 | 114.86 | 117.70 |
| 35 | E | 860 | U | O4'-C1'-N1 | 5.67 | 112.74 | 108.20 |
| 35 | E | 362 | C | N3-C4-C5 | -5.67 | 119.63 | 121.90 |
| 35 | E | 1915 | G | O4'-C1'-N9 | 5.67 | 112.73 | 108.20 |
| 35 | E | 492 | A | C4-C5-C6 | 5.67 | 119.83 | 117.00 |
| 35 | E | 500 | A | C5-C6-N6 | -5.67 | 119.17 | 123.70 |
| 35 | E | 1529 | A | C5-C6-N6 | -5.67 | 119.17 | 123.70 |
| 35 | E | 994 | G | O4'-C1'-N9 | 5.67 | 112.73 | 108.20 |
| 35 | E | 1815 | A | C5-C6-N1 | -5.67 | 114.87 | 117.70 |
| 35 | E | 1942 | A | C5-C6-N6 | -5.67 | 119.17 | 123.70 |
| 35 | E | 2048 | A | C5-C6-N6 | -5.67 | 119.17 | 123.70 |
| 35 | E | 293 | U | O4'-C1'-N1 | 5.66 | 112.73 | 108.20 |
| 35 | E | 516 | A | C5-C6-N6 | -5.66 | 119.17 | 123.70 |
| 35 | E | 858 | A | C5-C6-N1 | -5.66 | 114.87 | 117.70 |
| 35 | E | 861 | A | O4'-C1'-N9 | 5.66 | 112.73 | 108.20 |
| 35 | E | 959 | A | C5-C6-N1 | -5.66 | 114.87 | 117.70 |
| 35 | E | 1270 | A | C5-C6-N1 | -5.66 | 114.87 | 117.70 |
| 35 | E | 1959 | C | N3-C4-C5 | -5.66 | 119.63 | 121.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 62 | A | O4'-C1'-N9 | 5.66 | 112.73 | 108.20 |
| 35 | E | 174 | U | O4'-C1'-N1 | 5.66 | 112.73 | 108.20 |
| 35 | E | 366 | C | N3-C4-C5 | -5.66 | 119.64 | 121.90 |
| 35 | E | 2011 | A | C5-C6-N6 | -5.66 | 119.17 | 123.70 |
| 35 | E | 2098 | C | N3-C4-N4 | 5.66 | 121.96 | 118.00 |
| 35 | E | 765 | A | C5-C6-N1 | -5.66 | 114.87 | 117.70 |
| 35 | E | 1086 | A | C5-C6-N6 | -5.66 | 119.17 | 123.70 |
| 35 | E | 1181 | C | N3-C4-N4 | 5.66 | 121.96 | 118.00 |
| 35 | E | 1922 | G | O4'-C1'-N9 | 5.66 | 112.73 | 108.20 |
| 35 | E | 2065 | A | C5-C6-N1 | -5.66 | 114.87 | 117.70 |
| 35 | E | 434 | A | C5-C6-N1 | -5.66 | 114.87 | 117.70 |
| 35 | E | 571 | A | C5-C6-N1 | -5.66 | 114.87 | 117.70 |
| 35 | E | 707 | C | N3-C4-N4 | 5.66 | 121.96 | 118.00 |
| 35 | E | 990 | A | C5-C6-N6 | -5.66 | 119.17 | 123.70 |
| 35 | E | 852 | A | C5-C6-N6 | -5.66 | 119.18 | 123.70 |
| 35 | E | 1733 | A | C5-C6-N6 | -5.66 | 119.18 | 123.70 |
| 35 | E | 2236 | C | N3-C4-C5 | -5.66 | 119.64 | 121.90 |
| 35 | E | 910 | A | C4-C5-C6 | 5.65 | 119.83 | 117.00 |
| 35 | E | 1299 | U | O4'-C1'-N1 | 5.65 | 112.72 | 108.20 |
| 35 | E | 2141 | G | O4'-C1'-N9 | 5.65 | 112.72 | 108.20 |
| 35 | E | 2236 | C | N3-C4-N4 | 5.65 | 121.96 | 118.00 |
| 35 | E | 2299 | A | C5-C6-N6 | -5.65 | 119.18 | 123.70 |
| 35 | E | 300 | A | C5-C6-N1 | -5.65 | 114.88 | 117.70 |
| 35 | E | 647 | A | O4'-C1'-N9 | 5.65 | 112.72 | 108.20 |
| 35 | E | 728 | A | C5-C6-N6 | -5.65 | 119.18 | 123.70 |
| 35 | E | 771 | A | C5-C6-N6 | -5.65 | 119.18 | 123.70 |
| 35 | E | 1279 | A | C4-C5-C6 | 5.65 | 119.83 | 117.00 |
| 35 | E | 2173 | C | N3-C4-N4 | 5.65 | 121.95 | 118.00 |
| 35 | E | 1999 | A | O4'-C1'-N9 | 5.65 | 112.72 | 108.20 |
| 35 | E | 2264 | A | C5-C6-N1 | -5.65 | 114.88 | 117.70 |
| 35 | E | 1215 | A | C5-C6-N6 | -5.65 | 119.18 | 123.70 |
| 35 | E | 1383 | G | O4'-C1'-N9 | 5.65 | 112.72 | 108.20 |
| 35 | E | 2039 | A | C5-C6-N1 | -5.65 | 114.88 | 117.70 |
| 35 | E | 141 | A | C5-C6-N1 | -5.65 | 114.88 | 117.70 |
| 35 | E | 2169 | A | C5-C6-N6 | -5.65 | 119.18 | 123.70 |
| 35 | E | 237 | A | C4-C5-C6 | 5.64 | 119.82 | 117.00 |
| 35 | E | 633 | A | C4-C5-C6 | 5.64 | 119.82 | 117.00 |
| 35 | E | 941 | U | P-O3'-C3' | 5.64 | 126.47 | 119.70 |
| 35 | E | 2105 | C | N3-C4-N4 | 5.64 | 121.95 | 118.00 |
| 35 | E | 348 | A | C5-C6-N1 | -5.64 | 114.88 | 117.70 |
| 35 | E | 629 | C | N3-C4-N4 | 5.64 | 121.95 | 118.00 |
| 35 | E | 282 | C | N3-C4-N4 | 5.64 | 121.95 | 118.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 447 | A | C5-C6-N6 | -5.64 | 119.19 | 123.70 |
| 35 | E | 503 | A | C5-C6-N6 | -5.64 | 119.19 | 123.70 |
| 35 | E | 754 | G | O4'-C1'-N9 | 5.64 | 112.71 | 108.20 |
| 35 | E | 1637 | G | N3-C2-N2 | 5.64 | 123.85 | 119.90 |
| 35 | E | 407 | G | O4'-C1'-N9 | 5.64 | 112.71 | 108.20 |
| 35 | E | 865 | A | C5-C6-N6 | -5.64 | 119.19 | 123.70 |
| 35 | E | 880 | A | C4-C5-C6 | 5.64 | 119.82 | 117.00 |
| 35 | E | 1355 | A | C5-C6-N6 | -5.64 | 119.19 | 123.70 |
| 35 | E | 1574 | A | C5-C6-N1 | -5.64 | 114.88 | 117.70 |
| 35 | E | 1793 | G | O4'-C1'-N9 | 5.64 | 112.71 | 108.20 |
| 35 | E | 1904 | U | O4'-C1'-N1 | 5.64 | 112.71 | 108.20 |
| 35 | E | 1982 | C | N3-C4-N4 | 5.63 | 121.94 | 118.00 |
| 35 | E | 40 | A | C5-C6-N6 | -5.63 | 119.19 | 123.70 |
| 35 | E | 348 | A | C5-C6-N6 | -5.63 | 119.19 | 123.70 |
| 35 | E | 157 | G | O4'-C1'-N9 | 5.63 | 112.70 | 108.20 |
| 35 | E | 954 | G | O4'-C1'-N9 | 5.63 | 112.70 | 108.20 |
| 35 | E | 1343 | A | C5-C6-N1 | -5.63 | 114.88 | 117.70 |
| 35 | E | 1232 | C | N3-C4-N4 | 5.63 | 121.94 | 118.00 |
| 35 | E | 1261 | A | O4'-C1'-N9 | 5.63 | 112.70 | 108.20 |
| 35 | E | 355 | G | O4'-C1'-N9 | 5.63 | 112.70 | 108.20 |
| 35 | E | 1237 | G | O4'-C1'-N9 | 5.63 | 112.70 | 108.20 |
| 35 | E | 1357 | U | O4'-C1'-N1 | 5.63 | 112.70 | 108.20 |
| 35 | E | 1679 | A | C5-C6-N6 | -5.63 | 119.20 | 123.70 |
| 35 | E | 1833 | U | O4'-C1'-N1 | 5.63 | 112.70 | 108.20 |
| 35 | E | 2037 | A | O4'-C1'-N9 | 5.63 | 112.70 | 108.20 |
| 35 | E | 2137 | C | N3-C4-C5 | -5.63 | 119.65 | 121.90 |
| 35 | E | 1869 | G | O4'-C1'-N9 | 5.63 | 112.70 | 108.20 |
| 35 | E | 2036 | A | C5-C6-N6 | -5.63 | 119.20 | 123.70 |
| 35 | E | 2166 | C | N3-C4-C5 | -5.63 | 119.65 | 121.90 |
| 35 | E | 662 | C | N3-C4-N4 | 5.62 | 121.94 | 118.00 |
| 4 | t | 122 | TYR | CB-CG-CD1 | 5.62 | 124.37 | 121.00 |
| 35 | E | 160 | A | O4'-C1'-N9 | 5.62 | 112.70 | 108.20 |
| 35 | E | 444 | A | C5-C6-N6 | -5.62 | 119.20 | 123.70 |
| 35 | E | 1241 | A | C5-C6-N1 | -5.62 | 114.89 | 117.70 |
| 35 | E | 2199 | A | C5-C6-N6 | -5.62 | 119.20 | 123.70 |
| 35 | E | 727 | C | N3-C4-N4 | 5.62 | 121.94 | 118.00 |
| 35 | E | 771 | A | C4-C5-C6 | 5.62 | 119.81 | 117.00 |
| 35 | E | 1203 | G | O4'-C1'-N9 | 5.62 | 112.70 | 108.20 |
| 35 | E | 1987 | A | C5-C6-N6 | -5.62 | 119.20 | 123.70 |
| 35 | E | 2035 | A | O4'-C1'-N9 | 5.62 | 112.70 | 108.20 |
| 35 | E | 2198 | C | N3-C4-N4 | 5.62 | 121.93 | 118.00 |
| 35 | E | 499 | A | C5-C6-N6 | -5.62 | 119.20 | 123.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 781 | A | O4'-C1'-N9 | 5.62 | 112.70 | 108.20 |
| 30 | m | 144 | GLN | N-CA-CB | 5.62 | 120.71 | 110.60 |
| 35 | E | 180 | A | C5-C6-N6 | -5.62 | 119.20 | 123.70 |
| 35 | E | 367 | A | C4-C5-C6 | 5.62 | 119.81 | 117.00 |
| 35 | E | 760 | C | N3-C4-C5 | -5.62 | 119.65 | 121.90 |
| 35 | E | 928 | C | N3-C4-N4 | 5.62 | 121.93 | 118.00 |
| 35 | E | 1789 | A | C4-C5-C6 | 5.62 | 119.81 | 117.00 |
| 35 | E | 2050 | C | O4'-C1'-N1 | 5.62 | 112.69 | 108.20 |
| 35 | E | 1907 | C | N3-C4-N4 | 5.62 | 121.93 | 118.00 |
| 35 | E | 151 | A | C4-C5-C6 | 5.62 | 119.81 | 117.00 |
| 35 | E | 648 | A | C4-C5-C6 | 5.62 | 119.81 | 117.00 |
| 35 | E | 1170 | C | N3-C4-C5 | -5.62 | 119.65 | 121.90 |
| 35 | E | 1268 | A | C5-C6-N1 | -5.62 | 114.89 | 117.70 |
| 35 | E | 1824 | A | C4-C5-C6 | 5.62 | 119.81 | 117.00 |
| 35 | E | 2044 | G | O4'-C1'-N9 | 5.62 | 112.69 | 108.20 |
| 35 | E | 44 | C | N3-C4-N4 | 5.61 | 121.93 | 118.00 |
| 35 | E | 1605 | A | C5-C6-N1 | -5.61 | 114.89 | 117.70 |
| 35 | E | 1651 | A | C4-C5-C6 | 5.61 | 119.81 | 117.00 |
| 35 | E | 2278 | G | O4'-C1'-N9 | 5.61 | 112.69 | 108.20 |
| 35 | E | 2297 | U | O4'-C1'-N1 | 5.61 | 112.69 | 108.20 |
| 35 | E | 414 | A | C5-C6-N1 | -5.61 | 114.89 | 117.70 |
| 35 | E | 433 | G | O4'-C1'-N9 | 5.61 | 112.69 | 108.20 |
| 35 | E | 816 | C | N3-C4-N4 | 5.61 | 121.93 | 118.00 |
| 35 | E | 990 | A | O4'-C1'-N9 | 5.61 | 112.69 | 108.20 |
| 35 | E | 1312 | A | C5-C6-N6 | -5.61 | 119.21 | 123.70 |
| 35 | E | 1552 | A | C5-C6-N1 | -5.61 | 114.89 | 117.70 |
| 35 | E | 504 | A | C5-C6-N6 | -5.61 | 119.21 | 123.70 |
| 35 | E | 586 | A | O4'-C1'-N9 | 5.61 | 112.69 | 108.20 |
| 35 | E | 599 | A | C5-C6-N6 | -5.61 | 119.21 | 123.70 |
| 35 | E | 2260 | A | C5-C6-N1 | -5.61 | 114.89 | 117.70 |
| 2 | q | 30 | ALA | N-CA-CB | 5.61 | 117.95 | 110.10 |
| 35 | E | 1865 | A | O4'-C1'-N9 | 5.61 | 112.69 | 108.20 |
| 35 | E | 1881 | C | N3-C4-N4 | 5.61 | 121.93 | 118.00 |
| 35 | E | 254 | A | P-O3'-C3' | 5.61 | 126.43 | 119.70 |
| 35 | E | 268 | C | N3-C4-N4 | 5.61 | 121.92 | 118.00 |
| 35 | E | 879 | C | N3-C4-N4 | 5.61 | 121.92 | 118.00 |
| 35 | E | 1863 | C | N3-C4-C5 | -5.61 | 119.66 | 121.90 |
| 35 | E | 2049 | C | N3-C4-C5 | -5.61 | 119.66 | 121.90 |
| 35 | E | 2192 | A | C5-C6-N1 | -5.61 | 114.90 | 117.70 |
| 35 | E | 57 | G | O4'-C1'-N9 | 5.61 | 112.68 | 108.20 |
| 35 | E | 501 | A | C5-C6-N6 | -5.61 | 119.22 | 123.70 |
| 35 | E | 506 | A | C5-C6-N6 | -5.61 | 119.22 | 123.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 821 | C | O4'-C1'-N1 | 5.61 | 112.69 | 108.20 |
| 35 | E | 992 | A | C5-C6-N6 | -5.61 | 119.22 | 123.70 |
| 35 | E | 1248 | A | C5-C6-N6 | -5.61 | 119.22 | 123.70 |
| 35 | E | 2272 | A | C5-C6-N6 | -5.61 | 119.22 | 123.70 |
| 3 | r | 85 | TYR | CB-CG-CD2 | -5.60 | 117.64 | 121.00 |
| 35 | E | 1619 | A | C4-C5-C6 | 5.60 | 119.80 | 117.00 |
| 35 | E | 1919 | A | O4'-C1'-N9 | 5.60 | 112.68 | 108.20 |
| 35 | E | 2027 | C | C6-N1-C1' | -5.60 | 114.08 | 120.80 |
| 35 | E | 159 | G | N3-C2-N2 | 5.60 | 123.82 | 119.90 |
| 35 | E | 747 | U | O4'-C1'-N1 | 5.60 | 112.68 | 108.20 |
| 35 | E | 750 | C | N3-C4-C5 | -5.60 | 119.66 | 121.90 |
| 35 | E | 874 | C | N3-C4-N4 | 5.60 | 121.92 | 118.00 |
| 35 | E | 922 | C | N3-C4-C5 | -5.60 | 119.66 | 121.90 |
| 35 | E | 1829 | C | N3-C4-C5 | -5.60 | 119.66 | 121.90 |
| 35 | E | 1919 | A | C5-C6-N1 | -5.60 | 114.90 | 117.70 |
| 35 | E | 2076 | A | C5-C6-N1 | -5.60 | 114.90 | 117.70 |
| 35 | E | 2270 | C | N3-C4-N4 | 5.60 | 121.92 | 118.00 |
| 35 | E | 352 | A | C5-C6-N6 | -5.60 | 119.22 | 123.70 |
| 35 | E | 1211 | G | O4'-C1'-N9 | 5.60 | 112.68 | 108.20 |
| 35 | E | 1845 | C | N3-C4-C5 | -5.60 | 119.66 | 121.90 |
| 35 | E | 577 | A | C5-C6-N6 | -5.60 | 119.22 | 123.70 |
| 35 | E | 779 | A | C5-C6-N6 | -5.60 | 119.22 | 123.70 |
| 35 | E | 1784 | C | N3-C4-C5 | -5.60 | 119.66 | 121.90 |
| 35 | E | 2283 | A | C5-C6-N6 | -5.60 | 119.22 | 123.70 |
| 35 | E | 107 | A | C5-C6-N6 | -5.60 | 119.22 | 123.70 |
| 35 | E | 217 | C | N3-C4-N4 | 5.60 | 121.92 | 118.00 |
| 35 | E | 569 | A | C5-C6-N1 | -5.60 | 114.90 | 117.70 |
| 35 | E | 810 | U | C2'-C3'-O3' | 5.60 | 122.66 | 113.70 |
| 35 | E | 1823 | G | O4'-C1'-N9 | 5.60 | 112.68 | 108.20 |
| 35 | E | 2172 | G | O4'-C1'-N9 | 5.60 | 112.68 | 108.20 |
| 35 | E | 314 | A | C5-C6-N1 | -5.59 | 114.90 | 117.70 |
| 35 | E | 318 | C | N3-C4-N4 | 5.59 | 121.92 | 118.00 |
| 35 | E | 376 | C | N3-C4-N4 | 5.59 | 121.92 | 118.00 |
| 35 | E | 2104 | A | C5-C6-N1 | -5.59 | 114.90 | 117.70 |
| 35 | E | 56 | U | O4'-C1'-N1 | 5.59 | 112.67 | 108.20 |
| 35 | E | 364 | G | O4'-C1'-N9 | 5.59 | 112.67 | 108.20 |
| 35 | E | 587 | A | C5-C6-N6 | -5.59 | 119.23 | 123.70 |
| 35 | E | 778 | A | C5-C6-N6 | -5.59 | 119.23 | 123.70 |
| 35 | E | 1706 | A | O4'-C1'-N9 | 5.59 | 112.67 | 108.20 |
| 35 | E | 208 | G | O4'-C1'-N9 | 5.59 | 112.67 | 108.20 |
| 35 | E | 474 | C | N3-C4-N4 | 5.59 | 121.91 | 118.00 |
| 35 | E | 1196 | A | C5-C6-N6 | -5.59 | 119.23 | 123.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1323 | A | C5-C6-N1 | -5.59 | 114.91 | 117.70 |
| 35 | E | 2026 | A | C5-C6-N6 | -5.59 | 119.23 | 123.70 |
| 35 | E | 879 | C | O4'-C1'-N1 | 5.59 | 112.67 | 108.20 |
| 35 | E | 1255 | A | C5-C6-N6 | -5.59 | 119.23 | 123.70 |
| 35 | E | 1698 | A | C5-C6-N1 | -5.59 | 114.91 | 117.70 |
| 35 | E | 256 | A | C5-C6-N1 | -5.59 | 114.91 | 117.70 |
| 35 | E | 101 | C | N3-C4-N4 | 5.58 | 121.91 | 118.00 |
| 35 | E | 139 | G | O4'-C1'-N9 | 5.58 | 112.67 | 108.20 |
| 35 | E | 452 | C | N3-C4-N4 | 5.58 | 121.91 | 118.00 |
| 35 | E | 942 | C | N3-C4-N4 | 5.58 | 121.91 | 118.00 |
| 35 | E | 81 | A | C5-C6-N1 | -5.58 | 114.91 | 117.70 |
| 35 | E | 112 | A | C5-C6-N6 | -5.58 | 119.23 | 123.70 |
| 35 | E | 595 | A | C5-C6-N6 | -5.58 | 119.23 | 123.70 |
| 35 | E | 1180 | A | C5-C6-N6 | -5.58 | 119.23 | 123.70 |
| 35 | E | 1626 | C | N3-C4-C5 | -5.58 | 119.67 | 121.90 |
| 35 | E | 788 | A | C5-C6-N1 | -5.58 | 114.91 | 117.70 |
| 35 | E | 995 | C | N3-C4-C5 | -5.58 | 119.67 | 121.90 |
| 35 | E | 1312 | A | O4'-C1'-N9 | 5.58 | 112.67 | 108.20 |
| 35 | E | 43 | A | C5-C6-N6 | -5.58 | 119.24 | 123.70 |
| 35 | E | 1878 | A | C5-C6-N6 | -5.58 | 119.24 | 123.70 |
| 35 | E | 2060 | C | N3-C4-N4 | 5.58 | 121.91 | 118.00 |
| 35 | E | 124 | A | C5-C6-N1 | -5.58 | 114.91 | 117.70 |
| 35 | E | 675 | A | C4-C5-C6 | 5.58 | 119.79 | 117.00 |
| 35 | E | 833 | A | C5-C6-N1 | -5.58 | 114.91 | 117.70 |
| 35 | E | 2274 | A | C5-C6-N6 | -5.58 | 119.24 | 123.70 |
| 35 | E | 100 | A | C5-C6-N1 | -5.58 | 114.91 | 117.70 |
| 35 | E | 158 | C | N3-C4-N4 | 5.58 | 121.90 | 118.00 |
| 35 | E | 1684 | C | N3-C4-C5 | -5.58 | 119.67 | 121.90 |
| 35 | E | 2048 | A | C5-C6-N1 | -5.58 | 114.91 | 117.70 |
| 35 | E | 2107 | A | C4-C5-C6 | 5.58 | 119.79 | 117.00 |
| 35 | E | 2130 | C | N3-C4-C5 | -5.58 | 119.67 | 121.90 |
| 35 | E | 837 | C | N3-C4-N4 | 5.57 | 121.90 | 118.00 |
| 35 | E | 1215 | A | C5-C6-N1 | -5.57 | 114.91 | 117.70 |
| 35 | E | 1781 | A | C5-C6-N1 | -5.57 | 114.91 | 117.70 |
| 35 | E | 1812 | A | C5-C6-N1 | -5.57 | 114.91 | 117.70 |
| 35 | E | 1574 | A | O4'-C1'-N9 | 5.57 | 112.66 | 108.20 |
| 35 | E | 2259 | A | C5-C6-N6 | -5.57 | 119.24 | 123.70 |
| 35 | E | 279 | A | C5-C6-N1 | -5.57 | 114.92 | 117.70 |
| 20 | f | 172 | TYR | CB-CG-CD1 | 5.57 | 124.34 | 121.00 |
| 35 | E | 446 | A | C5-C6-N1 | -5.57 | 114.92 | 117.70 |
| 35 | E | 1670 | A | C5-C6-N6 | -5.57 | 119.25 | 123.70 |
| 35 | E | 425 | A | C5-C6-N6 | -5.57 | 119.25 | 123.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 577 | A | C5-C6-N1 | -5.57 | 114.92 | 117.70 |
| 35 | E | 1528 | C | N3-C4-N4 | 5.57 | 121.90 | 118.00 |
| 35 | E | 1631 | A | C5-C6-N6 | -5.57 | 119.25 | 123.70 |
| 35 | E | 257 | A | C5-C6-N6 | -5.56 | 119.25 | 123.70 |
| 35 | E | 960 | A | C5-C6-N6 | -5.56 | 119.25 | 123.70 |
| 35 | E | 821 | C | N3-C4-N4 | 5.56 | 121.89 | 118.00 |
| 35 | E | 1287 | A | O4'-C1'-N9 | 5.56 | 112.65 | 108.20 |
| 35 | E | 1960 | A | C5-C6-N6 | -5.56 | 119.25 | 123.70 |
| 35 | E | 2066 | C | N3-C4-C5 | -5.56 | 119.67 | 121.90 |
| 35 | E | 161 | A | C5-C6-N6 | -5.56 | 119.25 | 123.70 |
| 35 | E | 1530 | C | N3-C4-N4 | 5.56 | 121.89 | 118.00 |
| 35 | E | 1610 | A | C5-C6-N1 | -5.56 | 114.92 | 117.70 |
| 35 | E | 231 | A | O4'-C1'-N9 | 5.56 | 112.65 | 108.20 |
| 35 | E | 1999 | A | C5-C6-N6 | -5.56 | 119.25 | 123.70 |
| 35 | E | 2000 | C | N3-C4-C5 | -5.56 | 119.68 | 121.90 |
| 35 | E | 82 | A | C5-C6-N6 | -5.56 | 119.25 | 123.70 |
| 35 | E | 362 | C | N3-C4-N4 | 5.56 | 121.89 | 118.00 |
| 35 | E | 1255 | A | O4'-C1'-N9 | 5.56 | 112.65 | 108.20 |
| 35 | E | 1676 | A | C5-C6-N6 | -5.56 | 119.25 | 123.70 |
| 35 | E | 1866 | A | O4'-C1'-N9 | 5.56 | 112.65 | 108.20 |
| 35 | E | 251 | A | P-O3'-C3' | 5.56 | 126.37 | 119.70 |
| 35 | E | 1877 | U | O4'-C1'-N1 | 5.56 | 112.64 | 108.20 |
| 35 | E | 1991 | C | N3-C4-N4 | 5.56 | 121.89 | 118.00 |
| 35 | E | 2036 | A | C5-C6-N1 | -5.56 | 114.92 | 117.70 |
| 35 | E | 177 | A | C5-C6-N1 | -5.55 | 114.92 | 117.70 |
| 35 | E | 644 | C | O4'-C1'-N1 | 5.55 | 112.64 | 108.20 |
| 35 | E | 724 | A | C5'-C4'-O4' | 5.55 | 115.77 | 109.10 |
| 35 | E | 951 | U | O4'-C1'-N1 | 5.55 | 112.64 | 108.20 |
| 35 | E | 1689 | A | C5-C6-N1 | -5.55 | 114.92 | 117.70 |
| 35 | E | 704 | A | C5-C6-N1 | -5.55 | 114.92 | 117.70 |
| 35 | E | 873 | C | N3-C4-N4 | 5.55 | 121.89 | 118.00 |
| 35 | E | 1217 | A | O4'-C1'-N9 | 5.55 | 112.64 | 108.20 |
| 35 | E | 1670 | A | C4-C5-C6 | 5.55 | 119.78 | 117.00 |
| 35 | E | 1925 | A | O4'-C1'-N9 | 5.55 | 112.64 | 108.20 |
| 35 | E | 623 | C | N3-C4-N4 | 5.55 | 121.89 | 118.00 |
| 35 | E | 902 | A | C5-C6-N6 | -5.55 | 119.26 | 123.70 |
| 35 | E | 1523 | C | N3-C4-N4 | 5.55 | 121.89 | 118.00 |
| 35 | E | 1607 | A | O4'-C1'-N9 | 5.55 | 112.64 | 108.20 |
| 35 | E | 59 | C | N3-C4-N4 | 5.55 | 121.89 | 118.00 |
| 35 | E | 102 | A | O4'-C1'-N9 | 5.55 | 112.64 | 108.20 |
| 35 | E | 384 | G | O4'-C1'-N9 | 5.55 | 112.64 | 108.20 |
| 35 | E | 392 | A | C5-C6-N6 | -5.55 | 119.26 | 123.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 561 | A | O4'-C1'-N9 | 5.55 | 112.64 | 108.20 |
| 35 | E | 1525 | C | N3-C4-N4 | 5.55 | 121.89 | 118.00 |
| 35 | E | 1687 | A | C4-C5-C6 | 5.55 | 119.77 | 117.00 |
| 35 | E | 124 | A | C5-C6-N6 | -5.55 | 119.26 | 123.70 |
| 35 | E | 1724 | A | C5-C6-N1 | -5.55 | 114.93 | 117.70 |
| 35 | E | 2126 | A | C5-C6-N6 | -5.55 | 119.26 | 123.70 |
| 35 | E | 380 | U | O4'-C1'-N1 | 5.55 | 112.64 | 108.20 |
| 35 | E | 438 | A | C5-C6-N6 | -5.55 | 119.26 | 123.70 |
| 35 | E | 1192 | A | C5-C6-N1 | -5.55 | 114.93 | 117.70 |
| 35 | E | 1308 | A | C5-C6-N1 | -5.55 | 114.93 | 117.70 |
| 35 | E | 1662 | A | C5-C6-N6 | -5.55 | 119.26 | 123.70 |
| 35 | E | 1831 | C | N3-C4-N4 | 5.55 | 121.88 | 118.00 |
| 35 | E | 2050 | C | N3-C4-C5 | -5.55 | 119.68 | 121.90 |
| 35 | E | 2195 | G | O4'-C1'-N9 | 5.55 | 112.64 | 108.20 |
| 35 | E | 511 | G | O4'-C1'-N9 | 5.54 | 112.64 | 108.20 |
| 35 | E | 549 | A | C5-C6-N1 | -5.54 | 114.93 | 117.70 |
| 35 | E | 187 | C | N3-C4-N4 | 5.54 | 121.88 | 118.00 |
| 35 | E | 1264 | A | C5-C6-N6 | -5.54 | 119.27 | 123.70 |
| 35 | E | 1622 | G | O4'-C1'-N9 | 5.54 | 112.64 | 108.20 |
| 35 | E | 1728 | C | N3-C4-N4 | 5.54 | 121.88 | 118.00 |
| 35 | E | 2063 | A | C5-C6-N1 | -5.54 | 114.93 | 117.70 |
| 35 | E | 2189 | A | O4'-C1'-N9 | 5.54 | 112.64 | 108.20 |
| 35 | E | 19 | A | C5-C6-N1 | -5.54 | 114.93 | 117.70 |
| 35 | E | 831 | A | C5-C6-N1 | -5.54 | 114.93 | 117.70 |
| 35 | E | 2097 | U | C2-N1-C1' | 5.54 | 124.35 | 117.70 |
| 35 | E | 2100 | C | N3-C4-N4 | 5.54 | 121.88 | 118.00 |
| 35 | E | 2117 | C | O4'-C1'-N1 | 5.54 | 112.63 | 108.20 |
| 35 | E | 2267 | A | C5-C6-N6 | -5.54 | 119.27 | 123.70 |
| 35 | E | 527 | A | C5-C6-N1 | -5.54 | 114.93 | 117.70 |
| 35 | E | 972 | A | C5-C6-N6 | -5.54 | 119.27 | 123.70 |
| 35 | E | 61 | C | N3-C4-N4 | 5.54 | 121.88 | 118.00 |
| 35 | E | 107 | A | O4'-C1'-N9 | 5.54 | 112.63 | 108.20 |
| 35 | E | 215 | A | C5-C6-N1 | -5.54 | 114.93 | 117.70 |
| 35 | E | 793 | A | C4-C5-C6 | 5.54 | 119.77 | 117.00 |
| 35 | E | 1317 | G | O4'-C1'-N9 | 5.54 | 112.63 | 108.20 |
| 35 | E | 1951 | A | C4-C5-C6 | 5.54 | 119.77 | 117.00 |
| 35 | E | 216 | A | C5-C6-N6 | -5.54 | 119.27 | 123.70 |
| 35 | E | 735 | A | C5-C6-N1 | -5.54 | 114.93 | 117.70 |
| 35 | E | 2124 | G | O4'-C1'-N9 | 5.54 | 112.63 | 108.20 |
| 35 | E | 125 | A | O4'-C1'-N9 | 5.54 | 112.63 | 108.20 |
| 35 | E | 475 | A | C4-C5-C6 | 5.54 | 119.77 | 117.00 |
| 35 | E | 562 | A | C5-C6-N6 | -5.54 | 119.27 | 123.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 799 | A | C4-C5-C6 | 5.54 | 119.77 | 117.00 |
| 35 | E | 1241 | A | O4'-C1'-N9 | 5.54 | 112.63 | 108.20 |
| 35 | E | 1353 | A | C5-C6-N6 | -5.54 | 119.27 | 123.70 |
| 35 | E | 1749 | G | O4'-C1'-N9 | 5.54 | 112.63 | 108.20 |
| 35 | E | 1822 | A | C5-C6-N6 | -5.54 | 119.27 | 123.70 |
| 35 | E | 1996 | A | C5-C6-N1 | -5.54 | 114.93 | 117.70 |
| 35 | E | 2000 | C | N3-C4-N4 | 5.54 | 121.88 | 118.00 |
| 35 | E | 2007 | A | C4-C5-C6 | 5.54 | 119.77 | 117.00 |
| 35 | E | 2031 | A | C5-C6-N6 | -5.54 | 119.27 | 123.70 |
| 35 | E | 2076 | A | C5-C6-N6 | -5.54 | 119.27 | 123.70 |
| 35 | E | 914 | C | N3-C4-C5 | -5.53 | 119.69 | 121.90 |
| 35 | E | 968 | U | O4'-C1'-N1 | 5.53 | 112.63 | 108.20 |
| 35 | E | 1975 | A | C5-C6-N6 | -5.53 | 119.27 | 123.70 |
| 35 | E | 246 | A | O4'-C1'-N9 | 5.53 | 112.62 | 108.20 |
| 35 | E | 280 | C | N3-C4-C5 | -5.53 | 119.69 | 121.90 |
| 35 | E | 363 | A | C5-C6-N1 | -5.53 | 114.94 | 117.70 |
| 35 | E | 1818 | A | C5-C6-N6 | -5.53 | 119.28 | 123.70 |
| 35 | E | 1992 | A | C5-C6-N6 | -5.53 | 119.28 | 123.70 |
| 35 | E | 2126 | A | C5-C6-N1 | -5.53 | 114.94 | 117.70 |
| 35 | E | 580 | C | N3-C4-N4 | 5.53 | 121.87 | 118.00 |
| 35 | E | 832 | G | O4'-C1'-N9 | 5.53 | 112.62 | 108.20 |
| 35 | E | 1695 | A | C5-C6-N6 | -5.53 | 119.28 | 123.70 |
| 35 | E | 2088 | A | O4'-C1'-N9 | 5.53 | 112.62 | 108.20 |
| 35 | E | 1600 | A | O4'-C1'-N9 | 5.53 | 112.62 | 108.20 |
| 35 | E | 1620 | A | C5-C6-N1 | -5.53 | 114.94 | 117.70 |
| 35 | E | 1863 | C | N3-C4-N4 | 5.53 | 121.87 | 118.00 |
| 35 | E | 2168 | C | N3-C4-N4 | 5.53 | 121.87 | 118.00 |
| 35 | E | 2300 | A | C5-C6-N1 | -5.53 | 114.94 | 117.70 |
| 35 | E | 183 | C | N3-C4-N4 | 5.53 | 121.87 | 118.00 |
| 35 | E | 1624 | C | N3-C4-C5 | -5.53 | 119.69 | 121.90 |
| 35 | E | 2037 | A | C5-C6-N6 | -5.53 | 119.28 | 123.70 |
| 35 | E | 2267 | A | C5-C6-N1 | -5.53 | 114.94 | 117.70 |
| 35 | E | 627 | C | N3-C4-N4 | 5.52 | 121.87 | 118.00 |
| 35 | E | 644 | C | N3-C4-C5 | -5.52 | 119.69 | 121.90 |
| 35 | E | 1270 | A | C5-C6-N6 | -5.52 | 119.28 | 123.70 |
| 35 | E | 1374 | A | C5-C6-N1 | -5.52 | 114.94 | 117.70 |
| 35 | E | 1791 | C | N3-C4-C5 | -5.52 | 119.69 | 121.90 |
| 35 | E | 630 | G | O4'-C1'-N9 | 5.52 | 112.62 | 108.20 |
| 35 | E | 674 | A | C5-C6-N1 | -5.52 | 114.94 | 117.70 |
| 35 | E | 1229 | C | N3-C4-C5 | -5.52 | 119.69 | 121.90 |
| 35 | E | 1323 | A | O4'-C1'-N9 | 5.52 | 112.62 | 108.20 |
| 35 | E | 2035 | A | C5-C6-N6 | -5.52 | 119.28 | 123.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 2098 | C | O4'-C1'-N1 | 5.52 | 112.62 | 108.20 |
| 35 | E | 277 | U | O4'-C1'-N1 | 5.52 | 112.62 | 108.20 |
| 35 | E | 833 | A | C5-C6-N6 | -5.52 | 119.28 | 123.70 |
| 35 | E | 1275 | A | C5-C6-N1 | -5.52 | 114.94 | 117.70 |
| 35 | E | 1628 | A | C5-C6-N1 | -5.52 | 114.94 | 117.70 |
| 35 | E | 40 | A | O4'-C1'-N9 | 5.52 | 112.61 | 108.20 |
| 35 | E | 122 | A | C5-C6-N6 | -5.52 | 119.29 | 123.70 |
| 35 | E | 270 | C | N3-C4-N4 | 5.52 | 121.86 | 118.00 |
| 35 | E | 464 | C | N3-C4-C5 | -5.52 | 119.69 | 121.90 |
| 35 | E | 1605 | A | C4-C5-C6 | 5.52 | 119.76 | 117.00 |
| 35 | E | 418 | G | O4'-C1'-N9 | 5.52 | 112.61 | 108.20 |
| 35 | E | 369 | C | N3-C4-C5 | -5.51 | 119.69 | 121.90 |
| 35 | E | 607 | A | C5-C6-N6 | -5.51 | 119.29 | 123.70 |
| 35 | E | 2037 | A | C5-C6-N1 | -5.51 | 114.94 | 117.70 |
| 35 | E | 1688 | C | N3-C4-C5 | -5.51 | 119.69 | 121.90 |
| 35 | E | 2315 | A | O4'-C1'-N9 | 5.51 | 112.61 | 108.20 |
| 35 | E | 728 | A | C5-C6-N1 | -5.51 | 114.94 | 117.70 |
| 35 | E | 786 | A | C5-C6-N6 | -5.51 | 119.29 | 123.70 |
| 35 | E | 1189 | A | C5-C6-N6 | -5.51 | 119.29 | 123.70 |
| 35 | E | 1297 | C | N3-C4-N4 | 5.51 | 121.86 | 118.00 |
| 35 | E | 1978 | C | N3-C4-N4 | 5.51 | 121.86 | 118.00 |
| 35 | E | 2056 | A | O4'-C1'-N9 | 5.51 | 112.61 | 108.20 |
| 35 | E | 106 | G | O4'-C1'-N9 | 5.51 | 112.61 | 108.20 |
| 35 | E | 637 | C | N3-C4-C5 | -5.51 | 119.70 | 121.90 |
| 35 | E | 1249 | G | N3-C2-N2 | 5.51 | 123.75 | 119.90 |
| 35 | E | 135 | C | N3-C4-N4 | 5.51 | 121.86 | 118.00 |
| 35 | E | 300 | A | O4'-C1'-N9 | 5.51 | 112.61 | 108.20 |
| 35 | E | 655 | A | O4'-C1'-N9 | 5.51 | 112.61 | 108.20 |
| 35 | E | 1851 | C | N3-C4-N4 | 5.51 | 121.86 | 118.00 |
| 35 | E | 1977 | G | O4'-C1'-N9 | 5.51 | 112.61 | 108.20 |
| 35 | E | 2026 | A | C5-C6-N1 | -5.51 | 114.95 | 117.70 |
| 35 | E | 2136 | A | C5-C6-N1 | -5.51 | 114.95 | 117.70 |
| 35 | E | 255 | A | O4'-C1'-N9 | 5.50 | 112.60 | 108.20 |
| 35 | E | 1702 | A | C5-C6-N1 | -5.50 | 114.95 | 117.70 |
| 35 | E | 438 | A | O4'-C1'-N9 | 5.50 | 112.60 | 108.20 |
| 35 | E | 961 | A | C5-C6-N6 | -5.50 | 119.30 | 123.70 |
| 35 | E | 1313 | A | C5-C6-N6 | -5.50 | 119.30 | 123.70 |
| 35 | E | 1667 | G | O4'-C1'-N9 | 5.50 | 112.60 | 108.20 |
| 35 | E | 1959 | C | N3-C4-N4 | 5.50 | 121.85 | 118.00 |
| 35 | E | 38 | C | N3-C4-C5 | -5.50 | 119.70 | 121.90 |
| 35 | E | 120 | C | N3-C4-N4 | 5.50 | 121.85 | 118.00 |
| 35 | E | 250 | A | C5-C6-N6 | -5.50 | 119.30 | 123.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 270 | C | N3-C4-C5 | -5.50 | 119.70 | 121.90 |
| 35 | E | 870 | U | O4'-C1'-N1 | 5.50 | 112.60 | 108.20 |
| 35 | E | 993 | A | C5-C6-N6 | -5.50 | 119.30 | 123.70 |
| 35 | E | 1353 | A | C5-C6-N1 | -5.50 | 114.95 | 117.70 |
| 35 | E | 1548 | C | N3-C4-C5 | -5.50 | 119.70 | 121.90 |
| 35 | E | 2033 | C | N3-C4-N4 | 5.50 | 121.85 | 118.00 |
| 35 | E | 806 | C | N3-C4-N4 | 5.50 | 121.85 | 118.00 |
| 35 | E | 1328 | A | C5-C6-N6 | -5.50 | 119.30 | 123.70 |
| 35 | E | 197 | C | N3-C4-N4 | 5.50 | 121.85 | 118.00 |
| 35 | E | 846 | U | O4'-C1'-N1 | 5.50 | 112.60 | 108.20 |
| 35 | E | 1265 | A | C5-C6-N1 | -5.50 | 114.95 | 117.70 |
| 35 | E | 1286 | A | C4-C5-C6 | 5.50 | 119.75 | 117.00 |
| 35 | E | 2049 | C | N3-C4-N4 | 5.50 | 121.85 | 118.00 |
| 35 | E | 345 | A | O4'-C1'-N9 | 5.50 | 112.60 | 108.20 |
| 35 | E | 685 | G | O4'-C1'-N9 | 5.50 | 112.60 | 108.20 |
| 35 | E | 841 | C | N3-C4-N4 | 5.50 | 121.85 | 118.00 |
| 35 | E | 132 | G | O4'-C1'-N9 | 5.50 | 112.60 | 108.20 |
| 35 | E | 133 | G | O4'-C1'-N9 | 5.50 | 112.60 | 108.20 |
| 35 | E | 387 | C | N3-C4-C5 | -5.50 | 119.70 | 121.90 |
| 35 | E | 984 | A | C5-C6-N1 | -5.50 | 114.95 | 117.70 |
| 35 | E | 1681 | A | O4'-C1'-N9 | 5.50 | 112.60 | 108.20 |
| 35 | E | 184 | A | C5-C6-N1 | -5.49 | 114.95 | 117.70 |
| 35 | E | 233 | G | O4'-C1'-N9 | 5.49 | 112.59 | 108.20 |
| 35 | E | 749 | C | N3-C4-N4 | 5.49 | 121.85 | 118.00 |
| 35 | E | 1671 | A | C4-C5-C6 | 5.49 | 119.75 | 117.00 |
| 35 | E | 1920 | A | C5-C6-N6 | -5.49 | 119.31 | 123.70 |
| 35 | E | 2105 | C | N3-C4-C5 | -5.49 | 119.70 | 121.90 |
| 35 | E | 1937 | A | C5-C6-N6 | -5.49 | 119.31 | 123.70 |
| 35 | E | 769 | A | C5-C6-N6 | -5.49 | 119.31 | 123.70 |
| 35 | E | 1887 | U | C5'-C4'-C3' | -5.49 | 107.22 | 116.00 |
| 35 | E | 102 | A | C5-C6-N1 | -5.49 | 114.96 | 117.70 |
| 35 | E | 123 | A | C5-C6-N1 | -5.49 | 114.96 | 117.70 |
| 35 | E | 163 | C | N3-C4-N4 | 5.49 | 121.84 | 118.00 |
| 35 | E | 351 | A | O4'-C1'-N9 | 5.49 | 112.59 | 108.20 |
| 35 | E | 734 | G | N1-C2-N2 | 5.49 | 121.14 | 116.20 |
| 35 | E | 1217 | A | C5-C6-N1 | -5.49 | 114.96 | 117.70 |
| 35 | E | 258 | C | N3-C4-N4 | 5.49 | 121.84 | 118.00 |
| 35 | E | 703 | A | C5-C6-N6 | -5.49 | 119.31 | 123.70 |
| 35 | E | 780 | C | N3-C4-N4 | 5.49 | 121.84 | 118.00 |
| 35 | E | 1309 | A | O4'-C1'-N9 | 5.49 | 112.59 | 108.20 |
| 35 | E | 2133 | C | N3-C4-C5 | -5.49 | 119.70 | 121.90 |
| 35 | E | 62 | A | C5-C6-N1 | -5.49 | 114.96 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 621 | A | C5-C6-N6 | -5.49 | 119.31 | 123.70 |
| 35 | E | 1566 | A | C5-C6-N6 | -5.49 | 119.31 | 123.70 |
| 35 | E | 1738 | G | O4'-C1'-N9 | 5.49 | 112.59 | 108.20 |
| 35 | E | 1866 | A | C4-C5-C6 | 5.49 | 119.74 | 117.00 |
| 35 | E | 1906 | C | N3-C4-C5 | -5.49 | 119.71 | 121.90 |
| 35 | E | 2060 | C | N3-C4-C5 | -5.49 | 119.70 | 121.90 |
| 35 | E | 2262 | A | C5-C6-N6 | -5.49 | 119.31 | 123.70 |
| 35 | E | 254 | A | C5-C6-N1 | -5.48 | 114.96 | 117.70 |
| 35 | E | 2176 | G | O4'-C1'-N9 | 5.48 | 112.59 | 108.20 |
| 35 | E | 787 | C | N3-C4-C5 | -5.48 | 119.71 | 121.90 |
| 35 | E | 890 | C | N3-C4-N4 | 5.48 | 121.84 | 118.00 |
| 35 | E | 917 | A | C5-C6-N6 | -5.48 | 119.31 | 123.70 |
| 35 | E | 1348 | A | C5-C6-N1 | -5.48 | 114.96 | 117.70 |
| 35 | E | 2159 | A | C5-C6-N6 | -5.48 | 119.31 | 123.70 |
| 35 | E | 526 | A | O4'-C1'-N9 | 5.48 | 112.58 | 108.20 |
| 35 | E | 935 | A | C5-C6-N6 | -5.48 | 119.31 | 123.70 |
| 35 | E | 595 | A | C5-C6-N1 | -5.48 | 114.96 | 117.70 |
| 35 | E | 2248 | G | O4'-C1'-N9 | 5.48 | 112.58 | 108.20 |
| 35 | E | 97 | A | C5-C6-N6 | -5.48 | 119.32 | 123.70 |
| 35 | E | 403 | G | O4'-C1'-N9 | 5.48 | 112.58 | 108.20 |
| 35 | E | 673 | A | C5-C6-N6 | -5.48 | 119.32 | 123.70 |
| 35 | E | 732 | C | C6-N1-C1' | -5.48 | 114.23 | 120.80 |
| 35 | E | 2283 | A | C5-C6-N1 | -5.48 | 114.96 | 117.70 |
| 35 | E | 2299 | A | C5-C6-N1 | -5.48 | 114.96 | 117.70 |
| 35 | E | 425 | A | O4'-C1'-N9 | 5.48 | 112.58 | 108.20 |
| 35 | E | 181 | A | C5-C6-N6 | -5.47 | 119.32 | 123.70 |
| 35 | E | 585 | A | C5-C6-N6 | -5.47 | 119.32 | 123.70 |
| 35 | E | 2225 | C | N3-C4-N4 | 5.47 | 121.83 | 118.00 |
| 3 | r | 121 | TYR | CB-CG-CD2 | -5.47 | 117.72 | 121.00 |
| 35 | E | 184 | A | C5-C6-N6 | -5.47 | 119.32 | 123.70 |
| 35 | E | 185 | A | C5-C6-N6 | -5.47 | 119.32 | 123.70 |
| 35 | E | 428 | C | N3-C4-C5 | -5.47 | 119.71 | 121.90 |
| 35 | E | 482 | C | N3-C4-N4 | 5.47 | 121.83 | 118.00 |
| 35 | E | 269 | A | C5-C6-N6 | -5.47 | 119.32 | 123.70 |
| 35 | E | 859 | C | N3-C4-N4 | 5.47 | 121.83 | 118.00 |
| 35 | E | 1599 | A | C5-C6-N1 | -5.47 | 114.97 | 117.70 |
| 35 | E | 1996 | A | C5-C6-N6 | -5.47 | 119.32 | 123.70 |
| 35 | E | 97 | A | C5-C6-N1 | -5.47 | 114.97 | 117.70 |
| 35 | E | 853 | C | N3-C4-C5 | -5.47 | 119.71 | 121.90 |
| 35 | E | 1934 | G | O4'-C1'-N9 | 5.47 | 112.58 | 108.20 |
| 35 | E | 2163 | G | O4'-C1'-N9 | 5.47 | 112.58 | 108.20 |
| 35 | E | 181 | A | C5-C6-N1 | -5.47 | 114.97 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 604 | A | C5-C6-N1 | -5.47 | 114.97 | 117.70 |
| 35 | E | 1255 | A | C5-C6-N1 | -5.47 | 114.97 | 117.70 |
| 35 | E | 2260 | A | C5-C6-N6 | -5.47 | 119.33 | 123.70 |
| 35 | E | 2284 | A | C5-C6-N6 | -5.47 | 119.33 | 123.70 |
| 35 | E | 619 | C | N3-C4-C5 | -5.46 | 119.71 | 121.90 |
| 35 | E | 673 | A | C4-C5-C6 | 5.46 | 119.73 | 117.00 |
| 35 | E | 506 | A | C5-C6-N1 | -5.46 | 114.97 | 117.70 |
| 35 | E | 805 | C | N3-C4-C5 | -5.46 | 119.72 | 121.90 |
| 35 | E | 723 | C | N3-C4-C5 | -5.46 | 119.72 | 121.90 |
| 35 | E | 1286 | A | C5-C6-N6 | -5.46 | 119.33 | 123.70 |
| 35 | E | 7 | G | O4'-C1'-N9 | 5.46 | 112.57 | 108.20 |
| 35 | E | 55 | A | C5-C6-N6 | -5.46 | 119.33 | 123.70 |
| 35 | E | 141 | A | C5-C6-N6 | -5.46 | 119.33 | 123.70 |
| 35 | E | 482 | C | N3-C4-C5 | -5.46 | 119.72 | 121.90 |
| 35 | E | 709 | C | N3-C4-C5 | -5.46 | 119.72 | 121.90 |
| 35 | E | 1584 | A | C5-C6-N6 | -5.46 | 119.33 | 123.70 |
| 35 | E | 1609 | A | C5-C6-N1 | -5.46 | 114.97 | 117.70 |
| 35 | E | 1961 | A | C5-C6-N6 | -5.46 | 119.33 | 123.70 |
| 35 | E | 345 | A | C5-C6-N1 | -5.46 | 114.97 | 117.70 |
| 35 | E | 502 | A | C5-C6-N6 | -5.46 | 119.33 | 123.70 |
| 35 | E | 769 | A | C5-C6-N1 | -5.46 | 114.97 | 117.70 |
| 35 | E | 930 | G | O4'-C1'-N9 | 5.46 | 112.57 | 108.20 |
| 35 | E | 1561 | A | C5-C6-N6 | -5.46 | 119.33 | 123.70 |
| 35 | E | 1824 | A | C5-C6-N1 | -5.46 | 114.97 | 117.70 |
| 35 | E | 2251 | A | O4'-C1'-N9 | 5.46 | 112.56 | 108.20 |
| 5 | u | 43 | TYR | CB-CG-CD1 | 5.46 | 124.27 | 121.00 |
| 35 | E | 173 | A | C5-C6-N1 | -5.46 | 114.97 | 117.70 |
| 35 | E | 806 | C | N3-C4-C5 | -5.46 | 119.72 | 121.90 |
| 35 | E | 816 | C | N3-C4-C5 | -5.46 | 119.72 | 121.90 |
| 35 | E | 1578 | G | O4'-C1'-N9 | 5.46 | 112.56 | 108.20 |
| 35 | E | 1710 | A | C5-C6-N6 | -5.46 | 119.34 | 123.70 |
| 35 | E | 2014 | C | N3-C4-C5 | -5.45 | 119.72 | 121.90 |
| 35 | E | 812 | A | C5-C6-N6 | -5.45 | 119.34 | 123.70 |
| 35 | E | 2055 | A | C5-C6-N1 | -5.45 | 114.97 | 117.70 |
| 35 | E | 330 | A | C5-C6-N6 | -5.45 | 119.34 | 123.70 |
| 35 | E | 493 | A | C4-C5-C6 | 5.45 | 119.73 | 117.00 |
| 35 | E | 841 | C | N3-C4-C5 | -5.45 | 119.72 | 121.90 |
| 35 | E | 1180 | A | C5-C6-N1 | -5.45 | 114.97 | 117.70 |
| 35 | E | 1920 | A | C5-C6-N1 | -5.45 | 114.97 | 117.70 |
| 35 | E | 2199 | A | O4'-C1'-N9 | 5.45 | 112.56 | 108.20 |
| 35 | E | 170 | C | N3-C4-C5 | -5.45 | 119.72 | 121.90 |
| 35 | E | 1189 | A | C5-C6-N1 | -5.45 | 114.98 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1664 | A | O4'-C1'-N9 | 5.45 | 112.56 | 108.20 |
| 35 | E | 2008 | A | C5-C6-N6 | -5.45 | 119.34 | 123.70 |
| 35 | E | 2272 | A | C5-C6-N1 | -5.45 | 114.98 | 117.70 |
| 35 | E | 503 | A | C5-C6-N1 | -5.45 | 114.98 | 117.70 |
| 35 | E | 168 | A | C5-C6-N1 | -5.45 | 114.98 | 117.70 |
| 35 | E | 300 | A | C5-C6-N6 | -5.45 | 119.34 | 123.70 |
| 35 | E | 917 | A | C5-C6-N1 | -5.45 | 114.98 | 117.70 |
| 35 | E | 1683 | C | N3-C4-N4 | 5.45 | 121.81 | 118.00 |
| 35 | E | 2126 | A | O4'-C1'-N9 | 5.45 | 112.56 | 108.20 |
| 35 | E | 2167 | A | C5-C6-N1 | -5.45 | 114.98 | 117.70 |
| 35 | E | 502 | A | C5-C6-N1 | -5.44 | 114.98 | 117.70 |
| 35 | E | 644 | C | N3-C4-N4 | 5.44 | 121.81 | 118.00 |
| 35 | E | 1661 | A | C5-C6-N1 | -5.44 | 114.98 | 117.70 |
| 35 | E | 2009 | C | O4'-C1'-N1 | 5.44 | 112.56 | 108.20 |
| 35 | E | 6 | G | O4'-C1'-N9 | 5.44 | 112.55 | 108.20 |
| 35 | E | 61 | C | N3-C4-C5 | -5.44 | 119.72 | 121.90 |
| 35 | E | 578 | C | N3-C4-C5 | -5.44 | 119.72 | 121.90 |
| 35 | E | 688 | G | O4'-C1'-N9 | 5.44 | 112.55 | 108.20 |
| 35 | E | 710 | A | C5-C6-N1 | -5.44 | 114.98 | 117.70 |
| 35 | E | 1826 | U | O4'-C1'-N1 | 5.44 | 112.55 | 108.20 |
| 35 | E | 1960 | A | C5-C6-N1 | -5.44 | 114.98 | 117.70 |
| 35 | E | 2052 | C | P-O3'-C3' | 5.44 | 126.23 | 119.70 |
| 35 | E | 587 | A | C5-C6-N1 | -5.44 | 114.98 | 117.70 |
| 35 | E | 1330 | A | C5-C6-N6 | -5.44 | 119.35 | 123.70 |
| 35 | E | 2005 | A | O4'-C1'-N9 | 5.44 | 112.55 | 108.20 |
| 35 | E | 3 | U | O4'-C1'-N1 | 5.44 | 112.55 | 108.20 |
| 35 | E | 51 | A | C5-C6-N6 | -5.44 | 119.35 | 123.70 |
| 35 | E | 97 | A | O4'-C1'-N9 | 5.44 | 112.55 | 108.20 |
| 35 | E | 330 | A | C1'-O4'-C4' | -5.44 | 105.55 | 109.90 |
| 35 | E | 117 | C | N3-C4-N4 | 5.44 | 121.81 | 118.00 |
| 35 | E | 120 | C | N3-C4-C5 | -5.44 | 119.72 | 121.90 |
| 35 | E | 592 | A | C5-C6-N6 | -5.44 | 119.35 | 123.70 |
| 35 | E | 694 | A | C5-C6-N1 | -5.44 | 114.98 | 117.70 |
| 35 | E | 858 | A | C5-C6-N6 | -5.44 | 119.35 | 123.70 |
| 35 | E | 1806 | C | N3-C4-N4 | 5.44 | 121.81 | 118.00 |
| 35 | E | 1851 | C | N3-C4-C5 | -5.44 | 119.72 | 121.90 |
| 35 | E | 304 | A | C5-C6-N1 | -5.44 | 114.98 | 117.70 |
| 35 | E | 391 | C | N3-C4-N4 | 5.44 | 121.81 | 118.00 |
| 35 | E | 2171 | C | N3-C4-N4 | 5.44 | 121.81 | 118.00 |
| 35 | E | 483 | A | C5-C6-N1 | -5.43 | 114.98 | 117.70 |
| 35 | E | 766 | C | N3-C4-C5 | -5.43 | 119.73 | 121.90 |
| 35 | E | 825 | C | N3-C4-N4 | 5.43 | 121.81 | 118.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1596 | G | O4'-C1'-N9 | 5.43 | 112.55 | 108.20 |
| 35 | E | 2080 | A | O4'-C1'-N9 | 5.43 | 112.55 | 108.20 |
| 35 | E | 86 | G | O4'-C1'-N9 | 5.43 | 112.55 | 108.20 |
| 35 | E | 190 | A | C5-C6-N1 | -5.43 | 114.98 | 117.70 |
| 35 | E | 457 | A | C5-C6-N1 | -5.43 | 114.98 | 117.70 |
| 35 | E | 799 | A | C5-C6-N1 | -5.43 | 114.98 | 117.70 |
| 35 | E | 1259 | A | O4'-C1'-N9 | 5.43 | 112.55 | 108.20 |
| 35 | E | 2040 | G | O4'-C1'-N9 | 5.43 | 112.55 | 108.20 |
| 35 | E | 562 | A | C5-C6-N1 | -5.43 | 114.98 | 117.70 |
| 35 | E | 81 | A | C5-C6-N6 | -5.43 | 119.36 | 123.70 |
| 35 | E | 694 | A | C5-C6-N6 | -5.43 | 119.36 | 123.70 |
| 35 | E | 2315 | A | C5-C6-N1 | -5.43 | 114.98 | 117.70 |
| 35 | E | 195 | C | P-O3'-C3' | 5.43 | 126.21 | 119.70 |
| 35 | E | 765 | A | C5-C6-N6 | -5.43 | 119.36 | 123.70 |
| 35 | E | 1657 | A | C5-C6-N1 | -5.43 | 114.99 | 117.70 |
| 35 | E | 2027 | C | N3-C4-N4 | 5.43 | 121.80 | 118.00 |
| 35 | E | 480 | C | N3-C4-C5 | -5.43 | 119.73 | 121.90 |
| 35 | E | 527 | A | C5-C6-N6 | -5.43 | 119.36 | 123.70 |
| 35 | E | 1883 | C | N3-C4-C5 | -5.43 | 119.73 | 121.90 |
| 35 | E | 2030 | G | O4'-C1'-N9 | 5.43 | 112.54 | 108.20 |
| 35 | E | 177 | A | O4'-C1'-N9 | 5.42 | 112.54 | 108.20 |
| 35 | E | 187 | C | N3-C4-C5 | -5.42 | 119.73 | 121.90 |
| 35 | E | 900 | A | C5-C6-N6 | -5.42 | 119.36 | 123.70 |
| 35 | E | 1579 | G | O4'-C1'-N9 | 5.42 | 112.54 | 108.20 |
| 35 | E | 1644 | G | O4'-C1'-N9 | 5.42 | 112.54 | 108.20 |
| 35 | E | 1792 | G | O4'-C1'-N9 | 5.42 | 112.54 | 108.20 |
| 35 | E | 1265 | A | O4'-C1'-N9 | 5.42 | 112.54 | 108.20 |
| 35 | E | 564 | G | O4'-C1'-N9 | 5.42 | 112.54 | 108.20 |
| 35 | E | 566 | G | O4'-C1'-N9 | 5.42 | 112.54 | 108.20 |
| 35 | E | 2019 | C | N3-C4-C5 | -5.42 | 119.73 | 121.90 |
| 35 | E | 2111 | A | C5-C6-N1 | -5.42 | 114.99 | 117.70 |
| 35 | E | 504 | A | C5-C6-N1 | -5.42 | 114.99 | 117.70 |
| 35 | E | 829 | C | N3-C4-N4 | 5.42 | 121.79 | 118.00 |
| 35 | E | 942 | C | N3-C4-C5 | -5.42 | 119.73 | 121.90 |
| 35 | E | 2008 | A | C5-C6-N1 | -5.42 | 114.99 | 117.70 |
| 35 | E | 2055 | A | C5-C6-N6 | -5.42 | 119.36 | 123.70 |
| 35 | E | 203 | C | N3-C4-C5 | -5.42 | 119.73 | 121.90 |
| 35 | E | 743 | C | N3-C4-N4 | 5.42 | 121.79 | 118.00 |
| 35 | E | 1196 | A | C4-C5-C6 | 5.42 | 119.71 | 117.00 |
| 35 | E | 1298 | C | N3-C4-C5 | -5.42 | 119.73 | 121.90 |
| 35 | E | 1531 | G | O4'-C1'-N9 | 5.42 | 112.53 | 108.20 |
| 35 | E | 2186 | C | N3-C4-C5 | -5.42 | 119.73 | 121.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 38 | C | N3-C4-N4 | 5.42 | 121.79 | 118.00 |
| 35 | E | 89 | C | N3-C4-N4 | 5.42 | 121.79 | 118.00 |
| 35 | E | 607 | A | C5-C6-N1 | -5.42 | 114.99 | 117.70 |
| 35 | E | 1197 | A | C5-C6-N1 | -5.42 | 114.99 | 117.70 |
| 35 | E | 1660 | C | N3-C4-N4 | 5.42 | 121.79 | 118.00 |
| 35 | E | 1907 | C | N3-C4-C5 | -5.42 | 119.73 | 121.90 |
| 35 | E | 675 | A | C5-C6-N6 | -5.42 | 119.37 | 123.70 |
| 35 | E | 1378 | A | C5-C6-N6 | -5.42 | 119.37 | 123.70 |
| 35 | E | 1686 | G | P-O5'-C5' | -5.42 | 112.24 | 120.90 |
| 35 | E | 2068 | C | N3-C4-C5 | -5.42 | 119.73 | 121.90 |
| 35 | E | 19 | A | C5-C6-N6 | -5.41 | 119.37 | 123.70 |
| 35 | E | 141 | A | C4-C5-C6 | 5.41 | 119.71 | 117.00 |
| 35 | E | 175 | A | C5-C6-N1 | -5.41 | 114.99 | 117.70 |
| 35 | E | 1197 | A | C5-C6-N6 | -5.41 | 119.37 | 123.70 |
| 35 | E | 1857 | U | O4'-C1'-N1 | 5.41 | 112.53 | 108.20 |
| 35 | E | 1984 | A | C5-C6-N6 | -5.41 | 119.37 | 123.70 |
| 35 | E | 2034 | A | C5-C6-N6 | -5.41 | 119.37 | 123.70 |
| 35 | E | 2147 | U | C6-N1-C1' | -5.41 | 113.62 | 121.20 |
| 35 | E | 386 | A | C5-C6-N6 | -5.41 | 119.37 | 123.70 |
| 35 | E | 689 | A | C5-C6-N6 | -5.41 | 119.37 | 123.70 |
| 35 | E | 1803 | A | C5-C6-N6 | -5.41 | 119.37 | 123.70 |
| 35 | E | 1610 | A | C5-C6-N6 | -5.41 | 119.37 | 123.70 |
| 35 | E | 1742 | C | N3-C4-C5 | -5.41 | 119.74 | 121.90 |
| 35 | E | 1850 | C | N3-C4-C5 | -5.41 | 119.74 | 121.90 |
| 35 | E | 90 | A | C5-C6-N1 | -5.41 | 115.00 | 117.70 |
| 35 | E | 450 | A | C5-C6-N1 | -5.41 | 115.00 | 117.70 |
| 35 | E | 1177 | C | N3-C4-C5 | -5.41 | 119.74 | 121.90 |
| 35 | E | 367 | A | C5-C6-N6 | -5.41 | 119.38 | 123.70 |
| 35 | E | 585 | A | C5-C6-N1 | -5.41 | 115.00 | 117.70 |
| 35 | E | 641 | C | N3-C4-C5 | -5.41 | 119.74 | 121.90 |
| 35 | E | 945 | C | N3-C4-C5 | -5.41 | 119.74 | 121.90 |
| 35 | E | 1689 | A | C5-C6-N6 | -5.41 | 119.38 | 123.70 |
| 35 | E | 2065 | A | C5-C6-N6 | -5.41 | 119.38 | 123.70 |
| 35 | E | 2067 | C | N3-C4-C5 | -5.41 | 119.74 | 121.90 |
| 35 | E | 2259 | A | C5-C6-N1 | -5.41 | 115.00 | 117.70 |
| 35 | E | 1292 | A | C5-C6-N1 | -5.40 | 115.00 | 117.70 |
| 35 | E | 1340 | A | C5-C6-N6 | -5.40 | 119.38 | 123.70 |
| 35 | E | 1729 | C | N3-C4-N4 | 5.40 | 121.78 | 118.00 |
| 35 | E | 182 | C | N3-C4-C5 | -5.40 | 119.74 | 121.90 |
| 35 | E | 254 | A | C5-C6-N6 | -5.40 | 119.38 | 123.70 |
| 35 | E | 499 | A | C5-C6-N1 | -5.40 | 115.00 | 117.70 |
| 35 | E | 707 | C | N3-C4-C5 | -5.40 | 119.74 | 121.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1343 | A | C5-C6-N6 | -5.40 | 119.38 | 123.70 |
| 35 | E | 1658 | C | N3-C4-C5 | -5.40 | 119.74 | 121.90 |
| 35 | E | 2315 | A | C5-C6-N6 | -5.40 | 119.38 | 123.70 |
| 35 | E | 241 | A | O4'-C1'-N9 | 5.40 | 112.52 | 108.20 |
| 35 | E | 2204 | A | O4'-C1'-N9 | 5.40 | 112.52 | 108.20 |
| 35 | E | 51 | A | C5-C6-N1 | -5.40 | 115.00 | 117.70 |
| 35 | E | 214 | C | N3-C4-C5 | -5.40 | 119.74 | 121.90 |
| 35 | E | 101 | C | N3-C4-C5 | -5.40 | 119.74 | 121.90 |
| 35 | E | 444 | A | C5-C6-N1 | -5.40 | 115.00 | 117.70 |
| 35 | E | 586 | A | C5-C6-N1 | -5.40 | 115.00 | 117.70 |
| 35 | E | 966 | C | N3-C4-C5 | -5.40 | 119.74 | 121.90 |
| 35 | E | 1182 | G | O4'-C1'-N9 | 5.40 | 112.52 | 108.20 |
| 35 | E | 2092 | A | C5-C6-N1 | -5.40 | 115.00 | 117.70 |
| 35 | E | 2225 | C | N3-C4-C5 | -5.40 | 119.74 | 121.90 |
| 35 | E | 467 | A | C5-C6-N6 | -5.40 | 119.38 | 123.70 |
| 35 | E | 547 | G | O4'-C1'-N9 | 5.40 | 112.52 | 108.20 |
| 35 | E | 168 | A | O4'-C1'-N9 | 5.39 | 112.52 | 108.20 |
| 35 | E | 177 | A | C5-C6-N6 | -5.39 | 119.39 | 123.70 |
| 35 | E | 245 | A | O4'-C1'-N9 | 5.39 | 112.52 | 108.20 |
| 35 | E | 405 | G | O4'-C1'-N9 | 5.39 | 112.52 | 108.20 |
| 35 | E | 615 | G | O4'-C1'-N9 | 5.39 | 112.52 | 108.20 |
| 35 | E | 1214 | G | O4'-C1'-N9 | 5.39 | 112.52 | 108.20 |
| 35 | E | 1264 | A | C5-C6-N1 | -5.39 | 115.00 | 117.70 |
| 35 | E | 1797 | A | C5-C6-N1 | -5.39 | 115.00 | 117.70 |
| 35 | E | 2240 | A | C4-C5-C6 | 5.39 | 119.70 | 117.00 |
| 35 | E | 142 | A | C5-C6-N1 | -5.39 | 115.00 | 117.70 |
| 35 | E | 345 | A | C5-C6-N6 | -5.39 | 119.39 | 123.70 |
| 35 | E | 887 | C | N3-C4-N4 | 5.39 | 121.78 | 118.00 |
| 35 | E | 960 | A | C5-C6-N1 | -5.39 | 115.00 | 117.70 |
| 35 | E | 1172 | C | N3-C4-C5 | -5.39 | 119.74 | 121.90 |
| 35 | E | 1233 | A | C5-C6-N1 | -5.39 | 115.00 | 117.70 |
| 35 | E | 1338 | A | O4'-C1'-N9 | 5.39 | 112.51 | 108.20 |
| 35 | E | 1678 | C | N3-C4-C5 | -5.39 | 119.74 | 121.90 |
| 35 | E | 2052 | C | N3-C4-C5 | -5.39 | 119.74 | 121.90 |
| 35 | E | 2192 | A | C5-C6-N6 | -5.39 | 119.39 | 123.70 |
| 35 | E | 1077 | C | N3-C4-N4 | 5.39 | 121.77 | 118.00 |
| 35 | E | 1251 | C | N3-C4-C5 | -5.39 | 119.74 | 121.90 |
| 35 | E | 1536 | C | N3-C4-N4 | 5.39 | 121.77 | 118.00 |
| 35 | E | 485 | A | C5-C6-N1 | -5.39 | 115.01 | 117.70 |
| 35 | E | 784 | A | C5-C6-N6 | -5.39 | 119.39 | 123.70 |
| 35 | E | 1790 | A | C5-C6-N1 | -5.39 | 115.00 | 117.70 |
| 35 | E | 360 | A | C5-C6-N1 | -5.39 | 115.01 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 894 | A | C5-C6-N1 | -5.39 | 115.01 | 117.70 |
| 35 | E | 1995 | G | O4'-C1'-N9 | 5.39 | 112.51 | 108.20 |
| 35 | E | 30 | G | O4'-C1'-N9 | 5.38 | 112.51 | 108.20 |
| 35 | E | 962 | A | C5-C6-N1 | -5.38 | 115.01 | 117.70 |
| 35 | E | 990 | A | C5-C6-N1 | -5.38 | 115.01 | 117.70 |
| 35 | E | 1720 | C | N3-C4-N4 | 5.38 | 121.77 | 118.00 |
| 35 | E | 350 | C | N3-C4-C5 | -5.38 | 119.75 | 121.90 |
| 35 | E | 976 | U | O4'-C1'-N1 | 5.38 | 112.51 | 108.20 |
| 35 | E | 1684 | C | N3-C4-N4 | 5.38 | 121.77 | 118.00 |
| 35 | E | 2099 | G | C5-C6-O6 | -5.38 | 125.37 | 128.60 |
| 35 | E | 2200 | A | C5-C6-N1 | -5.38 | 115.01 | 117.70 |
| 35 | E | 22 | A | C5-C6-N1 | -5.38 | 115.01 | 117.70 |
| 35 | E | 926 | C | N3-C4-C5 | -5.38 | 119.75 | 121.90 |
| 35 | E | 1174 | C | N3-C4-C5 | -5.38 | 119.75 | 121.90 |
| 35 | E | 1576 | G | C5-C6-O6 | -5.38 | 125.37 | 128.60 |
| 35 | E | 2239 | A | C5-C6-N1 | -5.38 | 115.01 | 117.70 |
| 35 | E | 160 | A | C4-C5-C6 | 5.38 | 119.69 | 117.00 |
| 35 | E | 330 | A | C5-C6-N1 | -5.38 | 115.01 | 117.70 |
| 35 | E | 555 | G | O4'-C1'-N9 | 5.38 | 112.50 | 108.20 |
| 35 | E | 127 | C | N3-C4-C5 | -5.38 | 119.75 | 121.90 |
| 35 | E | 373 | G | O4'-C1'-N9 | 5.38 | 112.50 | 108.20 |
| 35 | E | 936 | C | C6-N1-C2 | -5.38 | 118.15 | 120.30 |
| 35 | E | 2158 | C | N3-C4-N4 | 5.38 | 121.77 | 118.00 |
| 35 | E | 309 | G | O4'-C1'-N9 | 5.38 | 112.50 | 108.20 |
| 35 | E | 1606 | A | C4-C5-C6 | 5.38 | 119.69 | 117.00 |
| 35 | E | 125 | A | C5-C6-N1 | -5.38 | 115.01 | 117.70 |
| 35 | E | 2312 | A | C5-C6-N1 | -5.38 | 115.01 | 117.70 |
| 35 | E | 158 | C | N3-C4-C5 | -5.37 | 119.75 | 121.90 |
| 35 | E | 704 | A | O4'-C1'-N9 | 5.37 | 112.50 | 108.20 |
| 35 | E | 1173 | U | O4'-C1'-N1 | 5.37 | 112.50 | 108.20 |
| 35 | E | 1288 | G | O4'-C1'-N9 | 5.37 | 112.50 | 108.20 |
| 35 | E | 2089 | A | C5-C6-N6 | -5.37 | 119.40 | 123.70 |
| 35 | E | 125 | A | C5-C6-N6 | -5.37 | 119.40 | 123.70 |
| 35 | E | 244 | G | O4'-C1'-N9 | 5.37 | 112.50 | 108.20 |
| 35 | E | 259 | C | O4'-C1'-N1 | 5.37 | 112.50 | 108.20 |
| 35 | E | 449 | U | O4'-C1'-N1 | 5.37 | 112.50 | 108.20 |
| 35 | E | 633 | A | C5-C6-N1 | -5.37 | 115.01 | 117.70 |
| 35 | E | 859 | C | N3-C4-C5 | -5.37 | 119.75 | 121.90 |
| 35 | E | 864 | A | C5-C6-N1 | -5.37 | 115.01 | 117.70 |
| 35 | E | 1803 | A | C5-C6-N1 | -5.37 | 115.02 | 117.70 |
| 35 | E | 2107 | A | C5-C6-N6 | -5.37 | 119.40 | 123.70 |
| 35 | E | 2197 | G | O4'-C1'-N9 | 5.37 | 112.50 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 855 | G | O4'-C1'-N9 | 5.37 | 112.50 | 108.20 |
| 35 | E | 916 | A | C5-C6-N1 | -5.37 | 115.02 | 117.70 |
| 35 | E | 1372 | C | N3-C4-C5 | -5.37 | 119.75 | 121.90 |
| 35 | E | 784 | A | C5-C6-N1 | -5.37 | 115.02 | 117.70 |
| 35 | E | 960 | A | O4'-C1'-N9 | 5.37 | 112.50 | 108.20 |
| 35 | E | 1239 | G | O4'-C1'-N9 | 5.37 | 112.49 | 108.20 |
| 35 | E | 1991 | C | N3-C4-C5 | -5.37 | 119.75 | 121.90 |
| 35 | E | 121 | A | C5-C6-N1 | -5.37 | 115.02 | 117.70 |
| 35 | E | 1176 | A | C5-C6-N1 | -5.37 | 115.02 | 117.70 |
| 35 | E | 1724 | A | C5-C6-N6 | -5.37 | 119.41 | 123.70 |
| 35 | E | 258 | C | N3-C4-C5 | -5.37 | 119.75 | 121.90 |
| 35 | E | 432 | A | C5-C6-N6 | -5.37 | 119.41 | 123.70 |
| 35 | E | 1662 | A | C5-C6-N1 | -5.37 | 115.02 | 117.70 |
| 34 | h | 218 | SER | N-CA-CB | 5.36 | 118.54 | 110.50 |
| 35 | E | 28 | A | C5-C6-N1 | -5.36 | 115.02 | 117.70 |
| 35 | E | 107 | A | C5-C6-N1 | -5.36 | 115.02 | 117.70 |
| 35 | E | 608 | C | N3-C4-C5 | -5.36 | 119.75 | 121.90 |
| 35 | E | 653 | A | O4'-C1'-N9 | 5.36 | 112.49 | 108.20 |
| 35 | E | 726 | C | N3-C4-N4 | 5.36 | 121.75 | 118.00 |
| 35 | E | 1861 | A | C5-C6-N1 | -5.36 | 115.02 | 117.70 |
| 35 | E | 2026 | A | O4'-C1'-N9 | 5.36 | 112.49 | 108.20 |
| 35 | E | 2033 | C | N3-C4-C5 | -5.36 | 119.75 | 121.90 |
| 35 | E | 11 | A | C5-C6-N6 | -5.36 | 119.41 | 123.70 |
| 35 | E | 571 | A | C5-C6-N6 | -5.36 | 119.41 | 123.70 |
| 35 | E | 1274 | A | O4'-C1'-N9 | 5.36 | 112.49 | 108.20 |
| 35 | E | 245 | A | C5-C6-N6 | -5.36 | 119.41 | 123.70 |
| 35 | E | 284 | C | N3-C4-C5 | -5.36 | 119.76 | 121.90 |
| 35 | E | 624 | A | O4'-C1'-N9 | 5.36 | 112.49 | 108.20 |
| 35 | E | 1697 | G | O4'-C1'-N9 | 5.36 | 112.49 | 108.20 |
| 35 | E | 2148 | A | C5-C6-N1 | -5.36 | 115.02 | 117.70 |
| 35 | E | 4 | C | N3-C4-C5 | -5.36 | 119.76 | 121.90 |
| 35 | E | 246 | A | C5-C6-N6 | -5.36 | 119.41 | 123.70 |
| 35 | E | 682 | G | N3-C2-N2 | 5.36 | 123.65 | 119.90 |
| 35 | E | 1313 | A | C5-C6-N1 | -5.36 | 115.02 | 117.70 |
| 35 | E | 1592 | A | C5-C6-N6 | -5.36 | 119.41 | 123.70 |
| 35 | E | 2097 | U | O4'-C1'-N1 | 5.36 | 112.49 | 108.20 |
| 35 | E | 638 | C | N3-C4-C5 | -5.36 | 119.76 | 121.90 |
| 35 | E | 814 | C | N3-C4-C5 | -5.36 | 119.76 | 121.90 |
| 35 | E | 998 | C | N3-C4-N4 | 5.36 | 121.75 | 118.00 |
| 35 | E | 1304 | C | N3-C4-C5 | -5.36 | 119.76 | 121.90 |
| 35 | E | 1658 | C | O4'-C1'-N1 | 5.36 | 112.48 | 108.20 |
| 35 | E | 2056 | A | C5-C6-N1 | -5.36 | 115.02 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 260 | A | C4-C5-C6 | 5.35 | 119.68 | 117.00 |
| 35 | E | 673 | A | C5-C6-N1 | -5.35 | 115.02 | 117.70 |
| 35 | E | 742 | A | C5-C6-N6 | -5.35 | 119.42 | 123.70 |
| 35 | E | 1365 | A | C5-C6-N6 | -5.35 | 119.42 | 123.70 |
| 3 | r | 135 | TRP | CA-C-N | 5.35 | 126.90 | 116.20 |
| 20 | f | 206 | PHE | CB-CG-CD1 | 5.35 | 124.55 | 120.80 |
| 35 | E | 82 | A | C5-C6-N1 | -5.35 | 115.02 | 117.70 |
| 35 | E | 92 | G | O4'-C1'-N9 | 5.35 | 112.48 | 108.20 |
| 35 | E | 397 | G | O4'-C1'-N9 | 5.35 | 112.48 | 108.20 |
| 35 | E | 854 | U | O4'-C1'-N1 | 5.35 | 112.48 | 108.20 |
| 35 | E | 1975 | A | C5-C6-N1 | -5.35 | 115.02 | 117.70 |
| 35 | E | 59 | C | N3-C4-C5 | -5.35 | 119.76 | 121.90 |
| 35 | E | 183 | C | N3-C4-C5 | -5.35 | 119.76 | 121.90 |
| 35 | E | 2102 | C | N3-C4-C5 | -5.35 | 119.76 | 121.90 |
| 35 | E | 250 | A | C5-C6-N1 | -5.35 | 115.03 | 117.70 |
| 35 | E | 404 | G | O4'-C1'-N9 | 5.35 | 112.48 | 108.20 |
| 35 | E | 689 | A | C5-C6-N1 | -5.35 | 115.03 | 117.70 |
| 35 | E | 727 | C | N3-C4-C5 | -5.35 | 119.76 | 121.90 |
| 35 | E | 1314 | A | C5-C6-N1 | -5.35 | 115.03 | 117.70 |
| 35 | E | 2202 | A | C5-C6-N1 | -5.35 | 115.03 | 117.70 |
| 35 | E | 108 | C | N3-C4-N4 | 5.35 | 121.74 | 118.00 |
| 35 | E | 179 | G | O4'-C1'-N9 | 5.35 | 112.48 | 108.20 |
| 35 | E | 220 | G | O4'-C1'-N9 | 5.35 | 112.48 | 108.20 |
| 35 | E | 285 | A | C5-C6-N6 | -5.35 | 119.42 | 123.70 |
| 35 | E | 509 | A | C5-C6-N1 | -5.35 | 115.03 | 117.70 |
| 35 | E | 830 | C | N3-C4-C5 | -5.35 | 119.76 | 121.90 |
| 35 | E | 875 | A | C5-C6-N1 | -5.35 | 115.03 | 117.70 |
| 35 | E | 1546 | C | N3-C4-N4 | 5.35 | 121.74 | 118.00 |
| 35 | E | 1627 | C | N3-C4-C5 | -5.35 | 119.76 | 121.90 |
| 35 | E | 889 | A | O4'-C1'-N9 | 5.35 | 112.48 | 108.20 |
| 35 | E | 1360 | A | C5-C6-N1 | -5.35 | 115.03 | 117.70 |
| 35 | E | 1999 | A | C5-C6-N1 | -5.35 | 115.03 | 117.70 |
| 35 | E | 463 | A | C5-C6-N6 | -5.34 | 119.42 | 123.70 |
| 35 | E | 484 | A | C5-C6-N1 | -5.34 | 115.03 | 117.70 |
| 35 | E | 812 | A | C5-C6-N1 | -5.34 | 115.03 | 117.70 |
| 35 | E | 1205 | A | C5-C6-N1 | -5.34 | 115.03 | 117.70 |
| 35 | E | 1322 | G | O4'-C1'-N9 | 5.34 | 112.48 | 108.20 |
| 35 | E | 1706 | A | C5-C6-N6 | -5.34 | 119.42 | 123.70 |
| 35 | E | 1731 | G | O4'-C1'-N9 | 5.34 | 112.47 | 108.20 |
| 35 | E | 25 | C | N3-C4-C5 | -5.34 | 119.76 | 121.90 |
| 35 | E | 417 | A | C5-C6-N1 | -5.34 | 115.03 | 117.70 |
| 35 | E | 1525 | C | N3-C4-C5 | -5.34 | 119.76 | 121.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1546 | C | N3-C4-C5 | -5.34 | 119.76 | 121.90 |
| 35 | E | 1631 | A | C5-C6-N1 | -5.34 | 115.03 | 117.70 |
| 35 | E | 1678 | C | N3-C4-N4 | 5.34 | 121.74 | 118.00 |
| 35 | E | 1766 | U | O4'-C1'-N1 | 5.34 | 112.47 | 108.20 |
| 35 | E | 783 | A | C5-C6-N1 | -5.34 | 115.03 | 117.70 |
| 35 | E | 1377 | A | C5-C6-N6 | -5.34 | 119.43 | 123.70 |
| 35 | E | 2239 | A | C5-C6-N6 | -5.34 | 119.43 | 123.70 |
| 35 | E | 2308 | C | N3-C4-C5 | -5.34 | 119.76 | 121.90 |
| 35 | E | 108 | C | N3-C4-C5 | -5.34 | 119.77 | 121.90 |
| 35 | E | 260 | A | C6-C5-N7 | -5.34 | 128.56 | 132.30 |
| 35 | E | 315 | A | C4-C5-C6 | 5.34 | 119.67 | 117.00 |
| 35 | E | 530 | G | O4'-C1'-N9 | 5.34 | 112.47 | 108.20 |
| 35 | E | 1338 | A | C5-C6-N1 | -5.34 | 115.03 | 117.70 |
| 35 | E | 1794 | A | C5-C6-N1 | -5.34 | 115.03 | 117.70 |
| 35 | E | 998 | C | N3-C4-C5 | -5.34 | 119.77 | 121.90 |
| 35 | E | 1832 | A | C5-C6-N1 | -5.34 | 115.03 | 117.70 |
| 35 | E | 444 | A | O4'-C1'-N9 | 5.34 | 112.47 | 108.20 |
| 35 | E | 632 | U | O4'-C1'-N1 | 5.34 | 112.47 | 108.20 |
| 35 | E | 643 | C | N3-C4-C5 | -5.34 | 119.77 | 121.90 |
| 35 | E | 1552 | A | O4'-C1'-N9 | 5.34 | 112.47 | 108.20 |
| 35 | E | 1743 | A | O4'-C1'-N9 | 5.34 | 112.47 | 108.20 |
| 35 | E | 2035 | A | C5-C6-N1 | -5.34 | 115.03 | 117.70 |
| 35 | E | 529 | A | C5-C6-N6 | -5.33 | 119.43 | 123.70 |
| 35 | E | 974 | A | C5-C6-N1 | -5.33 | 115.03 | 117.70 |
| 35 | E | 1302 | A | C5-C6-N1 | -5.33 | 115.03 | 117.70 |
| 35 | E | 1620 | A | C5-C6-N6 | -5.33 | 119.43 | 123.70 |
| 35 | E | 1919 | A | C5-C6-N6 | -5.33 | 119.43 | 123.70 |
| 35 | E | 2156 | G | O4'-C1'-N9 | 5.33 | 112.47 | 108.20 |
| 21 | d | 223 | TYR | CB-CG-CD2 | -5.33 | 117.80 | 121.00 |
| 35 | E | 40 | A | C5-C6-N1 | -5.33 | 115.03 | 117.70 |
| 35 | E | 1223 | C | N3-C4-C5 | -5.33 | 119.77 | 121.90 |
| 35 | E | 1325 | C | N3-C4-C5 | -5.33 | 119.77 | 121.90 |
| 35 | E | 2110 | A | C5-C6-N6 | -5.33 | 119.43 | 123.70 |
| 35 | E | 2312 | A | C5-C6-N6 | -5.33 | 119.44 | 123.70 |
| 35 | E | 116 | G | O4'-C1'-N9 | 5.33 | 112.46 | 108.20 |
| 35 | E | 269 | A | C5-C6-N1 | -5.33 | 115.03 | 117.70 |
| 35 | E | 316 | A | C5-C6-N1 | -5.33 | 115.03 | 117.70 |
| 35 | E | 659 | A | C5-C6-N1 | -5.33 | 115.03 | 117.70 |
| 35 | E | 690 | A | C5-C6-N6 | -5.33 | 119.44 | 123.70 |
| 35 | E | 11 | A | O4'-C1'-N9 | 5.33 | 112.46 | 108.20 |
| 35 | E | 2066 | C | N3-C4-N4 | 5.33 | 121.73 | 118.00 |
| 35 | E | 2238 | A | C5-C6-N6 | -5.33 | 119.44 | 123.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 135 | C | N3-C4-C5 | -5.33 | 119.77 | 121.90 |
| 35 | E | 779 | A | O4'-C1'-N9 | 5.33 | 112.46 | 108.20 |
| 35 | E | 1329 | G | O4'-C1'-N9 | 5.33 | 112.46 | 108.20 |
| 35 | E | 509 | A | O4'-C1'-N9 | 5.32 | 112.46 | 108.20 |
| 35 | E | 1352 | C | N3-C4-C5 | -5.32 | 119.77 | 121.90 |
| 35 | E | 1630 | A | C5-C6-N6 | -5.32 | 119.44 | 123.70 |
| 35 | E | 2203 | C | N3-C4-N4 | 5.32 | 121.73 | 118.00 |
| 35 | E | 429 | C | N3-C4-C5 | -5.32 | 119.77 | 121.90 |
| 35 | E | 1861 | A | O4'-C1'-N9 | 5.32 | 112.46 | 108.20 |
| 35 | E | 610 | A | C5-C6-N6 | -5.32 | 119.44 | 123.70 |
| 35 | E | 760 | C | O4'-C1'-N1 | 5.32 | 112.46 | 108.20 |
| 35 | E | 809 | A | C5-C6-N1 | -5.32 | 115.04 | 117.70 |
| 35 | E | 1323 | A | C5-C6-N6 | -5.32 | 119.44 | 123.70 |
| 35 | E | 1938 | C | N3-C4-C5 | -5.32 | 119.77 | 121.90 |
| 35 | E | 2168 | C | N3-C4-C5 | -5.32 | 119.77 | 121.90 |
| 35 | E | 2214 | A | O4'-C1'-N9 | 5.32 | 112.46 | 108.20 |
| 35 | E | 351 | A | C5-C6-N6 | -5.32 | 119.44 | 123.70 |
| 35 | E | 770 | C | N3-C4-C5 | -5.32 | 119.77 | 121.90 |
| 35 | E | 959 | A | C5-C6-N6 | -5.32 | 119.44 | 123.70 |
| 35 | E | 1963 | G | O4'-C1'-N9 | 5.32 | 112.45 | 108.20 |
| 35 | E | 89 | C | N3-C4-C5 | -5.32 | 119.77 | 121.90 |
| 35 | E | 185 | A | C5-C6-N1 | -5.32 | 115.04 | 117.70 |
| 35 | E | 1348 | A | C5-C6-N6 | -5.32 | 119.45 | 123.70 |
| 35 | E | 1348 | A | O4'-C1'-N9 | 5.32 | 112.45 | 108.20 |
| 35 | E | 2011 | A | C5-C6-N1 | -5.32 | 115.04 | 117.70 |
| 35 | E | 2305 | C | N3-C4-C5 | -5.32 | 119.77 | 121.90 |
| 35 | E | 46 | U | C2-N1-C1' | 5.32 | 124.08 | 117.70 |
| 35 | E | 84 | C | N3-C4-C5 | -5.32 | 119.77 | 121.90 |
| 35 | E | 241 | A | C5-C6-N1 | -5.32 | 115.04 | 117.70 |
| 35 | E | 278 | A | O4'-C1'-N9 | 5.32 | 112.45 | 108.20 |
| 35 | E | 1736 | G | O4'-C1'-N9 | 5.32 | 112.45 | 108.20 |
| 35 | E | 102 | A | C5-C6-N6 | -5.31 | 119.45 | 123.70 |
| 35 | E | 440 | C | N3-C4-C5 | -5.31 | 119.78 | 121.90 |
| 35 | E | 662 | C | N3-C4-C5 | -5.31 | 119.78 | 121.90 |
| 35 | E | 979 | G | C6-C5-N7 | -5.31 | 127.21 | 130.40 |
| 35 | E | 2077 | C | N3-C4-C5 | -5.31 | 119.77 | 121.90 |
| 35 | E | 2135 | A | C5-C6-N6 | -5.31 | 119.45 | 123.70 |
| 35 | E | 366 | C | N3-C4-N4 | 5.31 | 121.72 | 118.00 |
| 35 | E | 1584 | A | O4'-C1'-N9 | 5.31 | 112.45 | 108.20 |
| 35 | E | 1697 | G | C4-N9-C1' | 5.31 | 133.41 | 126.50 |
| 35 | E | 55 | A | C5-C6-N1 | -5.31 | 115.05 | 117.70 |
| 35 | E | 304 | A | O4'-C1'-N9 | 5.31 | 112.45 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 580 | C | N3-C4-C5 | -5.31 | 119.78 | 121.90 |
| 35 | E | 1959 | C | O4'-C1'-N1 | 5.31 | 112.45 | 108.20 |
| 35 | E | 1677 | C | N3-C4-C5 | -5.31 | 119.78 | 121.90 |
| 35 | E | 1916 | C | N3-C4-N4 | 5.31 | 121.72 | 118.00 |
| 35 | E | 80 | G | O4'-C1'-N9 | 5.31 | 112.44 | 108.20 |
| 35 | E | 127 | C | N3-C4-N4 | 5.31 | 121.72 | 118.00 |
| 35 | E | 581 | A | C5-C6-N1 | -5.31 | 115.05 | 117.70 |
| 35 | E | 1599 | A | C5-C6-N6 | -5.31 | 119.45 | 123.70 |
| 35 | E | 2268 | A | C5-C6-N1 | -5.31 | 115.05 | 117.70 |
| 35 | E | 467 | A | O4'-C1'-N9 | 5.30 | 112.44 | 108.20 |
| 35 | E | 597 | C | N3-C4-N4 | 5.30 | 121.71 | 118.00 |
| 35 | E | 1936 | A | C5-C6-N1 | -5.30 | 115.05 | 117.70 |
| 35 | E | 1966 | C | N3-C4-C5 | -5.30 | 119.78 | 121.90 |
| 35 | E | 2273 | A | C5-C6-N6 | -5.30 | 119.46 | 123.70 |
| 35 | E | 369 | C | N3-C4-N4 | 5.30 | 121.71 | 118.00 |
| 35 | E | 876 | A | C5-C6-N1 | -5.30 | 115.05 | 117.70 |
| 35 | E | 878 | G | O4'-C1'-N9 | 5.30 | 112.44 | 108.20 |
| 35 | E | 1619 | A | C5-C6-N6 | -5.30 | 119.46 | 123.70 |
| 35 | E | 1726 | C | N3-C4-C5 | -5.30 | 119.78 | 121.90 |
| 35 | E | 212 | G | O4'-C1'-N9 | 5.30 | 112.44 | 108.20 |
| 35 | E | 351 | A | C5-C6-N1 | -5.30 | 115.05 | 117.70 |
| 35 | E | 153 | C | N3-C4-C5 | -5.30 | 119.78 | 121.90 |
| 35 | E | 203 | C | N3-C4-N4 | 5.30 | 121.71 | 118.00 |
| 35 | E | 288 | A | C5-C6-N6 | -5.30 | 119.46 | 123.70 |
| 35 | E | 961 | A | C5-C6-N1 | -5.30 | 115.05 | 117.70 |
| 35 | E | 1728 | C | N3-C4-C5 | -5.30 | 119.78 | 121.90 |
| 35 | E | 1788 | C | N3-C4-C5 | -5.30 | 119.78 | 121.90 |
| 35 | E | 2142 | C | N3-C4-C5 | -5.30 | 119.78 | 121.90 |
| 35 | E | 55 | A | O4'-C1'-N9 | 5.29 | 112.44 | 108.20 |
| 35 | E | 287 | A | C5-C6-N1 | -5.29 | 115.05 | 117.70 |
| 35 | E | 441 | C | N3-C4-C5 | -5.29 | 119.78 | 121.90 |
| 35 | E | 476 | G | O4'-C1'-N9 | 5.29 | 112.44 | 108.20 |
| 35 | E | 571 | A | O4'-C1'-N9 | 5.29 | 112.44 | 108.20 |
| 35 | E | 1647 | G | O4'-C1'-N9 | 5.29 | 112.44 | 108.20 |
| 35 | E | 2215 | C | N3-C4-C5 | -5.29 | 119.78 | 121.90 |
| 35 | E | 352 | A | C5-C6-N1 | -5.29 | 115.05 | 117.70 |
| 35 | E | 425 | A | C5-C6-N1 | -5.29 | 115.05 | 117.70 |
| 35 | E | 521 | A | C5-C6-N1 | -5.29 | 115.05 | 117.70 |
| 35 | E | 898 | A | C5-C6-N6 | -5.29 | 119.47 | 123.70 |
| 35 | E | 1378 | A | C5-C6-N1 | -5.29 | 115.05 | 117.70 |
| 35 | E | 1902 | G | N3-C2-N2 | 5.29 | 123.60 | 119.90 |
| 35 | E | 1529 | A | C5-C6-N1 | -5.29 | 115.06 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1620 | A | O4'-C1'-N9 | 5.29 | 112.43 | 108.20 |
| 35 | E | 1961 | A | C5-C6-N1 | -5.29 | 115.06 | 117.70 |
| 20 | f | 206 | PHE | CB-CG-CD2 | -5.29 | 117.10 | 120.80 |
| 35 | E | 47 | A | C5-C6-N6 | -5.29 | 119.47 | 123.70 |
| 35 | E | 424 | G | O4'-C1'-N9 | 5.29 | 112.43 | 108.20 |
| 35 | E | 653 | A | C5-C6-N1 | -5.29 | 115.06 | 117.70 |
| 35 | E | 1178 | U | O4'-C1'-N1 | 5.29 | 112.43 | 108.20 |
| 35 | E | 1664 | A | C5-C6-N6 | -5.29 | 119.47 | 123.70 |
| 35 | E | 1709 | G | O4'-C1'-N9 | 5.29 | 112.43 | 108.20 |
| 35 | E | 1862 | C | N3-C4-C5 | -5.29 | 119.78 | 121.90 |
| 35 | E | 1992 | A | C5-C6-N1 | -5.29 | 115.06 | 117.70 |
| 35 | E | 2294 | A | C5-C6-N1 | -5.29 | 115.06 | 117.70 |
| 35 | E | 1188 | C | C5-C4-N4 | -5.29 | 116.50 | 120.20 |
| 35 | E | 163 | C | N3-C4-C5 | -5.29 | 119.78 | 121.90 |
| 35 | E | 1175 | A | C5-C6-N1 | -5.29 | 115.06 | 117.70 |
| 35 | E | 549 | A | O4'-C1'-N9 | 5.28 | 112.43 | 108.20 |
| 35 | E | 624 | A | C5-C6-N6 | -5.28 | 119.47 | 123.70 |
| 35 | E | 1927 | A | C5-C6-N1 | -5.28 | 115.06 | 117.70 |
| 35 | E | 2007 | A | C5-C6-N1 | -5.28 | 115.06 | 117.70 |
| 35 | E | 1307 | G | O4'-C1'-N9 | 5.28 | 112.43 | 108.20 |
| 35 | E | 2054 | G | O4'-C1'-N9 | 5.28 | 112.43 | 108.20 |
| 35 | E | 826 | A | O4'-C1'-N9 | 5.28 | 112.42 | 108.20 |
| 35 | E | 877 | A | C5-C6-N6 | -5.28 | 119.48 | 123.70 |
| 35 | E | 1523 | C | N3-C4-C5 | -5.28 | 119.79 | 121.90 |
| 35 | E | 1726 | C | N3-C4-N4 | 5.28 | 121.70 | 118.00 |
| 35 | E | 2052 | C | N3-C4-N4 | 5.28 | 121.70 | 118.00 |
| 35 | E | 2104 | A | C5-C6-N6 | -5.28 | 119.48 | 123.70 |
| 35 | E | 2170 | C | O4'-C1'-N1 | 5.28 | 112.42 | 108.20 |
| 35 | E | 2314 | C | N3-C4-N4 | 5.28 | 121.70 | 118.00 |
| 35 | E | 902 | A | C5-C6-N1 | -5.28 | 115.06 | 117.70 |
| 35 | E | 1630 | A | C5-C6-N1 | -5.28 | 115.06 | 117.70 |
| 35 | E | 699 | C | P-O3'-C3' | 5.28 | 126.03 | 119.70 |
| 35 | E | 1608 | G | O4'-C1'-N9 | 5.28 | 112.42 | 108.20 |
| 35 | E | 1700 | U | O4'-C1'-N1 | 5.28 | 112.42 | 108.20 |
| 35 | E | 1746 | G | O4'-C1'-N9 | 5.28 | 112.42 | 108.20 |
| 35 | E | 50 | C | N3-C4-C5 | -5.28 | 119.79 | 121.90 |
| 35 | E | 1282 | C | N3-C4-C5 | -5.28 | 119.79 | 121.90 |
| 35 | E | 1733 | A | C5-C6-N1 | -5.28 | 115.06 | 117.70 |
| 35 | E | 1811 | C | N3-C4-C5 | -5.28 | 119.79 | 121.90 |
| 35 | E | 2092 | A | O4'-C1'-N9 | 5.28 | 112.42 | 108.20 |
| 35 | E | 2294 | A | O4'-C1'-N9 | 5.28 | 112.42 | 108.20 |
| 35 | E | 516 | A | C5-C6-N1 | -5.27 | 115.06 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 545 | U | O4'-C1'-N1 | 5.27 | 112.42 | 108.20 |
| 35 | E | 605 | G | O4'-C1'-N9 | 5.27 | 112.42 | 108.20 |
| 35 | E | 771 | A | O4'-C1'-N9 | 5.27 | 112.42 | 108.20 |
| 35 | E | 884 | A | C5-C6-N1 | -5.27 | 115.06 | 117.70 |
| 35 | E | 186 | C | N3-C4-C5 | -5.27 | 119.79 | 121.90 |
| 35 | E | 622 | G | O4'-C1'-N9 | 5.27 | 112.42 | 108.20 |
| 35 | E | 711 | A | C5-C6-N6 | -5.27 | 119.48 | 123.70 |
| 35 | E | 1308 | A | O4'-C1'-N9 | 5.27 | 112.42 | 108.20 |
| 35 | E | 1789 | A | C5-C6-N6 | -5.27 | 119.48 | 123.70 |
| 35 | E | 1966 | C | C6-N1-C1' | -5.27 | 114.47 | 120.80 |
| 35 | E | 501 | A | C5-C6-N1 | -5.27 | 115.06 | 117.70 |
| 35 | E | 1821 | C | N3-C4-C5 | -5.27 | 119.79 | 121.90 |
| 35 | E | 104 | C | N3-C4-C5 | -5.27 | 119.79 | 121.90 |
| 35 | E | 1553 | A | O4'-C1'-N9 | 5.27 | 112.42 | 108.20 |
| 35 | E | 1580 | G | O4'-C1'-N9 | 5.27 | 112.42 | 108.20 |
| 35 | E | 2199 | A | C5-C6-N1 | -5.27 | 115.06 | 117.70 |
| 35 | E | 255 | A | C5-C6-N1 | -5.27 | 115.07 | 117.70 |
| 35 | E | 374 | G | O4'-C1'-N9 | 5.27 | 112.41 | 108.20 |
| 35 | E | 1626 | C | N3-C4-N4 | 5.27 | 121.69 | 118.00 |
| 35 | E | 1660 | C | N3-C4-C5 | -5.27 | 119.79 | 121.90 |
| 35 | E | 1698 | A | C5-C6-N6 | -5.27 | 119.49 | 123.70 |
| 35 | E | 1831 | C | N3-C4-C5 | -5.27 | 119.79 | 121.90 |
| 35 | E | 2284 | A | C5-C6-N1 | -5.27 | 115.07 | 117.70 |
| 35 | E | 1371 | C | N3-C4-C5 | -5.26 | 119.79 | 121.90 |
| 35 | E | 912 | A | C5-C6-N6 | -5.26 | 119.49 | 123.70 |
| 35 | E | 1077 | C | N3-C4-C5 | -5.26 | 119.80 | 121.90 |
| 35 | E | 845 | A | C5-C6-N1 | -5.26 | 115.07 | 117.70 |
| 35 | E | 915 | A | C5-C6-N1 | -5.26 | 115.07 | 117.70 |
| 35 | E | 1290 | A | O4'-C1'-N9 | 5.26 | 112.41 | 108.20 |
| 35 | E | 2039 | A | C5-C6-N6 | -5.26 | 119.49 | 123.70 |
| 35 | E | 2103 | A | O4'-C1'-N9 | 5.26 | 112.41 | 108.20 |
| 35 | E | 2174 | C | N3-C4-C5 | -5.26 | 119.80 | 121.90 |
| 35 | E | 2221 | A | C5-C6-N1 | -5.26 | 115.07 | 117.70 |
| 35 | E | 1543 | C | N3-C4-C5 | -5.26 | 119.80 | 121.90 |
| 35 | E | 1953 | G | O4'-C1'-N9 | 5.26 | 112.41 | 108.20 |
| 35 | E | 2209 | A | O4'-C1'-N9 | 5.26 | 112.41 | 108.20 |
| 35 | E | 284 | C | N3-C4-N4 | 5.26 | 121.68 | 118.00 |
| 35 | E | 1242 | A | C5-C6-N1 | -5.26 | 115.07 | 117.70 |
| 35 | E | 1528 | C | N3-C4-C5 | -5.26 | 119.80 | 121.90 |
| 35 | E | 1935 | C | N3-C4-N4 | 5.26 | 121.68 | 118.00 |
| 35 | E | 1361 | A | O4'-C1'-N9 | 5.25 | 112.40 | 108.20 |
| 35 | E | 1727 | C | N3-C4-N4 | 5.25 | 121.68 | 118.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 26 | A | C5-C6-N1 | -5.25 | 115.07 | 117.70 |
| 35 | E | 207 | G | O4'-C1'-N9 | 5.25 | 112.40 | 108.20 |
| 35 | E | 606 | G | O4'-C1'-N9 | 5.25 | 112.40 | 108.20 |
| 35 | E | 887 | C | N3-C4-C5 | -5.25 | 119.80 | 121.90 |
| 35 | E | 928 | C | N3-C4-C5 | -5.25 | 119.80 | 121.90 |
| 35 | E | 179 | G | N3-C2-N2 | 5.25 | 123.58 | 119.90 |
| 35 | E | 598 | A | C5-C6-N1 | -5.25 | 115.08 | 117.70 |
| 35 | E | 786 | A | C5-C6-N1 | -5.25 | 115.08 | 117.70 |
| 35 | E | 826 | A | C5-C6-N1 | -5.25 | 115.08 | 117.70 |
| 35 | E | 862 | A | C4-C5-C6 | 5.25 | 119.62 | 117.00 |
| 35 | E | 900 | A | C5-C6-N1 | -5.25 | 115.07 | 117.70 |
| 35 | E | 142 | A | O4'-C1'-N9 | 5.25 | 112.40 | 108.20 |
| 35 | E | 353 | C | N3-C4-C5 | -5.25 | 119.80 | 121.90 |
| 35 | E | 483 | A | O4'-C1'-N9 | 5.25 | 112.40 | 108.20 |
| 35 | E | 533 | C | N3-C4-N4 | 5.25 | 121.67 | 118.00 |
| 35 | E | 792 | G | O4'-C1'-N9 | 5.25 | 112.40 | 108.20 |
| 35 | E | 122 | A | C5-C6-N1 | -5.25 | 115.08 | 117.70 |
| 35 | E | 166 | C | N3-C4-C5 | -5.25 | 119.80 | 121.90 |
| 35 | E | 169 | G | O4'-C1'-N9 | 5.25 | 112.40 | 108.20 |
| 35 | E | 874 | C | N3-C4-C5 | -5.25 | 119.80 | 121.90 |
| 35 | E | 2002 | A | C5-C6-N1 | -5.25 | 115.08 | 117.70 |
| 35 | E | 240 | G | O4'-C1'-N9 | 5.25 | 112.40 | 108.20 |
| 35 | E | 263 | G | O4'-C1'-N9 | 5.25 | 112.40 | 108.20 |
| 35 | E | 35 | U | O4'-C1'-N1 | 5.24 | 112.39 | 108.20 |
| 35 | E | 68 | A | C5-C6-N1 | -5.24 | 115.08 | 117.70 |
| 35 | E | 765 | A | O4'-C1'-N9 | 5.24 | 112.39 | 108.20 |
| 35 | E | 1185 | A | N1-C2-N3 | 5.24 | 131.92 | 129.30 |
| 35 | E | 1575 | G | O4'-C1'-N9 | 5.24 | 112.39 | 108.20 |
| 35 | E | 2300 | A | C5-C6-N6 | -5.24 | 119.50 | 123.70 |
| 35 | E | 1539 | A | C5-C6-N1 | -5.24 | 115.08 | 117.70 |
| 35 | E | 1903 | A | C5-C6-N1 | -5.24 | 115.08 | 117.70 |
| 35 | E | 2056 | A | C5-C6-N6 | -5.24 | 119.51 | 123.70 |
| 35 | E | 825 | C | N3-C4-C5 | -5.24 | 119.80 | 121.90 |
| 35 | E | 1878 | A | C5-C6-N1 | -5.24 | 115.08 | 117.70 |
| 35 | E | 112 | A | C5-C6-N1 | -5.24 | 115.08 | 117.70 |
| 35 | E | 695 | G | O4'-C1'-N9 | 5.24 | 112.39 | 108.20 |
| 35 | E | 795 | U | C2'-C3'-O3' | 5.24 | 122.08 | 113.70 |
| 35 | E | 842 | G | O4'-C1'-N9 | 5.24 | 112.39 | 108.20 |
| 35 | E | 895 | A | C5-C6-N1 | -5.24 | 115.08 | 117.70 |
| 35 | E | 1683 | C | N3-C4-C5 | -5.24 | 119.81 | 121.90 |
| 35 | E | 2271 | A | O4'-C1'-N9 | 5.24 | 112.39 | 108.20 |
| 35 | E | 785 | A | C5-C6-N1 | -5.24 | 115.08 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1888 | A | C5-C6-N6 | -5.24 | 119.51 | 123.70 |
| 35 | E | 1935 | C | N3-C4-C5 | -5.24 | 119.81 | 121.90 |
| 35 | E | 2078 | C | N3-C4-C5 | -5.24 | 119.81 | 121.90 |
| 35 | E | 228 | G | O4'-C1'-N9 | 5.24 | 112.39 | 108.20 |
| 35 | E | 291 | G | O4'-C1'-N9 | 5.24 | 112.39 | 108.20 |
| 35 | E | 463 | A | C5-C6-N1 | -5.24 | 115.08 | 117.70 |
| 35 | E | 648 | A | C5-C6-N6 | -5.24 | 119.51 | 123.70 |
| 35 | E | 793 | A | C5-C6-N6 | -5.24 | 119.51 | 123.70 |
| 35 | E | 2204 | A | C5-C6-N6 | -5.24 | 119.51 | 123.70 |
| 35 | E | 90 | A | C5-C6-N6 | -5.23 | 119.51 | 123.70 |
| 35 | E | 668 | C | N3-C4-C5 | -5.23 | 119.81 | 121.90 |
| 35 | E | 414 | A | O4'-C1'-N9 | 5.23 | 112.39 | 108.20 |
| 35 | E | 432 | A | O4'-C1'-N9 | 5.23 | 112.39 | 108.20 |
| 35 | E | 576 | A | O4'-C1'-N9 | 5.23 | 112.39 | 108.20 |
| 35 | E | 682 | G | O4'-C1'-N9 | 5.23 | 112.39 | 108.20 |
| 35 | E | 782 | A | C5-C6-N1 | -5.23 | 115.08 | 117.70 |
| 35 | E | 1309 | A | C5-C6-N1 | -5.23 | 115.08 | 117.70 |
| 35 | E | 1910 | G | O4'-C1'-N9 | 5.23 | 112.39 | 108.20 |
| 35 | E | 798 | U | O4'-C1'-N1 | 5.23 | 112.39 | 108.20 |
| 35 | E | 920 | A | C5-C6-N1 | -5.23 | 115.08 | 117.70 |
| 35 | E | 2050 | C | C5'-C4'-O4' | 5.23 | 115.38 | 109.10 |
| 35 | E | 1739 | G | O4'-C1'-N9 | 5.23 | 112.38 | 108.20 |
| 35 | E | 123 | A | O4'-C1'-N9 | 5.23 | 112.38 | 108.20 |
| 35 | E | 288 | A | C5-C6-N1 | -5.23 | 115.09 | 117.70 |
| 35 | E | 360 | A | C5-C6-N6 | -5.23 | 119.52 | 123.70 |
| 35 | E | 452 | C | N3-C4-C5 | -5.23 | 119.81 | 121.90 |
| 35 | E | 1877 | U | C4'-C3'-C2' | 5.23 | 107.83 | 102.60 |
| 35 | E | 1944 | G | O4'-C1'-N9 | 5.23 | 112.38 | 108.20 |
| 35 | E | 2069 | A | C5-C6-N6 | -5.23 | 119.52 | 123.70 |
| 35 | E | 2103 | A | C5-C6-N6 | -5.23 | 119.52 | 123.70 |
| 35 | E | 1591 | C | N3-C4-C5 | -5.23 | 119.81 | 121.90 |
| 35 | E | 1846 | C | N3-C4-C5 | -5.23 | 119.81 | 121.90 |
| 35 | E | 2050 | C | N3-C4-N4 | 5.23 | 121.66 | 118.00 |
| 35 | E | 295 | A | C5-C6-N1 | -5.22 | 115.09 | 117.70 |
| 35 | E | 1378 | A | O4'-C1'-N9 | 5.22 | 112.38 | 108.20 |
| 35 | E | 347 | G | O4'-C1'-N9 | 5.22 | 112.38 | 108.20 |
| 35 | E | 629 | C | N3-C4-C5 | -5.22 | 119.81 | 121.90 |
| 35 | E | 931 | G | O4'-C1'-N9 | 5.22 | 112.38 | 108.20 |
| 35 | E | 992 | A | C5-C6-N1 | -5.22 | 115.09 | 117.70 |
| 35 | E | 1780 | G | O4'-C1'-N9 | 5.22 | 112.38 | 108.20 |
| 35 | E | 2241 | G | O4'-C1'-N9 | 5.22 | 112.38 | 108.20 |
| 35 | E | 2299 | A | O4'-C1'-N9 | 5.22 | 112.38 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 94 | C | N3-C4-C5 | -5.22 | 119.81 | 121.90 |
| 35 | E | 1568 | A | C5-C6-N1 | -5.22 | 115.09 | 117.70 |
| 35 | E | 2314 | C | N3-C4-C5 | -5.22 | 119.81 | 121.90 |
| 35 | E | 281 | A | C5-C6-N1 | -5.22 | 115.09 | 117.70 |
| 35 | E | 308 | C | N3-C4-N4 | 5.22 | 121.65 | 118.00 |
| 35 | E | 498 | A | C5-C6-N1 | -5.22 | 115.09 | 117.70 |
| 35 | E | 515 | C | N3-C4-C5 | -5.22 | 119.81 | 121.90 |
| 35 | E | 1264 | A | O4'-C1'-N9 | 5.22 | 112.38 | 108.20 |
| 35 | E | 1361 | A | C5-C6-N1 | -5.22 | 115.09 | 117.70 |
| 35 | E | 1359 | C | N3-C4-C5 | -5.22 | 119.81 | 121.90 |
| 35 | E | 491 | C | N3-C4-C5 | -5.22 | 119.81 | 121.90 |
| 35 | E | 658 | A | C5-C6-N1 | -5.22 | 115.09 | 117.70 |
| 35 | E | 1206 | G | O4'-C1'-N9 | 5.22 | 112.37 | 108.20 |
| 35 | E | 1743 | A | C4-C5-C6 | 5.22 | 119.61 | 117.00 |
| 35 | E | 659 | A | O4'-C1'-N9 | 5.21 | 112.37 | 108.20 |
| 35 | E | 991 | C | N3-C4-C5 | -5.21 | 119.81 | 121.90 |
| 35 | E | 1201 | G | C5'-C4'-C3' | 5.21 | 124.34 | 116.00 |
| 35 | E | 1273 | G | O4'-C1'-N9 | 5.21 | 112.37 | 108.20 |
| 35 | E | 1312 | A | C5-C6-N1 | -5.21 | 115.09 | 117.70 |
| 35 | E | 1825 | A | C5-C6-N6 | -5.21 | 119.53 | 123.70 |
| 35 | E | 1946 | C | N3-C4-N4 | 5.21 | 121.65 | 118.00 |
| 35 | E | 2275 | G | O4'-C1'-N9 | 5.21 | 112.37 | 108.20 |
| 35 | E | 538 | A | C5-C6-N1 | -5.21 | 115.09 | 117.70 |
| 35 | E | 569 | A | O4'-C1'-N9 | 5.21 | 112.37 | 108.20 |
| 35 | E | 1741 | G | O4'-C1'-N9 | 5.21 | 112.37 | 108.20 |
| 35 | E | 2109 | G | O4'-C1'-N9 | 5.21 | 112.37 | 108.20 |
| 35 | E | 64 | A | C5-C6-N6 | -5.21 | 119.53 | 123.70 |
| 35 | E | 1625 | A | C5-C6-N6 | -5.21 | 119.53 | 123.70 |
| 35 | E | 2046 | A | C5-C6-N1 | -5.21 | 115.09 | 117.70 |
| 35 | E | 72 | C | N3-C4-C5 | -5.21 | 119.82 | 121.90 |
| 35 | E | 454 | A | C5-C6-N6 | -5.21 | 119.53 | 123.70 |
| 35 | E | 626 | C | N3-C4-C5 | -5.21 | 119.82 | 121.90 |
| 35 | E | 1548 | C | N3-C4-N4 | 5.21 | 121.65 | 118.00 |
| 35 | E | 2258 | C | N3-C4-C5 | -5.21 | 119.82 | 121.90 |
| 26 | j | 97 | ALA | N-CA-CB | 5.21 | 117.39 | 110.10 |
| 35 | E | 48 | G | O4'-C1'-N9 | 5.21 | 112.36 | 108.20 |
| 35 | E | 1311 | C | N3-C4-C5 | -5.21 | 119.82 | 121.90 |
| 35 | E | 1601 | A | O4'-C1'-N9 | 5.21 | 112.36 | 108.20 |
| 35 | E | 1812 | A | C5-C6-N6 | -5.21 | 119.53 | 123.70 |
| 35 | E | 2248 | G | N3-C2-N2 | 5.21 | 123.54 | 119.90 |
| 35 | E | 180 | A | C5-C6-N1 | -5.21 | 115.10 | 117.70 |
| 35 | E | 65 | A | C5-C6-N1 | -5.20 | 115.10 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 533 | C | N3-C4-C5 | -5.20 | 119.82 | 121.90 |
| 35 | E | 1300 | C | C6-N1-C2 | -5.20 | 118.22 | 120.30 |
| 35 | E | 1359 | C | N3-C4-N4 | 5.20 | 121.64 | 118.00 |
| 35 | E | 879 | C | N3-C4-C5 | -5.20 | 119.82 | 121.90 |
| 35 | E | 1633 | A | C5-C6-N6 | -5.20 | 119.54 | 123.70 |
| 35 | E | 501 | A | O4'-C1'-N9 | 5.20 | 112.36 | 108.20 |
| 35 | E | 525 | A | C5-C6-N6 | -5.20 | 119.54 | 123.70 |
| 35 | E | 584 | C | N3-C4-C5 | -5.20 | 119.82 | 121.90 |
| 35 | E | 903 | G | O4'-C1'-N9 | 5.20 | 112.36 | 108.20 |
| 35 | E | 2274 | A | C5-C6-N1 | -5.20 | 115.10 | 117.70 |
| 35 | E | 248 | G | O4'-C1'-N9 | 5.20 | 112.36 | 108.20 |
| 35 | E | 505 | A | C5-C6-N1 | -5.20 | 115.10 | 117.70 |
| 35 | E | 801 | C | N3-C4-C5 | -5.20 | 119.82 | 121.90 |
| 35 | E | 922 | C | N3-C4-N4 | 5.20 | 121.64 | 118.00 |
| 35 | E | 963 | G | O4'-C1'-N9 | 5.20 | 112.36 | 108.20 |
| 35 | E | 1358 | G | O4'-C1'-N9 | 5.20 | 112.36 | 108.20 |
| 35 | E | 1368 | A | C5-C6-N1 | -5.20 | 115.10 | 117.70 |
| 35 | E | 2234 | A | C5-C6-N1 | -5.20 | 115.10 | 117.70 |
| 35 | E | 389 | G | O4'-C1'-N9 | 5.20 | 112.36 | 108.20 |
| 35 | E | 674 | A | C5-C6-N6 | -5.20 | 119.54 | 123.70 |
| 35 | E | 729 | C | N3-C4-N4 | 5.20 | 121.64 | 118.00 |
| 35 | E | 1987 | A | C5-C6-N1 | -5.20 | 115.10 | 117.70 |
| 35 | E | 2251 | A | C5-C6-N1 | -5.20 | 115.10 | 117.70 |
| 35 | E | 268 | C | N3-C4-C5 | -5.20 | 119.82 | 121.90 |
| 35 | E | 904 | C | N3-C4-C5 | -5.20 | 119.82 | 121.90 |
| 35 | E | 1937 | A | C5-C6-N1 | -5.20 | 115.10 | 117.70 |
| 35 | E | 2255 | C | N3-C4-C5 | -5.20 | 119.82 | 121.90 |
| 35 | E | 561 | A | C5-C6-N1 | -5.19 | 115.10 | 117.70 |
| 35 | E | 972 | A | C5-C6-N1 | -5.19 | 115.10 | 117.70 |
| 35 | E | 325 | U | O4'-C1'-N1 | 5.19 | 112.35 | 108.20 |
| 35 | E | 539 | G | O4'-C1'-N9 | 5.19 | 112.35 | 108.20 |
| 35 | E | 925 | C | N3-C4-C5 | -5.19 | 119.82 | 121.90 |
| 35 | E | 1340 | A | C5-C6-N1 | -5.19 | 115.10 | 117.70 |
| 35 | E | 1581 | A | C5-C6-N1 | -5.19 | 115.10 | 117.70 |
| 35 | E | 1607 | A | C5-C6-N1 | -5.19 | 115.10 | 117.70 |
| 35 | E | 1727 | C | N3-C4-C5 | -5.19 | 119.82 | 121.90 |
| 35 | E | 2007 | A | C5-C6-N6 | -5.19 | 119.55 | 123.70 |
| 35 | E | 744 | C | C2-N1-C1' | 5.19 | 124.51 | 118.80 |
| 35 | E | 993 | A | C5-C6-N1 | -5.19 | 115.11 | 117.70 |
| 35 | E | 1266 | C | N3-C4-C5 | -5.19 | 119.82 | 121.90 |
| 35 | E | 1954 | C | N3-C4-C5 | -5.19 | 119.82 | 121.90 |
| 35 | E | 2013 | U | P-O3'-C3' | 5.19 | 125.93 | 119.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 237 | A | C5-C6-N6 | -5.19 | 119.55 | 123.70 |
| 35 | E | 575 | A | C5-C6-N6 | -5.19 | 119.55 | 123.70 |
| 35 | E | 1633 | A | O4'-C1'-N9 | 5.19 | 112.35 | 108.20 |
| 35 | E | 2296 | G | O4'-C1'-N9 | 5.19 | 112.35 | 108.20 |
| 35 | E | 590 | C | N3-C4-C5 | -5.19 | 119.83 | 121.90 |
| 35 | E | 966 | C | N3-C4-N4 | 5.19 | 121.63 | 118.00 |
| 35 | E | 1218 | A | C5-C6-N1 | -5.19 | 115.11 | 117.70 |
| 35 | E | 1982 | C | N3-C4-C5 | -5.19 | 119.83 | 121.90 |
| 35 | E | 1658 | C | N3-C4-N4 | 5.19 | 121.63 | 118.00 |
| 30 | m | 146 | ALA | N-CA-CB | 5.18 | 117.36 | 110.10 |
| 35 | E | 554 | C | N3-C4-C5 | -5.18 | 119.83 | 121.90 |
| 35 | E | 945 | C | O4'-C1'-N1 | 5.18 | 112.35 | 108.20 |
| 35 | E | 751 | C | N3-C4-N4 | 5.18 | 121.63 | 118.00 |
| 35 | E | 914 | C | N3-C4-N4 | 5.18 | 121.63 | 118.00 |
| 35 | E | 1248 | A | C5-C6-N1 | -5.18 | 115.11 | 117.70 |
| 35 | E | 1292 | A | O4'-C1'-N9 | 5.18 | 112.35 | 108.20 |
| 35 | E | 1903 | A | C4-C5-C6 | 5.18 | 119.59 | 117.00 |
| 35 | E | 596 | A | C5-C6-N1 | -5.18 | 115.11 | 117.70 |
| 35 | E | 2087 | C | N3-C4-C5 | -5.18 | 119.83 | 121.90 |
| 35 | E | 450 | A | O4'-C1'-N9 | 5.18 | 112.34 | 108.20 |
| 35 | E | 1599 | A | O4'-C1'-N9 | 5.18 | 112.34 | 108.20 |
| 35 | E | 419 | G | O4'-C1'-N9 | 5.18 | 112.34 | 108.20 |
| 35 | E | 923 | A | C5-C6-N1 | -5.18 | 115.11 | 117.70 |
| 35 | E | 1199 | G | O4'-C1'-N9 | 5.18 | 112.34 | 108.20 |
| 35 | E | 1663 | C | N3-C4-C5 | -5.18 | 119.83 | 121.90 |
| 35 | E | 1946 | C | N3-C4-C5 | -5.18 | 119.83 | 121.90 |
| 35 | E | 2005 | A | C5-C6-N1 | -5.18 | 115.11 | 117.70 |
| 35 | E | 435 | G | O4'-C1'-N9 | 5.17 | 112.34 | 108.20 |
| 35 | E | 1626 | C | O4'-C1'-N1 | 5.17 | 112.34 | 108.20 |
| 35 | E | 1925 | A | C5-C6-N1 | -5.17 | 115.11 | 117.70 |
| 35 | E | 2114 | U | O4'-C1'-N1 | 5.17 | 112.34 | 108.20 |
| 35 | E | 2134 | A | C5-C6-N6 | -5.17 | 119.56 | 123.70 |
| 35 | E | 210 | A | C5-C6-N1 | -5.17 | 115.11 | 117.70 |
| 35 | E | 392 | A | O4'-C1'-N9 | 5.17 | 112.34 | 108.20 |
| 35 | E | 588 | A | C5-C6-N1 | -5.17 | 115.11 | 117.70 |
| 35 | E | 684 | A | C5-C6-N1 | -5.17 | 115.11 | 117.70 |
| 35 | E | 1087 | A | C5-C6-N6 | -5.17 | 119.56 | 123.70 |
| 35 | E | 1566 | A | C5-C6-N1 | -5.17 | 115.11 | 117.70 |
| 35 | E | 1611 | A | C5-C6-N6 | -5.17 | 119.56 | 123.70 |
| 35 | E | 834 | G | P-O5'-C5' | 5.17 | 129.17 | 120.90 |
| 35 | E | 863 | A | C5-C6-N6 | -5.17 | 119.56 | 123.70 |
| 35 | E | 821 | C | N3-C4-C5 | -5.17 | 119.83 | 121.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1526 | A | C5-C6-N1 | -5.17 | 115.12 | 117.70 |
| 35 | E | 1898 | G | O4'-C1'-N9 | 5.17 | 112.33 | 108.20 |
| 35 | E | 2171 | C | N3-C4-C5 | -5.17 | 119.83 | 121.90 |
| 35 | E | 308 | C | N3-C4-C5 | -5.17 | 119.83 | 121.90 |
| 35 | E | 1543 | C | C5-C4-N4 | -5.17 | 116.58 | 120.20 |
| 35 | E | 1798 | G | O4'-C1'-N9 | 5.17 | 112.33 | 108.20 |
| 35 | E | 303 | C | N3-C4-C5 | -5.16 | 119.83 | 121.90 |
| 35 | E | 379 | G | O4'-C1'-N9 | 5.16 | 112.33 | 108.20 |
| 35 | E | 932 | G | N1-C2-N3 | -5.16 | 120.80 | 123.90 |
| 35 | E | 1665 | C | N3-C4-C5 | -5.16 | 119.83 | 121.90 |
| 35 | E | 2202 | A | O4'-C1'-N9 | 5.16 | 112.33 | 108.20 |
| 35 | E | 463 | A | O4'-C1'-N9 | 5.16 | 112.33 | 108.20 |
| 35 | E | 455 | C | N3-C4-C5 | -5.16 | 119.84 | 121.90 |
| 35 | E | 1184 | C | N3-C4-C5 | -5.16 | 119.84 | 121.90 |
| 35 | E | 1552 | A | C5-C6-N6 | -5.16 | 119.57 | 123.70 |
| 35 | E | 317 | G | O4'-C1'-N9 | 5.16 | 112.33 | 108.20 |
| 35 | E | 658 | A | O4'-C1'-N9 | 5.16 | 112.33 | 108.20 |
| 35 | E | 1377 | A | C5-C6-N1 | -5.16 | 115.12 | 117.70 |
| 35 | E | 2004 | A | C5-C6-N1 | -5.16 | 115.12 | 117.70 |
| 35 | E | 282 | C | N3-C4-C5 | -5.16 | 119.84 | 121.90 |
| 35 | E | 681 | C | N3-C4-C5 | -5.16 | 119.84 | 121.90 |
| 35 | E | 908 | G | O4'-C1'-N9 | 5.16 | 112.32 | 108.20 |
| 35 | E | 493 | A | O4'-C1'-N9 | 5.15 | 112.32 | 108.20 |
| 35 | E | 1367 | G | O4'-C1'-N9 | 5.15 | 112.32 | 108.20 |
| 35 | E | 218 | C | N3-C4-C5 | -5.15 | 119.84 | 121.90 |
| 35 | E | 336 | C | N3-C4-C5 | -5.15 | 119.84 | 121.90 |
| 35 | E | 1209 | C | N3-C4-C5 | -5.15 | 119.84 | 121.90 |
| 35 | E | 1362 | A | C5-C6-N1 | -5.15 | 115.12 | 117.70 |
| 35 | E | 1530 | C | N3-C4-C5 | -5.15 | 119.84 | 121.90 |
| 35 | E | 1563 | G | O4'-C1'-N9 | 5.15 | 112.32 | 108.20 |
| 35 | E | 447 | A | C5-C6-N1 | -5.15 | 115.12 | 117.70 |
| 35 | E | 738 | G | C6-C5-N7 | -5.15 | 127.31 | 130.40 |
| 35 | E | 1259 | A | C5-C6-N6 | -5.15 | 119.58 | 123.70 |
| 35 | E | 2234 | A | C4'-C3'-C2' | -5.15 | 97.45 | 102.60 |
| 35 | E | 740 | U | O4'-C1'-N1 | 5.15 | 112.32 | 108.20 |
| 35 | E | 117 | C | N3-C4-C5 | -5.15 | 119.84 | 121.90 |
| 35 | E | 367 | A | C5-C6-N1 | -5.15 | 115.13 | 117.70 |
| 35 | E | 746 | A | C5-C6-N6 | -5.15 | 119.58 | 123.70 |
| 35 | E | 1801 | C | N3-C4-C5 | -5.15 | 119.84 | 121.90 |
| 35 | E | 272 | G | O4'-C1'-N9 | 5.14 | 112.32 | 108.20 |
| 35 | E | 917 | A | O4'-C1'-N9 | 5.14 | 112.31 | 108.20 |
| 35 | E | 1301 | A | O4'-C1'-N9 | 5.14 | 112.31 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 779 | A | C5-C6-N1 | -5.14 | 115.13 | 117.70 |
| 35 | E | 784 | A | O4'-C1'-N9 | 5.14 | 112.31 | 108.20 |
| 35 | E | 1538 | G | O4'-C1'-N9 | 5.14 | 112.31 | 108.20 |
| 35 | E | 2120 | A | O4'-C1'-N9 | 5.14 | 112.31 | 108.20 |
| 35 | E | 2204 | A | C5-C6-N1 | -5.14 | 115.13 | 117.70 |
| 35 | E | 43 | A | C5-C6-N1 | -5.14 | 115.13 | 117.70 |
| 35 | E | 781 | A | C5-C6-N1 | -5.14 | 115.13 | 117.70 |
| 35 | E | 1666 | G | O4'-C1'-N9 | 5.14 | 112.31 | 108.20 |
| 35 | E | 975 | U | P-O3'-C3' | 5.14 | 125.87 | 119.70 |
| 35 | E | 1642 | G | O4'-C1'-N9 | 5.14 | 112.31 | 108.20 |
| 35 | E | 1956 | C | N3-C4-C5 | -5.14 | 119.84 | 121.90 |
| 35 | E | 1370 | A | C5-C6-N1 | -5.14 | 115.13 | 117.70 |
| 35 | E | 1894 | C | N3-C4-N4 | 5.14 | 121.60 | 118.00 |
| 35 | E | 1986 | A | C5-C6-N1 | -5.14 | 115.13 | 117.70 |
| 35 | E | 2136 | A | O4'-C1'-N9 | 5.14 | 112.31 | 108.20 |
| 35 | E | 401 | A | C5-C6-N1 | -5.14 | 115.13 | 117.70 |
| 35 | E | 475 | A | O4'-C1'-N9 | 5.14 | 112.31 | 108.20 |
| 35 | E | 1190 | G | O4'-C1'-N9 | 5.14 | 112.31 | 108.20 |
| 35 | E | 1287 | A | C5-C6-N1 | -5.14 | 115.13 | 117.70 |
| 35 | E | 1891 | C | N3-C4-C5 | -5.14 | 119.84 | 121.90 |
| 35 | E | 261 | A | C5-C6-N1 | -5.13 | 115.13 | 117.70 |
| 35 | E | 316 | A | C5-C6-N6 | -5.13 | 119.59 | 123.70 |
| 35 | E | 1916 | C | N3-C4-C5 | -5.13 | 119.85 | 121.90 |
| 35 | E | 2189 | A | C5-C6-N6 | -5.13 | 119.59 | 123.70 |
| 35 | E | 2229 | A | O4'-C1'-N9 | 5.13 | 112.31 | 108.20 |
| 35 | E | 2288 | A | O4'-C1'-N9 | 5.13 | 112.31 | 108.20 |
| 15 | W | 165 | TRP | CA-CB-CG | 5.13 | 123.45 | 113.70 |
| 35 | E | 406 | A | C5-C6-N1 | -5.13 | 115.13 | 117.70 |
| 35 | E | 861 | A | C5-C6-N6 | -5.13 | 119.59 | 123.70 |
| 35 | E | 865 | A | C5-C6-N1 | -5.13 | 115.13 | 117.70 |
| 35 | E | 2238 | A | O4'-C1'-N9 | 5.13 | 112.31 | 108.20 |
| 35 | E | 526 | A | C5-C6-N1 | -5.13 | 115.13 | 117.70 |
| 35 | E | 905 | A | C5-C6-N6 | -5.13 | 119.59 | 123.70 |
| 35 | E | 67 | C | N3-C4-N4 | 5.13 | 121.59 | 118.00 |
| 35 | E | 315 | A | C5-C6-N6 | -5.13 | 119.60 | 123.70 |
| 35 | E | 676 | G | O4'-C1'-N9 | 5.13 | 112.30 | 108.20 |
| 35 | E | 965 | C | N3-C4-C5 | -5.13 | 119.85 | 121.90 |
| 35 | E | 2264 | A | O4'-C1'-N9 | 5.13 | 112.30 | 108.20 |
| 35 | E | 203 | C | P-O3'-C3' | 5.13 | 125.85 | 119.70 |
| 35 | E | 1220 | G | O4'-C1'-N9 | 5.13 | 112.30 | 108.20 |
| 35 | E | 1864 | C | N3-C4-C5 | -5.13 | 119.85 | 121.90 |
| 35 | E | 2071 | U | O4'-C1'-N1 | 5.13 | 112.30 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 2222 | G | O4'-C1'-N9 | 5.13 | 112.30 | 108.20 |
| 35 | E | 54 | C | N3-C4-C5 | -5.12 | 119.85 | 121.90 |
| 35 | E | 446 | A | C5-C6-N6 | -5.12 | 119.60 | 123.70 |
| 35 | E | 485 | A | C5-C6-N6 | -5.12 | 119.60 | 123.70 |
| 35 | E | 537 | C | N3-C4-C5 | -5.12 | 119.85 | 121.90 |
| 35 | E | 759 | C | C5'-C4'-O4' | -5.12 | 102.95 | 109.10 |
| 35 | E | 2063 | A | C5-C6-N6 | -5.12 | 119.60 | 123.70 |
| 35 | E | 2 | A | C5-C6-N1 | -5.12 | 115.14 | 117.70 |
| 35 | E | 78 | A | C5-C6-N1 | -5.12 | 115.14 | 117.70 |
| 35 | E | 237 | A | C5-C6-N1 | -5.12 | 115.14 | 117.70 |
| 35 | E | 445 | G | O4'-C1'-N9 | 5.12 | 112.30 | 108.20 |
| 35 | E | 1242 | A | C5-C6-N6 | -5.12 | 119.60 | 123.70 |
| 35 | E | 1385 | A | O4'-C1'-N9 | 5.12 | 112.30 | 108.20 |
| 35 | E | 1565 | U | O4'-C1'-N1 | 5.12 | 112.30 | 108.20 |
| 35 | E | 1695 | A | C5-C6-N1 | -5.12 | 115.14 | 117.70 |
| 35 | E | 1729 | C | N3-C4-C5 | -5.12 | 119.85 | 121.90 |
| 35 | E | 2143 | C | N3-C4-C5 | -5.12 | 119.85 | 121.90 |
| 35 | E | 2208 | G | O4'-C1'-N9 | 5.12 | 112.30 | 108.20 |
| 35 | E | 51 | A | O4'-C1'-N9 | 5.12 | 112.30 | 108.20 |
| 35 | E | 517 | G | O4'-C1'-N9 | 5.12 | 112.30 | 108.20 |
| 20 | f | 205 | PHE | CB-CG-CD1 | 5.12 | 124.38 | 120.80 |
| 35 | E | 684 | A | C5-C6-N6 | -5.12 | 119.61 | 123.70 |
| 35 | E | 916 | A | O4'-C1'-N9 | 5.12 | 112.30 | 108.20 |
| 35 | E | 1257 | C | N3-C4-C5 | -5.12 | 119.85 | 121.90 |
| 35 | E | 140 | C | N3-C4-C5 | -5.12 | 119.85 | 121.90 |
| 35 | E | 1336 | A | C5-C6-N1 | -5.12 | 115.14 | 117.70 |
| 35 | E | 143 | C | N3-C4-C5 | -5.12 | 119.85 | 121.90 |
| 35 | E | 848 | U | O4'-C1'-N1 | 5.12 | 112.29 | 108.20 |
| 35 | E | 1165 | G | O4'-C1'-N9 | 5.12 | 112.29 | 108.20 |
| 35 | E | 1232 | C | N3-C4-C5 | -5.12 | 119.85 | 121.90 |
| 35 | E | 1981 | A | O4'-C1'-N9 | 5.12 | 112.29 | 108.20 |
| 35 | E | 2283 | A | O4'-C1'-N9 | 5.12 | 112.29 | 108.20 |
| 35 | E | 53 | G | O4'-C1'-N9 | 5.11 | 112.29 | 108.20 |
| 35 | E | 724 | A | O4'-C1'-N9 | 5.11 | 112.29 | 108.20 |
| 35 | E | 1340 | A | O4'-C1'-N9 | 5.11 | 112.29 | 108.20 |
| 35 | E | 2178 | C | N3-C4-C5 | -5.11 | 119.86 | 121.90 |
| 35 | E | 2203 | C | N3-C4-C5 | -5.11 | 119.86 | 121.90 |
| 35 | E | 1778 | U | O4'-C1'-N1 | 5.11 | 112.29 | 108.20 |
| 35 | E | 732 | C | N3-C4-N4 | 5.11 | 121.58 | 118.00 |
| 35 | E | 829 | C | N3-C4-C5 | -5.11 | 119.86 | 121.90 |
| 35 | E | 902 | A | O4'-C1'-N9 | 5.11 | 112.29 | 108.20 |
| 35 | E | 1353 | A | O4'-C1'-N9 | 5.11 | 112.29 | 108.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1873 | G | O4'-C1'-N9 | 5.11 | 112.29 | 108.20 |
| 35 | E | 1240 | A | O4'-C1'-N9 | 5.11 | 112.29 | 108.20 |
| 35 | E | 2215 | C | P-O3'-C3' | 5.11 | 125.83 | 119.70 |
| 35 | E | 87 | C | N3-C4-C5 | -5.11 | 119.86 | 121.90 |
| 35 | E | 588 | A | O4'-C1'-N9 | 5.11 | 112.29 | 108.20 |
| 35 | E | 1623 | G | O4'-C1'-N9 | 5.11 | 112.29 | 108.20 |
| 35 | E | 1760 | G | O4'-C1'-N9 | 5.11 | 112.29 | 108.20 |
| 35 | E | 2059 | A | O4'-C1'-N9 | 5.11 | 112.29 | 108.20 |
| 35 | E | 2216 | A | C5-C6-N6 | -5.11 | 119.61 | 123.70 |
| 24 | a | 104 | PHE | CB-CG-CD1 | 5.11 | 124.37 | 120.80 |
| 34 | h | 206 | ALA | N-CA-CB | 5.11 | 117.25 | 110.10 |
| 35 | E | 49 | C | N3-C4-C5 | -5.11 | 119.86 | 121.90 |
| 35 | E | 523 | A | C5-C6-N6 | -5.11 | 119.61 | 123.70 |
| 35 | E | 603 | G | O4'-C1'-N9 | 5.11 | 112.28 | 108.20 |
| 35 | E | 1360 | A | O4'-C1'-N9 | 5.11 | 112.28 | 108.20 |
| 35 | E | 1799 | A | O4'-C1'-N9 | 5.11 | 112.28 | 108.20 |
| 35 | E | 39 | A | C5-C6-N6 | -5.10 | 119.62 | 123.70 |
| 35 | E | 409 | G | O4'-C1'-N9 | 5.10 | 112.28 | 108.20 |
| 35 | E | 1610 | A | O4'-C1'-N9 | 5.10 | 112.28 | 108.20 |
| 35 | E | 209 | C | N3-C4-C5 | -5.10 | 119.86 | 121.90 |
| 35 | E | 1788 | C | N3-C4-N4 | 5.10 | 121.57 | 118.00 |
| 35 | E | 242 | A | O4'-C1'-N9 | 5.10 | 112.28 | 108.20 |
| 35 | E | 877 | A | C5-C6-N1 | -5.10 | 115.15 | 117.70 |
| 35 | E | 583 | C | N3-C4-C5 | -5.10 | 119.86 | 121.90 |
| 35 | E | 817 | A | C5-C6-N6 | -5.10 | 119.62 | 123.70 |
| 35 | E | 822 | A | C5-C6-N1 | -5.10 | 115.15 | 117.70 |
| 35 | E | 983 | C | N3-C4-C5 | -5.10 | 119.86 | 121.90 |
| 35 | E | 1365 | A | C5-C6-N1 | -5.10 | 115.15 | 117.70 |
| 35 | E | 214 | C | O4'-C1'-N1 | 5.10 | 112.28 | 108.20 |
| 35 | E | 661 | G | O4'-C1'-N9 | 5.10 | 112.28 | 108.20 |
| 35 | E | 1269 | C | C2-N3-C4 | 5.10 | 122.45 | 119.90 |
| 35 | E | 1546 | C | P-O5'-C5' | 5.10 | 129.06 | 120.90 |
| 35 | E | 1878 | A | O4'-C1'-N9 | 5.10 | 112.28 | 108.20 |
| 35 | E | 1936 | A | O4'-C1'-N9 | 5.10 | 112.28 | 108.20 |
| 35 | E | 1976 | C | N3-C4-C5 | -5.10 | 119.86 | 121.90 |
| 35 | E | 2213 | G | C2'-C3'-O3' | 5.10 | 121.86 | 113.70 |
| 35 | E | 2220 | G | O4'-C1'-N9 | 5.10 | 112.28 | 108.20 |
| 35 | E | 250 | A | O4'-C1'-N9 | 5.10 | 112.28 | 108.20 |
| 35 | E | 711 | A | C6-N1-C2 | 5.09 | 121.66 | 118.60 |
| 35 | E | 1274 | A | C4-C5-C6 | 5.09 | 119.55 | 117.00 |
| 35 | E | 2214 | A | C5-C6-N1 | -5.09 | 115.15 | 117.70 |
| 35 | E | 1354 | C | N3-C4-C5 | -5.09 | 119.86 | 121.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 35 | E | 2148 | A | C5-C6-N6 | -5.09 | 119.63 | 123.70 |
| 35 | E | 2158 | C | N3-C4-C5 | -5.09 | 119.86 | 121.90 |
| 35 | E | 764 | A | C5-C6-N1 | -5.09 | 115.15 | 117.70 |
| 35 | E | 1547 | A | O4'-C1'-N9 | 5.09 | 112.27 | 108.20 |
| 35 | E | 2120 | A | C5-C6-N6 | -5.09 | 119.63 | 123.70 |
| 35 | E | 43 | A | O4'-C1'-N9 | 5.09 | 112.27 | 108.20 |
| 35 | E | 352 | A | O4'-C1'-N9 | 5.09 | 112.27 | 108.20 |
| 35 | E | 913 | A | C5-C6-N6 | -5.09 | 119.63 | 123.70 |
| 35 | E | 1827 | U | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |
| 35 | E | 408 | C | N3-C4-C5 | -5.09 | 119.87 | 121.90 |
| 35 | E | 655 | A | C5-C6-N1 | -5.09 | 115.16 | 117.70 |
| 35 | E | 1222 | A | O4'-C1'-N9 | 5.09 | 112.27 | 108.20 |
| 35 | E | 1808 | G | O4'-C1'-N9 | 5.08 | 112.27 | 108.20 |
| 35 | E | 2152 | C | N3-C4-C5 | -5.08 | 119.87 | 121.90 |
| 35 | E | 131 | C | N3-C4-C5 | -5.08 | 119.87 | 121.90 |
| 35 | E | 294 | G | O4'-C1'-N9 | 5.08 | 112.27 | 108.20 |
| 35 | E | 299 | A | C5-C6-N6 | -5.08 | 119.63 | 123.70 |
| 35 | E | 862 | A | C5-C6-N6 | -5.08 | 119.63 | 123.70 |
| 35 | E | 2159 | A | C5-C6-N1 | -5.08 | 115.16 | 117.70 |
| 35 | E | 231 | A | C5-C6-N6 | -5.08 | 119.64 | 123.70 |
| 35 | E | 381 | A | C5-C6-N1 | -5.08 | 115.16 | 117.70 |
| 35 | E | 1939 | A | C5-C6-N6 | -5.08 | 119.64 | 123.70 |
| 35 | E | 2200 | A | O4'-C1'-N9 | 5.08 | 112.26 | 108.20 |
| 5 | u | 9 | GLN | C-N-CA | 5.08 | 134.39 | 121.70 |
| 35 | E | 734 | G | N3-C4-N9 | -5.08 | 122.95 | 126.00 |
| 35 | E | 1374 | A | O4'-C1'-N9 | 5.08 | 112.26 | 108.20 |
| 35 | E | 2081 | G | O4'-C1'-N9 | 5.08 | 112.26 | 108.20 |
| 35 | E | 137 | C | N3-C4-C5 | -5.08 | 119.87 | 121.90 |
| 35 | E | 406 | A | O4'-C1'-N9 | 5.08 | 112.26 | 108.20 |
| 35 | E | 17 | C | N3-C4-C5 | -5.08 | 119.87 | 121.90 |
| 35 | E | 1338 | A | C5-C6-N6 | -5.08 | 119.64 | 123.70 |
| 35 | E | 349 | A | C5-C6-N1 | -5.07 | 115.16 | 117.70 |
| 35 | E | 518 | C | N3-C4-C5 | -5.07 | 119.87 | 121.90 |
| 35 | E | 1258 | A | O4'-C1'-N9 | 5.07 | 112.26 | 108.20 |
| 35 | E | 1573 | C | N3-C4-C5 | -5.07 | 119.87 | 121.90 |
| 35 | E | 778 | A | O4'-C1'-N9 | 5.07 | 112.26 | 108.20 |
| 35 | E | 2280 | A | C5-C6-N1 | -5.07 | 115.16 | 117.70 |
| 35 | E | 500 | A | C5-C6-N1 | -5.07 | 115.17 | 117.70 |
| 35 | E | 782 | A | O4'-C1'-N9 | 5.07 | 112.26 | 108.20 |
| 35 | E | 1235 | A | O4'-C1'-N9 | 5.07 | 112.26 | 108.20 |
| 35 | E | 1540 | C | N3-C4-N4 | 5.07 | 121.55 | 118.00 |
| 35 | E | 1262 | C | N3-C4-C5 | -5.07 | 119.87 | 121.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1630 | A | O4'-C1'-N9 | 5.07 | 112.25 | 108.20 |
| 11 | S | 53 | SER | N-CA-CB | 5.07 | 118.10 | 110.50 |
| 35 | E | 242 | A | C5-C6-N1 | -5.07 | 115.17 | 117.70 |
| 35 | E | 271 | C | N3-C4-C5 | -5.07 | 119.87 | 121.90 |
| 35 | E | 454 | A | O4'-C1'-N9 | 5.07 | 112.25 | 108.20 |
| 35 | E | 575 | A | C5-C6-N1 | -5.07 | 115.17 | 117.70 |
| 35 | E | 1887 | U | O4'-C1'-N1 | 5.07 | 112.25 | 108.20 |
| 35 | E | 2022 | A | C5-C6-N1 | -5.07 | 115.17 | 117.70 |
| 35 | E | 278 | A | C5-C6-N1 | -5.07 | 115.17 | 117.70 |
| 35 | E | 490 | C | N3-C4-C5 | -5.07 | 119.87 | 121.90 |
| 35 | E | 1368 | A | O4'-C1'-N9 | 5.07 | 112.25 | 108.20 |
| 35 | E | 224 | C | N3-C4-C5 | -5.06 | 119.87 | 121.90 |
| 35 | E | 349 | A | O4'-C1'-N9 | 5.06 | 112.25 | 108.20 |
| 35 | E | 2067 | C | N3-C4-N4 | 5.06 | 121.55 | 118.00 |
| 35 | E | 1075 | G | C5'-C4'-O4' | -5.06 | 103.03 | 109.10 |
| 35 | E | 2211 | C | N3-C4-C5 | -5.06 | 119.88 | 121.90 |
| 35 | E | 149 | A | C3'-C2'-C1' | 5.06 | 105.55 | 101.50 |
| 35 | E | 1606 | A | O4'-C1'-N9 | 5.06 | 112.25 | 108.20 |
| 35 | E | 2006 | A | C5-C6-N1 | -5.06 | 115.17 | 117.70 |
| 35 | E | 2271 | A | C5-C6-N6 | -5.06 | 119.65 | 123.70 |
| 35 | E | 488 | G | O4'-C1'-N9 | 5.06 | 112.25 | 108.20 |
| 35 | E | 763 | G | O4'-C1'-N9 | 5.06 | 112.25 | 108.20 |
| 35 | E | 1639 | A | C5-C6-N1 | -5.06 | 115.17 | 117.70 |
| 35 | E | 472 | A | O4'-C1'-N9 | 5.06 | 112.25 | 108.20 |
| 35 | E | 1569 | G | O4'-C1'-N9 | 5.06 | 112.25 | 108.20 |
| 30 | m | 178 | ALA | N-CA-CB | 5.05 | 117.17 | 110.10 |
| 35 | E | 597 | C | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 35 | E | 1978 | C | N3-C4-C5 | -5.05 | 119.88 | 121.90 |
| 35 | E | 1586 | G | O4'-C1'-N9 | 5.05 | 112.24 | 108.20 |
| 35 | E | 1237 | G | N3-C2-N2 | 5.05 | 123.44 | 119.90 |
| 35 | E | 1326 | G | O4'-C1'-N9 | 5.05 | 112.24 | 108.20 |
| 35 | E | 576 | A | C5-C6-N1 | -5.05 | 115.17 | 117.70 |
| 35 | E | 866 | A | C5-C6-N6 | -5.05 | 119.66 | 123.70 |
| 35 | E | 1702 | A | O4'-C1'-N9 | 5.05 | 112.24 | 108.20 |
| 35 | E | 456 | C | N3-C4-C5 | -5.04 | 119.88 | 121.90 |
| 35 | E | 513 | G | O4'-C1'-N9 | 5.04 | 112.24 | 108.20 |
| 35 | E | 575 | A | O4'-C1'-N9 | 5.04 | 112.24 | 108.20 |
| 35 | E | 1245 | C | N3-C4-C5 | -5.04 | 119.88 | 121.90 |
| 35 | E | 1976 | C | N3-C4-N4 | 5.04 | 121.53 | 118.00 |
| 35 | E | 2107 | A | O4'-C1'-N9 | 5.04 | 112.24 | 108.20 |
| 35 | E | 1602 | C | N3-C4-C5 | -5.04 | 119.88 | 121.90 |
| 35 | E | 1651 | A | C5-C6-N1 | -5.04 | 115.18 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 2034 | A | C5-C6-N1 | -5.04 | 115.18 | 117.70 |
| 35 | E | 2302 | C | N3-C4-C5 | -5.04 | 119.88 | 121.90 |
| 35 | E | 1183 | G | O4'-C1'-N9 | 5.04 | 112.23 | 108.20 |
| 35 | E | 299 | A | O4'-C1'-N9 | 5.04 | 112.23 | 108.20 |
| 35 | E | 845 | A | O4'-C1'-N9 | 5.04 | 112.23 | 108.20 |
| 35 | E | 1385 | A | C5-C6-N1 | -5.04 | 115.18 | 117.70 |
| 35 | E | 1595 | A | O4'-C1'-N9 | 5.04 | 112.23 | 108.20 |
| 35 | E | 2038 | G | O4'-C1'-N9 | 5.04 | 112.23 | 108.20 |
| 35 | E | 26 | A | O4'-C1'-N9 | 5.04 | 112.23 | 108.20 |
| 35 | E | 1540 | C | N3-C4-C5 | -5.04 | 119.89 | 121.90 |
| 35 | E | 2131 | A | C5-C6-N1 | -5.04 | 115.18 | 117.70 |
| 35 | E | 813 | U | O4'-C1'-N1 | 5.03 | 112.23 | 108.20 |
| 35 | E | 1699 | U | O4'-C1'-N1 | 5.03 | 112.23 | 108.20 |
| 35 | E | 1768 | A | C5-C6-N6 | -5.03 | 119.67 | 123.70 |
| 35 | E | 1802 | C | N3-C4-C5 | -5.03 | 119.89 | 121.90 |
| 35 | E | 2149 | C | N3-C4-C5 | -5.03 | 119.89 | 121.90 |
| 35 | E | 2233 | G | O4'-C1'-N9 | 5.03 | 112.23 | 108.20 |
| 35 | E | 216 | A | C5-C6-N1 | -5.03 | 115.18 | 117.70 |
| 35 | E | 249 | A | C5-C6-N1 | -5.03 | 115.19 | 117.70 |
| 35 | E | 600 | U | O4'-C1'-N1 | 5.03 | 112.22 | 108.20 |
| 35 | E | 877 | A | O4'-C1'-N9 | 5.03 | 112.22 | 108.20 |
| 35 | E | 1252 | C | N3-C4-C5 | -5.03 | 119.89 | 121.90 |
| 35 | E | 1547 | A | C5-C6-N6 | -5.03 | 119.68 | 123.70 |
| 35 | E | 721 | C | N3-C4-C5 | -5.03 | 119.89 | 121.90 |
| 35 | E | 2187 | C | N3-C4-C5 | -5.03 | 119.89 | 121.90 |
| 35 | E | 2247 | C | N3-C4-C5 | -5.03 | 119.89 | 121.90 |
| 35 | E | 983 | C | N3-C4-N4 | 5.03 | 121.52 | 118.00 |
| 35 | E | 1261 | A | C5-C6-N1 | -5.03 | 115.19 | 117.70 |
| 35 | E | 1310 | C | N3-C4-C5 | -5.03 | 119.89 | 121.90 |
| 35 | E | 2287 | U | O4'-C1'-N1 | 5.03 | 112.22 | 108.20 |
| 35 | E | 738 | G | C5-C6-N1 | -5.03 | 108.99 | 111.50 |
| 35 | E | 2012 | C | N3-C4-C5 | -5.03 | 119.89 | 121.90 |
| 35 | E | 2290 | C | N3-C4-C5 | -5.03 | 119.89 | 121.90 |
| 35 | E | 1580 | G | N3-C2-N2 | 5.02 | 123.42 | 119.90 |
| 35 | E | 202 | C | N3-C4-C5 | -5.02 | 119.89 | 121.90 |
| 3 | r | 121 | TYR | CB-CG-CD1 | 5.02 | 124.01 | 121.00 |
| 35 | E | 2095 | G | C4-N9-C1' | 5.02 | 133.02 | 126.50 |
| 35 | E | 211 | G | O4'-C1'-N9 | 5.02 | 112.21 | 108.20 |
| 35 | E | 1254 | C | N3-C4-C5 | -5.02 | 119.89 | 121.90 |
| 35 | E | 436 | G | O4'-C1'-N9 | 5.02 | 112.21 | 108.20 |
| 35 | E | 623 | C | N3-C4-C5 | -5.02 | 119.89 | 121.90 |
| 35 | E | 771 | A | C5-C6-N1 | -5.02 | 115.19 | 117.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 35 | E | 1250 | A | O4'-C1'-N9 | 5.01 | 112.21 | 108.20 |
| 35 | E | 1589 | C | N3-C4-C5 | -5.01 | 119.89 | 121.90 |
| 35 | E | 206 | C | N3-C4-C5 | -5.01 | 119.89 | 121.90 |
| 35 | E | 616 | G | O4'-C1'-N9 | 5.01 | 112.21 | 108.20 |
| 35 | E | 1074 | C | N3-C4-C5 | -5.01 | 119.89 | 121.90 |
| 35 | E | 2169 | A | C5-C6-N1 | -5.01 | 115.19 | 117.70 |
| 35 | E | 411 | G | O4'-C1'-N9 | 5.01 | 112.21 | 108.20 |
| 35 | E | 2088 | A | C5-C6-N1 | -5.01 | 115.19 | 117.70 |
| 35 | E | 111 | A | C5-C6-N1 | -5.01 | 115.20 | 117.70 |
| 35 | E | 1980 | C | N3-C4-C5 | -5.01 | 119.90 | 121.90 |
| 35 | E | 313 | G | C8-N9-C1' | -5.01 | 120.49 | 127.00 |
| 35 | E | 295 | A | O4'-C1'-N9 | 5.00 | 112.20 | 108.20 |
| 35 | E | 1194 | U | O4'-C1'-N1 | 5.00 | 112.20 | 108.20 |
| 35 | E | 522 | A | C5-C6-N6 | -5.00 | 119.70 | 123.70 |
| 35 | E | 534 | C | N3-C4-C5 | -5.00 | 119.90 | 121.90 |
| 35 | E | 542 | C | N3-C4-C5 | -5.00 | 119.90 | 121.90 |
| 35 | E | 1072 | G | O4'-C1'-N9 | 5.00 | 112.20 | 108.20 |
| 35 | E | 1230 | G | O4'-C1'-N9 | 5.00 | 112.20 | 108.20 |
| 35 | E | 1328 | A | C5-C6-N1 | -5.00 | 115.20 | 117.70 |
| 35 | E | 2023 | C | N3-C4-N4 | 5.00 | 121.50 | 118.00 |
| 35 | E | 189 | G | O4'-C1'-N9 | 5.00 | 112.20 | 108.20 |
| 35 | E | 232 | C | N3-C4-C5 | -5.00 | 119.90 | 121.90 |
| 35 | E | 271 | C | P-O5'-C5' | 5.00 | 128.90 | 120.90 |
| 35 | E | 484 | A | C5-C6-N6 | -5.00 | 119.70 | 123.70 |
| 35 | E | 1998 | A | C5-C6-N1 | -5.00 | 115.20 | 117.70 |
| 35 | E | 2121 | G | O4'-C1'-N9 | 5.00 | 112.20 | 108.20 |

All (4) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 35 | E | 325 | U | C3' |
| 35 | E | 702 | U | C1' |
| 35 | E | 810 | U | C3' |
| 35 | E | 1903 | A | C3' |

All (180) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 35 | E | 1080 | U | Sidechain |
| 35 | E | 1084 | G | Sidechain |
| 35 | E | 1169 | U | Sidechain |
| 35 | E | 1170 | C | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 35 | E | 1171 | C | Sidechain |
| 35 | E | 1182 | G | Sidechain |
| 35 | E | 1186 | U | Sidechain |
| 35 | E | 1187 | C | Sidechain |
| 35 | E | 1188 | C | Sidechain |
| 35 | E | 1190 | G | Sidechain |
| 35 | E | 1253 | G | Sidechain |
| 35 | E | 1271 | G | Sidechain |
| 35 | E | 1300 | C | Sidechain |
| 35 | E | 1358 | G | Sidechain |
| 35 | E | 1376 | G | Sidechain |
| 35 | E | 143 | C | Sidechain |
| 35 | E | 1542 | U | Sidechain |
| 35 | E | 1543 | C | Sidechain |
| 35 | E | 1559 | U | Sidechain |
| 35 | E | 1560 | G | Sidechain |
| 35 | E | 159 | G | Sidechain |
| 35 | E | 1625 | A | Sidechain |
| 35 | E | 1638 | G | Sidechain |
| 35 | E | 1651 | A | Sidechain |
| 35 | E | 1652 | A | Sidechain |
| 35 | E | 1667 | G | Sidechain |
| 35 | E | 1670 | A | Sidechain |
| 35 | E | 1686 | G | Sidechain |
| 35 | E | 1714 | U | Sidechain |
| 35 | E | 172 | A | Sidechain |
| 35 | E | 1735 | G | Sidechain |
| 35 | E | 1737 | U | Sidechain |
| 35 | E | 1825 | A | Sidechain |
| 35 | E | 1867 | G | Sidechain |
| 35 | E | 1870 | G | Sidechain |
| 35 | E | 1872 | G | Sidechain |
| 35 | E | 1873 | G | Sidechain |
| 35 | E | 1874 | C | Sidechain |
| 35 | E | 1876 | G | Sidechain |
| 35 | E | 1880 | U | Sidechain |
| 35 | E | 1886 | G | Sidechain |
| 35 | E | 1903 | A | Sidechain |
| 35 | E | 1924 | G | Sidechain |
| 35 | E | 1925 | A | Sidechain |
| 35 | E | 1928 | U | Sidechain |
| 35 | E | 1941 | C | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 35 | E | 1989 | G | Sidechain |
| 35 | E | 2003 | G | Sidechain |
| 35 | E | 2012 | C | Sidechain |
| 35 | E | 2019 | C | Sidechain |
| 35 | E | 202 | C | Sidechain |
| 35 | E | 2044 | G | Sidechain |
| 35 | E | 2075 | G | Sidechain |
| 35 | E | 2113 | G | Sidechain |
| 35 | E | 2129 | U | Sidechain |
| 35 | E | 213 | G | Sidechain |
| 35 | E | 2153 | C | Sidechain |
| 35 | E | 2215 | C | Sidechain |
| 35 | E | 2239 | A | Sidechain |
| 35 | E | 2240 | A | Sidechain |
| 35 | E | 226 | A | Sidechain |
| 35 | E | 228 | G | Sidechain |
| 35 | E | 2283 | A | Sidechain |
| 35 | E | 249 | A | Sidechain |
| 35 | E | 259 | C | Sidechain |
| 35 | E | 260 | A | Sidechain |
| 35 | E | 344 | G | Sidechain |
| 35 | E | 361 | U | Sidechain |
| 35 | E | 39 | A | Sidechain |
| 35 | E | 476 | G | Sidechain |
| 35 | E | 481 | G | Sidechain |
| 35 | E | 512 | A | Sidechain |
| 35 | E | 60 | U | Sidechain |
| 35 | E | 600 | U | Sidechain |
| 35 | E | 667 | G | Sidechain |
| 35 | E | 700 | U | Sidechain |
| 35 | E | 701 | C | Sidechain |
| 35 | E | 706 | G | Sidechain |
| 35 | E | 708 | G | Sidechain |
| 35 | E | 710 | A | Sidechain |
| 35 | E | 712 | U | Sidechain |
| 35 | E | 713 | G | Sidechain |
| 35 | E | 717 | U | Sidechain |
| 35 | E | 718 | A | Sidechain |
| 35 | E | 719 | G | Sidechain |
| 35 | E | 720 | U | Sidechain |
| 35 | E | 721 | C | Sidechain |
| 35 | E | 724 | A | Sidechain |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 35 | E | 726 | C | Sidechain |
| 35 | E | 733 | G | Sidechain |
| 35 | E | 734 | G | Sidechain |
| 35 | E | 735 | A | Sidechain |
| 35 | E | 738 | G | Sidechain |
| 35 | E | 739 | G | Sidechain |
| 35 | E | 741 | G | Sidechain |
| 35 | E | 744 | C | Sidechain |
| 35 | E | 746 | A | Sidechain |
| 35 | E | 754 | G | Sidechain |
| 35 | E | 756 | G | Sidechain |
| 35 | E | 758 | U | Sidechain |
| 35 | E | 759 | C | Sidechain |
| 35 | E | 774 | C | Sidechain |
| 35 | E | 776 | G | Sidechain |
| 35 | E | 788 | A | Sidechain |
| 35 | E | 792 | G | Sidechain |
| 35 | E | 796 | G | Sidechain |
| 35 | E | 807 | U | Sidechain |
| 35 | E | 824 | G | Sidechain |
| 35 | E | 828 | G | Sidechain |
| 35 | E | 834 | G | Sidechain |
| 35 | E | 849 | U | Sidechain |
| 35 | E | 874 | C | Sidechain |
| 35 | E | 936 | C | Sidechain |
| 35 | E | 937 | C | Sidechain |
| 35 | E | 953 | G | Sidechain |
| 35 | E | 954 | G | Sidechain |
| 35 | E | 966 | C | Sidechain |
| 35 | E | 979 | G | Sidechain |
| 35 | E | 982 | G | Sidechain |
| 35 | E | 984 | A | Sidechain |
| 35 | E | 989 | G | Sidechain |
| 8 | O | 138 | TYR | Sidechain |
| 8 | O | 150 | ARG | Peptide |
| 8 | O | 57 | ARG | Sidechain |
| 27 | P | 44 | ASP | Peptide |
| 27 | P | 9 | ARG | Peptide |
| 9 | Q | 112 | TYR | Sidechain |
| 9 | Q | 119 | ARG | Sidechain |
| 9 | Q | 37 | LYS | Peptide |
| 15 | W | 81 | ASP | Peptide |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 18 | Z | 56 | ARG | Sidechain |
| 24 | a | 107 | TYR | Sidechain |
| 24 | a | 46 | VAL | Peptide |
| 33 | c | 62 | PRO | Peptide |
| 33 | c | 65 | ALA | Peptide |
| 22 | e | 57 | ARG | Sidechain |
| 34 | h | 111 | ALA | Peptide |
| 34 | h | 120 | LEU | Peptide |
| 34 | h | 139 | THR | Peptide |
| 34 | h | 147 | ASN | Peptide |
| 34 | h | 154 | SER | Peptide |
| 34 | h | 155 | PRO | Peptide |
| 34 | h | 157 | PHE | Peptide |
| 34 | h | 158 | ARG | Peptide |
| 34 | h | 159 | ALA | Peptide |
| 34 | h | 160 | SER | Peptide |
| 34 | h | 174 | LYS | Peptide |
| 34 | h | 179 | ARG | Peptide |
| 34 | h | 180 | THR | Peptide |
| 34 | h | 182 | ARG | Peptide |
| 34 | h | 183 | ASN | Peptide |
| 34 | h | 184 | ASN | Peptide |
| 34 | h | 203 | LYS | Peptide |
| 34 | h | 207 | GLU | Peptide |
| 34 | h | 217 | LEU | Peptide |
| 34 | h | 77 | GLN | Peptide |
| 34 | h | 93 | VAL | Peptide |
| 34 | h | 94 | VAL | Peptide |
| 26 | j | 99 | LYS | Peptide |
| 28 | k | 173 | ARG | Sidechain |
| 30 | m | 142 | LYS | Peptide |
| 30 | m | 145 | ARG | Peptide |
| 32 | o | 63 | ALA | Peptide |
| 32 | o | 89 | TYR | Sidechain |
| 1 | p | 110 | LYS | Peptide |
| 1 | p | 261 | ARG | Sidechain |
| 1 | p | 43 | TRP | Peptide |
| 3 | r | 120 | LYS | Peptide |
| 3 | r | 121 | TYR | Peptide |
| 3 | r | 141 | ARG | Peptide |
| 3 | r | 142 | THR | Peptide |
| 3 | r | 147 | SER | Peptide |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 3 | r | 32 | GLN | Peptide |
| 3 | r | 42 | VAL | Peptide |
| 4 | t | 104 | TYR | Sidechain |
| 4 | t | 128 | MET | Peptide |
| 5 | u | 43 | TYR | Sidechain |
| 5 | u | 48 | LYS | Peptide |
| 5 | u | 56 | ARG | Peptide |
| 5 | u | 9 | GLN | Peptide |

## 5.2 Too-close contacts (i)

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 | p | 2405 | 0 | 2323 | 0 | 0 |
| 2 | q | 311 | 0 | 319 | 0 | 0 |
| 3 | r | 1113 | 0 | 1175 | 0 | 0 |
| 4 | t | 969 | 0 | 1003 | 0 | 0 |
| 5 | u | 981 | 0 | 1021 | 0 | 0 |
| 6 | L | 2038 | 0 | 2142 | 0 | 0 |
| 7 | M | 1116 | 0 | 1169 | 0 | 0 |
| 8 | O | 1493 | 0 | 1562 | 0 | 0 |
| 9 | Q | 1670 | 0 | 1778 | 1 | 0 |
| 10 | R | 1143 | 0 | 1226 | 1 | 0 |
| 11 | S | 630 | 0 | 630 | 0 | 0 |
| 12 | T | 829 | 0 | 866 | 0 | 0 |
| 13 | U | 526 | 0 | 550 | 0 | 0 |
| 14 | V | 1011 | 0 | 1019 | 0 | 0 |
| 15 | W | 1781 | 0 | 1853 | 0 | 0 |
| 16 | X | 1212 | 0 | 1250 | 0 | 0 |
| 17 | Y | 989 | 0 | 1065 | 0 | 0 |
| 18 | Z | 1404 | 0 | 1503 | 1 | 0 |
| 19 | b | 1365 | 0 | 1410 | 0 | 0 |
| 20 | f | 1658 | 0 | 1704 | 0 | 0 |
| 21 | d | 1726 | 0 | 1774 | 0 | 0 |
| 22 | e | 1019 | 0 | 1050 | 0 | 0 |
| 23 | g | 635 | 0 | 631 | 0 | 0 |
| 24 | a | 553 | 0 | 608 | 0 | 0 |
| 25 | i | 958 | 0 | 981 | 0 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 26 | j | 518 | 0 | 513 | 0 | 0 |
| 27 | P | 1983 | 0 | 2131 | 0 | 0 |
| 28 | k | 972 | 0 | 1031 | 0 | 0 |
| 29 | l | 784 | 0 | 848 | 0 | 0 |
| 30 | m | 1587 | 0 | 1662 | 0 | 0 |
| 31 | n | 780 | 0 | 771 | 0 | 0 |
| 32 | o | 1116 | 0 | 1166 | 0 | 0 |
| 33 | c | 480 | 0 | 532 | 0 | 0 |
| 34 | h | 1358 | 0 | 1419 | 0 | 0 |
| 35 | E | 43106 | 0 | 21756 | 87 | 0 |
| All | All | 82219 | 0 | 62441 | 87 | 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 1.

All (87) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 35:E:725:U:H3 | 35:E:733:G:H1 | 1.12 | 0.96 |
| 35:E:1849:U:H3 | 35:E:1869:G:H1 | 1.26 | 0.83 |
| 35:E:207:G:H1 | 35:E:222:U:H3 | 1.30 | 0.78 |
| 35:E:2220:G:H1 | 35:E:2232:U:H3 | 1.32 | 0.77 |
| 35:E:711:A:N1 | 35:E:746:A:N1 | 2.33 | 0.77 |
| 35:E:1085:G:H1 | 35:E:1169:U:H3 | 1.33 | 0.76 |
| 35:E:322:G:H1 | 35:E:331:U:H3 | 1.31 | 0.76 |
| 35:E:546:U:H2' | 35:E:547:G:H5' | 1.68 | 0.75 |
| 35:E:539:G:H1 | 35:E:550:U:H3 | 1.35 | 0.74 |
| 35:E:259:C:N3 | 35:E:954:G:N1 | 2.35 | 0.73 |
| 35:E:724:A:C4 | 35:E:735:A:C2 | 2.80 | 0.70 |
| 35:E:216:A:H2' | 35:E:217:C:H5' | 1.74 | 0.69 |
| 35:E:1088:A:N1 | 35:E:1166:C:N3 | 2.41 | 0.69 |
| 35:E:532:G:H1 | 35:E:558:U:H3 | 1.38 | 0.69 |
| 35:E:1089:U:H3 | 35:E:1165:G:H1 | 1.39 | 0.68 |
| 35:E:1381:G:H1 | 35:E:1537:U:H3 | 1.40 | 0.67 |
| 35:E:880:A:H62 | 35:E:892:U:H3 | 1.43 | 0.64 |
| 35:E:546:U:C2' | 35:E:547:G:H5' | 2.28 | 0.63 |
| 35:E:724:A:C2 | 35:E:734:G:N1 | 2.65 | 0.63 |
| 35:E:259:C:C2 | 35:E:954:G:C2 | 2.88 | 0.62 |
| 35:E:2124:G:H22 | 35:E:2140:U:H3 | 1.48 | 0.61 |
| 35:E:1852:G:C2 | 35:E:1866:A:C2 | 2.93 | 0.57 |
| 35:E:216:A:C2' | 35:E:217:C:H5' | 2.35 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 35:E:1872:G:C6 | 35:E:1873:G:C6 | 2.94 | 0.55 |
| 35:E:724:A:C2 | 35:E:725:U:C2 | 2.96 | 0.54 |
| 35:E:2004:A:H61 | 35:E:2052:C:H41 | 1.57 | 0.53 |
| 35:E:259:C:N3 | 35:E:954:G:C6 | 2.77 | 0.53 |
| 35:E:817:A:C2 | 35:E:828:G:C2 | 2.97 | 0.52 |
| 35:E:1856:G:H3' | 35:E:1857:U:H5" | 1.92 | 0.52 |
| 35:E:989:G:H1 | 35:E:1177:C:H42 | 1.57 | 0.51 |
| 35:E:1689:A:H1' | 35:E:1691:G:H1 | 1.74 | 0.51 |
| 35:E:718:A:C2 | 35:E:719:G:C2 | 2.99 | 0.51 |
| 35:E:1911:U:H3 | 35:E:1917:G:H1 | 1.59 | 0.50 |
| 35:E:1852:G:N1 | 35:E:1866:A:C2 | 2.80 | 0.50 |
| 35:E:1184:C:H2' | 35:E:1185:A:C8 | 2.46 | 0.50 |
| 35:E:724:A:N1 | 35:E:734:G:C6 | 2.80 | 0.50 |
| 35:E:1866:A:C2 | 35:E:1867:G:C4 | 3.00 | 0.49 |
| 35:E:260:A:N1 | 35:E:953:G:C6 | 2.81 | 0.49 |
| 35:E:744:C:H2' | 35:E:745:C:C6 | 2.47 | 0.49 |
| 35:E:259:C:C4 | 35:E:954:G:N1 | 2.81 | 0.48 |
| 35:E:202:C:N3 | 35:E:226:A:N1 | 2.61 | 0.48 |
| 35:E:1200:A:N1 | 35:E:1300:C:C4 | 2.81 | 0.48 |
| 35:E:1848:U:H3 | 35:E:1870:G:H1 | 1.60 | 0.48 |
| 35:E:1384:G:N1 | 35:E:1534:A:C2 | 2.82 | 0.48 |
| 35:E:2091:U:H3' | 35:E:2092:A:H5" | 1.96 | 0.48 |
| 35:E:1987:A:H3' | 35:E:1988:U:H5' | 1.96 | 0.47 |
| 35:E:260:A:C6 | 35:E:953:G:N1 | 2.82 | 0.47 |
| 35:E:711:A:C2 | 35:E:746:A:C2 | 3.03 | 0.47 |
| 35:E:120:C:H3' | 35:E:121:A:H5" | 1.97 | 0.47 |
| 35:E:1908:U:H3' | 35:E:1909:U:H5' | 1.98 | 0.46 |
| 35:E:734:G:C6 | 35:E:735:A:C6 | 3.04 | 0.46 |
| 35:E:1375:U:H3 | 35:E:1543:C:N4 | 2.13 | 0.45 |
| 35:E:774:C:H1' | 35:E:775:A:H5" | 1.98 | 0.45 |
| 35:E:259:C:C2 | 35:E:954:G:C4 | 3.05 | 0.45 |
| 35:E:2051:C:H3' | 35:E:2052:C:H4' | 1.99 | 0.45 |
| 35:E:1846:C:C2 | 35:E:1873:G:N2 | 2.85 | 0.44 |
| 35:E:1923:U:H3 | 35:E:1927:A:H62 | 1.66 | 0.44 |
| 35:E:156:G:H3' | 35:E:157:G:H5" | 1.99 | 0.44 |
| 35:E:1169:U:C4 | 35:E:1170:C:C4 | 3.05 | 0.44 |
| 35:E:743:C:H2' | 35:E:744:C:C6 | 2.52 | 0.43 |
| 35:E:999:U:H3 | 35:E:1072:G:H1 | 1.66 | 0.43 |
| 35:E:1872:G:N1 | 35:E:1873:G:N1 | 2.66 | 0.43 |
| 35:E:824:G:H5" | 35:E:825:C:H5" | 1.99 | 0.43 |
| 35:E:711:A:C5 | 35:E:712:U:C4 | 3.07 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:Z:64:ASN:HD21 | 35:E:305:U:H2' | 1.83 | 0.43 |
| 35:E:1380:U:H3 | 35:E:1538:G:H1 | 1.65 | 0.43 |
| 35:E:1542:U:H2' | 35:E:1543:C:H5" | 2.01 | 0.43 |
| 10:R:16:LEU:HD11 | 35:E:1196:A:H5" | 2.01 | 0.43 |
| 35:E:711:A:N1 | 35:E:746:A:C2 | 2.86 | 0.42 |
| 35:E:1905:U:H3 | 35:E:1922:G:H22 | 1.68 | 0.42 |
| 35:E:714:G:H2' | 35:E:718:A:H62 | 1.84 | 0.42 |
| 35:E:1629:C:H1' | 35:E:2153:C:H41 | 1.84 | 0.42 |
| 35:E:1852:G:C6 | 35:E:1866:A:N1 | 2.88 | 0.42 |
| 35:E:260:A:C2 | 35:E:953:G:C2 | 3.08 | 0.42 |
| 35:E:1993:G:H21 | 35:E:1994:U:H2' | 1.84 | 0.41 |
| 35:E:703:A:C2 | 35:E:704:A:C5 | 3.09 | 0.41 |
| 35:E:260:A:C2 | 35:E:953:G:C4 | 3.08 | 0.41 |
| 35:E:724:A:C6 | 35:E:735:A:N1 | 2.88 | 0.41 |
| 35:E:1825:A:C2 | 35:E:1879:U:O4 | 2.73 | 0.41 |
| 35:E:1852:G:N2 | 35:E:1866:A:C2 | 2.89 | 0.41 |
| 35:E:817:A:N1 | 35:E:828:G:N1 | 2.69 | 0.41 |
| 35:E:718:A:C2 | 35:E:744:C:O2 | 2.73 | 0.41 |
| 35:E:602:G:N1 | 35:E:645:A:N1 | 2.69 | 0.41 |
| 35:E:1856:G:C3' | 35:E:1857:U:H5" | 2.51 | 0.41 |
| 9:Q:103:LYS:HA | 35:E:763:G:H1 | 1.85 | 0.41 |
| 35:E:1384:G:C2 | 35:E:1534:A:C2 | 3.09 | 0.40 |
| 35:E:216:A:C2 | 35:E:217:C:C6 | 3.10 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | p | 308/318 (97%) | 288 (94%) | 18 (6%) | 2 (1%) | 25 63 |
| 2 | q | 36/57 (63%) | 28 (78%) | 6 (17%) | 2 (6%) | 2 20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 3 | r | 138/149 (93%) | 113 (82%) | 18 (13%) | 7 (5%) | 2 | 22 |
| 4 | t | 117/152 (77%) | 105 (90%) | 8 (7%) | 4 (3%) | 3 | 30 |
| 5 | u | 118/153 (77%) | 102 (86%) | 13 (11%) | 3 (2%) | 5 | 35 |
| 6 | L | 256/273 (94%) | 239 (93%) | 16 (6%) | 1 (0%) | 34 | 71 |
| 7 | M | 140/143 (98%) | 131 (94%) | 8 (6%) | 1 (1%) | 22 | 61 |
| 8 | O | 188/190 (99%) | 165 (88%) | 16 (8%) | 7 (4%) | 3 | 28 |
| 9 | Q | 198/211 (94%) | 178 (90%) | 16 (8%) | 4 (2%) | 7 | 40 |
| 10 | R | 139/151 (92%) | 127 (91%) | 11 (8%) | 1 (1%) | 22 | 61 |
| 11 | S | 80/86 (93%) | 73 (91%) | 5 (6%) | 2 (2%) | 5 | 35 |
| 12 | T | 102/112 (91%) | 90 (88%) | 12 (12%) | 0 | 100 | 100 |
| 13 | U | 66/112 (59%) | 62 (94%) | 3 (4%) | 1 (2%) | 10 | 45 |
| 14 | V | 133/144 (92%) | 116 (87%) | 16 (12%) | 1 (1%) | 19 | 58 |
| 15 | W | 215/261 (82%) | 200 (93%) | 13 (6%) | 2 (1%) | 17 | 55 |
| 16 | X | 146/173 (84%) | 133 (91%) | 11 (8%) | 2 (1%) | 11 | 46 |
| 17 | Y | 121/137 (88%) | 113 (93%) | 8 (7%) | 0 | 100 | 100 |
| 18 | Z | 171/221 (77%) | 157 (92%) | 12 (7%) | 2 (1%) | 13 | 49 |
| 19 | b | 162/190 (85%) | 143 (88%) | 17 (10%) | 2 (1%) | 13 | 49 |
| 20 | f | 205/245 (84%) | 190 (93%) | 12 (6%) | 3 (2%) | 10 | 45 |
| 21 | d | 221/263 (84%) | 205 (93%) | 14 (6%) | 2 (1%) | 17 | 55 |
| 22 | e | 127/130 (98%) | 118 (93%) | 8 (6%) | 1 (1%) | 19 | 58 |
| 23 | g | 81/236 (34%) | 78 (96%) | 3 (4%) | 0 | 100 | 100 |
| 24 | a | 68/110 (62%) | 58 (85%) | 6 (9%) | 4 (6%) | 1 | 19 |
| 25 | i | 119/141 (84%) | 111 (93%) | 7 (6%) | 1 (1%) | 19 | 58 |
| 26 | j | 62/150 (41%) | 47 (76%) | 11 (18%) | 4 (6%) | 1 | 18 |
| 27 | P | 247/250 (99%) | 226 (92%) | 21 (8%) | 0 | 100 | 100 |
| 28 | k | 116/196 (59%) | 102 (88%) | 13 (11%) | 1 (1%) | 17 | 55 |
| 29 | l | 97/117 (83%) | 82 (84%) | 15 (16%) | 0 | 100 | 100 |
| 30 | m | 198/214 (92%) | 179 (90%) | 14 (7%) | 5 (2%) | 5 | 35 |
| 31 | n | 91/161 (56%) | 83 (91%) | 5 (6%) | 3 (3%) | 4 | 30 |
| 32 | o | 138/167 (83%) | 112 (81%) | 21 (15%) | 5 (4%) | 3 | 28 |
| 33 | c | 58/66 (88%) | 53 (91%) | 4 (7%) | 1 (2%) | 9 | 43 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 34 | h | 171/257 (66%) | 123 (72%) | 31 (18%) | 17 (10%) | 0 9 |
| All | All | 4833/5936 (81%) | 4330 (90%) | 412 (8%) | 91 (2%) | 11 40 |

All (91) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | r | 121 | TYR |
| 3 | r | 124 | ILE |
| 5 | u | 120 | VAL |
| 9 | Q | 138 | CYS |
| 21 | d | 81 | SER |
| 26 | j | 95 | MET |
| 26 | j | 97 | ALA |
| 30 | m | 144 | GLN |
| 34 | h | 77 | GLN |
| 34 | h | 121 | PHE |
| 34 | h | 155 | PRO |
| 34 | h | 158 | ARG |
| 34 | h | 162 | THR |
| 34 | h | 183 | ASN |
| 34 | h | 184 | ASN |
| 34 | h | 204 | ASN |
| 2 | q | 31 | VAL |
| 3 | r | 119 | ASP |
| 3 | r | 146 | LYS |
| 4 | t | 45 | HIS |
| 5 | u | 35 | LYS |
| 8 | O | 10 | ASN |
| 8 | O | 114 | VAL |
| 9 | Q | 122 | THR |
| 11 | S | 53 | SER |
| 11 | S | 71 | LYS |
| 19 | b | 136 | ALA |
| 24 | a | 101 | SER |
| 24 | a | 103 | LYS |
| 24 | a | 105 | ARG |
| 30 | m | 141 | ILE |
| 30 | m | 187 | ILE |
| 32 | o | 81 | VAL |
| 34 | h | 94 | VAL |
| 34 | h | 164 | LYS |
| 34 | h | 191 | ASP |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | p | 131 | ASN |
| 2 | q | 30 | ALA |
| 3 | r | 127 | PRO |
| 8 | O | 155 | LEU |
| 9 | Q | 51 | VAL |
| 16 | X | 43 | MET |
| 18 | Z | 69 | THR |
| 20 | f | 36 | ALA |
| 20 | f | 116 | GLN |
| 26 | j | 105 | GLU |
| 26 | j | 115 | ARG |
| 32 | o | 13 | ARG |
| 32 | o | 15 | ILE |
| 34 | h | 128 | GLY |
| 34 | h | 163 | LYS |
| 4 | t | 60 | ALA |
| 4 | t | 128 | MET |
| 7 | M | 86 | PRO |
| 8 | O | 25 | SER |
| 8 | O | 39 | ALA |
| 10 | R | 134 | GLN |
| 13 | U | 108 | ALA |
| 14 | V | 57 | ALA |
| 18 | Z | 29 | LEU |
| 24 | a | 45 | ALA |
| 25 | i | 103 | LEU |
| 28 | k | 141 | PRO |
| 31 | n | 32 | THR |
| 31 | n | 36 | SER |
| 31 | n | 68 | TRP |
| 34 | h | 161 | THR |
| 1 | p | 122 | ARG |
| 3 | r | 143 | ARG |
| 5 | u | 9 | GLN |
| 8 | O | 2 | SER |
| 8 | O | 11 | LYS |
| 9 | Q | 39 | LEU |
| 15 | W | 56 | ILE |
| 19 | b | 137 | LYS |
| 20 | f | 9 | LYS |
| 21 | d | 238 | ALA |
| 32 | o | 77 | ILE |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | h | 175 | VAL |
| 34 | h | 206 | ALA |
| 30 | m | 92 | VAL |
| 32 | o | 63 | ALA |
| 33 | c | 23 | LYS |
| 34 | h | 111 | ALA |
| 22 | e | 29 | PRO |
| 4 | t | 61 | PRO |
| 3 | r | 61 | VAL |
| 30 | m | 47 | ILE |
| 6 | L | 167 | VAL |
| 15 | W | 223 | PRO |
| 16 | X | 89 | VAL |

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 |
|---|---|---|---|---|---|
| 1 | p | 262/268 (98%) | 260 (99%) | 2 (1%) | 81 89 |
| 2 | q | 34/49 (69%) | 34 (100%) | 0 | 100 100 |
| 3 | r | 113/121 (93%) | 113 (100%) | 0 | 100 100 |
| 4 | t | 102/131 (78%) | 102 (100%) | 0 | 100 100 |
| 5 | u | 104/132 (79%) | 104 (100%) | 0 | 100 100 |
| 6 | L | 217/230 (94%) | 217 (100%) | 0 | 100 100 |
| 7 | M | 116/117 (99%) | 116 (100%) | 0 | 100 100 |
| 8 | O | 160/160 (100%) | 160 (100%) | 0 | 100 100 |
| 9 | Q | 188/195 (96%) | 188 (100%) | 0 | 100 100 |
| 10 | R | 125/132 (95%) | 124 (99%) | 1 (1%) | 81 89 |
| 11 | S | 70/73 (96%) | 70 (100%) | 0 | 100 100 |
| 12 | T | 87/93 (94%) | 87 (100%) | 0 | 100 100 |
| 13 | U | 57/97 (59%) | 57 (100%) | 0 | 100 100 |
| 14 | V | 103/112 (92%) | 102 (99%) | 1 (1%) | 76 86 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 15 | W | 194/223 (87%) | 192 (99%) | 2 (1%) | 76 | 86 |
| 16 | X | 137/157 (87%) | 137 (100%) | 0 | 100 | 100 |
| 17 | Y | 104/116 (90%) | 104 (100%) | 0 | 100 | 100 |
| 18 | Z | 143/184 (78%) | 143 (100%) | 0 | 100 | 100 |
| 19 | b | 148/165 (90%) | 148 (100%) | 0 | 100 | 100 |
| 20 | f | 182/211 (86%) | 181 (100%) | 1 (0%) | 88 | 93 |
| 21 | d | 187/208 (90%) | 187 (100%) | 0 | 100 | 100 |
| 22 | e | 110/111 (99%) | 109 (99%) | 1 (1%) | 78 | 88 |
| 23 | g | 68/186 (37%) | 68 (100%) | 0 | 100 | 100 |
| 24 | a | 64/96 (67%) | 63 (98%) | 1 (2%) | 62 | 79 |
| 25 | i | 103/120 (86%) | 99 (96%) | 4 (4%) | 32 | 58 |
| 26 | j | 55/123 (45%) | 54 (98%) | 1 (2%) | 59 | 77 |
| 27 | P | 204/205 (100%) | 204 (100%) | 0 | 100 | 100 |
| 28 | k | 108/172 (63%) | 108 (100%) | 0 | 100 | 100 |
| 29 | l | 89/104 (86%) | 89 (100%) | 0 | 100 | 100 |
| 30 | m | 167/179 (93%) | 166 (99%) | 1 (1%) | 86 | 92 |
| 31 | n | 84/125 (67%) | 83 (99%) | 1 (1%) | 71 | 84 |
| 32 | o | 118/139 (85%) | 117 (99%) | 1 (1%) | 81 | 89 |
| 33 | c | 49/53 (92%) | 49 (100%) | 0 | 100 | 100 |
| 34 | h | 138/191 (72%) | 133 (96%) | 5 (4%) | 35 | 61 |
| All | All | 4190/4978 (84%) | 4168 (100%) | 22 (0%) | 89 | 93 |

All (22) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | p | 29 | ILE |
| 1 | p | 175 | ASP |
| 10 | R | 16 | LEU |
| 14 | V | 44 | GLU |
| 15 | W | 89 | VAL |
| 15 | W | 165 | TRP |
| 20 | f | 72 | GLU |
| 22 | e | 57 | ARG |
| 24 | a | 106 | LEU |
| 25 | i | 69 | GLU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 25 | i | 121 | VAL |
| 25 | i | 128 | GLU |
| 25 | i | 133 | LEU |
| 26 | j | 119 | GLU |
| 30 | m | 137 | VAL |
| 31 | n | 48 | GLN |
| 32 | o | 116 | LEU |
| 34 | h | 94 | VAL |
| 34 | h | 103 | TYR |
| 34 | h | 181 | TYR |
| 34 | h | 217 | LEU |
| 34 | h | 222 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | p | 307 | ASN |
| 3 | r | 13 | GLN |
| 6 | L | 33 | HIS |
| 8 | O | 27 | HIS |
| 9 | Q | 36 | HIS |
| 9 | Q | 47 | HIS |
| 14 | V | 25 | HIS |
| 15 | W | 193 | ASN |
| 16 | X | 11 | HIS |
| 16 | X | 37 | ASN |
| 18 | Z | 64 | ASN |
| 20 | f | 121 | GLN |
| 30 | m | 163 | HIS |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 35 | E | 2017/2319 (86%) | 437 (21%) | 86 (4%) |

All (437) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 35 | E | 4 | C |
| 35 | E | 5 | U |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 35 | E | 17 | C |
| 35 | E | 25 | C |
| 35 | E | 26 | A |
| 35 | E | 34 | G |
| 35 | E | 35 | U |
| 35 | E | 45 | U |
| 35 | E | 46 | U |
| 35 | E | 47 | A |
| 35 | E | 56 | U |
| 35 | E | 65 | A |
| 35 | E | 74 | U |
| 35 | E | 75 | U |
| 35 | E | 76 | G |
| 35 | E | 82 | A |
| 35 | E | 83 | U |
| 35 | E | 90 | A |
| 35 | E | 111 | A |
| 35 | E | 121 | A |
| 35 | E | 137 | C |
| 35 | E | 143 | C |
| 35 | E | 144 | A |
| 35 | E | 145 | U |
| 35 | E | 157 | G |
| 35 | E | 163 | C |
| 35 | E | 170 | C |
| 35 | E | 184 | A |
| 35 | E | 191 | U |
| 35 | E | 193 | U |
| 35 | E | 194 | U |
| 35 | E | 196 | U |
| 35 | E | 198 | U |
| 35 | E | 199 | G |
| 35 | E | 200 | U |
| 35 | E | 202 | C |
| 35 | E | 203 | C |
| 35 | E | 204 | G |
| 35 | E | 227 | U |
| 35 | E | 228 | G |
| 35 | E | 249 | A |
| 35 | E | 252 | G |
| 35 | E | 253 | U |
| 35 | E | 255 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 35 | E | 257 | A |
| 35 | E | 258 | C |
| 35 | E | 271 | C |
| 35 | E | 284 | C |
| 35 | E | 286 | G |
| 35 | E | 287 | A |
| 35 | E | 288 | A |
| 35 | E | 309 | G |
| 35 | E | 311 | G |
| 35 | E | 313 | G |
| 35 | E | 316 | A |
| 35 | E | 322 | G |
| 35 | E | 325 | U |
| 35 | E | 326 | U |
| 35 | E | 327 | U |
| 35 | E | 329 | U |
| 35 | E | 331 | U |
| 35 | E | 357 | C |
| 35 | E | 362 | C |
| 35 | E | 364 | G |
| 35 | E | 385 | G |
| 35 | E | 386 | A |
| 35 | E | 408 | C |
| 35 | E | 427 | U |
| 35 | E | 447 | A |
| 35 | E | 449 | U |
| 35 | E | 450 | A |
| 35 | E | 463 | A |
| 35 | E | 464 | C |
| 35 | E | 465 | G |
| 35 | E | 471 | C |
| 35 | E | 472 | A |
| 35 | E | 473 | G |
| 35 | E | 486 | U |
| 35 | E | 491 | C |
| 35 | E | 507 | A |
| 35 | E | 520 | A |
| 35 | E | 529 | A |
| 35 | E | 531 | A |
| 35 | E | 532 | G |
| 35 | E | 533 | C |
| 35 | E | 560 | C |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 35 | E | 564 | G |
| 35 | E | 570 | U |
| 35 | E | 571 | A |
| 35 | E | 585 | A |
| 35 | E | 586 | A |
| 35 | E | 590 | C |
| 35 | E | 592 | A |
| 35 | E | 593 | G |
| 35 | E | 596 | A |
| 35 | E | 613 | C |
| 35 | E | 634 | A |
| 35 | E | 648 | A |
| 35 | E | 665 | U |
| 35 | E | 673 | A |
| 35 | E | 674 | A |
| 35 | E | 676 | G |
| 35 | E | 677 | G |
| 35 | E | 678 | G |
| 35 | E | 698 | C |
| 35 | E | 699 | C |
| 35 | E | 702 | U |
| 35 | E | 703 | A |
| 35 | E | 704 | A |
| 35 | E | 705 | G |
| 35 | E | 706 | G |
| 35 | E | 707 | C |
| 35 | E | 708 | G |
| 35 | E | 710 | A |
| 35 | E | 713 | G |
| 35 | E | 714 | G |
| 35 | E | 717 | U |
| 35 | E | 718 | A |
| 35 | E | 720 | U |
| 35 | E | 721 | C |
| 35 | E | 726 | C |
| 35 | E | 727 | C |
| 35 | E | 728 | A |
| 35 | E | 729 | C |
| 35 | E | 730 | U |
| 35 | E | 731 | U |
| 35 | E | 732 | C |
| 35 | E | 733 | G |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 35 | E | 736 | U |
| 35 | E | 737 | U |
| 35 | E | 738 | G |
| 35 | E | 739 | G |
| 35 | E | 740 | U |
| 35 | E | 741 | G |
| 35 | E | 742 | A |
| 35 | E | 745 | C |
| 35 | E | 747 | U |
| 35 | E | 748 | G |
| 35 | E | 749 | C |
| 35 | E | 750 | C |
| 35 | E | 751 | C |
| 35 | E | 752 | U |
| 35 | E | 757 | G |
| 35 | E | 760 | C |
| 35 | E | 762 | U |
| 35 | E | 766 | C |
| 35 | E | 768 | G |
| 35 | E | 769 | A |
| 35 | E | 770 | C |
| 35 | E | 771 | A |
| 35 | E | 772 | U |
| 35 | E | 773 | U |
| 35 | E | 774 | C |
| 35 | E | 775 | A |
| 35 | E | 776 | G |
| 35 | E | 777 | A |
| 35 | E | 778 | A |
| 35 | E | 785 | A |
| 35 | E | 786 | A |
| 35 | E | 789 | C |
| 35 | E | 793 | A |
| 35 | E | 795 | U |
| 35 | E | 796 | G |
| 35 | E | 798 | U |
| 35 | E | 799 | A |
| 35 | E | 804 | U |
| 35 | E | 806 | C |
| 35 | E | 808 | G |
| 35 | E | 809 | A |
| 35 | E | 810 | U |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 35 | E | 811 | U |
| 35 | E | 812 | A |
| 35 | E | 813 | U |
| 35 | E | 814 | C |
| 35 | E | 815 | G |
| 35 | E | 821 | C |
| 35 | E | 822 | A |
| 35 | E | 823 | U |
| 35 | E | 824 | G |
| 35 | E | 825 | C |
| 35 | E | 827 | U |
| 35 | E | 829 | C |
| 35 | E | 830 | C |
| 35 | E | 834 | G |
| 35 | E | 835 | G |
| 35 | E | 836 | G |
| 35 | E | 844 | G |
| 35 | E | 847 | U |
| 35 | E | 848 | U |
| 35 | E | 858 | A |
| 35 | E | 861 | A |
| 35 | E | 871 | G |
| 35 | E | 872 | A |
| 35 | E | 877 | A |
| 35 | E | 880 | A |
| 35 | E | 881 | G |
| 35 | E | 884 | A |
| 35 | E | 885 | U |
| 35 | E | 886 | U |
| 35 | E | 887 | C |
| 35 | E | 888 | G |
| 35 | E | 889 | A |
| 35 | E | 891 | U |
| 35 | E | 892 | U |
| 35 | E | 893 | G |
| 35 | E | 895 | A |
| 35 | E | 901 | A |
| 35 | E | 919 | G |
| 35 | E | 920 | A |
| 35 | E | 921 | G |
| 35 | E | 922 | C |
| 35 | E | 923 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 35 | E | 924 | G |
| 35 | E | 925 | C |
| 35 | E | 935 | A |
| 35 | E | 936 | C |
| 35 | E | 940 | U |
| 35 | E | 941 | U |
| 35 | E | 942 | C |
| 35 | E | 943 | G |
| 35 | E | 944 | G |
| 35 | E | 945 | C |
| 35 | E | 946 | U |
| 35 | E | 947 | U |
| 35 | E | 950 | G |
| 35 | E | 966 | C |
| 35 | E | 969 | U |
| 35 | E | 975 | U |
| 35 | E | 976 | U |
| 35 | E | 977 | A |
| 35 | E | 979 | G |
| 35 | E | 980 | G |
| 35 | E | 983 | C |
| 35 | E | 986 | U |
| 35 | E | 988 | U |
| 35 | E | 989 | G |
| 35 | E | 994 | G |
| 35 | E | 999 | U |
| 35 | E | 1074 | C |
| 35 | E | 1077 | C |
| 35 | E | 1078 | U |
| 35 | E | 1079 | U |
| 35 | E | 1081 | G |
| 35 | E | 1082 | U |
| 35 | E | 1083 | G |
| 35 | E | 1171 | C |
| 35 | E | 1172 | C |
| 35 | E | 1175 | A |
| 35 | E | 1177 | C |
| 35 | E | 1178 | U |
| 35 | E | 1187 | C |
| 35 | E | 1188 | C |
| 35 | E | 1189 | A |
| 35 | E | 1191 | G |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 35 | E | 1192 | A |
| 35 | E | 1193 | A |
| 35 | E | 1194 | U |
| 35 | E | 1195 | G |
| 35 | E | 1197 | A |
| 35 | E | 1207 | U |
| 35 | E | 1208 | U |
| 35 | E | 1211 | G |
| 35 | E | 1221 | U |
| 35 | E | 1247 | U |
| 35 | E | 1268 | A |
| 35 | E | 1270 | A |
| 35 | E | 1295 | U |
| 35 | E | 1301 | A |
| 35 | E | 1339 | G |
| 35 | E | 1340 | A |
| 35 | E | 1356 | C |
| 35 | E | 1359 | C |
| 35 | E | 1360 | A |
| 35 | E | 1361 | A |
| 35 | E | 1363 | C |
| 35 | E | 1375 | U |
| 35 | E | 1524 | U |
| 35 | E | 1541 | U |
| 35 | E | 1542 | U |
| 35 | E | 1543 | C |
| 35 | E | 1544 | U |
| 35 | E | 1545 | U |
| 35 | E | 1546 | C |
| 35 | E | 1547 | A |
| 35 | E | 1559 | U |
| 35 | E | 1560 | G |
| 35 | E | 1561 | A |
| 35 | E | 1606 | A |
| 35 | E | 1618 | G |
| 35 | E | 1626 | C |
| 35 | E | 1627 | C |
| 35 | E | 1628 | A |
| 35 | E | 1631 | A |
| 35 | E | 1638 | G |
| 35 | E | 1653 | U |
| 35 | E | 1659 | U |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 35 | E | 1661 | A |
| 35 | E | 1664 | A |
| 35 | E | 1668 | G |
| 35 | E | 1669 | G |
| 35 | E | 1671 | A |
| 35 | E | 1672 | C |
| 35 | E | 1685 | G |
| 35 | E | 1689 | A |
| 35 | E | 1690 | G |
| 35 | E | 1691 | G |
| 35 | E | 1695 | A |
| 35 | E | 1696 | G |
| 35 | E | 1701 | G |
| 35 | E | 1711 | G |
| 35 | E | 1712 | U |
| 35 | E | 1724 | A |
| 35 | E | 1725 | U |
| 35 | E | 1727 | C |
| 35 | E | 1738 | G |
| 35 | E | 1782 | U |
| 35 | E | 1783 | U |
| 35 | E | 1789 | A |
| 35 | E | 1813 | G |
| 35 | E | 1815 | A |
| 35 | E | 1829 | C |
| 35 | E | 1830 | C |
| 35 | E | 1831 | C |
| 35 | E | 1832 | A |
| 35 | E | 1833 | U |
| 35 | E | 1857 | U |
| 35 | E | 1872 | G |
| 35 | E | 1873 | G |
| 35 | E | 1874 | C |
| 35 | E | 1875 | G |
| 35 | E | 1876 | G |
| 35 | E | 1877 | U |
| 35 | E | 1878 | A |
| 35 | E | 1880 | U |
| 35 | E | 1881 | C |
| 35 | E | 1882 | G |
| 35 | E | 1883 | C |
| 35 | E | 1884 | U |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 35 | E | 1885 | U |
| 35 | E | 1886 | G |
| 35 | E | 1887 | U |
| 35 | E | 1903 | A |
| 35 | E | 1904 | U |
| 35 | E | 1905 | U |
| 35 | E | 1909 | U |
| 35 | E | 1910 | G |
| 35 | E | 1914 | U |
| 35 | E | 1927 | A |
| 35 | E | 1930 | U |
| 35 | E | 1943 | G |
| 35 | E | 1947 | U |
| 35 | E | 1950 | G |
| 35 | E | 1951 | A |
| 35 | E | 1955 | U |
| 35 | E | 1956 | C |
| 35 | E | 1959 | C |
| 35 | E | 1961 | A |
| 35 | E | 1965 | U |
| 35 | E | 1966 | C |
| 35 | E | 1974 | C |
| 35 | E | 1976 | C |
| 35 | E | 1977 | G |
| 35 | E | 1988 | U |
| 35 | E | 1990 | U |
| 35 | E | 1991 | C |
| 35 | E | 1992 | A |
| 35 | E | 1993 | G |
| 35 | E | 1994 | U |
| 35 | E | 2000 | C |
| 35 | E | 2002 | A |
| 35 | E | 2007 | A |
| 35 | E | 2008 | A |
| 35 | E | 2009 | C |
| 35 | E | 2010 | G |
| 35 | E | 2012 | C |
| 35 | E | 2013 | U |
| 35 | E | 2016 | U |
| 35 | E | 2018 | U |
| 35 | E | 2019 | C |
| 35 | E | 2020 | G |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 35 | E | 2021 | G |
| 35 | E | 2022 | A |
| 35 | E | 2030 | G |
| 35 | E | 2032 | U |
| 35 | E | 2033 | C |
| 35 | E | 2034 | A |
| 35 | E | 2048 | A |
| 35 | E | 2049 | C |
| 35 | E | 2050 | C |
| 35 | E | 2051 | C |
| 35 | E | 2052 | C |
| 35 | E | 2053 | G |
| 35 | E | 2054 | G |
| 35 | E | 2060 | C |
| 35 | E | 2061 | G |
| 35 | E | 2063 | A |
| 35 | E | 2064 | G |
| 35 | E | 2068 | C |
| 35 | E | 2070 | C |
| 35 | E | 2071 | U |
| 35 | E | 2072 | U |
| 35 | E | 2075 | G |
| 35 | E | 2077 | C |
| 35 | E | 2087 | C |
| 35 | E | 2090 | U |
| 35 | E | 2091 | U |
| 35 | E | 2092 | A |
| 35 | E | 2097 | U |
| 35 | E | 2099 | G |
| 35 | E | 2102 | C |
| 35 | E | 2103 | A |
| 35 | E | 2107 | A |
| 35 | E | 2108 | G |
| 35 | E | 2118 | G |
| 35 | E | 2135 | A |
| 35 | E | 2153 | C |
| 35 | E | 2165 | A |
| 35 | E | 2214 | A |
| 35 | E | 2216 | A |
| 35 | E | 2217 | G |
| 35 | E | 2218 | U |
| 35 | E | 2225 | C |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 35 | E | 2226 | U |
| 35 | E | 2228 | C |
| 35 | E | 2235 | C |
| 35 | E | 2275 | G |
| 35 | E | 2278 | G |
| 35 | E | 2280 | A |
| 35 | E | 2283 | A |
| 35 | E | 2284 | A |
| 35 | E | 2287 | U |
| 35 | E | 2288 | A |
| 35 | E | 2310 | G |
| 35 | E | 2311 | G |
| 35 | E | 2312 | A |
| 35 | E | 2314 | C |
| 35 | E | 2317 | U |

All (86) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 35 | E | 56 | U |
| 35 | E | 68 | A |
| 35 | E | 193 | U |
| 35 | E | 227 | U |
| 35 | E | 325 | U |
| 35 | E | 531 | A |
| 35 | E | 701 | C |
| 35 | E | 702 | U |
| 35 | E | 703 | A |
| 35 | E | 712 | U |
| 35 | E | 713 | G |
| 35 | E | 717 | U |
| 35 | E | 719 | G |
| 35 | E | 727 | C |
| 35 | E | 729 | C |
| 35 | E | 756 | G |
| 35 | E | 765 | A |
| 35 | E | 769 | A |
| 35 | E | 771 | A |
| 35 | E | 774 | C |
| 35 | E | 775 | A |
| 35 | E | 777 | A |
| 35 | E | 785 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 35 | E | 788 | A |
| 35 | E | 792 | G |
| 35 | E | 795 | U |
| 35 | E | 797 | G |
| 35 | E | 807 | U |
| 35 | E | 808 | G |
| 35 | E | 810 | U |
| 35 | E | 812 | A |
| 35 | E | 813 | U |
| 35 | E | 814 | C |
| 35 | E | 822 | A |
| 35 | E | 828 | G |
| 35 | E | 829 | C |
| 35 | E | 847 | U |
| 35 | E | 885 | U |
| 35 | E | 890 | C |
| 35 | E | 891 | U |
| 35 | E | 892 | U |
| 35 | E | 918 | G |
| 35 | E | 919 | G |
| 35 | E | 921 | G |
| 35 | E | 922 | C |
| 35 | E | 923 | A |
| 35 | E | 935 | A |
| 35 | E | 939 | U |
| 35 | E | 940 | U |
| 35 | E | 942 | C |
| 35 | E | 968 | U |
| 35 | E | 975 | U |
| 35 | E | 982 | G |
| 35 | E | 988 | U |
| 35 | E | 998 | C |
| 35 | E | 1076 | C |
| 35 | E | 1186 | U |
| 35 | E | 1187 | C |
| 35 | E | 1188 | C |
| 35 | E | 1191 | G |
| 35 | E | 1192 | A |
| 35 | E | 1526 | A |
| 35 | E | 1545 | U |
| 35 | E | 1546 | C |
| 35 | E | 1695 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 35 | E | 1712 | U |
| 35 | E | 1872 | G |
| 35 | E | 1875 | G |
| 35 | E | 1876 | G |
| 35 | E | 1882 | G |
| 35 | E | 1886 | G |
| 35 | E | 1903 | A |
| 35 | E | 1904 | U |
| 35 | E | 1913 | U |
| 35 | E | 2006 | A |
| 35 | E | 2017 | G |
| 35 | E | 2020 | G |
| 35 | E | 2048 | A |
| 35 | E | 2049 | C |
| 35 | E | 2050 | C |
| 35 | E | 2051 | C |
| 35 | E | 2052 | C |
| 35 | E | 2152 | C |
| 35 | E | 2213 | G |
| 35 | E | 2227 | U |
| 35 | E | 2234 | A |

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

There are no ligands in this entry.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

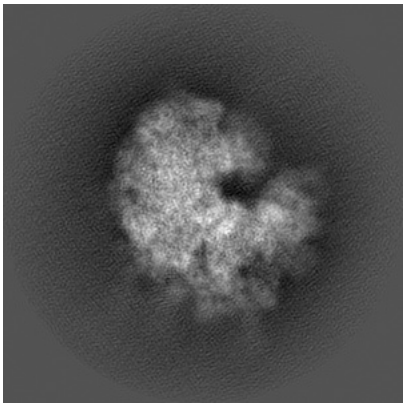
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-3844. These allow visual inspection of the internal detail of the map and identification of artifacts.

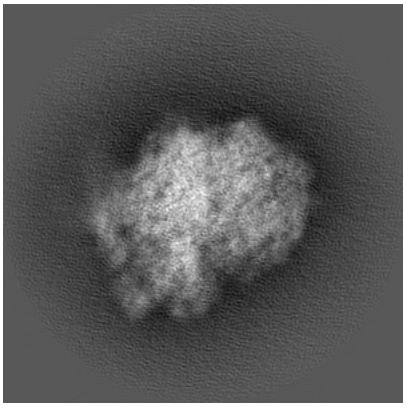
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections (i)

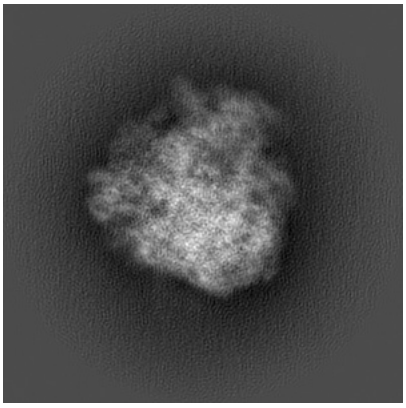
### 6.1.1 Primary map



X



Y

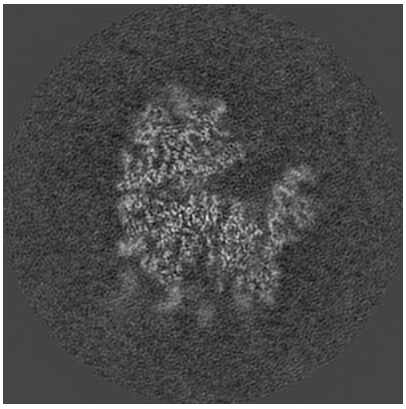


Z

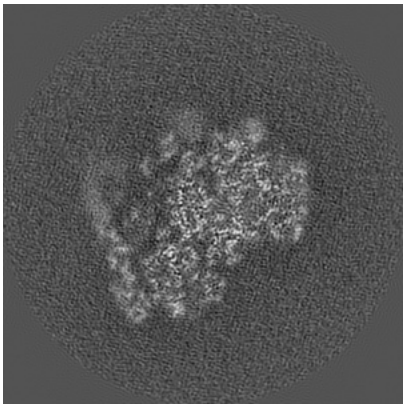
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

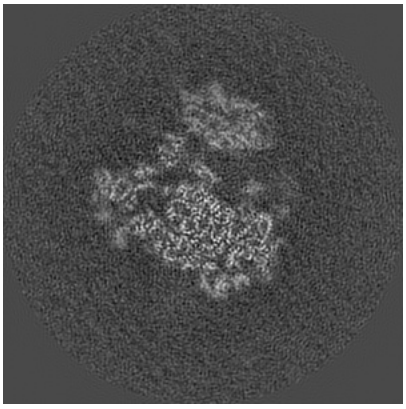
### 6.2.1 Primary map



X Index: 160



Y Index: 160

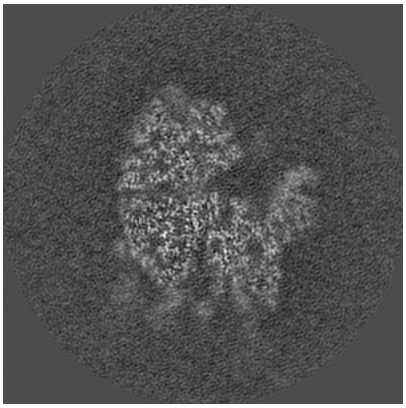


Z Index: 160

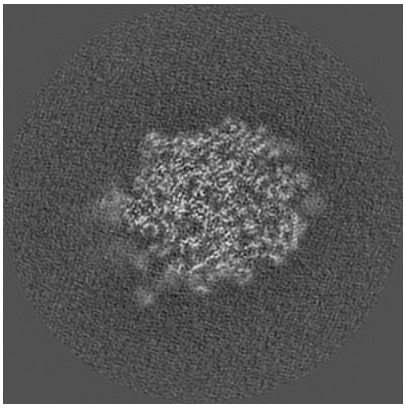
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

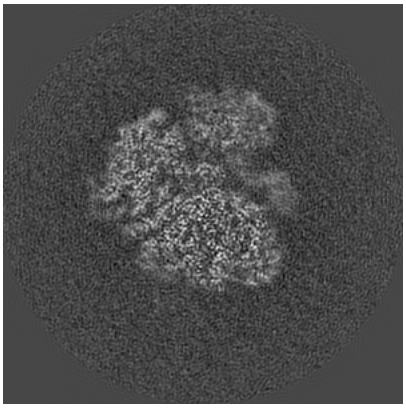
### 6.3.1 Primary map



X Index: 157



Y Index: 134



Z Index: 147

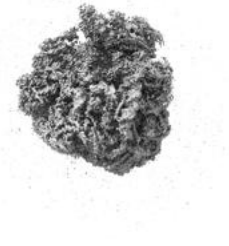
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views (i)

### 6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0549. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

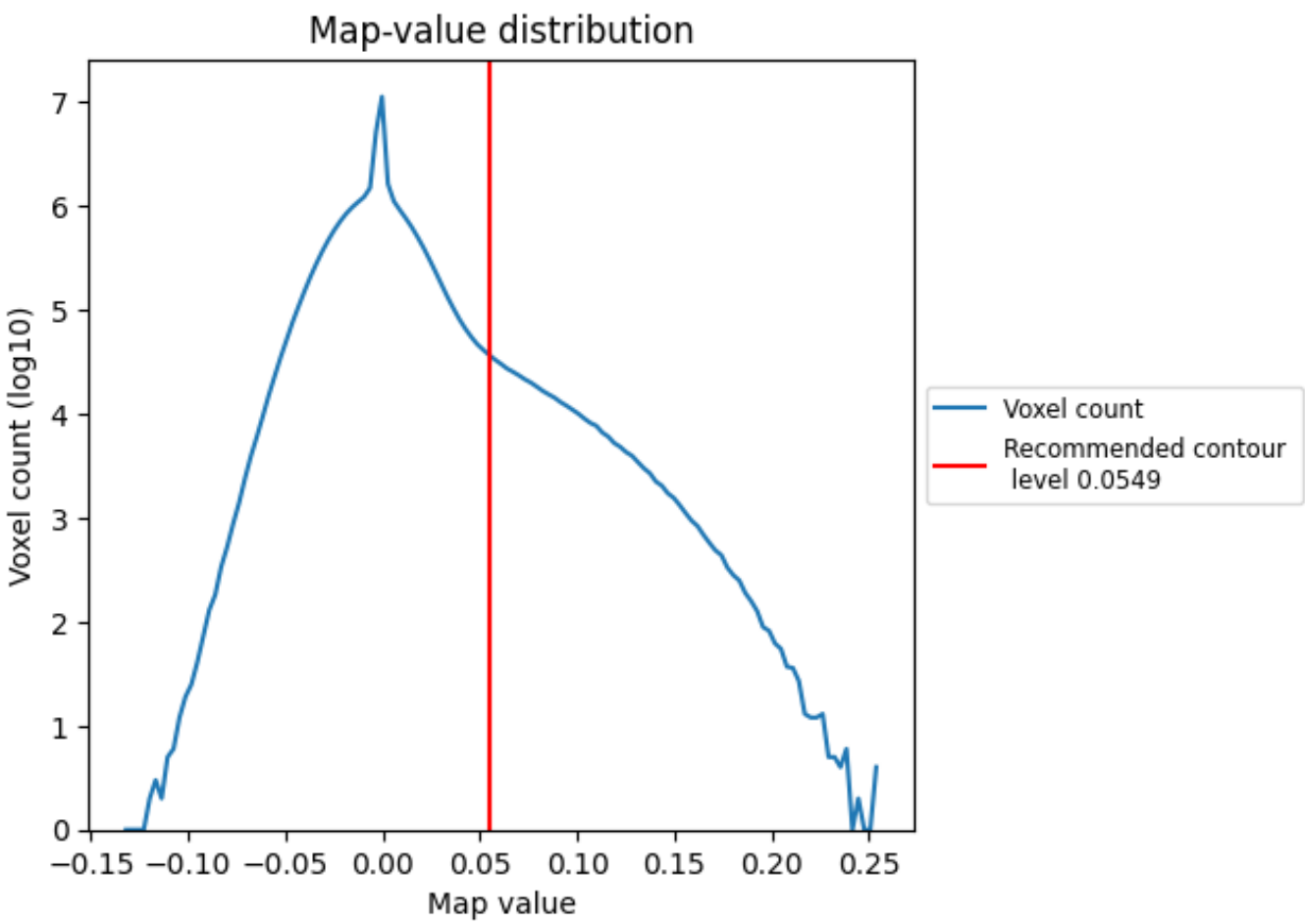
## 6.5 Mask visualisation (i)

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

# 7 Map analysis (i)

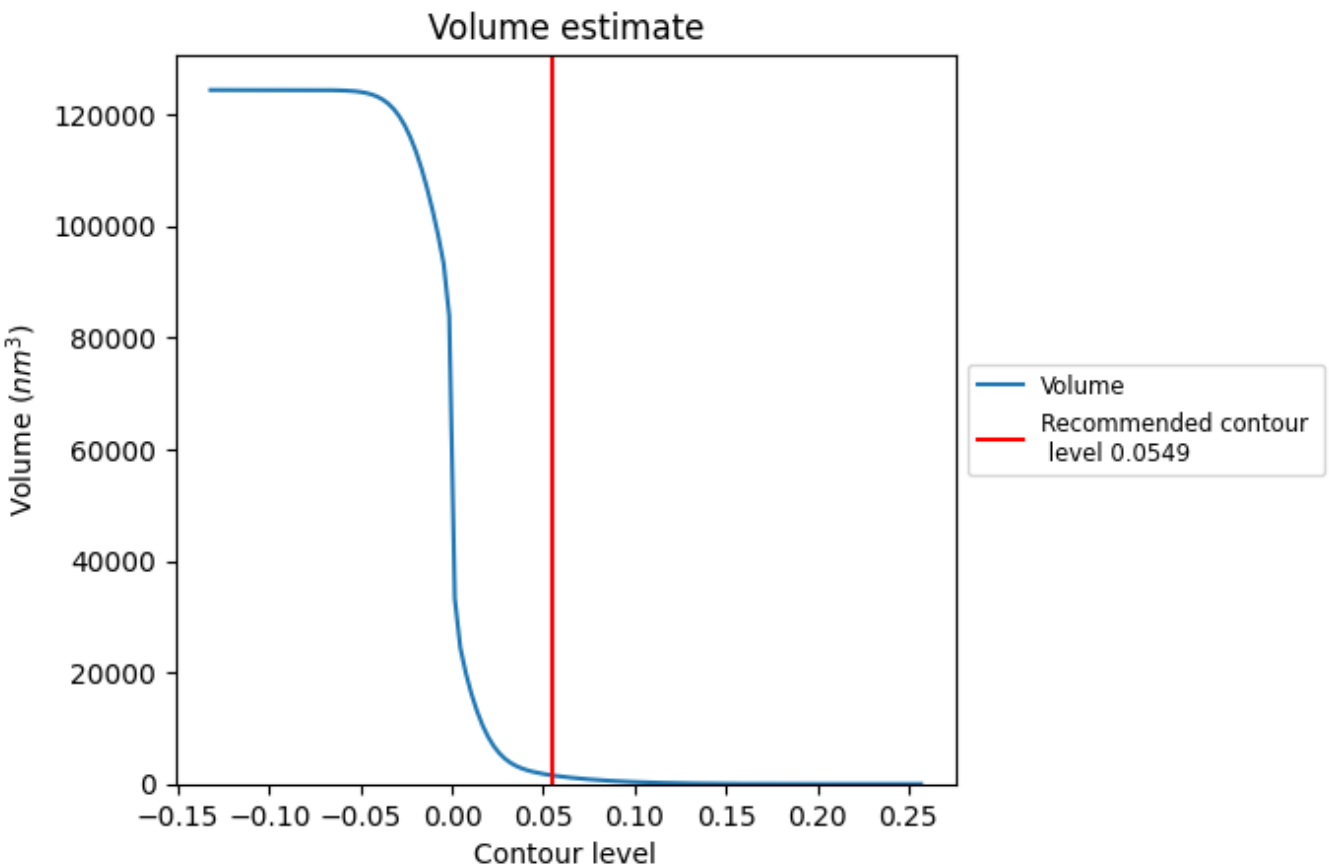
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution (i)




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

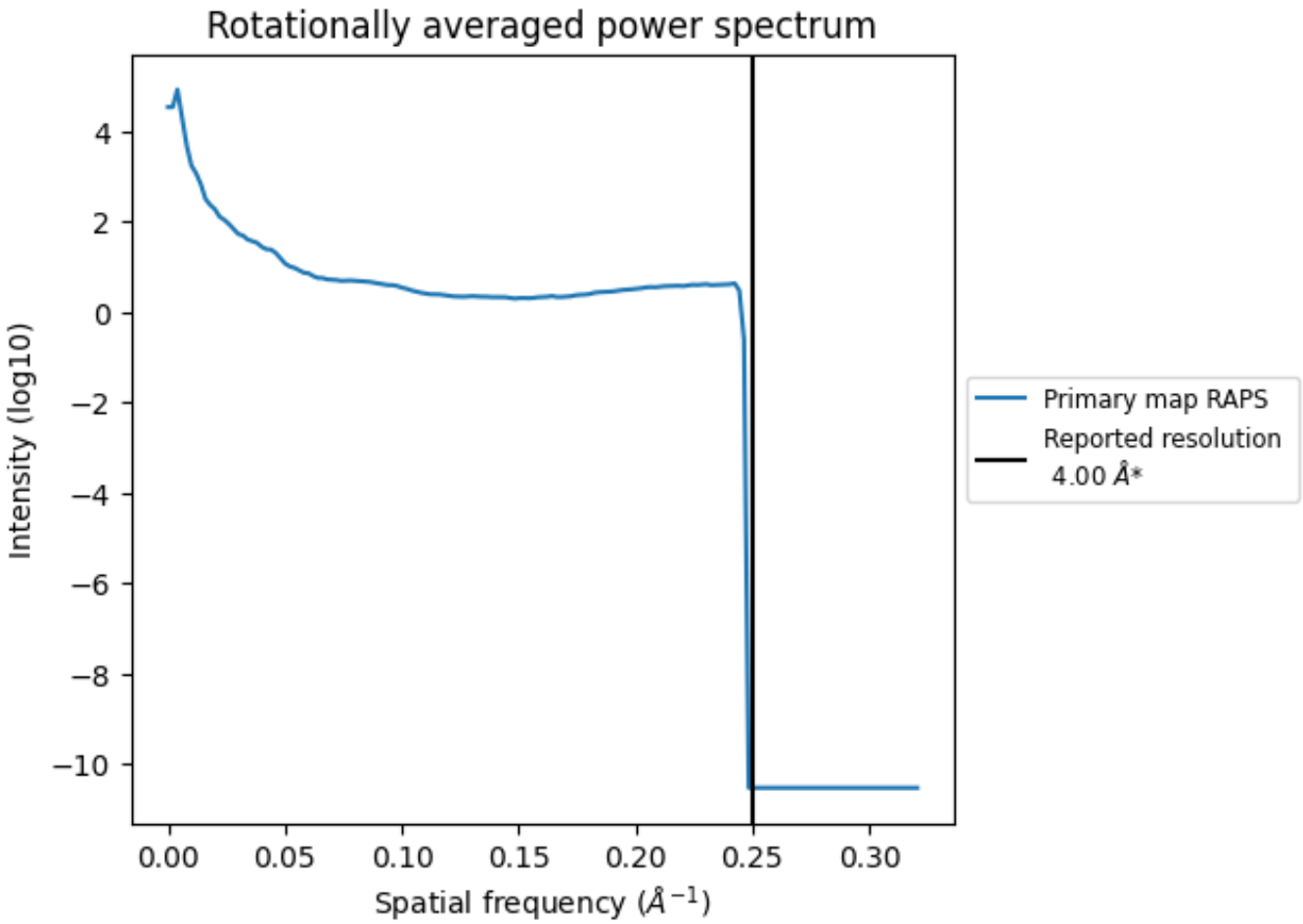
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 1549 $nm^3$; this corresponds to an approximate mass of 1400 kDa.

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

## 7.3 Rotationally averaged power spectrum (i)




*Reported resolution corresponds to spatial frequency of 0.250 Å$^{-1}$

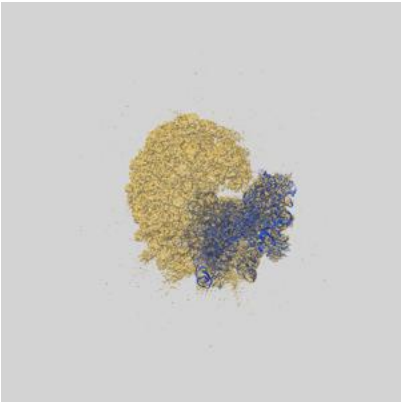
# 8 Fourier-Shell correlation (i)

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

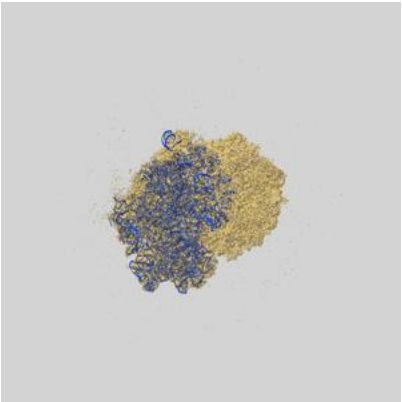
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-3844 and PDB model 5OPT. Per-residue inclusion information can be found in section 3 on page 11.

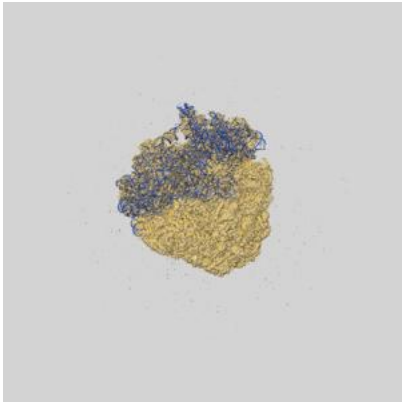
## 9.1 Map-model overlay (i)



X



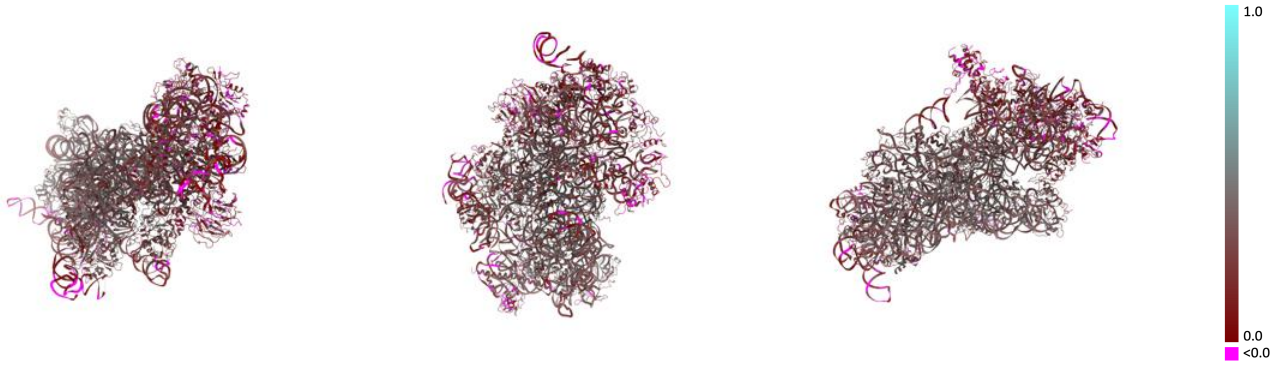
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0549 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

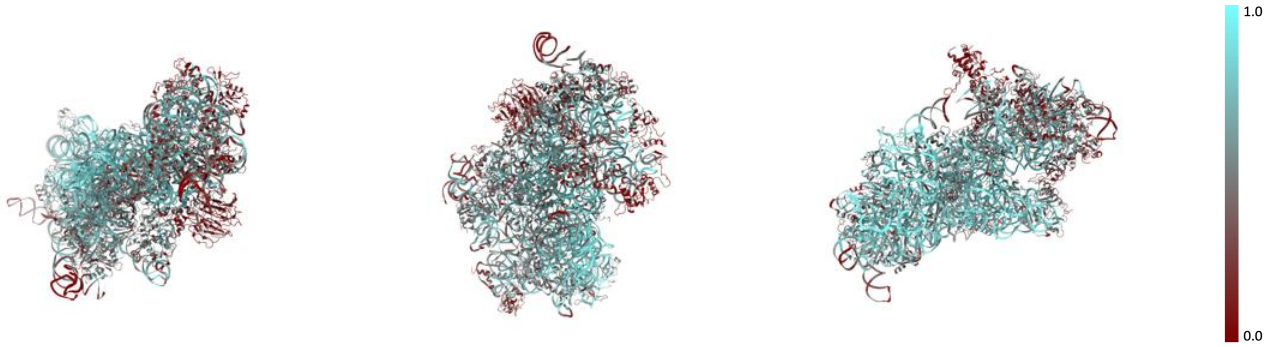
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

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

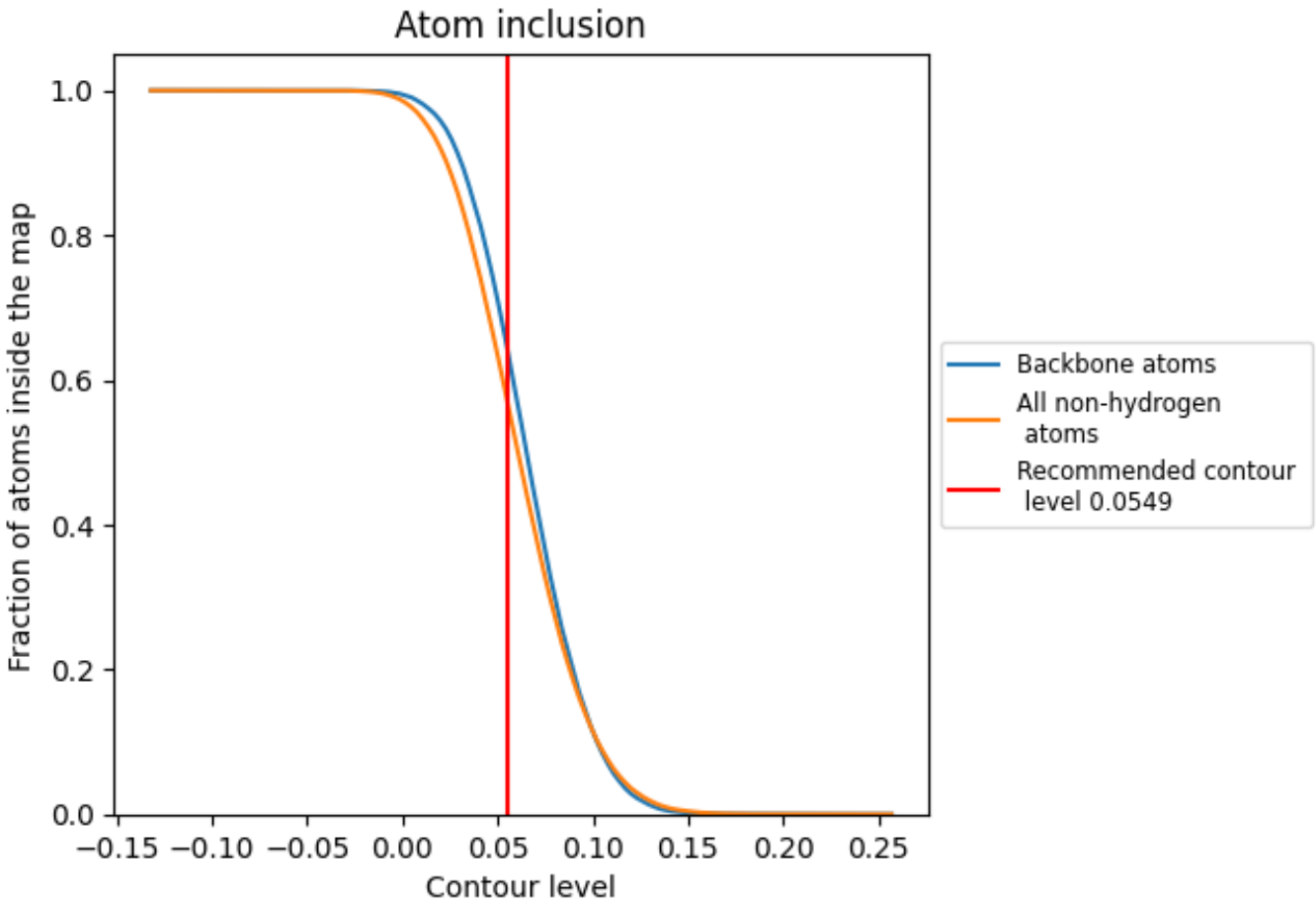
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0549).

## 9.4 Atom inclusion (i)




At the recommended contour level, 65% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0549) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.5724 | 0.2840 |
| E | 0.6987 | 0.2970 |
| L | 0.5232 | 0.3590 |
| M | 0.5606 | 0.3500 |
| O | 0.3579 | 0.2240 |
| P | 0.5280 | 0.2910 |
| Q | 0.5311 | 0.3060 |
| R | 0.5204 | 0.3280 |
| S | 0.4421 | 0.3200 |
| T | 0.5044 | 0.3360 |
| U | 0.2609 | 0.2090 |
| V | 0.4923 | 0.3140 |
| W | 0.5513 | 0.3340 |
| X | 0.5149 | 0.3370 |
| Y | 0.5848 | 0.3250 |
| Z | 0.5968 | 0.3600 |
| a | 0.2983 | 0.1260 |
| b | 0.5505 | 0.3240 |
| c | 0.4765 | 0.2910 |
| d | 0.5234 | 0.3260 |
| e | 0.5473 | 0.3480 |
| f | 0.5207 | 0.3120 |
| g | 0.5169 | 0.3330 |
| h | 0.2966 | 0.1270 |
| i | 0.1113 | 0.0940 |
| j | 0.1861 | 0.1000 |
| k | 0.3771 | 0.2550 |
| l | 0.2936 | 0.2240 |
| m | 0.2931 | 0.2600 |
| n | 0.2964 | 0.2120 |
| o | 0.3843 | 0.1690 |
| p | 0.1712 | 0.1680 |
| q | 0.3767 | 0.2290 |
| r | 0.3924 | 0.2380 |
| t | 0.2790 | 0.1820 |
| u | 0.3231 | 0.1910 |